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ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА

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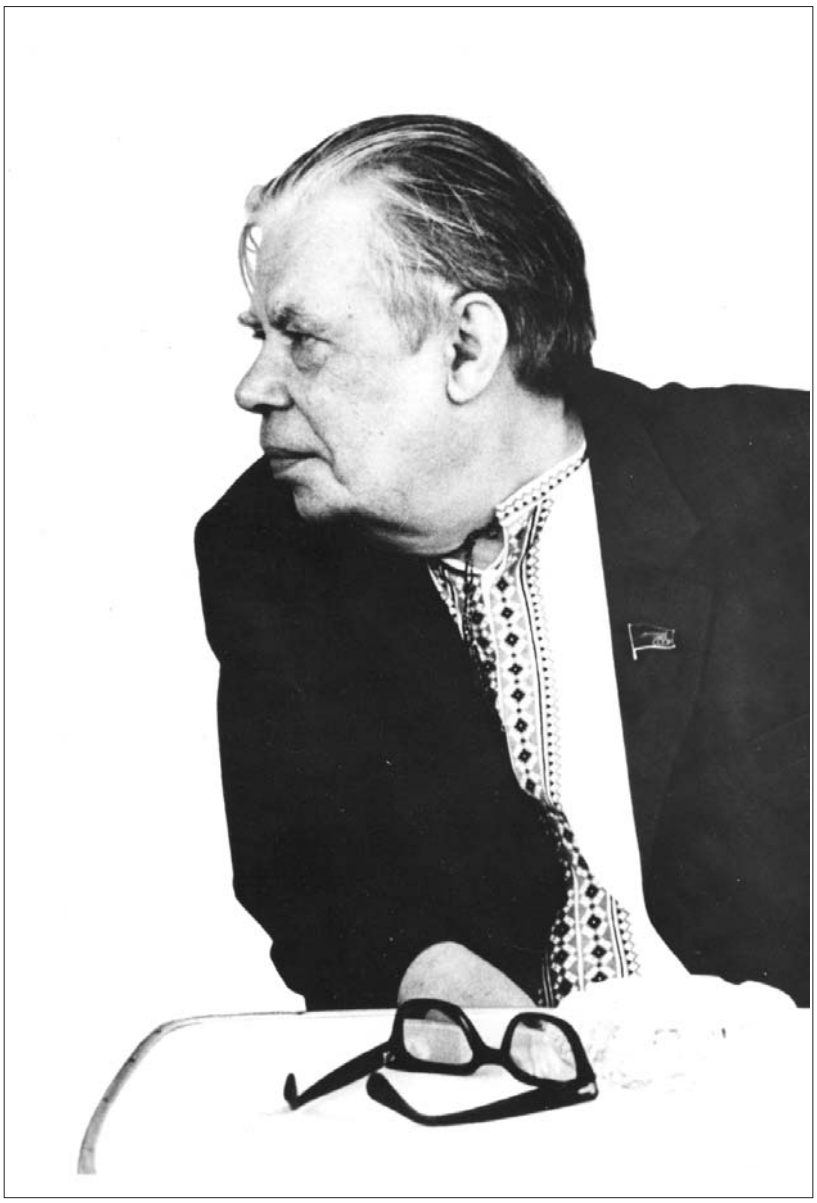

РОССИЙСКАЯ АКАДЕМИЯ НАУК
НАЦИОНАЛЬНАЯ АКАДЕМИЯ НАУК УКРАИНЫ
ОБЪЕДИНЕННЫЙ ИНСТИТУТ ЯДЕРНЫХ ИССЛЕДОВАНИЙ

БОГОЛЮБОВСКАЯ КОНФЕРЕНЦИЯ «ПРОБЛЕМЫ ТЕОРЕТИЧЕСКОЙ И МАТЕМАТИЧЕСКОЙ ФИЗИКИ»

Москва – Дубна – Киев,
27 сентября – 6 октября 1999 г.

ТРУДЫ КОНФЕРЕНЦИИ

Под общей редакцией
В.Г.Кадышевского
А.Н.Сисакяна

BOGOLYUBOV CONFERENCE «PROBLEMS OF THEORETICAL AND MATHEMATICAL PHYSICS»

Moscow – Dubna – Kyiv
27 September – 6 October 1999

PROCEEDINGS

Editors
V.G.Kadyshevsky
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«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
2000, ТОМ 31, ВЫП. 7Б

FOREWORD

The Bogolyubov Conference on Problems of Theoretical and Mathematical Physics organized by the Russian Academy of Sciences (RAS), the National Academy of Sciences of Ukraine (NASU) and the Joint Institute for Nuclear Research (JINR) was held on September 27 – October 6, 1999 in Moscow (27.09–28.09), Dubna (29.09–2.10) and Kyiv (3.10–6.10).

The Conference was devoted to the commemoration of the 90th anniversary of the birth of the outstanding scientist Nikolai Nikolaevich Bogolyubov (1909–1992).

The programme of the Conference has covered the problems of mathematics, mechanics, theoretical and mathematical physics to which N.N. Bogolyubov made a fundamental contribution. The Bogolyubov meetings in Moscow, Dubna and Kyiv shared the common interdisciplinary spirit of the Bogolyubov Conferences, and brought together many scientists with the interests ranging from mathematics to nonlinear mechanics, quantum field theory, particle physics, statistical physics, kinetics and nuclear physics.

The Conference programme included memory sessions, plenary talks and parallel sessions. Many of the speakers sent their contributions. We thank them for having allowed us to collect such a large amount of papers in a short time.

The number of participants overtook our optimistic expectations and we were forced to refuse to some late applications in order to limit the talks. More than 40 plenary talks were devoted to the most actual problems from mathematics to nuclear physics. About two hundred original investigations of fundamental aspect of physics, mechanics and mathematics were presented at parallel sessions.

We thank all the participants who, attracted by their interest to the Bogolyubov Meeting, came together to make this Conference such a success. We thank the heads of Moscow State University, the V.A. Steklov Mathematical Institute of RAS, the Joint Institute for Nuclear Research, the Bogolyubov Institute of Theoretcal Physics of NASU and the Mathematical Institute of NASU in Kyiv for hosting the Conference and providing the administrative help and secretary staff.

On behalf of the Organizing Committee we acknowledge and thank for financial support:
UNESCO
INTAS

International Mathematical Union
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ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ

«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
2000, ТОМ 31, ВЫП. 7Б

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NONLOCAL QUARK AND GLUON CONDENSATES WITHIN A CONSTRAINED INSTANTON MODEL

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We suggest a constrained instanton (CI) solution in the physical QCD vacuum which is described by large-scale vacuum field fluctuations. This solution decays exponentially at large distances. It is stable only if the interaction of the instanton with the background vacuum field is small and additional constraints are introduced. The CI solution is explicitly constructed in the ansatz form, and the two-point vacuum correlator of gluon field strengths is calculated in the framework of the effective instanton vacuum model. At small distances the results are qualitatively similar to the single instanton case, in particular, the form factor D_1 is small, which is in agreement with the lattice calculations.

The nonperturbative vacuum of QCD is densely populated by long-wave fluctuations of gluon and quark fields. The order parameters of this complicated state are characterized by the vacuum matrix elements of various singlet combinations of quark and gluon fields, condensates: $\langle : \bar{q}q : \rangle$, $\left\langle : F^a_{\mu\nu}F^a_{\mu\nu} : \right\rangle$, $\left\langle : \bar{q}(\sigma_{\mu\nu}F^a_{\mu\nu}\frac{\lambda^a}{2})q : \right\rangle$, *etc*. The nonzero quark condensate $\langle : \bar{q}q : \rangle$ is responsible for the spontaneous breakdown of chiral symmetry, and its value was estimated a long time ago within the current algebra approach. The nonzero gluon condensate $\left\langle : F^a_{\mu\nu}F^a_{\mu\nu} : \right\rangle$ through trace anomaly provides the mass scale for hadrons, and its value was estimated within the QCD sum rule (SR) approach. The values of low-dimensional condensates were obtained phenomenologically from the QCD SR analysis of various hadron channels.

The nonlocal vacuum condensates or vacuum correlators [1, 2] describe the distribution of quarks and gluons in the nonperturbative vacuum. Physically, it means that vacuum quarks and gluons can flow through the vacuum with nonzero momentum. From this point of view the standard vacuum expectation values (VEVs) like $\langle : \bar{q}q : \rangle$, $\left\langle : \bar{q}D^2q : \right\rangle$, $\left\langle : g^2F^2 : \right\rangle$, ... appear as expansion coefficients of the quark $M(x) = \left\langle : \bar{q}(0)\hat{E}(0,x)q(x) : \right\rangle$ and gluon $D^{\mu\nu,\rho\sigma}(x)$

correlators in a Taylor series in the variable $x^2/4$. The correlator $D^{\mu\nu,\rho\sigma}(x)$ of gluonic field strengths

$$D^{\mu\nu,\rho\sigma}(x-y) \equiv \left\langle : TrF^{\mu\nu}(x)\hat{E}(x,y)F^{\rho\sigma}(y)\hat{E}(y,x) : \right\rangle , \tag{1}$$

may be parameterized in the form consistent with general requirements of the gauge and Lorentz symmetries as

$$\begin{aligned} D^{\mu\nu,\rho\sigma}(x) \quad &\equiv \quad \frac{1}{24}\left\langle : F^2 : \right\rangle \Big\{ (\delta_{\mu\rho}\delta_{\nu\sigma} - \delta_{\mu\sigma}\delta_{\nu\rho})[D(x^2) + D_1(x^2)] + \\ &+ \quad (x_\mu x_\rho \delta_{\nu\sigma} - x_\mu x_\sigma \delta_{\nu\rho} + x_\nu x_\sigma \delta_{\mu\rho} - x_\nu x_\rho \delta_{\mu\sigma}) \frac{\partial D_1(x^2)}{\partial x^2} \Big\}, \end{aligned} \tag{2}$$

where $\hat{E}(x,y) = P\exp\left(i\int_x^y A_\mu(z)dz^\mu\right)$ is the path-ordered Schwinger phase factor (the integration is performed along the *straight* line) required for gauge invariance and $A_\mu(z) = A^a_\mu(z)\dfrac{\lambda^a}{2}$, $F_{\mu\nu}(x) = F^a_{\mu\nu}(x)\dfrac{\lambda^a}{2}$, $F^a_{\mu\nu}(x) = \partial_\mu A^a_\nu(x) - \partial_\nu A^a_\mu(x) + f^{abc}A^b_\mu(x)A^c_\nu(x)$. The P-exponential ensures the parallel transport of color from one point to another. In (2), $\left\langle : F^2 : \right\rangle = \left\langle : F^a_{\mu\nu}(0)F^a_{\mu\nu}(0) : \right\rangle$ is a gluon condensate, and $D(x^2)$ and $D_1(x^2)$ are invariant functions which characterize nonlocal properties of the condensate in different directions. The form factors are normalized at zero by the conditions $D(0) = \kappa$, $D_1(0) = 1 - \kappa$, that depend on the dynamics considered. For example, for the self-dual fields $\kappa = 1$, while in the Abelian theory without monopoles the Bianchi identity provides $\kappa = 0$.

In [3], one has shown that the instanton model of the QCD vacuum provides a way to construct nonlocal vacuum condensates. Within the effective single instanton (SI) approximation one has obtained the expressions for the nonlocal gluon $D_I^{\mu\nu,\rho\sigma}(x)$ and quark $M_I(x)$ condensates and derived the average virtualities of quarks λ_q^2 and gluons λ_g^2 in the QCD vacuum. The behavior of the correlation functions demonstrates that in the SI approximation the model of nonlocal condensates can well reproduce the behavior of the quark and gluon correlators at *short distances*. Really, the quark and gluon average virtualities, defined via the first derivatives of the nonlocal condensates $M_I(x^2)$, $D_I(x)$ at the origin,

$$\lambda_q^2 \equiv -\frac{8}{M_I(0)}\frac{dM_I(x^2)}{dx^2}\bigg|_{x=0} = 2\frac{1}{\rho_c^2}\,, \qquad \lambda_g^2 \equiv -8\frac{dD_I(x^2)}{dx^2}\bigg|_{x=0} = \frac{24}{5}\frac{1}{\rho_c^2}\,, \tag{3}$$

are connected with vacuum expectation values that parameterize the QCD SR,

$$\lambda_q^2 \equiv \frac{\left\langle : \bar{q}D^2 q : \right\rangle}{\left\langle : \bar{q}q : \right\rangle}, \quad \lambda_g^2 \equiv \frac{\left\langle : F^a_{\mu\nu}\tilde{D}^2 F^a_{\mu\nu} : \right\rangle}{\left\langle : F^2 : \right\rangle} = 2\frac{\left\langle : fF^3 : \right\rangle}{\left\langle : F^2 : \right\rangle} - 2\frac{\left\langle : g^4 J^2 : \right\rangle}{\left\langle : F^2 : \right\rangle}, \tag{4}$$

where $\left\langle : fF^3 : \right\rangle = \left\langle : f^{abc} F^a_{\mu\nu} F^b_{\nu\rho} F^c_{\rho\mu} : \right\rangle$, $J^2 = J^a_\mu J^a_\mu$ and $J^a_\mu = \bar{q}(x)\dfrac{\lambda^a}{2}\gamma_\mu q(x)$. The value of $\lambda_q^2 \approx 0.5\ \ \mathrm{GeV}^2$ estimated in the QCD SR analysis [4] is reproduced at $\rho_c \approx 2\ \mathrm{GeV}^{-1}$. This number is close to the estimate from the phenomenology of the QCD vacuum in the instanton liquid model. Nevertheless, the SI approximation used evidently fails in the description of physically argued distributions at large distances.

In [5], it was suggested that the instanton $A^{CI}_\mu(x)$ is developed in the physical vacuum field $b_\mu(x)$ interpolating large-scale vacuum fluctuations. One has found that at small distances the instanton field dominates, and at large distances it decreases exponentially. This solution is called constraint instanton (CI). The long-wave vacuum field $b_\mu(x)$ is specified by the correlation function $\widetilde{B}(x^2)$ determined by its strength $\left\langle F_b^2 \right\rangle_b$ and the correlation length R. Within this model, by averaging over random color vector orientations of the background field with respect to the fixed instanton field orientation, one has found the equation

$$D^{ab}_\mu \left[A^{CI}\right] F^{CI,b}_{\mu\nu}(x) - \frac{N_c \left\langle F_b^2 \right\rangle_b}{24(N_c^2-1)} x^2 \Phi\left(x^2\right) A^{CI,a}_\mu(x) + \text{Constraint term} = 0, \tag{5}$$

governing the deformation of the instanton under the influence of the weak background vacuum field. The constraint term is added to stabilize the instanton against shrinking [6]. In (5)

$$\Phi\left(x^2\right) = 4\int_0^1 d\alpha \int_0^1 d\beta \alpha\beta \widetilde{B}\left[(\alpha-\beta)^2 x^2\right], \qquad \Phi(0) = 1, \tag{6}$$

and N_c is the number of colors. The constraint independent asymptotics of the instanton solution at large distances is found as

$$A^{CI,a}_{\mu,\mathrm{asympt}}(x) = \overline{\eta}^a_{\nu\mu} \frac{2x_\nu}{x^2} a_{4/3} (\rho\eta_g)^2 K_{4/3}\left[\frac{2}{3}\left(\eta_g |x|\right)^{3/2}\right],$$

where

$$a_{4/3} = \frac{2}{\Gamma(1/3)\, 3^{1/3}} \tag{7}$$

is the normalization coefficient, $K_{4/3}(z)$ is modified Bessel function and $\Gamma(z)$ is the Gamma-function. This solution is exponentially suppressed at large distances $\sim \exp\left[-\dfrac{2}{3}\left(\eta_g |x|\right)^{3/2}\right]$ unlike the powerful decreasing SI. It is important to note that the form of this asymptotics is also independent of the model for the background field and the driven parameter $\eta_g \sim \left(\dfrac{N_c}{9\left(N_c^2-1\right)} R \left\langle F_b^2 \right\rangle_b\right)^{\frac{1}{3}}$

only weakly depends on it. Assuming that the external field is weak, the CI profile function is close to SI profile at distances smaller than ρ_c and it decreases exponentially at distances larger than η_g^{-1}. The knowledge of the constraint-independent parts of CI allowed to construct the solution in the ansatz form

$$A_\mu^{CI,a}(x) = \overline{\eta}^a_{\nu\mu}\frac{x_\nu}{x^2}\varphi_g\left(x^2\right), \qquad \varphi_g\left(x^2\right) = \frac{\overline{\rho}^2\left(x^2\right)}{x^2+\overline{\rho}^2\left(x^2\right)}, \tag{8}$$

where the notation

$$\overline{\rho}^2\left(x^2\right) \;=\; a_{4/3}\eta_g^2 x^2 K_{4/3}\left[\frac{2}{3}(\eta_g x)^{3/2}\right], \qquad \overline{\rho}^2\left(0\right) = \rho^2$$

is introduced. By translational invariance the centre of CI can be shifted in (8) from the origin to an arbitrary position x_0: $x \to x - x_0$.

By averaging over the instanton orientations in the color space and taking the trace over color matrices the invariant functions $D\left(x^2\right)$ and $D_1\left(x^2\right)$ can be extracted. It is convenient to define the combinations of functions $D\left(x^2\right)$ and $D_1\left(x^2\right)$

$$A\left(x^2\right) = \delta_{\mu\rho}\delta_{\nu\sigma}\frac{D^{\mu\nu,\rho\sigma}(x)}{\left\langle 0\left|F^2_{\mu\nu}\right|0\right\rangle^{CI}} = D\left(x^2\right) + D_1\left(x^2\right) + \frac{1}{2}x^2\frac{\partial D_1\left(x^2\right)}{\partial x^2},$$

$$B\left(x^2\right) = 4\frac{x_\mu x_\rho}{x^2}\delta_{\nu\sigma}\frac{D^{\mu\nu,\rho\sigma}(x)}{\left\langle 0\left|F^2_{\mu\nu}\right|0\right\rangle^{CI}} = D\left(x^2\right) + D_1\left(x^2\right) + x^2\frac{\partial D_1\left(x^2\right)}{\partial x^2}, \tag{9}$$

taking the boundary condition, $D(0) + D_1(0) = 1$ and the asymptotic conditions $D(\infty) = D_1(\infty) = 0$. The final expressions for form factors A and B [5] are:

$$\begin{aligned} A(x^2) = \frac{8}{\pi}N_D\int_0^\infty dr r^2\int_0^\infty dt\,\{&[\omega_1(z_+)\,\omega_1(z_-) + \omega_3(z_+)\,\omega_3(z_-)] \\ &\times\left(3-4\sin^2(\alpha_z)\right) - 2\omega_2(z_+)\,\omega_2(z_-) \\ &\times\left[r^2x^2\left(1-2\sin^2(\alpha_z)\right) - rx\,(z_+\cdot z_-)\sin(2\alpha_z)\right]\}, \end{aligned} \tag{10}$$

$$\begin{aligned} B(x^2) = \frac{16}{\pi}N_D\int_0^\infty dr r^2\int_0^\infty dt\,\{&\omega_1(z_+)\,\omega_1(z_-)\left(3-4\sin^2(\alpha_z)\right) \\ &-\omega_1(z_+)\,\omega_2(z_-)\left[z_-^2 + 2t_-^2\left(1-2\sin^2(\alpha_z)\right) + 2rt_-\sin(2\alpha_z)\right] \\ &-\omega_2(z_+)\,\omega_1(z_-)\left[z_+^2 + 2t_+^2\left(1-2\sin^2(\alpha_z)\right) - 2rt_+\sin(2\alpha_z)\right] \\ &+\omega_2(z_+)\,\omega_2(z_-)\left[z_+^2z_-^2 + 2t_+t_-\,(z_+\cdot z_-)\left(1-2\sin^2(\alpha_z)\right)\right. \\ &\left.+2rxt_+t_-\sin(2\alpha_z)\right]\}, \end{aligned} \tag{11}$$

where

$$\omega_1(x) = x^2\varphi_g^2\left(x^2\right) - \varphi_g\left(x^2\right), \qquad \omega_2(x) = \varphi_g^2\left(x^2\right) + \frac{\partial\varphi_g\left(x^2\right)}{\partial x^2}, \tag{12}$$

$$x_\rho^2 = x^2 + \rho^2,$$

$z_\pm = (r, t_\pm)$, $t_\pm = t \pm \dfrac{x}{2}$, N_D is the normalization factor

$$N_D^{-1} = 6\int_0^\infty dy y^3\left(\omega_1^2(y) + \omega_3^2(y)\right), \tag{13}$$

and the phase factor

$$\alpha_z = r\int_{-\frac{x}{2}}^{\frac{x}{2}} d\tau\varphi_g\left(r^2 + (t+\tau)^2\right),$$

reflects the presence of the $\hat{E}$ exponent in the definition of the bilocal correlator. The form factors $D(x^2)$ and $D_1(x^2)$ are determined numerically by solving the equations (9) and plotted in the Figure in coordinate space. As it turns out, at a reasonable set of parameters, guaranteeing the smallness of the large-scale vacuum field fluctuations, the $D\left(x^2\right)$ structure is close to the SI induced function with the exponential asymptotics being developed at large distances. At the same time, the $D_1\left(x^2\right)$ structure is about two orders smaller than the $D\left(x^2\right)$ function at any reasonable choice of the parameter $\rho_c\eta_g$. The lattice data are in qualitative agreement with predictions of the constrained instanton model.

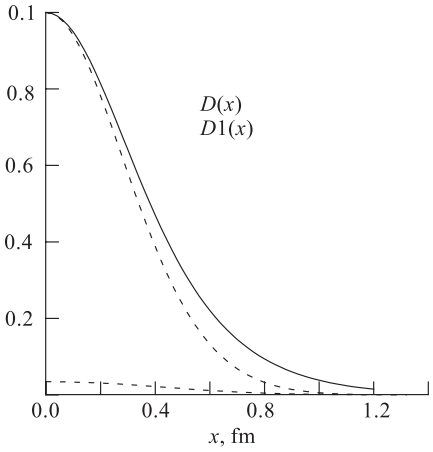

Fig. 1. The form factors D (top lines) and D_1 (bottom lines) (all normalized by $D(0)$) versus physical distance x, for the instanton size $\rho = 0.3$ fm and parameters $(\rho\eta_g)^2 = 0$ (solid lines) and $(\rho\eta_g)^2 = 1$ (dashed lines)

The nonperturbative part of the invariant functions $A(x^2)$ and $B(x^2)$ are the sum of short-range instanton induced contributions (10) and (11), multiplied by the weight factor $n_c 32\pi^2/\left\langle 0\left|F^2\right|0\right\rangle_{\text{total}}$, and the long-range contribution

$$\widetilde{B}\left(z^2\right) = \widetilde{D}\left(z^2\right) + \widetilde{D}_1\left(z^2\right) + z^2\partial\widetilde{D}_1\left(z^2\right)/\partial z^2 \tag{14}$$

modeled by exponentially decreasing function $\widetilde{B}_E\left(x^2\right) = \exp(-|x|/R)$, with the weight factor $\left\langle F_b^2 \right\rangle_b / \left\langle 0 \left| F^2 \right| 0 \right\rangle_{\rm total}$. The constrained instanton model introduces two characteristic scales (correlation lengths). One is related to short distance behavior of the correlation functions and another with long range distance behavior. The first one, λ_g^{-1}, is predictable and expressed in terms of physical quantities.

The instanton model predicts the behaviour of nonpertirbative part of gluon correlation functions in the short and intermediate region assuming that it is dominated by instanton vacuum component, while the large-scale asymptotics is dominated by the background field.

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BOUND STATES IN QUANTUM FIELD THEORY

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The method called «the Bosonization of Nonlocal Currents» (BNC), used for calculations of bound states in a quark model, is demonstrated within the simplest relativistic quantum field model of two scalar fields with the Yukawa type interaction.

Hadronization of quarks and gluons is one of the most important and interesting problems of QCD. In papers [1] we have formulated «the Model of Induced Nonlocal Quark Currents», based on the assumption that QCD vacuum is realized by the (anti-)self-dual homogeneous vacuum field. All calculations of the meson spectrum and other characteristics of light mesons in this model were done by the method of «Bosonization of Nonlocal Currents» and quite good agreement with experimental data was obtained. Our method is quite close to the so-called $Z_2 = 0$ method (see, for example, [2–4]) and differs from the known axiomatic methods (see, for example, [5–7]). In this talk I would like to demonstrate our method on a simple but nontrivial QFT model.

Our initial idea is based on the standard physical interpretation of a Lagrangian of a system of fields (for example, ϕ). Usually the Lagrangian can be represented in the form $L = L_0[\phi] + gL_I[\phi]$. The physical particles ϕ are described by the «free Lagrangian» $L_0[\phi]$, which is quadratic over fields ϕ. The interactions of particles are described by the «interaction Lagrangian» $L_I[\phi]$, which contains the field operators ϕ in the third or more degree. This interpretation can be reasonable if the coupling constant g is small enough. The generating functional, or partition function contains amplitudes of all physical processes and can be written in the form of the functional integral

$$Z[J] = Z[J;\phi] = \int D\phi \; e^{i\int dx L_0[\phi] + ig\int dx L_I[\phi] + \int dx \phi J}. \qquad (1)$$

Usually we can perform calculations expanding the generating functional over the coupling constant g.

Let us suppose that we are able after some functional transformations and changing the functional variables to rewrite the representation (1) in the form

$$Z[J] = Z[J;B] = \int DB \; e^{i\int dx \mathrm{L}_0[B] + ig_{\mathrm{eff}}\int dx \mathrm{L}_I[B] + W[B,J]}. \qquad (2)$$

Here the «free Lagrangian» $\mathrm{L}_0[B]$ is quadratic over fields B and the «interaction Lagrangian» $\mathrm{L}_I[B]$ contains the field B in the third or more degree. The effective coupling constant g_{eff} should be small enough. Then we can say that the new Lagrangian $\mathrm{L} = \mathrm{L}_0[B] + g_{\mathrm{eff}}\mathrm{L}_I[B]$ describes the physical particles B and these paricles can be considered as bound states of the initial particles ϕ.

Let us demonstrate our method on the simple quantum field model describing the Yukawa interaction of charged scalar bosons Φ and neutral bosons ϕ. The Lagrangian density is

$$L(x) \quad = \quad \Phi^+(\Box - M^2)\Phi + \frac{1}{2}\phi(\Box - m^2)\phi + g\Phi^+\Phi\phi. \tag{3}$$

In this model it is possible to retrace all details of bound states arising in quantum field theory. Generalization to the case of the Dirac field presents no difficulties of principle and leads to technical problems connected with the algebra of γ-matrices only. This model is superrenormalizable so that the renormalization procedure has the simplest form.

1. The Initial Representation. Let us put the Lagrangian (3) into the representation (1) and integrate over the field ϕ, we get

$$Z \quad = \quad \int\int D\Phi D\Phi^+ \cdot e^{-(\Phi^+ D_M^{-1}\Phi) + \frac{g^2}{2}(\Phi^+\Phi D_m \Phi^+\Phi)}, \tag{4}$$

$$\begin{aligned} (\Phi^+ D_M^{-1}\Phi) \quad &= \quad \int dx\ \Phi^+(x)(-\Box + M^2)\Phi(x), \\ \frac{g^2}{2}(\Phi^+\Phi D_m\Phi^+\Phi) \quad &= \quad \int dx \int dy\ \Phi^+(x)\Phi(x)D_m(x-y)\Phi^+(y)\Phi(y). \end{aligned}$$

For simplicity we have omitted the term with the current J, which can be restored without any problems.

Let us introduce the bilocal current:

$$J(y_1, y_2) = \sqrt{D_m(y_1 - y_2)}(\Phi^+(y_1)\Phi(y_2)),$$

and use the Gaussian representation

$$e^{\frac{g^2}{2}(\Phi^+\Phi D_m\Phi^+\Phi)} = e^{\frac{g^2}{2}(J^+J)} = \int DA\ e^{-\frac{1}{2}(A^+A) - g\ (A^+J)}.$$

Here $A = A(x_1, x_2)$ is a bilocal field. Now we can calculate in (4) the Gaussian integral over Φ and Φ^+:

$$Z = \int DA\ e^{-\frac{1}{2}(A^+A) - \mathrm{tr}\ln\left[1 + g(A^+\sqrt{D_m})D_M\right]}. \tag{5}$$

2. Linear Term. Our problem is to give the standard particle interpretation to the action $S[A]$ in (5). For this aim this action should be represented in the form

$$S[A] = -\frac{1}{2}(A^+ R^{-1} A) + I_{int}[A], \qquad I_{int}[A] = O(A^3).$$

It means that we have to remove the term linear in A and extract the quadratic term out of $S[A]$. Let us introduce the displacement

$$A(y_1, y_2) = A_1(y_1, y_2) + \frac{a(x_1 - x_2)}{g\sqrt{D_m(x_1 - x_2)}}.$$

The term linear in A will be equal to zero if

$$a(x_1 - x_2) = -g^2 D_m(x_1 - x_2)\mathcal{D}(x_1 - x_2),$$

where

$$\mathcal{D} = D_M \cdot \frac{1}{1 + aD_M}, \qquad \tilde{\mathcal{D}}(k^2) = \frac{1}{M^2 + k^2 + \tilde{a}(k^2)},$$

which is the Schwinger–Dyson equation. In the momentum representation this Schwinger–Dyson equation contains the logarithmic ultraviolet divergence which can be removed by the renormalization of the mass M. It means that we should put

$$M^2 + \tilde{a}(k^2) = M_r^2 + \tilde{a}_r(k^2), \qquad \tilde{a}_r(k^2) = \tilde{a}(k^2) - \tilde{a}(-M_r^2),$$

where M_r is the «physical» mass of the constituent particle Φ and the renormalized function $a_r(k^2) = \tilde{a}(k^2) - \tilde{a}(-M_r^2)$ satisfies the equation

$$\begin{aligned} a_r(k^2) &= g^2 \int \frac{dp}{(2\pi)^4} \cdot \left[\frac{1}{(m^2 + (q-p)^2)(M_r^2 + p^2 + a_r(p^2))}\bigg|_{q^2 = -M_r^2} \right. \\ &- \left. \frac{1}{(m^2 + (k-p)^2)(M_r^2 + p^2 + a_r(p^2))} \right]. \end{aligned} \tag{6}$$

This functional equation is of the type $a_r(k^2) = F[a_r, k^2]$ and can be solved by the fixed point method, i.e., we choose the initial «point» $a_r^{(0)}(k^2)$ and calculate

$$a_r^{(n+1)}(k^2) = F[a_r^{(n)}, k^2], \quad \text{and} \quad \lim_{n\to\infty} a_r^{(n)}(k^2) = a_r(k^2).$$

In subsequent calculations we use the zeroth approximation

$$\tilde{\mathcal{D}}(k^2) = \tilde{D}_r = \frac{1}{M_r^2 + k^2}$$

which gives quite acceptable qualitative semiquantitative estimations.

3. From Bilocal to Local Fields. After removing the linear term we have

$$\begin{aligned} S[A] &= -\frac{1}{2}(A^+A) - \mathrm{tr}\ln_1\left[1 + g(A^+\sqrt{D_m})D_r\right], \\ &\ln_1(1+s) = \ln(1+s) - s. \end{aligned}$$

Let a system of functions $\{U_Q(y)\}$ with quantum numbers $Q = (nl\{\mu\})$, where n, l and $\{\mu\}$ are radial, orbital and magnetic quantum numbers, be orthonormal, i.e.,

$$\begin{aligned} &(U_Q U^*_{Q'}) = \int d^4y\ U_Q(y)U^*_{Q'}(y) = \delta_{QQ'} = \delta_{nn'}\delta_{ll'}\delta_{\{\mu\}\{\mu'\}}, \\ &\sum_Q U_Q(y)U^*_Q(y') = \delta(y-y'). \end{aligned} \tag{7}$$

Let us introduce in the «$\mathrm{tr}\ln_1\left[1 + g(A^+\sqrt{D_m})D_r\right]$» new variables

$$x_j = z_j + \frac{y_j}{2}, \qquad x_{j+1} = z_j - \frac{y_j}{2},$$

and represent the bilocal functions in the form:

$$A(x_j, x_{j+1}) = \sum_Q W_Q(z_j)U_Q(-y_j). \tag{8}$$

Then we have

$$\begin{aligned} &(A^+\sqrt{D_m}) = (WV) = \sum_Q W_Q(z)V_Q\left(\overleftrightarrow{p}_x\right), \qquad \overleftrightarrow{p}_x = \frac{1}{i}\left(\overleftarrow{\partial}_x - \overrightarrow{\partial}_x\right), \\ &V_Q\left(\overleftrightarrow{p}_x\right) = \int dy\sqrt{D_m(y)}U_Q(y)e^{-i\frac{y}{2}\overleftrightarrow{p}_x}. \end{aligned} \tag{9}$$

The basic representation for the partition function gets the form

$$Z = \int\prod_Q DW_Q \cdot e^{-\frac{1}{2}(WW) - \mathrm{tr}\ln_1[1+g_r(WV)D_r]}. \tag{10}$$

4. Particle Interpretation of the Quadratic Term. Let us extract the quadratic form from $\mathcal{S}[W]$

$$\begin{aligned} \mathcal{S}[W] &= -\frac{1}{2}(W[I - g_r^2\Pi]W) - \mathrm{tr}\ln_2[1 + g_r(WV)D_r], \\ &\ln_2(1+s) = \ln(1+s) - s + \frac{s^2}{2}. \end{aligned} \tag{11}$$

Here

$$(Wg_r^2\Pi W) = \sum_{QQ'}\int\int dxdx'\ W_Q(x)g_r^2\Pi_{QQ'}(x-x')W_{Q'}(x').$$

The polarization operator $g_r^2\tilde{\Pi}_{QQ'}$ looks

$$\begin{aligned} g_r^2\Pi_{QQ'}(x-x') &= g_r^2\iint dydy'\ U_Q(y)P(x-x';y,y')U^*_{Q'}(y'),\\ P(x;y,y') &= \sqrt{D_m(y)}D_r\left(x-\frac{y-y'}{2}\right)D_r\left(x+\frac{y-y'}{2}\right)\sqrt{D_m(y')},\\ \tilde{P}(p;y,y') &= \int dx\ e^{ipx}P(x;y,y'). \end{aligned}$$

In the momentum space we get

$$g_r^2\tilde{\Pi}_{QQ'}(p) = g_r^2\int\frac{dk}{(2\pi)^4}\cdot\frac{V_Q(k)V_{Q'}(k)}{\left(M_r^2+\left(k+\frac{p}{2}\right)^2\right)\left(M_r^2+\left(k-\frac{p}{2}\right)^2\right)}. \quad (12)$$

The orthonormal system $\{U_Q(x)\}$ should be chosen so that the polarization operator $\tilde{\Pi}_{QQ'}(p)$ should be diagonal in radial (n,n') and orbital (l,l') quantum numbers. The index structure of the diagonal polarization operator $\tilde{\Pi}^{(nl)}_{\{\mu\}\{\mu'\}}(p)$ looks like

$$\tilde{\Pi}^{(nl)}_{\{\mu\}\{\mu'\}}(p) = \tilde{\Pi}^{(nl)}(p^2)\cdot\delta_{\{\mu\}\{\mu'\}} + \sum_j\tilde{\Pi}^{(nl)}_j(p^2)\cdot t^j_{\{\mu\}\{\mu'\}}(p), \quad (13)$$

where the tensors $t^j_{\{\mu\}\{\mu'\}}(p)$ contain combinations of the vectors $p_\mu p_{\mu'}$.

The diagonal quadratic form of (11) gives the equation of motion for the field $W_Q(x) = W^{(nl)}_{\{\nu\mu_2\ldots\mu_l\}}(x)$

$$\left[\delta_{QQ'} - g_r^2\tilde{\Pi}_{QQ'}\left(\frac{\partial}{i\partial x}\right)\right]W_{Q'}(x) = 0, \quad \left[\delta_{QQ'} - g_r^2\tilde{\Pi}_{QQ'}(p)\right]\tilde{W}_{Q'}(p) = 0.$$

The requirement that this equation on the mass shell should be the Klein–Gordon equation gives the constraint

$$\frac{\partial}{\partial x_\nu}W^{(nl)}_{\nu\mu_2\ldots\mu_l}(x) = 0 \qquad \text{or} \qquad p_\nu\tilde{W}^{(nl)}_{\{\nu\mu_2\ldots\mu_l\}}(p) = 0$$

on the mass shell. Thus, the function $\tilde{W}^{(nl)}_{\{\mu\}}(p)$ satisfies the equation

$$\left[1 - g_r^2\tilde{\Pi}^{(nl)}(p^2)\right]\tilde{W}^{(nl)}_{\{\mu_1\ldots\mu_l\}}(p) = 0. \quad (14)$$

The mass of the state with quantum numbers $Q = (nl)$ is defined by

$$1 - g_r^2 \tilde{\Pi}^{(nl)}(-M^2_{(nl)}) = 0. \tag{15}$$

Let us write

$$-1 + g_r^2 \tilde{\Pi}^{(nl)}(p^2) = -Z_{(nl)}(p^2 + M^2_{(nl)}) + \Sigma^{(nl)}(p^2),$$
$$Z_{(nl)} = g_r^2 \left[-\tilde{\Pi}'_{(nl)}(-M^2_{(nl)}) \right], \quad \Sigma^{(nl)}(p^2) = O((p^2 + M^2_{(nl)})^2).$$

The constant $Z_{(nl)}$ is positive.

New field variables can be introduced as follows:

$$W_Q(x) = \frac{\varphi_Q(x)}{\sqrt{Z_{(nl)}}}. \tag{16}$$

The representation (10) assumes the form

$$Z = \int \prod_Q D\varphi_Q \; e^{-\frac{1}{2}(\varphi \mathcal{D}^{-1} \varphi) - \mathcal{I}_{\rm int}[\varphi]}. \tag{17}$$

Here the kinetic term is

$$\begin{aligned} (\varphi \mathcal{D}^{-1} \varphi) &= (\varphi \left[-\Box + M_b^2 + \Sigma_b \right] \varphi) \\ &= \int dp \sum_{\mathcal{Q}} \tilde{\varphi}^+_Q(p) \left[p^2 + M^2_{(nl)} + \Sigma^{(nl)}(p^2) \right] \tilde{\varphi}_Q(p) \end{aligned} \tag{18}$$

and the interaction term is

$$\mathcal{I}_{\rm int}[\varphi] = \mathrm{tr} \ln_2 \left[1 + (h\varphi V)\mathcal{D} \right], \tag{19}$$
$$(h\varphi V) = \sum_Q h_Q \varphi_Q V_Q, \qquad h_Q = \frac{1}{\sqrt{-\Pi'_Q(-M^2_Q)}}.$$

The effective dimensionless coupling constants are defined as

$$\lambda_Q^{(\rm eff)} = \frac{h_Q^2}{16\pi M_r^2} = \frac{1}{16\pi[-M_r^2 \tilde{\Pi}'_{(nl)}(-M^2_{(nl)})]}. \tag{20}$$

As a result, the final representation (17) can be interpreted as a partition function of the quantum field system of bosonic fields $\{\phi_Q\}$ which have masses M_Q and interact by means of the nonlocal interaction Lagrangian (19).

We would like to stress that the resulting representation for the generating functional does not contain the initial coupling constant g.

All calculations with the generating functional (17) can be performed by perturbation expansions in coupling constants h_Q. We can trust these calculations if and only if the effective coupling constants (20) are small enough:

$$\lambda_Q^{(\mathrm{eff})} \ll 1.$$

5. The Orthonormal System. The next step is to determine the orthonormal system (7). The problem is to find the spectrum and eigenfunctions of the operator $\tilde{P}(p; y, y')$ in (12), i.e.,

$$\int dy' \tilde{\mathcal{P}}(p; y, y') U_Q(y', p) = E_Q(p) U_Q(y, p), \qquad Q = (n, l, \{\mu\}). \quad (21)$$

This equation can be represented in a standard form of the Bethe–Salpeter equation in the one-boson exchange approximation. Using the relation

$$K_+ K_- \cdot \int dx\ e^{ipx} D_r \left(x - \frac{y - y'}{2} \right) D_r \left(x + \frac{y - y'}{2} \right) = \delta(y - y')$$

with

$$K_\pm = \left[M_r^2 + \left(i \frac{\partial}{\partial y} \pm \frac{p}{2} \right)^2 \right]$$

and introducing the functions

$$\Psi_Q(y, p) = \frac{1}{\sqrt{D_m(y)}} \cdot U_Q(y, p)$$

we get the standard form of the Bethe–Salpeter equation (see, for example, [10])

$$\left[M_r^2 + \left(i \frac{\partial}{\partial y} + \frac{p}{2} \right)^2 \right] \cdot \left[M_r^2 + \left(i \frac{\partial}{\partial y} - \frac{p}{2} \right)^2 \right] \Psi_Q(y, p) = g_r^2 D_m(y) \Psi_Q(y, p),$$

where the spectrum is defined by the equation

$$g_r^2 E_Q(-M_Q^2) = 1.$$

Thus the diagonalization of the operator $\tilde{P}(p; y, y')$ is equivalent to the solution of the Bethe–Salpeter equation in one-boson exchange approximation.

Now we would like to remark the following. Our mathematical task is to diagonalize an operator and we are not able to do it analytically. There exist two ways to overcome this difficulty and these ways are defined by physical problems under consideration. If we calculate corrections to precision experiments (for example, quantum electrodynamics phenomena), which require quite high

accuracy, we have to get solutions, accuracy of which should be around $10^{-5} \div 10^{-6}$ %. This accuracy can be obtained by numerical methods using quite powerful computers only. If we consider particle physics phenomena where required accuracy is not so high, then the mathematical method with accuracy $1 \div 5$ % is completely acceptable. Our method formulated in the given paper is relative to the second point of view.

The main problem to use the Bethe–Salpeter basis is that the Bethe–Salpeter equation can only be solved by numerical methods. Even the solution obtained by Wick and Cutkosky [8,10] is reduced to the differential equation which should be numerically computed. Our aim is to continue analytic calculations as long as possible in order to get a visible general picture of arising bound states in the system under consideration. Therefore we choose a more practical way, namely, we use an orthonormal basis that is simple enough from an analytic point of view and is directly connected with the problem under consideration. In this case the operators $g_r^2\tilde{\Pi}_{QQ'}$ are not diagonal so that we should diagonalize them. The idea consists in finding an effective basis for diagonalization of $g_r^2\tilde{\Pi}_{QQ'}$ such that its lowest function would provide a good qualitative description for the eigenvalues $E_{(nl)}$ and the next two or three functions only give a good quantitative description for those eigenvalues.

This effective basis $\{U_Q(x)\}$ can be constructed using the standard boson Green function $D_a(u)$ with a mass a as a weight function inducing uniquely the system of orthonormal polynomials in the space R^4. Thus, the full orthonormal system of functions (7) can be chosen in the form

$$U_Q(x,a) = i^l\sqrt{D_a(x)}aP_Q(ax). \tag{22}$$

Here $P_Q(u)$ are real polynomials. The mass parameter a that enters into the orthonormal system is fixed by a variation condition formulated below.

The construction of this basis is presented in the Appendix A in [11].

6. The Polarization Operator. The problem is that our basis does not diagonalize the polarization operators (12) for states $Q = (nl\{\mu\})$ and $Q' = (n'l\{\mu'\})$ and does not have the form (13), so that the diagonalization procedure should be performed. In the momentum space the nondiagonal polarization operators (12) for states $Q = (nl\{\mu\})$ and $Q' = (n'l\{\mu'\})$ according to the representation (13) for $p^2 = -M_b^2$ look like

$$g_r^2\tilde{\Pi}^{(nn',l)}(p^2|a) = \frac{32\lambda_r M_r^2}{(2\pi)^2}\cdot\frac{2^l(l!)^2}{(2l+1)!}\cdot\int\limits_0^\infty dk\ k^{3+2l}\cdot V_{(nl)}(k^2|a)V_{(n'l)}(k^2|a)\times$$

$$\times\int\limits_0^1\frac{dt\ (1-t^2)^{\frac{1}{2}+l}}{\left(M_r^2-\frac{M_b^2}{4}+k^2\right)^2+k^2M_b^2t^2},$$

where $\lambda_r = \frac{g_r^2}{16\pi M_r^2}$ and the vertex looks

$$V_{(nl)}(k^2|m,a) \quad = \quad \int dx \ \sqrt{D_m(x)D_a(x)}a^{1+l}P_{(nl)}(a^2x^2)e^{ixp}. \qquad (23)$$

We shall use the approximation

$$\sqrt{D_m(x)D_a(x)} \approx D_{\frac{m+a}{2}}(x), \qquad (24)$$

the accuracy of which is quite acceptable for our consideration. In particular

$$V_{(0l)}(k^2|m,a) = \frac{a^{1+l}\,2^{l/2}}{M_r^{2+2l}\left(\left(\frac{m+a}{2M_r}\right)^2 + \frac{k^2}{M_r^2}\right)^{1+l}}. \qquad (25)$$

Now we formulate the variational principle which defines the parameter a. The mass $M_{(nl)}$ of the bound state with quantum numbers (nl) should be defined by the equation

$$1 = \lambda_r \tilde{\Pi}_{(nn,l)}(M_{(nl)}|m,a).$$

The function $\tilde{\Pi}_{(nl)} = \tilde{\Pi}_{(nn,l)}$ is the largest eigenvalue of the matrix $\tilde{\Pi}^{(n_1n_2,l)}$ for $n_1, n_2 \geq n$, therefore the parameter $a = a_n$ can be defined by the variation requirement

$$\tilde{\Pi}_{(nl)}(b,\xi) = \max_a \ \tilde{\Pi}_{(nn,l)}(M_b|m,a), \qquad (26)$$

which gives $a = a_{(nl)}(b,\xi)$ where the notions $b = \left(\frac{M_b}{2M_r}\right)^2$, $\xi = \frac{m}{M_r}$ are used. Thus, the parameter $a_{(nl)}(b,\xi)$ is a function of m and M_b. The mass

$$M_{(nl)} = M_{(nl)}(\lambda_r,\xi) = 2M_r \cdot b_{(nl)}(\lambda_r,\xi)$$

is defined by the equation

$$1 = \lambda_r \tilde{\Pi}_{(n,l)}(b_{(nl)},\xi). \qquad (27)$$

In order to show that this orthonormal functions with the parameter $\eta = \frac{a}{M_r}$ give quite good approximation for the eigenvalues of the matrix $\tilde{\Pi}_{(nn')}(p^2)$ we have calculated the matrix

$$\mathcal{P}^{(N)} = \left\{\tilde{\Pi}_{(n_1n_2)}(b,\xi,\eta), \quad (n_1,n_2 = 0,1,2,...,N)\right\}$$

and their eigenvalues

$$\mathcal{E}_n^{(N)} = \mathrm{diag}\left\{\mathcal{P}^{(N)}\right\} = \mathrm{diag}\left\{E_0^{(N)}, E_1^{(N)}, ..., E_N^{(N)}\right\}.$$

Then we have to compare $E_n^{(N)}$ for different $N = 0, 1, ...$

The numerical results are given in the Table: the first case for $\xi = .5,\ b = .25,\ \eta = 2.451$ and the second case for $\xi = .2,\ b = .9,\ \eta = 1.22$. One can see that for the lowest eigenvalue practically the first lowest eigenfunction can be used, i.e., our choice of the orthonormal system gives quite a good accuracy.

Table. Diagonalization of the matrix $\mathcal{P}_N$

N	E_0	E_1	E_2	E_3	E_0	E_1	E_2	E_3
0	.04165				.1239			
1	.04166	.009941			.1262	.03564		
2	.04173	.010279	.002755		.1262	.03616	.01162	
3	.04175	.010368	.003295	.0007482	.1263	.03645	.01298	.003789
4	.04175	.010402	.003546	.0010336	.1263	.03655	.01373	.004710

In conclusion we can say that the representations (4) and (17) are equivalent and the representation (17) contains the bound states of the initial system (3) of particles Φ and ϕ.

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THE INTERPLAY BETWEEN PERTURBATIVE QCD AND POWER CORRECTIONS: THE DESCRIPTION OF SCALING OR AUTOMODELLING LIMIT VIOLATION IN DEEP-INELASTIC SCATTERING

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The summary of the results of our next-to-next-to-leading fits of the Tevatron experimental data for xF_3 structure function of the νN deep-inelastic scattering is given. The special attention is paid to the extraction of twist-4 contributions and demonstration of the interplay between these effects and higher order perturbative QCD corrections. The factorization and renormalization scale uncertainties of the results obtained are analyzed.

1. The study of deep-inelastic scattering (DIS) processes has a rather long and inspiring history. One of the first realizations that the analysis of νN DIS could play an important role in investigations of the properties of the nucleon came in Ref. 1. The fundamental concept of scaling of DIS structure functions (SFs) [2] has lead to many subsequent investigations. Other important stages in the development of both theoretical and experimental studies of various characteristics of DIS processes in this productive period were reviewed in detail recently [3].

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In particular, it was stressed that after the experimental confirmation of scaling and indications of the existence of point-like constituents of the nucleon, the more rigorous theoretical explanation of the behaviour of DIS form factors came onto the agenda. A series of works by N.N.Bogoliubov and coauthors [4], were devoted to the development of the new method, which made it possible to analyse the asymptotics of the form factors of eN DIS using the Jost–Lehmann–Dyson integral representation, and explain the property of scaling (or as called by the authors of Ref. 4 «automodelling») behaviour of the corresponding SFs in the framework of general principles of local quantum field theory [5].

We now know that this property is true only in the asymptotic regime and that it is violated within the framework of QCD (see, e.g., the extensive discussions in a number of books on the subject [6]). Indeed, the theory of QCD predicts that scaling or automodelling behaviour of SFs is violated by the logarithmically decreasing perturbative QCD contributions to the leading twist operators. However, in the intermediate and low Q^2 regime the higher twist operators, which give rise to scaling violations of the form $1/Q^2$, $1/Q^4$, etc., might also be important [7,8]. Indeed, the NLO DGLAP fits [9] of the BCDMS data of DIS of charged leptons on nucleons [10] and reanalysed SLAC eN data [11] resulted in the detection of the signals from the twist-4 contributions.

During the last few years there has been considerable progress in modelling these effects with the help of the infrared renormalon (IRR) approach (for the review see Ref. 12) and the dispersive method [13] (see also Ref. 14). Using these methods the authors of Ref. 15 explained the behaviour of the twist-4 contributions to the F_2 SF observed in Ref. 9 and constructed a model for the similar power-suppressed corrections to xF_3 SF. In view of this it became important to check the predictions of Ref. 15 and to study the possibility of extracting higher-twist contributions from the new more precise experimental data for νN DIS, obtained by the CCFR collaboration at Fermilab Tevatron [16], and also to exploit the considerable progress in calculations of the perturbative QCD corrections to characteristics of DIS, achieved in the last decade.

Indeed, the analytic expressions for the next-to-next-to-leading order (NNLO) perturbative QCD corrections to the coefficient functions of SFs F_2 [17] and xF_3 [18] are now known. Moreover, the expressions for the NNLO corrections to the anomalous dimensions of nonsinglet (NS) even Mellin moments of F_2 SF with $n = 2, 4, 6, 8, 10$ and for the N^{3}LO corrections to the coefficient functions of these moments are also available [19]. In this report we will summarize the results of the series of the works of Refs. 20–22, devoted to the analysis of the CCFR data at NNLO, which has the aim to determine the NNLO value of the QCD coupling constant $\alpha_s(M_Z)$ and to extract the effects of the twist-4 contributions to SF xF_3 [21, 22]. In particular, we will concentrate on the discussion of the factorization and renormalization scale uncertainties of the results obtained.

2. Our analysis of Refs. 20–22 is based on reconstruction of the SF xF_3 from its Mellin moments $M_n(Q^2) = \int_0^1 x^{n-1} F_3(x,Q^2)dx$ using the Jacobi polynomials method, proposed in Ref. 23 and further developed in the works of Ref. 24. Within this framework one has:

$$xF_3(x,Q^2) = x^{\alpha}(1-x)^{\beta} \sum_{n=0}^{N_{max}} \Theta_n^{\alpha,\beta}(x) \sum_{j=0}^{n} c_j^{(n)}(\alpha,\beta) M_{j+2}(Q^2), \qquad (1)$$

where $\Theta_n^{\alpha,\beta}$ are the Jacobi polynomials, $c_j^{(n)}(\alpha,\beta)$ are combinatorial coefficients given in terms of Euler Γ-functions of the α and β weight parameters. In view of the reasons discussed in Ref. 22, they were fixed to 0.7 and 3, respectively. The QCD evolution of the moments is defined by the solution of the corresponding renormalization group equation:

$$\frac{M_n(Q^2)}{M_n(Q_0^2)} = exp\Big[- \int_{A_s(Q_0^2)}^{A_s(Q^2)} \frac{\gamma_{NS}^{(n)}(x)}{\beta(x)} dx \Big] \frac{C_{NS}^{(n)}(A_s(Q^2))}{C_{NS}^{(n)}(A_s(Q_0^2)}. \qquad (2)$$

The QCD running coupling constant enters this equation through $A_s(Q^2) = \frac{\alpha_s(Q^2)}{(4\pi)}$ and is defined as the expansion in terms of inverse powers of $ln(Q^2/\Lambda^{(4)\ 2}_{\overline{MS}})$. For the initial scale Q_0^2, from which the evolution is started, the moments in Eq.(2) were parametrized as $M_n(Q_0^2) = \int_0^1 x^{n-2} A(Q_0^2) x^{b(Q_0^2)}(1-x)^{c(Q_0^2)}(1+ +\gamma(Q_0^2)x)dx$. In the process of our analysis we took into account both target mass corrections and twist-4 contributions. The latter were modeled using the IRR approach as $M_n^{IRR} = C(n)M_n(Q^2)A_2^{'}/Q^2$ [15] and by adding into the r.h.s. of Eq.(1) the term $h(x)/Q^2$ with $h(x)$ considered as a free parameter for each x-bin of the experimental data.

For arbitrary factorization and renormalization scales the NNLO expression for the NS Mellin moments reads:

$$M_n(Q^2) \sim (A_s(Q^2 k_F))^a \times \overline{AD}(n, A_s(Q^2 k_F)) \times C_{NS}^{(n)}(A_s(Q^2 k_R)), \qquad (3)$$

where $a{=}\gamma_{NS}^{(0)}/(2\beta_0)$, $\overline{AD}{=}1{+}[p(n){+}ak_1^F]A_s(Q^2k_F){+}[q(n){+}p(n)(a{+}1)k_1^F{+}$ $+(\beta_1/\beta_0)ak_1^F{+}a(a{+}1)(k_1^F)^2/2]A_s^2(Q^2k_F)$ and $C_{NS}^{(n)}{=}1{+}C^{(1)}(n)A_s(Q^2k_R){+}$ $+[C^{(2)}(n){+}C^{(1)}(n)k_1^R]A_s^2(Q^2k_R)$. Here $\gamma_{NS}^{(0)}$, β_0, and β_1 are the scheme-independent coefficients of the anomalous dimension function $\gamma_{NS}(x)$ and QCD β-function $\beta(x)$, $p(n)$ and $q(n)$-terms are expressed through the NLO and NNLO coefficients of $\gamma_{NS}(x)$ and $\beta(x)$ via equations, given in Refs. 20,22. Within the $\overline{MS}$-like schemes the factorization and renormalization scale ambiguities are parameterized by the terms $k_1^F = \beta_0 ln(k_F)$ and $k_1^R = \beta_0 ln(k_R)$, where k_F (k_R) is the ratio of the factorization (renormalization) scale and the scale of the $\overline{MS}$-scheme. Following the analysis of Ref. 25 we take $k_R = k_F = k$, fixing

identically the factorization scale and the renormalization scale. We performed our fits for the case of $k = 1$ (namely, in the pure $\overline{MS}$-scheme) and then determine the scale uncertainties of $\Lambda^{(4)}_{\overline{MS}}$, the twist-4 parameter $A_2^{'}$ and the x-shape of $h(x)$ by choosing $k = 1/4$ and $k = 4$ and repeating the fits for these two cases.

3. In the process of our analysis of CCFR'97 data we applied the same kinematic cuts as in Ref. 16, namely $Q^2 > 5$ GeV^2, $x < 0.7$ and $W^2 > 10$ GeV^2. We started the QCD evolution from the initial scale $Q_0^2 = 20$ GeV^2, which we consider as more appropriate from the point of view of stability of the NLO and NNLO results for $\Lambda^{(4)}_{\overline{MS}}$ due to variation of the initial scale [22]. In order to estimate the uncertainties of the NNLO results, we also performed the N^{3}LO fits with the help of the expanded Padé approximations technique (for the detailed discussions see Ref. 22). The results are presented in Table 1.

Table 1. The results of the fits of CCFR'97 data with the cut $Q^2 > 5$ GeV^2

	$\Lambda^{(4)}_{\overline{MS}}$ (MeV)	$A_2^{'}$ (GeV^2)	χ^2/points
LO	264±37	–	113.1/86
	433±53	-0.33±0.06	83.1/86
	331±162	h(x) in Fig.1	66.3/86
NLO	339±42	–	87.6/86
	369±39	-0.12±0.06	82.3/86
	440±183	h(x) in Fig.1	65.8/86
NNLO	326±35	–	77.0/86
	327±35	-0.01±0.05	76.9/86
	372±133	h(x) in Fig.1	65.0/86
N^{3}LO	332±28	–	76.9/86
Pade	333±27	-0.04±0.05	76.3/86
	371±127	h(x) in Fig.1	64.8/86

At NLO the value for $\Lambda^{(4)}_{\overline{MS}}$ is in good agreement with the NLO result $\Lambda^{(4)}_{\overline{MS}} = 337 \pm 28$ MeV, obtained by the CCFR collaboration with the help of DGLAP NLO analysis of both F_2 and xF_3 SFs data in the case when HT-corrections were neglected [16]. The obtained NLO value of the IRR-model parameter $A_2^{'}$ is in agreement with the estimates of Ref. 15 and of Ref. 26 especially. However, at NNLO a significant decrease of the magnitude of the parameter $A_2^{'}$ is observed. In view of this the results for $\Lambda^{(4)}_{\overline{MS}}$ obtained at the NNLO without HT corrections and with IRR-model of twist-4 term almost coincide. A similar tendency was observed in the process of the N^{3}LO Padé fits. To study this feature in more detail we extracted the x-shape of the model-independent function $h(x)$ (see Fig. 1) and analyzed the factorization/renormalization scale uncertainties of the outcomes of our fits [22]. The corresponding results are presented in Table 2,

where Δ_k is defined as $\Delta_k = \Lambda^{(4)}_{\overline{MS}}(k) - \Lambda^{(4)}_{\overline{MS}}(k=1)$. The related x-shapes of $h(x)$ are presented in Fig. 2.

Table 2. The results of NLO and NNLO fits of CCFR'97 data for different values of factorization/renormalization scales

Order	k	Δ_k (MeV)	$A_2^{'}$ (GeV^2)	χ^2/points
NLO	4	116	–	99.1/86
	4	213	-0.22±0.006	84.2/86
	1/4	-61	–	80.4/86
	1/4	-99	+0.02±0.005	80.2/86
NNLO	4	35	–	83.5/86
	4	66	-0.11±0.06	83.5/86
	1/4	-51	–	87.3/86
	1/4	-45	+0.09±0.05	84.5/86

4. We will concentrate first on discussing the presented behaviour of the twist-4 parameter $h(x)$ of xF_3 SF, presented in Figs. 1,2. In the case of $k = 1$, namely in the pure $\overline{MS}$-scheme, x-shape of $h(x)$ obtained from the LO and NLO analysis of Refs. 21,22 is in agreement with the IRR-model predictions of Ref. 15. Note also that the combination of the quark counting rules [27] with the results of Ref. 7 predict the following x-form of $h(x)$: $h(x) \sim A_2^{'}(1-x)^2$. Taking into account the negative values of $A_2^{'}$, obtained in the process of our LO and NLO fits (see Table 1), we conclude that the related behaviour of $h(x)$ is in qualitative agreement with these predictions.

At the NNLO the situation is more intriguing. Indeed, though a certain indication of the twist-4 term survives even at this level, the NNLO part of Fig. 1 demonstrates that its extracted x-shape starts to deviate both from the IRR prediction of Ref. 15 and from the quark-parton model picture, mentioned above. Notice also that within the statistical error bars the NNLO value of $A_2^{'}$ is indistinguishable from zero. These conclusions are confirmed by the studies of the factorization/renormalization scale dependence of the NLO and NNLO outcomes of the fits [22].

Indeed, it is known that the variation of the related scales is simulating in part the effects of the higher-order perturbative QCD corrections. In view of this the NLO (NNLO) results, obtained in the case of $k = 1/4$ (see Table 2 and Fig. 2 in particular), are almost identical to the NNLO (Padé motivated N^{3}LO) extractions of $h(x)$ and of the IRR model parameter $A_2^{'}$ from the fits with $k = 1$ (see Fig. 1 and Table 1). Thus, we conclude, that as the result of analysis of the CCFR'97 data, the NNLO and beyond we observe the minimization of the twist-4 contributions to xF_3 SF. This feature is related to the interplay between NNLO

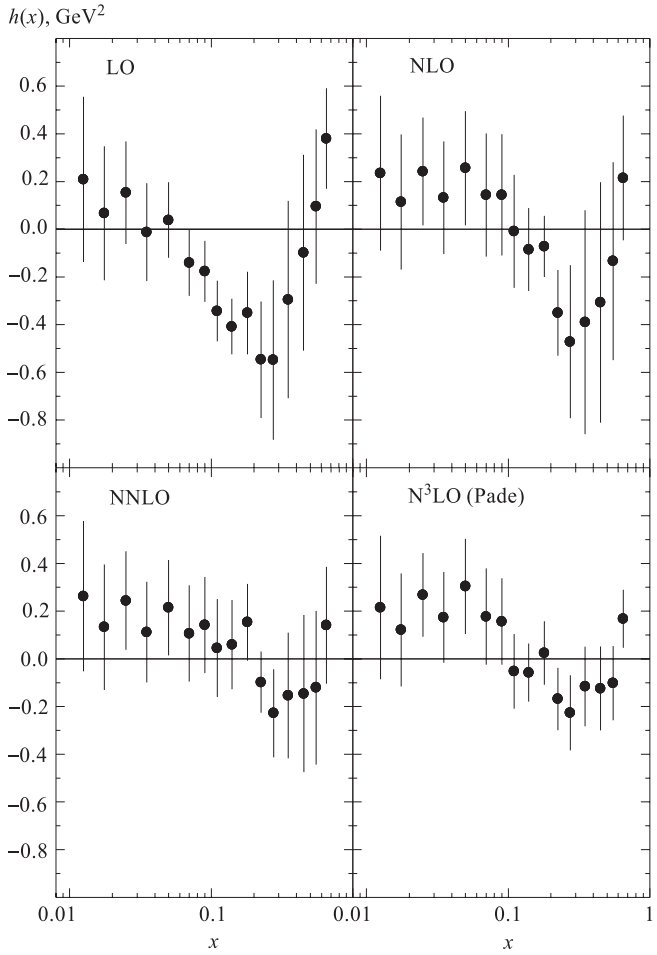

Fig. 1. $h(x)$ extracted from the CCFR'97 data

perturbative QCD and twist-4 $1/Q^2$ corrections. The recent studies of the scale-dependence of the NLO DGLAP extraction of the twist-4 terms from different recent DIS experimental data [28] are supporting the foundations of Refs. 21,22. This means that the higher-twist parameters cannot be defined independently of the effects of perturbation theory and that the NNLO corrections can mimick the contributions of higher twists [29] provided the experimental data are not precise enough for the clear separation of the nonperturbative from perturbative effects. Thus, it is highly desirable to have new experimental data for xF_3 SF, which are more precise than the ones given by the CCFR collaboration.

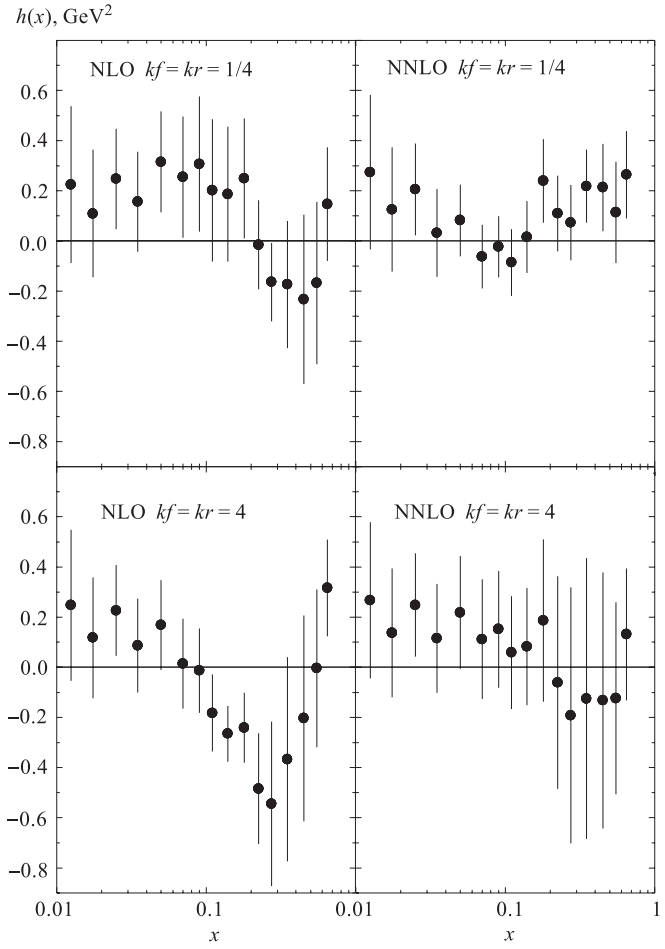

Fig. 2. Scale dependence of $h(x)$

In conclusion we present also the NLO and NNLO values of $\alpha_s(M_Z)$, obtained by us in Ref. 22 from the fits of CCFR'97 data for xF_3 SF with twist-4 terms modelled through the IRR approach:

$$\begin{aligned} NLO \quad \alpha_s(M_Z) &= 0.120 \pm 0.003(\text{stat}) \pm 0.005(\text{syst})^{+0.009}_{-0.007} \\ NNLO \quad \alpha_s(M_Z) &= 0.118 \pm 0.003(\text{stat}) \pm 0.005(\text{syst}) \pm 0.003. \end{aligned} \tag{4}$$

The systematical uncertainties in these results are determined by the systematical uncertainties of the CCFR'97 data, and the theoretical errors are fixed from the numbers for Δ_k (see Table 2), which reflect the factorization/renormalization scale

uncertainties of the values of $\Lambda^{(4)}_{\overline{MS}}$. The incorporation into the $\overline{MS}$-matching formula [30] of the proposals of Ref. 31 for estimates of the ambiguities due to smooth transition to the world with $f = 5$ numbers of active flavours was also taken into account. The theoretical uncertainties presented are in agreement with the ones, obtained in Ref. 25, while the NNLO value of $\alpha_s(M_Z)$ is in agreement with another NNLO result $\alpha_s(M_Z) = 0.1172 \pm 0.0024$, which was obtained from the analysis of SLAC, BCDMS, E665 and HERA data for F_2 SF with the help of the Bernstein polynomial technique [32]. It might be of interest to verify the theoretical errors of these two available phenomenological NNLO analysis using different variants of fixing scheme-dependence ambiguities. The first steps towards the analysis of this problem are already made [33].

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«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
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RESIPE — RENORMALIZATION SCHEME INDEPENDENT PERTURBATION THEORY

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A new approach to perturbation theory for renormalizable quantum field theories, developed in the last few years, is briefly reviewed. Our method gives finite perturbative predictions, which are free from renormalization scheme ambiguities, for any quantity of interest (like a cross section or Green's function) starting from the bare regularized Lagrangian.

1. INTRODUCTION

I will present a new approach to perturbation theory [1–4] for renormalizable quantum field theories (QFTs) which gives renormalization scheme (RS) independent predictions for observable and other quantities of interest (e.g., Green's functions). The resulting REnormalization Scheme Independent PErturbation theory will be called RESIPE for short.

In the time available I will illustrate how RESIPE works for a renormalizable QFT with one dimensionless coupling constant (see Ref. 2). Applications of 2nd order RESIPE to some specific physical measurables, for massless QCD, are to be found in Ref. 3. Generalization of the RESIPE formalism to QFT's with masses and more than one coupling constant and its connection with the renormalization group (RG) formalism is given in Ref. 4. Here, in addition, a new scheme-independent perturbation expansion, without reference to RG techniques, is given which is valid for the general case with masses, several kinematic variables and more than one coupling constant. These references may be consulted for more detail.

2. RESIPE FORMALISM FOR A RENORMALIZABLE QFT WITH ONE COUPLING CONSTANT

Consider a QFT which is renormalizable and has one dimensionless bare coupling constant g_0 (e.g., QCD). For simplicity, consider a physical quantity which depends on only one external energy scale Q. Corresponding to it, one can

always construct a dimensionless measurable quantity R (see sec. 2.2) such that its regularized unrenomalized perturbation expansion is of the form

$$R = a_0 + r_{10}\, a_0^2 + r_{20}\, a_0^3 + ... \tag{1}$$

Here the bare couplant $a_0 \equiv g_0^2/4\pi^2$ and the subscript '0' denotes bare or unrenormalized quantities. The bare perturbation series is not well defined since the coefficients of the expansion are infinite. In a renormalizable theory finite results are extracted by absorbing the infinities in the bare parameters (coupling constant, masses, etc.) and the fields present in the Lagrangian. The definitions of the renormalized fields and parameters in terms of the corresponding bare quantities are, however, not unique because of the possibility of finite renormalizations. After renormalization, since the measurable R has no anomalous dimensions, Eq.(1) becomes

$$R = a + r_1 a^2 + r_2 a^3 + ... \tag{2}$$

where the renormalized couplant $a \equiv g^2/4\pi^2$ and g = renormalized coupling constant. The coefficients r_n are finite but their values depend on the RS used to define g. Consequently, finite-order predictions for R in the renormalized theory will depend on the RS used. Thus the conventional renormalization procedure gives predictions for R which, although finite, are still ambiguous. Can this problem of RS-dependent perturbative predictions (present for all QFT's) be solved? Does the fact that the perturbative predictions based on Eq. (1) or Eq. (2) are not well defined mean that R itself is not directly computable in the theory, but instead the theory predicts some function f(R) uniqueley? How, in what form does the theory determine f(R)? RESIPE provides the answers. We will see that for a renormalizable QFT with a single dimensionless coupling constant g_0 the theory, at best, determines the Q dependence of R through the differential equation

$$\begin{aligned} Q\frac{dR}{dQ} \equiv R'(Q) &= f(R(Q)) \\ &= -f_0 R^2(1 + f_1 R + f_2 R^2 + ...). \end{aligned} \tag{3}$$

The second line expresses f(R) as a series in R with finite RS-invariant coefficients $f_0, f_1, ...$. Each term in this series is RS-invariant and therefore so is any finite order truncation. The convergence of perturbative approximations to f(R) is now controlled by the magnitude of R itself. For practical application, one may approximate the r.h.s. by the first 2 or 3 terms if $|f_n R^n| \ll 1$ for $n \geq 2$ or 3. These would give the second or third order RESIPE prediction. Since these finite order predictions are RS-independent, their confrontation with experiment provides an *unambiguous* probe for higher-order corrections.

2.1. Determination of the RS-Invariants f_n's. Since the coefficients r_{no} depend on Q through the regularization scale (e.g., an ultraviolet cut-off), Eq. (1) gives

$$R' = r'_{10}a_0^2 + r'_{20}a_0^3 + ... \tag{4}$$

where $$r'_{no} \equiv Q\frac{\partial r_{no}}{\partial Q}.$$

Eliminate a_0 between Eqs. (1) and (4) to express R' as a series in R and compare with Eq. (3)., or equivalently, substitute Eq. (1) into Eq. (3) and compare the resulting series in a_0 for R' with Eq. (4). The resulting expressions for f_n's in terms of r_{no} and r'_{no} are given in Eq. (6) below. Since the theory is renormalizable, one can start with Eq. (2) to obtain

$$R' = r'_1a^2 + r'_2a^3 + ..., \tag{5}$$

where $$r'_n \equiv Q\frac{\partial r_n}{\partial Q}.$$

Manipulating Eqs. (2), (3) and (5) as indicated above yields expressions for f_n's in terms of r_n and r'_n. Note the algebra is the same whether one starts with Eq. (1) or Eq. (2). Thus, we find:

$$-f_o = r'_{10} = r'_1$$

$$-f_of_1 = r'_{20} - 2r'_{10}r_{10} = r'_2 - 2r'_1r_1$$

$$-f_of_2 = r'_{30} - 3r'_{20}r_{10} - 2r'_{10}r_{20} + 5r'_{10}r^2_{10} = r'_3 - 3r'_2r_1 - 2r'_1r_2 + 5r'_1r^2_1, \tag{6}$$

etc. Since r_{n0} and r'_{no} are RS-independent, while r_n and r'_n are finite (by definition) Eq. (6) proves that f_n's are both finite and RS-invariant. These properties for the f_n's are, in a sense, obvious from Eq. (3), since both R and R' possess these two properties being measurables. Note that f_0, f_1..., etc., can be directly calculated from the combinations of the bare series coefficients (in Eq. (6)) without having to renormalize them. The finiteness of f_n's is guaranteed by the renormalizability of the theory. Note that f_0 and f_1 are universal in the sense that they are independent of the process under consideration. Of course, f_n, $n \geq 2$, do depend on the process, that is R, though this has not been explicitly indicated in Eq. (3) for notational simplicity.

2.2. Testing RESIPE. Eq. (3) requires the knowledge of R at some $Q = Q_0$ (which has to be obtained from experiment) to predict it at any other Q. This boundary condition on Eq. (3) provides the process dependent scale Λ_R for R to have a nontrivial dependence on Q. Dependence of R on the RS-independent scale Λ_R (undetermined by the theory) is consistent with the fact that the starting

Lagrangian contained the undetermined parameter g_0. The dependence of R on the dimensionless g_0 has now appeared, by «dimensional transmutation» [5] trough Λ_R. In the present approach, different physical quantities $R, \tilde{R}$,..., will automatically have scales $\Lambda_R, \Lambda_{\tilde{R}}$, which are specific to them. Does that mean the theory has many independent scales? The answer is no [2]. For the massless case, one can integrate Eq. (3) for the process R and the corresponding equation

$$\tilde{R}' = -f_0\tilde{R}^2(1 + f_1\tilde{R} + \tilde{f}_2\tilde{R}^2 + ...) \tag{7}$$

for the process $\tilde{R} = a + \tilde{r}_1 a^2 + ...$, since the RS-invariants f_n's and $\tilde{f}_n$'s are constants independent of Q. One can show [2] that the two scales Λ_R and $\Lambda_{\tilde{R}}$ are related:

$$\Lambda_{\tilde{R}} = \Lambda_R \, \exp\,[f_0^{-1}(\tilde{r}_{10} - r_{10})]. \tag{8}$$

Also,

$$\Lambda_R = \Lambda \, \exp\,[f_0^{-1}(r_1)_{\mu=Q}], \tag{9}$$

where Λ is the usual RS-dependent scale parameter and μ is the renormalization point. Note r_n's and $\tilde{r}_n$'s are functions of Q/μ only and $\tilde{r}_{10} - r_{10} = \tilde{r}_1 - r_1$.

To test the theory using RESIPE one can extract Λ_R and $\Lambda_{\tilde{R}}$ to a given order and see how well Eq. (8) is satisfied. Alternatively, one can use Eq. (9) and compare the value of Λ obtained in the two cases.

Some examples of processes from (massless) QCD to which 2nd order RESIPE has been applied [3] are presented. These examples also show how to construct the appropriate dimensionless R which has the perturbation expansion of the required form (viz. Eq. (1) or (2))) and which will obey Eq. (3).

2.2.1. $e^+e^- \to$ *Hadrons.* Experiment gives the dimensionless ratio

$$\Re \equiv \frac{\sigma(e^+e^- \to \text{hadrons})}{\sigma(e^+e^- \to \mu^+\mu^-)} = \Re_0\,(1 + s_1 a + s_2 a^2 + ...).$$

The theorical prediction with QCD corrections is given by the second term where $\Re_0 = 3\sum e_q^2$ is the parton model value and $\mathbf{a}$ is the QCD couplant. The one-loop coefficient s_1 is finite and RS-independent, so in this case RESIPE is to be applied to

$$R \equiv \frac{1}{s_1}(\frac{\Re}{\Re_0} - 1) = a + \frac{s_2}{s_1}\,a^2 + ...$$

2.2.2. Deep Inelastic Scattering. The moments of a nonsinglet structure function $M^{(n)}(Q^2)$ with QCD perturbative corrections has the form:

$$M^{(n)}(Q^2) = A_n(a)^{d^{(n)}}[1 + s_1^{(n)}a + s_2^{(n)}a^2 + ...].$$

Since the unknown nonperturbative matrix element A_n is independent of Q^2, the appropriate quantity here is

$$R^{(n)}(q^2) \equiv -\frac{2}{b_0 d^{(n)}} \frac{d \ln M^{(n)}(Q^2)}{d \ln Q^2} = a[1 + \alpha_1^{(n)} a + ...],$$

where b_0 is defined in Eq. (13) below. It can be seen that corresponding to different processes the appropriate quantities which satisfy an equation like Eq. (3) are quite different. As shown earlier [3], second order RESIPE gives novel tests which involve only measurable quantities.

2.3. Extension of RESIPE to Quantities with Anomalous Dimensions. This is necessary if RESIPE is to apply to all quantities of interest in QFT. For application to Green's function, which has anomalous dimensions, one must first construct an object out of G (analogous to R) which does not get explicitly renormalized and thus is independent of any RS. For example, let $G(p^2)$ be a renormalized propagator (in a massless theory) corresponding to the bare propagator $G_0(p^2)$, so that

$$G(p^2) = Z_G G_0(p^2). \tag{10}$$

Since the infinite constant Z_G is independent of p^2, one has

$$R_G(p^2) = p^2 \frac{d}{dp^2}[\ln G(p^2)] = p^2 \frac{d}{dp^2}[\ln G_0(p^2)]. \tag{11}$$

Thus, R_G in this case is the analogue of a physical quantity. We may now construct from it a quantity which has a perturbation expansion of the form Eq. (1) or Eq. (2) to be able to apply the RESIPE formalism. The second-order RESIPE prediction for the gluon propagator in the Landau gauge is given in Ref. 2.

3. CONNECTION OF RESIPE WITH THE RENORMALIZATION GROUP (RG)

In showing this connection for a renormalizable QFT with one dimensionless renormalized couplant a we will obtain alternative expressions for the RS-invariants f_n's.

3.1. QFT with no Masses. Dimensionless R can depend on Q only through the ratio Q/μ, where μ is the renormalization scale. Since R is a physical quantity, we have the RG equation

$$\mu \frac{d}{d\mu} R(Q/\mu, a(\mu)) = 0 = \mu \frac{\partial R}{\partial \mu} + b(a) \frac{\partial R}{\partial a}, \tag{12}$$

where $b(a)$ is the beta-function for a, defined as

$$\mu\frac{\partial a}{\partial \mu} = b(a) \equiv -b_0 a^2[1 + b_1 a + b_2 a^2 + ...]. \tag{13}$$

Since, $\mu\frac{\partial R}{\partial \mu} = -R'$, we obtain, using Eq. (2)

$$R' = b(a)\frac{\partial R}{\partial a} = b(a)[1 + r_1 a + 2r_2 a^2 + ...]. \tag{14}$$

Now, eliminating the couplant **a** in favour of R by inverting Eq. (2) we obtain

$$R' = b(a)\frac{\partial R}{\partial a} = -b_0 R^2[1 + \rho R_1 + \rho_2 R^2 + ...]. \tag{15}$$

Comparing this with Eq. (3), gives

$$f_0 = b_0, f_1 = \rho_1 = b_1, f_2 = \rho_2 = b_2 + r_2 - b_1 r_1 - r_1^2, \text{ etc.} \tag{16}$$

These relations give an additional proof of the finiteness and regularization independence of the f_n's since, for a renormalizable QFT, the coefficients b_n and r_n are by definition finite and independent of the regularization procedure. The first two relations in Eq. (16), tell us that f_0 and f_1 are process independent and b_0 and b_1 are RS-invariant. The latter is well known to be true for massless QCD.

3.2. QFT with Masses. For our purpose, we choose to define the physical mass of a particle as the pole in its propagator. Let the masses in the theory be m_i, $i = 1, 2, ...$ Now R can be taken to be a function of Q/μ, m_i/μ and the couplant a. Since $\mu dR/d\mu = 0$, the RG equation reads

$$Q\frac{\partial R}{\partial Q} + \sum_i m_i \frac{\partial R}{\partial m_i} = b(a)\frac{\partial R}{\partial a}. \tag{17}$$

The f_n's in the expansion of R' in Eq. (3) are RS-invariant, as argued earlier. But the coefficients in the expansion of r.h.s. of Eq. (17) (see Eq. (15) viz. b_0, b_1 and $\rho_n (n \geq 2)$ are no longer RS-independent as they depend on m_i/μ. Using Eq. (2) one can expand $m_i\frac{\partial R}{\partial m_i}$ as a series in R:

$$m_i\frac{\partial R}{\partial m_i} = h_{0i} R^2[1 + h_{1i} R + ...] \tag{18}$$

with

$$h_{0i} = m_i\frac{\partial r_1}{\partial m_i},\ h_{0i}h_{1i} = m_i\frac{\partial}{\partial m_i}(r_2 - r_1^2), \text{ etc.} \tag{19}$$

Eq. (18) and Eq. (19) will hold for each m_i and so no sum over i is implied. From Eqs. (3), (15), (17) and (18), one obtains

$$f_0 = b_0 + \sum_i h_{0i};\ f_0 f_n = b_0 \rho_n + \sum_i h_{0i} h_{ni},\ n \geq 1. \tag{20}$$

Due to the presence of masses the h_{ni}'s and r_n's will depend on Q/μ and m_i/μ while b_n's will depend on m_i/μ so that all these will be RS-dependent. However, their combinations on the r.h.s. of Eqs. (19), which give the f_n's are RS-independent an will be functions of m_i/Q. The above formulation of the RESIPE program is equivalent to the RG formalism developed by Bogoliubov and Shirkov [6]. Recently, higher order corrections, to the total decay width $\Gamma(H^0 \rightarrow hadrons)$ of the Higgs boson H^0 have been calculated [7] keeping quark masses. Their calculations of QCD corrections in three different schemes provide an explicit example of the emergence of RS-invariants in theories with masses.

4. CONCLUDING REMARKS

The central idea of RESIPE is to use some observable quantity as the perturbation expansion parameter instead of the usual RS-dependent coupling constant, as is normally done in conventional renormalized perturbation theory (CRPT). It is because of this key ingredient, namely expanding a physical quantity as series in an RS-independent quantity, that the RESIPE formalism yields RS-indendent perturbative predictions at finite order. This central idea can be implemented in different ways depending on the technique used [4, 8]. I have presented one of these in the context of a renormalizable QFT with a single dimensionless coupling constant and shown that it can be applied to any quantity of interest, may it be a measurable or Green's function. RESIPE can be considered as a full-fledged RS-independent substitute for CRPT.

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ANALYTIC MODEL OF A REGGE TRAJECTORY IN THE SPACE-LIKE AND TIME-LIKE REGIONS

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A model for a Regge trajectory compatible with the threshold behavior required by unitarity and asymptotics in agreement with Mandelstam analyticity is analyzed and confronted with the experimental data on the spectrum of the ρ trajectory as well as those on the $\pi^- p \to \pi^0 n$ charge-exchange reaction. The fitted trajectory deviates considerably from a linear one both in the space-like and time-like regions, matching nicely between the two.

Regge trajectories may be considered as building blocks in the framework of the analytic S-matrix theory. We dedicate this contribution to the late N.N.Bogolyubov, whose contribution in this field is enormous, on the occasion of his 90th anniversary. The model to be presented is an example of the realization of the ideas of the analytic S-matrix theory.

There is a renewed interest in the studies of the dynamics of the Regge trajectories [1–3]. There are various reasons for this phenomenon.

The hadronic string model (see, e.g., [4]) was successful as a mechanical analogy, generating a spectrum similar to that of a linear trajectory, but it fails to incorporate the interaction between the strings. Although intuitively it seems

clear that hadron production corresponds to breakdown of the strings, the theory of interacting strings faces many problems. Paradoxically, the final goal of the hadronic string theory and, in a sense of the modern strong interaction theory, is the reconstruction of the dual (e.g., Veneziano) amplitude from the interacting strings, originated by the former.

Nonlinear trajectories were derived also from potential models. The saturation of the spectrum of resonances was shown [5] to be connected to a screening quark-antiquark potential.

A relatively new development is that connected with various quantum deformations, although the relation between q deformations and nonlinear (logarithmic) trajectories was first derived by Baker and Coon [6]. q-deformations of the dual amplitudes (or harmonic oscillators) resulted [7, 8] in deviations from linear trajectories, although the results are rather ambiguous. By a different, so-called k-deformation, the authors [3] arrived at rather exotic hyperbolic trajectories.

All these developments were preceded by earlier studies of general properties of the trajectories [9], that culminated in classical papers of the early 70ies by E. Predazzi and co-workers [10], followed by the paper of late A.A. Trushevsky [11], who were able to show, on quite general grounds, that the asymptotic rise of the Regge trajectories cannot exceed $|t|^{1/2}$. This result, later confirmed in the framework of dual amplitudes with Mandelstam analyticity [12], is of fundamental importance. Moreover, wide-angle scaling behavior of the dual amplitudes imposes an even stronger, logarithmic asymptotic upper bound on the trajectories. The combination of a rapid, nearly linear rise at small $|t|$ with the logarithmic asymptotics may be comprised in the following form of the trajectory:

$$\alpha(t) = \alpha(0) - \gamma \ln(1 - \beta t), \tag{1}$$

where γ and β are constants.

The threshold behavior of the trajectories is constrained by unitarity:

$$\mathcal{I}m\, \alpha_n(t) \sim (t - t_n)^{\mathcal{R}e\, \alpha(t_n)+1/2}, \tag{2}$$

where t_n is the mass of the nth threshold. The combination of this threshold behavior with the square-root and/or logarithmic behavior is far from trivial, unless one assumes a simplified square root threshold behavior that, combined with the logarithmic asymptotics, results in the following form [13]

$$\alpha(t) = \alpha_0 - \gamma \ln(1 + \beta\sqrt{t - t_n}). \tag{3}$$

The next question is how do various thresholds enter the trajectory. In a long series of papers N.A. Kobylinsky with his co-workers [14] advocated the additivity idea

$$\alpha(t) = \alpha(0) + \sum_n \alpha_n(t), \tag{4}$$

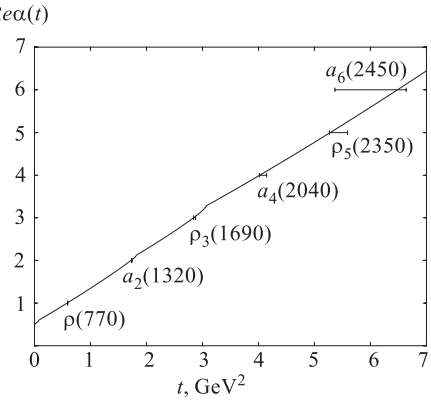

Fig. 1. Chew–Frautschi plot for the six low-lying $I = 1$ parity even mesons (ρ-trajectory). The masses of the resonances were taken from [20]

with $\alpha_n(t)$ having only one threshold branch point on the physical sheet. The choice of the threshold masses is another controversial problem. Kobylinsky et al. [14] assumed that the thresholds are made only of the lowest-lying particles (and their antiparticles), appearing in the $SU(3)$ octet and decuplet — π and K mesons and baryons (N, eventually Σ and/or Ξ). We prefer to include the physical $4m_\pi$ threshold, an intermediate one at 1 GeV, as well as a heavy one accounting for the observed (nearly linear) spectrum of resonances on the ρ trajectory. The masses of the latter will be fitted to the data.

Figure 1 shows the Chew–Frautschi plot with the trajectory (3), (4) and four thresholds [14] included. This trajectory matches well with the scattering data [16–18], as shown in Figs. 2,*a,b,c*, where fits to the scattering data based on the model [19] are presented.

The construction of a trajectory with a correct threshold behaviour and Mandelstam analyticity, or its reconstruction from a dispersion relation is a formidable challenge for the theory. This problem can be approached by starting from the following simple analytical model where the imaginary part of the trajectory is chosen as a sum of terms like

$$\mathcal{I}m\,\alpha_n(t) = \gamma_n \left(\frac{t - t_n}{t}\right)^{\mathcal{R}e\,\alpha(t_n)+1/2} \theta(t - t_n). \tag{5}$$

A rough estimate of $Re\,\alpha(t_n)$ can be obtained from a linear trajectory adapted to the experimental data.

We have checked this approximation *a posteriori* and found that it works. It could be improved by iterating the zeroth order approximation. From the dispersion relation for the trajectory, the real part can be easily calculated [15]

$$\mathcal{R}e\,\alpha(t) = \alpha(0) + \frac{t}{\sqrt{\pi}} \sum_n \gamma_n \frac{\Gamma(\lambda_n + 3/2)}{\sqrt{t_n}\Gamma(\lambda_n + 2)} \times$$

$$\times\, {}_2F_1\left(1, \frac{1}{2}; \lambda_n + 2; \frac{t}{t_n}\right) \theta(t_n - t) +$$

$$+\frac{2}{\sqrt{\pi}}\sum_n \gamma_n \frac{\Gamma(\lambda_n+3/2)}{\Gamma(\lambda_n+1)}\sqrt{t_n}\;{}_2F_1\left(-\lambda_n,1;3/2;\frac{t_n}{t}\right)\theta(t-t_n), \qquad (6)$$

where $\lambda_n = \mathcal{R}e\,\alpha(t_n)$. Work in this direction is in progress.

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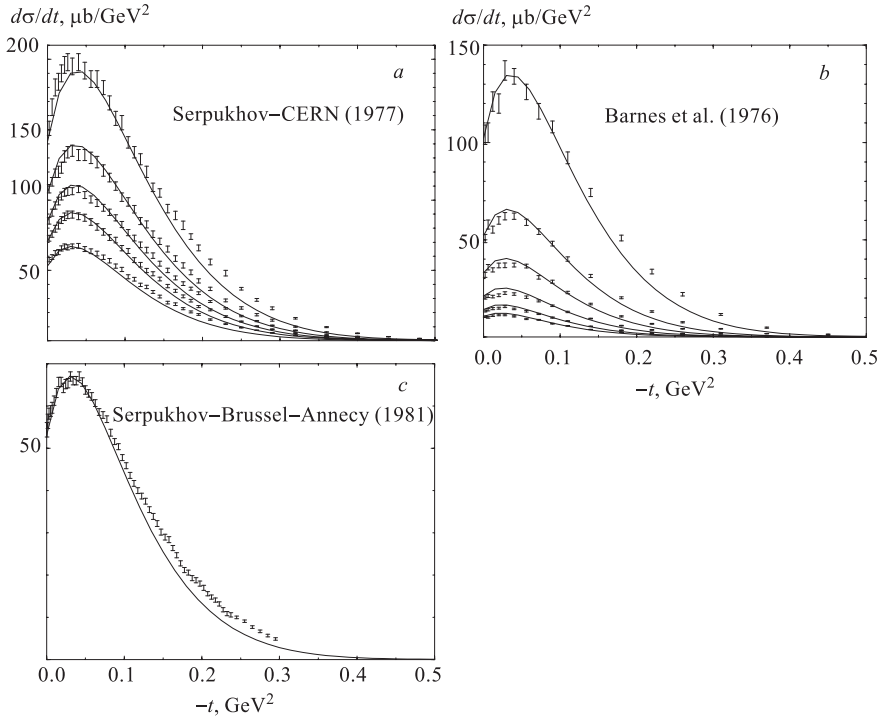

Fig. 2. *a*) Differential cross section $d\sigma/dt$ [μb/GeV^2] versus $-t$ [GeV^2]. The solid curves represent the result of a fit with the model by Arbab and Chiu [19] using the trajectory defined in Eqs. (3) and (4). Data are taken from Ref. 16. *b*) The same as in *a*, with data taken from Ref. 17. *c*) The same as in *a*, with data taken from Ref. 18

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2000, ТОМ 31, ВЫП. 7Б

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DIFFRACTIVE HADRON PRODUCTION AND POMERON COUPLING STRUCTURE

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Large-distance effects, which lead to the spin-flip part of the hadron-pomeron coupling in QCD-models, are discussed. We study spin asymmetries in exclusive reactions and in diffractive $Q\bar{Q}$ and vector meson production which are sensitive to the spin-dependent part of the pomeron coupling.

Investigation of hard diffractive processes is now a problem of topical interest. Experimental study of reactions with a large rapidity gap [1] gives information on the pomeron structure. Theoretically, it is important to find a possible way to test different model approaches which have been proposed for the pomeron and its couplings with quarks and hadrons. The pomeron has mainly the gluon contents and can be represented in QCD as a two-gluon exchange [2]. Thus, the diffractive reactions may be a significant tool to study the gluon distributions in the nucleon at small x [3]. Actually, these processes can be expressed in terms of skewed gluon distribution in the nucleon $\mathcal{F}_X(X+\Delta X)$, where $X+\Delta X$ is a fraction of the proton momentum carried by the outgoing gluon ($\Delta X \ll X$) and the difference between the gluon momenta (skewedness) is equal to X [4].

The pomeron is a color singlet object which describes high energy reactions at fixed momentum transfer. Usually, the pomeron exchange is written in the factorized form as a product of the function $\boldsymbol{P}$, which absorbs s-dependence of the amplitude, and the pomeron-hadron vertices $V^{h\boldsymbol{P}}$

$$\hat{T}(s,t) = i\boldsymbol{P}(s,t)V_{h_1\boldsymbol{P}} \otimes V^{h_2\boldsymbol{P}}. \tag{1}$$

The model approaches [5, 6] lead to the quark-pomeron couplings in a simple form:

$$V^{\mu}_{h\boldsymbol{P}} = B_{h\boldsymbol{P}}(t)\,\gamma^{\mu}, \tag{2}$$

which looks like a $C=+1$ isoscalar photon vertex [7]. In this case, the spin-flip effects are suppressed as a power of s.

In QCD-based models, which consider large-distance contributions in hadrons, a more general form of the pomeron coupling with the proton has been obtained. In the model [8], which was found to be valid for momentum transfer

$|t| <$ few GeV^2, the $Q\bar{Q}$ sea effects have been approximated by a meson cloud of the hadron. The model results in the pomeron-hadron coupling in the form

$$V^{\mu}_{pI\!P}(p,t,x_P) = 2p^{\mu}A(t,x_P) + \gamma^{\mu}B(t,x_P). \tag{3}$$

Here x_P is a fraction of the initial pomeron momentum carried by the pomeron ($x_P = 0$ for elastic scattering). The large-distance meson cloud contributions in the nucleon produce the A term in (3). It leads to the transverse spin effects in the pomeron coupling which does not vanish at high energies. This means that the pomeron might not conserve the s-channel helicity. Within this model, a quantitative description of meson-nucleon and nucleon-nucleon polarized scattering at high energies has been obtained [8]. The model predictions for polarization at RHIC energies are shown in Fig. 1 [9]. Error bars in the Figure indicate expected statistical errors for the PP2PP experiment at RHIC. The expected errors are quite small and the information about the spin-flip part of the proton-pomeron coupling can be obtained experimentally.

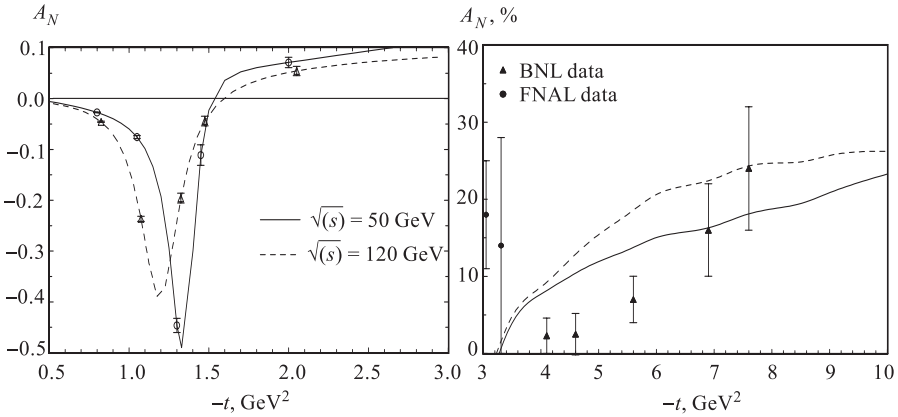

Fig. 1. Meson cloud model predictions for single-spin transverse asymmetry of the pp scattering at RHIC energies

Fig. 2. Diquark model predictions for single-spin asymmetry at high energy pp scattering

The similar structure of the proton coupling with the two-gluon system has been found for moderate momentum transfer in a QCD-based diquark model [10]. Diquarks provide an effective description of nonperturbative effects in the proton. The spin-dependent A contribution in (3) is determined in the model by the effects of vector diquarks. The predicted A_N asymmetry (Fig. 2) is of the same order of magnitude as has been observed in the model [8, 9] for $|t| \sim 3$GeV^2 and found in the BNL [11] and FNAL experiments [12]. A similar form of the proton-pomeron coupling has been used in [13]. Generally, the spin-dependent

pomeron coupling (3) can be obtained if one considers together with the Dirac the Pauli form factors [14] in the electromagnetic nucleon current. In all the cases, the spin-flip A contribution is determined by the nonperturbative effects in the proton.

Let us analyze now what polarized diffractive experiments might be sensitive to the pomeron coupling structure (3). We shall consider double spin asymmetry of the J/Ψ and $Q\bar{Q}$ production. The cross section of these reactions can be decomposed into the following important parts: leptonic and hadronic tensors and the amplitude of the $\gamma^\star P \to J/\Psi(Q\bar{Q})$ transition. The hadronic tensor for the vertex (3) can be written as

$$W^{\mu;\nu}(s_p) = \sum_{s_{fin}} \bar{u}(p', s_{fin}) V^{\mu}_{pgg}(p, t, x_P) u(p, s_p) \bar{u}(p, s_p) \tag{4}$$

$$\times V^{\star\,\nu}_{pgg}(p, t, x_P) u(p', s_{fin}),$$

where p and p' are the initial and final proton momenta, and s_p is a spin of the initial proton.

The spin-average and spin dependent cross sections with parallel and antiparallel longitudinal polarization of a lepton and a proton are determined by the relation

$$\sigma(\pm) = \frac{1}{2}\left(\sigma(\overrightarrow{\Leftarrow}) \pm \sigma(\overrightarrow{\Rightarrow})\right). \tag{5}$$

These cross sections can be expressed in terms of spin-average and spin dependent values of the leptonic and hadronic tensors. The structure of the leptonic tensor is well known [15]. For the hadronic tensor one can write

$$W^{\mu;\nu}(\pm) = \frac{1}{2}(W^{\mu;\nu}(+\frac{1}{2}) \pm W^{\mu;\nu}(-\frac{1}{2})), \tag{6}$$

where $W(\pm\frac{1}{2})$ are the hadronic tensors with the helicity of the initial proton equal to $\pm 1/2$. The explicit forms of the hadronic tensors can be found in [16].

A simple model is considered for the amplitude of the $\gamma^\star \to J/\Psi$ transition. The virtual photon is going to the $q\bar{q}$ state and the $q\bar{q} \to V$ amplitude is described by a nonrelativistic wave function [3]. In this approximation, quarks have the same momenta equal to half of the vector meson momentum and $m_c = m_J/2$. The gluons from the pomeron are coupled to the single and different quarks in the $c\bar{c}$ loop. This ensures gauge invariance of the final result.

The cross section of the J/Ψ leptoproduction can be written in the form

$$\frac{d\sigma^{\pm}}{dQ^2 dy dt} = \frac{|T^{\pm}|^2}{32(2\pi)^3 Q^2 s^2 y}. \tag{7}$$

For the spin-average amplitude square we find

$$|T^+|^2 = N((2-2y+y^2)m_J^2 + 2(1-y)Q^2)s^2[|B+2mA|^2 + |A|^2|t|]I^2. \quad (8)$$

Here N is a known normalization factor and I is the integral over transverse momentum of the gluon

$$I = \frac{1}{(m_J^2+Q^2+|t|)} \int \frac{d^2 l_\perp (l_\perp^2 + \vec{l}_\perp \vec{\Delta})}{(l_\perp^2+\lambda^2)((\vec{l}_\perp+\vec{\Delta})^2+\lambda^2)[l_\perp^2 + \vec{l}_\perp\vec{\Delta} + (m_J^2+Q^2+|t|)/4]}. \quad (9)$$

The term proportional to $(2-2y+y^2)m_J^2$ in (8) represents the contribution of the virtual photon with transverse polarization. The $2(1-y)Q^2$ term describes the effect of longitudinal photons.

The spin-dependent amplitude square looks like

$$|T^-|^2 = N(2-y)s|t|[|B|^2 + m(A^\star B + AB^\star)]m_J^2 I^2. \quad (10)$$

As a result, we find the following form of asymmetry [16]:

$$A_{ll} = \sigma(-)/\sigma(+) \sim \frac{|t|}{s} \frac{(2-y)[|B|^2 + m(A^\star B + AB^\star)]}{(2-2y+y^2)[|B+2mA|^2 + |t||A|^2]}. \quad (11)$$

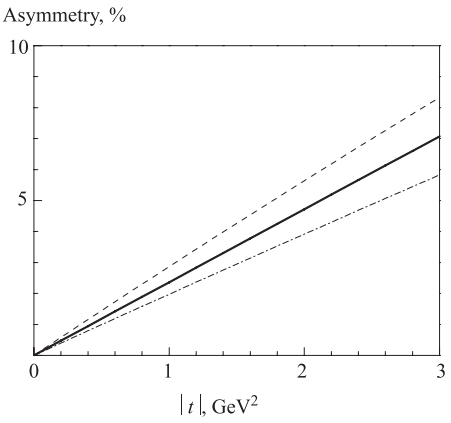

Fig. 3. The predicted A_{ll} asymmetry of the J/Ψ production at HERMES: solid line — for $\alpha = 0$; dot-dashed and dashed lines — for $\alpha = \pm 0.1$ GeV^{-1}

The A_{ll} asymmetry of vector meson production is equal to zero for the forward direction ($t = 0$). It depends on the ratio of the spin-flip to the nonflip parts of the pomeron coupling $\alpha = A/B$. The absolute value of α is proportional to the ratio of helicity-flip and nonflip amplitudes which have been found in [8,10] to be of about 0.1 and weakly dependent on energy. The predicted asymmetry at HERMES energies is shown in Fig. 3. At HERA energies, the asymmetry will be negligible. The value of asymmetry for $\alpha = 0$ is not equal to zero. This term of the asymmetry is determined by the γ_μ part of the pomeron coupling (3). It gives the predominated contribution to the asymmetry of vector meson production in our model.

Let us pass now to spin effects in $Q\bar{Q}$ leptoproduction. In the two-gluon picture of the pomeron, we consider all the graphs where the gluons from the

pomeron couple to a different quark as well to the single one. The spin-average and spin-dependent cross section can be written in the form

$$\frac{d^5\sigma(\pm)}{dQ^2dydx_pdtdk_\perp^2} = \binom{(2-2y+y^2)}{(2-y)} \frac{N(x_p,Q^2)\ C(\pm)}{\sqrt{1-4k_\perp^2\beta/Q^2}}. \tag{12}$$

Here, $N(x_p, Q^2)$ is a normalization function which is common for spin average and spin dependent cross section and

$$C(\pm) = \int \frac{d^2l_\perp d^2l'_\perp D^\pm(t,Q^2,l_\perp,l'_\perp,\cdots)}{(l_\perp^2+\lambda^2)((\vec{l}_\perp+\vec{r}_\perp)^2+\lambda^2)(l_\perp'^2+\lambda^2)((\vec{l'}_\perp+\vec{r}_\perp)^2+\lambda^2)}, \tag{13}$$

where $D^\pm$ function comprises a sum of the $\gamma P \to Q\bar{Q}$ production diagrams and the corresponding crossed contributions convoluted with the spin average and spin-dependent tensors. The obtained diffractive A_{ll} asymmetry has weak energy dependence and is proportional to x_p which is typically of about $.05 - .1$. The predicted asymmetry is quite small and does not exceed 1-1.5% [17]. We find that the asymmetry is not equal to zero for $\alpha = 0$. The value of the asymmetry for nonzero α is determined by the spin–dependent part of the pomeron coupling. However, as in the case of J/Ψ production, sensitivity of the asymmetry to α is not very strong.

Another object, which can be studied at polarized $Q\bar{Q}$ production, is the A_{lT} asymmetry with longitudinal lepton and transverse proton polarization. It has been found that the A_{lT} asymmetry is proportional to the scalar production of the proton spin vector and the transverse jet momentum. Thus, the asymmetry integrated over the azimuthal jet angle is zero. We have calculated the A_{lT} asymmetry for the case when the proton spin vector is perpendicular to the lepton scattering plane and the jet momentum is parallel to this spin vector. The estimated Q^2 dependence of the A_{lT} asymmetry integrated over t for $\alpha = 0.1\text{GeV}^{-1}$ is shown in Fig. 4. The predicted asymmetry is huge and has a strong $k_\perp^2$ dependence. The large value of A_{lT} asymmetry is caused by the fact that it does not have a small factor x_p as a coefficient.

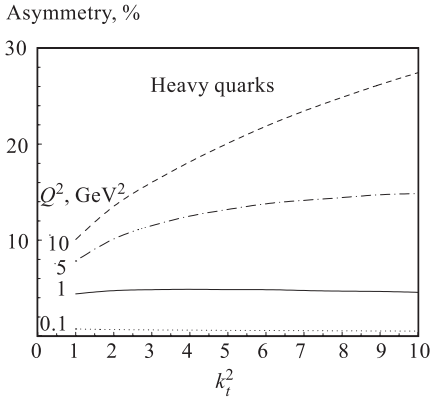

Fig. 4. The predicted Q^2 dependence of A_{lT} asymmetry for the $c\bar{c}$ production at HERA for $\alpha = 0.1$ GeV^{-1}, $x_p = 0.1$, $y = 0.5$

In the present report, the polarized cross section of the diffractive hadron leptoproduction at high energies has been studied. The spin asymmetries are expressed in terms of the A and B structures of the pomeron coupling (3). Generally, the function B should be determined by the spin–average and the function A — by the polarized skewed gluon distribution in the proton. The $B\gamma^\mu$ term of the pomeron coupling (3) contributes to both $\sigma(+)$ and $\sigma(-)$ cross sections which for $\alpha = 0$ are proportional to B^2. This gives the nonzero $A_{ll}(\alpha = 0)$ asymmetry which is independent of the gluon density. We predict not small value of the A_{ll} asymmetry of the diffractive vector meson production at the HERMES energy. The obtained asymmetry is independent of the mass of a produced meson. So, we can expect a similar value of the asymmetry in the polarized diffractive ϕ –meson leptoproduction. The predicted A_{ll} asymmetry in the $Q\bar{Q}$ leptoproduction is smaller than 1.5%. The $A_{ll}(\alpha = 0)$ contribution is predominated in asymmetry, and sensitivity of the asymmetry on α for $\alpha \neq 0$ is rather weak. Thus, the A_{ll} asymmetry in diffractive reactions is not a good tool to study polarized gluon distributions of the proton and the spin structure of the pomeron. Otherwise, it has been found not small A_{lT} asymmetry in diffractive $Q\bar{Q}$ production. This asymmetry is proportional to α and can be used to obtain direct information about the spin–dependent part A of the pomeron coupling. Experimental analyses of energy dependence of the A_{lT} asymmetry as well as of the A_N asymmetry in elastic pp scattering, which have a weak energy dependence in the model, can throw light on the spin structure of the pomeron coupling. They are appropriate objects to study the polarized gluon structure of the proton too. Thus, the pomeron coupling structure can be investigated in diffractive processes. This gives important information on the spin structure of QCD at large distances.

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ABSENCE OF AXIAL ANOMALY IN THE BACKGROUND OF THE BOHM–AHARONOV VECTOR POTENTIAL

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The problem of the axial anomaly in the presence of the Bohm–Aharonov gauge vector field is exactly solved.

The axial anomaly arises as a violation of the classical conservation law for the axial-current at the quantum level. Since its discovery [1–3] the anomaly has played a more and more significant role in the development of contemporary quantum field theory, and has led to a number of important phenomenological consequences in particle physics. Although the first anomalies were found in studies by means of the diagram technique of perturbations in coupling constant, it was soon recognized that the results do not depend on the use of perturbative methods. The nonperturbative (i.e., not describable in the framework of perturbation theory) nature of the anomalies can be revealed by means of an approach in which the gauge vector field is treated as a classical external one and the problem of quantizing massless fermions in this background is solved. Such a treatment makes it possible to regard the anomaly as a manifestation of nontrivial topology of configurations of the gauge vector field and establish a connection between the anomaly and the topological invariant of the spectrum of the massless Dirac operator in an external-field background.

Singular (or contact, or zero-range) interaction potentials were introduced in quantum mechanics more than sixty years ago [4–6]. A mathematically consistent and rigorous treatment of the subject was developed [7], basing on the notion of self-adjoint extension of a Hermitian operator (for a review see monograph [8]). Singular external-field background can act on the quantized spinor field in a rather unusual manner: a leak of quantum numbers from the singularity point into the vacuum occurs [9–14]. This is due to the fact that a solution to the Dirac equation, unlike that to the Schrödinger one, does not obey a condition of regularity at the singularity point. It is necessary then to specify a boundary condition at this point, and the least restrictive, but still physically acceptable, condition is such that guarantees self-adjointness of the operator of the appropriate dynamical variable.

In the present paper the problem of the axial anomaly in the singular background of the Bohm–Aharonov [15] gauge vector field is comprehensively studied. We show that, contrary to the leak of vacuum quantum numbers, the leak of anomaly from the singularity point does not occur.

Let us consider the effective action functional for quantized massless spinor field $\Psi(x)$ in external classical vector field $V_\mu(x)$ in the Wick-rotated (Euclidean) d-dimensional space-time

$$S^{\rm eff}[V_\mu(x)] = 3D - \ln \int d\Psi(x)\, d\Psi^\dagger(x)\, \exp[-\int d^d x\, L(x)] =$$

$$= 3D - \ln Det(-i\gamma^\mu \nabla_\mu), \tag{1}$$

where

$$L(x) = 3D - \frac{i}{2}\Psi^\dagger(x)\gamma^\mu[\nabla_\mu \Psi(x)] + \frac{i}{2}[\nabla_\mu \Psi(x)]^\dagger \gamma^\mu \Psi(x) \tag{2}$$

is the Lagrangian density, $\nabla_\mu = 3D\partial_\mu - iV_\mu(x)$ is the covariant differentiation operator, and γ^μ $(\mu = 3D\overline{1,d})$ are the Dirac matrices,

$$[\gamma^\mu, \gamma^\nu]_+ = 3D2g^{\mu\nu}, \qquad \mathrm{tr}\,\gamma^\mu = 3D0, \qquad g_{\mu\nu} = 3Ddiag(1, ..., 1). \tag{3}$$

If there exists matrix Γ anticommuting with the Dirac matrices,

$$[\Gamma, \gamma^\mu]_+ = 3D0, \qquad \mathrm{tr}\,\Gamma = 3D0, \qquad \Gamma^2 = 3DI, \tag{4}$$

then one can define local chiral transformation

$$\Psi(x) \to e^{i\omega(x)\Gamma}\Psi(x), \qquad \Psi^\dagger(x) \to \Psi^\dagger(x)e^{i\omega(x)\Gamma},$$
$$V_\mu(x) \to e^{i\omega(x)\Gamma}V_\mu(x)e^{-i\omega(x)\Gamma} + \partial_\mu\omega(x)\Gamma. \tag{5}$$

The invariance of functional (1) under this transformation corresponds to conservation law

$$\nabla_\mu J^\mu_{d+1}(x) = 3D0, \tag{6}$$

where

$$J^\mu_{d+1}(x) = 3Di\mathrm{tr}\,\langle x|\gamma^\mu\Gamma(-i\gamma^\nu\nabla_\nu)^{-1}|x\rangle. \tag{7}$$

However, functional (1), as well as current (7), is ill-defined, suffering from both ultraviolet and infrared divergences. Performing the regularization of divergencies in a way which is consistent with gauge invariance, one may arrive at the violation of conservation law (6) (i.e., at the axial anomaly) [1–3].

An example of a singular background field configuration is provided by that of the Bohm–Aharonov [15] vortex represented by a point for $d = 3D2$, a line for $d = 3D3$, and a $(d-2)$-dimensional hypersurface for $d > 3$:

$$V^1(x) = 3D - \Phi^{(0)} \frac{x^2}{(x^1)^2 + (x^2)^2}, \quad V^2(x) = 3D\Phi^{(0)} \frac{x^1}{(x^1)^2 + (x^2)^2},$$
$$V^\nu(x) = 3D0, \qquad \nu = 3D\overline{3, d}, \tag{8}$$

$$B^{3\cdots d}(x) = 3D2\pi\Phi^{(0)}\delta(x), \tag{9}$$

where $\Phi^{(0)}$ is the vortex flux in 2π units, i.e., in the London ($2\pi\hbar ce^{-1}$) units, since we use conventional units $\hbar = 3Dc = 3D1$ and coupling constant e is included into vector potential $V_\mu(x)$.

In the $d = 3D2$ case, the γ-matrices are chosen as $\gamma^1 = 3D\sigma_1, \gamma^2 = 3D\sigma_2$, and, consequently, $\Gamma = 3D\sigma_3$, where σ_1, σ_2 and σ_3 are the Pauli matrices. Then the complete set of solutions to Dirac equation

$$(-i\gamma^\mu\nabla_\mu - E)\langle x|E\rangle = 3D0 \tag{10}$$

in background (8) takes the form

$$\langle x|E\rangle = 3D \sum_{n\in \mathrm{Z}} \begin{pmatrix} f_n(r)\exp(in\varphi) \\ g_n(r)\exp[i(n+1)\varphi] \end{pmatrix}, \tag{11}$$

where Z is the set of integer numbers, r and φ are the polar coordinates, and the radial functions, in general, are

$$\begin{pmatrix} f_n(r) \\ g_n(r) \end{pmatrix} =$$

$$= 3D \begin{pmatrix} C_n^{(1)}(E)J_{n-\Phi^{(0)}}(|E|r) + C_n^{(2)}(E)Y_{n-\Phi^{(0)}}(|E|r) \\ i(E/|E|)\big[C_n^{(1)}(E)J_{n+1-\Phi^{(0)}}(|E|r) + C_n^{(2)}(E)Y_{n+1-\Phi^{(0)}}(|E|r)\big] \end{pmatrix}, \tag{12}$$

$J_\rho(u)$ and $Y_\rho(u)$ are the Bessel and the Neumann functions of order ρ. It is clear that the condition of regularity at $r = 3D0$ can be imposed on both f_n and g_n for all n in the case of integer values of quantity $\Phi^{(0)}$ only. Otherwise, the condition of regularity at $r = 3D0$ can be imposed on both f_n and g_n for all but $n = 3Dn_0$, where n_0 is the integer part of the quantity $\Phi^{(0)}$ (i.e., the integer which is less than or equal to $\Phi^{(0)}$); in this case at least one of the functions, f_{n_0} or g_{n_0}, remains irregular, although square integrable, with the asymptotics r^{-p}

$(p < 1)$ at $r \to 0$. The question arises then, what boundary condition, instead of regularity, is to be imposed on f_{n_0} and g_{n_0} at $r = 3D0$ in the latter case?

To answer this question, one has to find the self-adjoint extension for the partial Dirac operator corresponding to the mode with $n = 3Dn_0$. If this operator is defined on the domain of regular at $r = 3D0$ functions, then it is Hermitian, but not self-adjoint, having the deficiency index equal to (1,1). The use of the Weyl–von Neumann theory of self-adjoint operators (see, e.g., Ref. 8) yields that, for the partial Dirac operator to be self-adjoint extended, it has to be defined on the domain of functions satisfying the boundary condition

$$\begin{aligned} & i\cos\left(\frac{\theta}{2}+\frac{\pi}{4}\right)2^{1-F}\,\Gamma(1-F)\,\lim_{r\to 0}\left(\mu r\right)^{F} f_{n_0}(r) \\ & = 3D\sin\left(\frac{\theta}{2}+\frac{\pi}{4}\right)2^{F}\,\Gamma(F)\,\lim_{r\to 0}\left(\mu r\right)^{1-F} g_{n_0}(r), \end{aligned} \tag{13}$$

where $\Gamma(u)$ is the Euler gamma function,

$$F = 3D\Phi^{(0)} - n_0 \tag{14}$$

is the fractional part of quantity $\Phi^{(0)}$ $(0 \leq F < 1)$, θ is the self-adjoint extension parameter, and $\mu > 0$ is inserted merely for the dimension reasons. Note that Eq.(13) implies that $0 < F < 1$, since in the case of $F = 3D0$ both f_{n_0} and g_{n_0} satisfy the condition of regularity at $r = 3D0$. Note also that, since Eq.(13) is periodic in θ with period 2π, all permissible values of θ can be restricted, without a loss of generality, to range $0 \leq \theta \leq 2\pi$.

The gauge invariant regularization of $\nabla_\mu J^\mu_{d+1}(x)$ can be achieved by means of the zeta function method [16–18], yielding, instead of Eq.(6), the following relation

$$\nabla_\mu J^\mu_{d+1}(x) = 3D2 \lim_{z\to 0}\lim_{M\to 0}\tilde{\zeta}_x(z|M), \tag{15}$$

where

$$\tilde{\zeta}_x(z|M) = 3D\mathrm{tr}\,\langle x|\Gamma\left\{\nabla^\mu\nabla_\mu + \frac{i}{2}[\gamma^\mu,\gamma^\nu]_-[\nabla_\mu V_\nu(x)] + M^2\right\}^{-z}|x\rangle \tag{16}$$

is the modified zeta function density.

In the $d = 3D2$ case, using the explicit form of the solution to the Dirac equation in background (8), it is straightforward to compute the modified zeta function density. As follows already from the preceding discussion, the modified zeta function density vanishes in the case of integer values of $\Phi^{(0)}$ $(F = 3D0)$, since this case is indistinguishable from the case of the trivial background

($\Phi^{(0)} = 3D0$). In the case of noninteger values of $\Phi^{(0)}$ ($0 < F < 1$) we get

$$\tilde{\zeta}_x(z|M) = 3D\frac{\sin(F\pi)}{\pi^3}\sin(z\pi)r^{2(z-1)}\int\limits_{|M|r}^{\infty} dw\, w(w^2 - M^2r^2)^{-z}$$
$$\times\Big\{K_F^2(w) - K_{1-F}^2(w) + \big[K_F^2(w) + K_{1-F}^2(w)\big]$$
$$\times\tanh\ln\big[\big(\frac{w}{\mu r}\big)^{2F-1}\mathrm{cotan}\,\big(\frac{\theta}{2} - \frac{\pi}{4}\big)\big]\Big\}. \qquad (17)$$

Taking limit $M \to 0$, we get

$$\tilde{\zeta}_x(z|0) = 3D\frac{\sin(F\pi)}{\pi^3}\sin(z\pi)r^{2(z-1)}$$
$$\times\Big\{\frac{\sqrt{\pi}}{2}\,\frac{\Gamma(1-z)}{\Gamma(\frac{3}{2}-z)}\big(F - \frac{1}{2}\big)\Gamma(F-z)\Gamma(1-F-z)$$
$$+\int\limits_0^{\infty} dw\, w^{1-2z}\big[K_F^2(w) + K_{1-F}^2(w)\big]\tanh\ln\big[\big(\frac{w}{\mu r}\big)^{2F-1}\mathrm{cotan}\,\big(\frac{\theta}{2} - \frac{\pi}{4}\big)\big]\Big\}; \qquad (18)$$

in particular, at half-integer values of the vortex flux:

$$\tilde{\zeta}_x(z|0)\big|_{F=3D\frac{1}{2}} = 3D\frac{\sin\theta}{2\pi^{\frac{3}{2}}}\,\frac{\Gamma(\frac{1}{2}-z)}{\Gamma(z)}r^{2(z-1)}; \qquad (19)$$

and at $\cos\theta = 3D0$:

$$\tilde{\zeta}_x(z|0) = 3D \pm \frac{\sin(F\pi)}{2\pi^{\frac{3}{2}}}\,\frac{\Gamma(\frac{3}{2}-z\pm F\mp\frac{1}{2})\Gamma(\frac{1}{2}-z\mp F\pm\frac{1}{2})}{\Gamma(z)\Gamma(\frac{3}{2}-z)}\,r^{2(z-1)}, \qquad (20)$$

$$\theta = 3D\pi(1 \mp \frac{1}{2}).$$

Consequently, we obtain

$$\tilde{\zeta}_x(0|0) = 3D0, \qquad x \neq 0. \qquad (21)$$

Thus the anomaly is absent everywhere on the plane with the puncture at $x = 3D0$. This looks rather natural, since two-dimensional anomaly $2\tilde{\zeta}_x(0|0)$ is usually identified with quantity $\frac{1}{\pi}B(x)$, and background field strength $B(x)$ vanishes everywhere on the punctured plane, see Eq. (9) at $d = 3D2$. We see that natural anticipations are confirmed, provided that the boundary conditions

at the puncture are chosen to be physically acceptable, i.e., compatible with the self-adjointness of the Dirac operator.

We might finish here the discussion of the anomaly problem in the background of the Bohm–Aharonov vortex. However, there remains a purely academic question: what is the anomaly in background (8)–(9) on the whole plane (without puncturing $x = 3D0$)? Just due to a confusion persisting in the literature [19,20], we shall waste now some time to clarify this, otherwise inessential, point.

Background field strength (9), when considered on the whole plane, is interpreted in the sense of a distribution (generalized function), i.e., a functional on a set of suitable test functions $f(x)$:

$$\int d^2x\, f(x)\, \frac{1}{\pi} B(x) = 3D f(0)\, 2\Phi^{(0)}; \tag{22}$$

here $f(x)$ is a continuous function. In particular, choosing $f(x) = 3D1$, one gets

$$\int d^2x\, \frac{1}{\pi} B(x) = 3D2\Phi^{(0)}. \tag{23}$$

Considering the anomaly on the whole plane, one is led to study different limiting procedures as $r \to 0$ and $z \to 0$ in Eq.(18). So, the notorious question is, whether anomaly $2\tilde{\zeta}_x$ can be interpreted in the sense of a distribution which coincides with distribution $\frac{1}{\pi} B(x)$? The answer is resolutely negative, and this will be immediately demonstrated below.

First, using explicit form (18), we get

$$\int d^2x\, 2\tilde{\zeta}_x(z|0) = 3D \begin{cases} \infty, & z \neq 0 \\ 0, & z = 3D0 \end{cases} ; \tag{24}$$

therefore, the anomaly functional cannot be defined on the same set of test functions as that used in Eq.(22) (for example, the test functions have to decrease rapidly enough at large (small) distances in the case of $z > 0$ ($z < 0$)). Moreover, if one neglects the requirement of self-consistency, permitting a different (more specified) set of test functions for the anomaly functional, then even this will not save the situation. Let us take $z > 0$ for definiteness and use the test functions which are adjusted in such a way that the quantity

$$A = 3D \lim_{z \to 0_+} \int d^2x\, f(x)\, 2\tilde{\zeta}_x(z|0) \tag{25}$$

is finite. Certainly, this quantity can take values in a rather wide range, but it cannot be made equal to the right-hand side of Eq.(23). Really, the only source of the dependence on $\Phi^{(0)}$ in the integral in Eq.(25) is the factor $\tilde{\zeta}_x(z|0)$, and the latter, as is evident from Eq.(18), depends rather on F, than on $\Phi^{(0)}$ itself, thus

forbidding the linear dependence of A on $\Phi^{(0)}$. In particular, let us choose test function $f(x)$ in the form

$$f(x) = 3D \exp(-\tilde{\mu}^2 r^2), \tag{26}$$

where $\tilde{\mu}$ is the parameter of the dimension of mass. Then, choosing the case of $\cos\theta = 3D0$ for simplicity and using Eq.(20), one gets that Eq. (25) takes the form

$$A = 3D2\left(F - \frac{1}{2} \pm \frac{1}{2}\right), \qquad \theta = 3D\pi(1 \mp \frac{1}{2}), \tag{27}$$

which differs clearly from $2\Phi^{(0)}$.

We have proved that, in a singular background, the conventional relation between the axial anomaly and the background field strength is valid only in the space with punctured singularities; consequently, wherever the field strength is zero the anomaly always is absent. If singularities are not punctured, then the anomaly and the field strength can be interpreted in the sense of distributions, but, contrary to the assertions of the authors of Refs. 19,20, the conventional relation is not valid.

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THE GRAVITY THEORY ON A BACKGROUND OF THE LOBACHEVSKY GEOMETRY

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In this paper four models are being discussed, concerning the gravitational field of a star at rest and the equations of motion of the companion planet. The first model has been created by Newton; and the second model, by Lobachevsky. The third model has been initiated by Einstein, further developed by Schwarzschild and completed by Fock. The fourth model has been created by the author of this paper. In the second and in the fourth models the Lobachevsky geometry with the characteristic constant k is introduced in the background space. The constant k is the absolute measure of the length in the background space. In the third and in the fourth models the Lobachevsky geometry with the characteristic constant c is introduced in the velocity space. The constant c is the absolute measure of the rapidity in the velocity space. It equals the light velocity. In the first and in the third models the gravitational field of the star obeys the Einstein's equations. In the second and in the fourth models the gravitational field of the star obeys new equations, proposed by the author. The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

1. INTRODUCTION

Much can be understood, considering the gravitational theory on the background of the Lobachevsky geometry. For example, it can be understood why, despite all the achievements of relativistic theory of gravitation, some shortcomings in this theory can also be found. It can be understood also how one can remove these shortcomings.

As is known, Einstein has set up all the achievements of relativistic theory of gravitation, replacing in Newton's model the gravitational potential U with the gravitational metrics $g_{mn}dx^m dx^n$, and replacing the gravitational connection, given in the nonrelativistic case by the symbol $\mathrm{grad}\, U$, by the relativistic gravitational connection, expressed by the Christoffell's symbol for the tensor g_{mn}.

It is true that because of such a replacement the energy density of the gravitational field has turned out to depend on the choice of coordinate map, and the reason for this is the loss of the background connection. Without noticing this loss, the gravitationalists declared that the energy of the gravitational field is *non-localized*, thus damaging the relativistic theory of gravitation. From here come all the shortcomings in the theory.

Seemingly, such a loss has been performed under milder circumstances, because in Newton's model the background connection is primitive. But here is an intricate and subtle danger: in some coordinate maps all components of primitive connection equal zero, while in other coordinate maps the components of the same connection are not equal to zero. Therefore, it is more reliable to deal with a nonprimitive connection: the aggregate of its components does not equal zero in all the coordinate maps.

The Lobachevsky model [1], [2] helps to restore the background connection in the relativistic theory of gravitation. In this model the background connection is nonprimitive, but one can again return in the framework of Einstein's theory, keeping the restored background connection. For the purpose one has to set up to infinity the characteristic length for the Lobachevsky geometry. The restored connection in this limit will be, as in Newton's model, the primitive one.

As a result of the introduction of the Lobachevsky geometry in the background connection, during the last years some difficult questions in gravity theory become more clear. For example, the problem about the choice of harmonical coordinates has been clarified. The situation is analogous to the one, which Bogoliubov [3] has solved in statistical mechanics by applying the method of quasi-average quantities. The role, which in Bogoliubov's method is played by the magnetic field, in the current case is transferred to the length measure.

I have found the following method for the restored background connection [4].

Let us denote by Γ^a_{mn} the gravitational connection, by $\breve{\Gamma}^a_{mn}$ the background connection and by $P^a_{mn} = \breve{\Gamma}^a_{mn} - \Gamma^a_{mn}$ their affine deformation tensor.

And let us denote by R_{mn} the gravitational Ricci tensor, by $\breve{R}_{mn}$ the background Ricci tensor and by $S_{mn} = \breve{R}_{mn} - R_{mn}$ their difference.

According to the method, on that place, where (in the pseudoscalar Lagrangian and in the energy-momentum pseudotensor) a geometrical object with components $(-\Gamma^a_{mn})$ stands, (according to Manoff [5], it is called a covariant affine connection) we must put the tensor P^a_{mn}, and also on the place, where (in the Einstein equations of gravity) the tensor $(-R_{mn})$ stands, we must put the tensor S_{mn}.

In the new equations of the gravitational field

$$S_{mn} - \frac{1}{2}\, S\, g_{mn} = -\frac{8\pi\gamma}{c^4}\, M_{mn}, \qquad S = g^{mn} S_{mn},$$

the background connection is given, but the gravitational connection is to be found.

In the region, where $M_{mn} = 0$, the new equations of gravitational field take the form $S_{mn} = 0$.

The trivial solution $\Gamma^a_{mn} = \breve{\Gamma}^a_{mn}$ means that the background connection is the gravitational connection in its trivial form. In this case there is no gravitational field.

The background connection is defined by the equations of motion for a free particle.

The gravitational connection is defined by the equations of motion for a particle in a gravitational field, when there are no any other forces.

The condition of harmonicity for the background connection in respect of the gravitational field has a form $\Phi^a = 0$, where

$$\Phi^a = g^{mn} P^a_{mn}.$$

I have shown in my works [6], that any physical theory is founded on the concept of velocity space and that the geometry of this space is the Euclidean or the Lobachevsky one. In the first case the theory is named nonrelativistic and in the second case it is named relativistic. It is strange, of course, but it has been named in this way.

In the first case there is no characteristic measure of velocity. In the second case there is such a measure. It equals the light velocity c. The constant c is the analogue of the length measure k. The nonrelativistic case we shall denote by $c = \infty$. The relativistic case we shall denote by $c < \infty$.

The gravitational metrics may be transformed to the following sum

$$g_{mn} dx^m dx^n = f^1 f^1 + f^2 f^2 + f^3 f^3 - c^2 \ f^4 f^4,$$

where f^m are linear differential forms.

If the gravitational field is absent, we put

$$g_{mn} dx^m dx^n = \breve{g}_{mn} dx^m dx^n = h_{\mu\nu} dx^\mu dx^\nu - c^2 \ dtdt,$$

where $h_{\mu\nu}$ do not depend on $x^4 = t$.

The quadratic form $h_{\mu\nu} dx^\mu dx^\nu$ is either the metrics of the Euclidean space in the Newton's model (the case $k = \infty$), or the metrics of the Lobachevsky space in the Lobachevsky model (the case $k < \infty$).

The components of Christoffell's connection for the metrics $h_{\mu\nu} dx^\mu dx^\nu$ we shall denote by $h^\alpha_{\mu\nu}$.

The Ricci tensor $r_{\mu\nu}$ for the connection $h^\alpha_{\mu\nu}$ equals $r_{\mu\nu} = -k^{-2} \ h_{\mu\nu}$ in the case $k < 0$ and it equals zero ($r_{\mu\nu} = 0$) in the case $k = \infty$.

It is interesting, that the background connection $\breve{\Gamma}^a_{mn}$ does not depend on the light velocity c. Consequently it refers to the Absolute Geometry of Bolyai in velocity space. Indeed, the equations of geodesical lines in the case of the metrics $h_{\mu\nu} dx^\mu dx^\nu - c^2 \ dtdt$, may be written as

$$\frac{d^2 x^\alpha}{d\tau^2} + h^\alpha_{\mu\nu} \frac{dx^\mu}{d\tau} \frac{dx^\nu}{d\tau} = 0, \quad \frac{d^2 t}{d\tau^2} = 0.$$

But in such a form the equations of motion for a particle may be written if Lagrangian equals

$$\frac{1}{2}\, h_{\mu\nu}\frac{dx^\mu}{dt}\frac{dx^\nu}{dt}\ .$$

Consequently, both in the relativistic case and in the nonrelativistic case

$$\breve{\Gamma}^\alpha_{\mu\nu} = h^\alpha_{\mu\nu}, \quad \breve{\Gamma}^\alpha_{\mu 4} = 0, \quad \breve{\Gamma}^\alpha_{4\nu} = 0, \quad \breve{\Gamma}^\alpha_{44} = 0, \quad \breve{\Gamma}^4_{mn} = 0.$$

Accordingly, both in the relativistic and in the nonrelativistic case the background Ricci tensor equals

$$\breve{R}_{\mu\nu} = r_{\mu\nu}, \quad \breve{R}_{4n} = 0, \quad \breve{R}_{m4} = 0.$$

Further we consider a star at rest with its planet. As coordinates x^1, $x^2 < x^3$ we choose the distance ρ from the star, the polar angle θ and the azimuth ϕ on a sphere $\rho = \mathrm{const}$; the notation $x^4 = t$ we will preserve. With such a restriction we must solve the equations

$$S_{mn} = 0.$$

2. THE NEWTON'S MODEL: THE CASE $(k = \infty,\ c = \infty)$

According to Newton, the equations of motion for a planet are:

$$\frac{d^2\rho}{d\tau^2} - \rho\frac{d\theta}{d\tau}\frac{d\theta}{d\tau} - \rho\sin^2\theta\frac{d\phi}{d\tau}\frac{d\phi}{d\tau} + \frac{\gamma M}{\rho^2}\frac{dt}{d\tau}\frac{dt}{d\tau} = 0,$$

$$\frac{d^2\theta}{d\tau^2} + \frac{2}{\rho}\frac{d\rho}{d\tau}\frac{d\theta}{d\tau} - \sin\theta\cos\theta\frac{d\phi}{d\tau}\frac{d\phi}{d\tau} = 0,$$

$$\frac{d^2\phi}{d\tau^2} + \frac{2}{\rho}\frac{d\rho}{d\tau}\frac{d\phi}{d\tau} - 2\cot\theta\frac{d\theta}{d\tau}\frac{d\phi}{d\tau} = 0, \quad \frac{d^2t}{d\tau^2} = 0.$$

Here γ is the Newton's constant, M is a mass of the star.

From here we find the gravitational connection Γ^a_{mn} in the Newton's case. If $M = 0$, it coincides with the background connection. In this case all components of the affine deformation tensor equal zero except

$$P^1_{44} = -\frac{\gamma M}{\rho^2},$$

which equals the force, with which the star attracts the planet's unit mass.

It is remarkable that the Newton's gravitational connection with an arbitrary constant γM is an exact solution of Einstein equations

$$R_{mn} = 0.$$

3. THE LOBACHEVSKY MODEL: THE CASE $(k < \infty,\ c = \infty)$

In the Lobachevsky geometry the length of a circle of radius ρ equals $2\pi r$, and the area of a sphere of the same radius equals $4\pi r^2$, where $r = k \sinh \frac{\rho}{k}$. Because of it Lobachevsky has shown [1, c. 159] that in the new model the force, with which the star attracts the planet's unit mass should equal

$$P^1_{44} = -\frac{\gamma M}{r^2}.$$

The rest components of tensor P^a_{mn} must be equal to zero. The force of attraction in the Lobachevsky model has potential [2], which equals

$$U = \frac{\gamma M}{k}\left(1 - \coth\frac{\rho}{k}\right).$$

In order to find the background connection in the Lobachevsky model we must write down the equations of motion for a particle in the case when the Lagrangian equals

$$\frac{1}{2}\frac{d\rho}{dt}\frac{d\rho}{dt} + \frac{1}{2}\, r^2\, \frac{d\theta}{dt}\frac{d\theta}{dt} + \frac{1}{2}\, r^2\, \sin^2\theta\, \frac{d\phi}{dt}\frac{d\phi}{dt}.$$

From these equations we receive

$$\breve{\Gamma}^1_{22} = -k\sinh\frac{\rho}{k}\,\cosh\frac{\rho}{k}, \qquad \breve{\Gamma}^1_{33} = \breve{\Gamma}^1_{22}\sin^2\theta,$$
$$\breve{\Gamma}^2_{12} = k^{-1}\coth\frac{\rho}{k} = \breve{\Gamma}^2_{21}, \quad \breve{\Gamma}^2_{33} = -\sin\theta\cos\theta,$$
$$\breve{\Gamma}^3_{13} = k^{-1}\coth\frac{\rho}{k} = \breve{\Gamma}^3_{31}, \quad \breve{\Gamma}^3_{23} = \cot\theta = \breve{\Gamma}^3_{32},$$

the remaining components $\breve{\Gamma}^a_{mn}$ being equal to zero.

The background Ricci tensor in the coordinates ρ, θ, ϕ, t is a diagonal one. Its diagonal elements are

$$\breve{R}_{11} = -2k^{-2},$$
$$\breve{R}_{22} = -2k^{-2}r^2,$$
$$\breve{R}_{33} = -2k^{-2}r^2\sin^2\theta,$$
$$\breve{R}_{44} = 0.$$

The Lobachevsky gravitational connection with an arbitrary constant γM is an exact solution of the equations $R_{\mu\nu} = -2k^{-2}h_{\mu\nu}, R_{m4} = R_{4m} = 0$.

4. THE EINSTEIN–SCHWARZSCHILD–FOCK MODEL: THE CASE $(k = \infty,\ c < \infty)$

Einstein began the construction of this model, and it was continued by Schwarzschild, and completed by Fock, who insisted on the application of the harmonicity condition. The gravitational metrics in this case equals

$$\left(\frac{\rho+\alpha}{\rho-\alpha}\right) d\rho^2 + (\rho+\alpha)^2(d\theta^2 + \sin^2\theta\, d\phi^2) - \left(\frac{\rho-\alpha}{\rho+\alpha}\right) c^2 dt^2,$$

where $\alpha = \gamma M c^{-2}$ is the gravitational radius of mass M. This metrics satisfies the equation $R_{mn} = 0$. (See [7, c.263]).

In the case of the static spherical symmetric metrics

$$g_{mn}dx^m dx^n = F^2 d\rho^2 + H^2(d\theta^2 + \sin^2\theta d\phi^2) - V^2 dt^2$$

the components $\Phi^2,\ \Phi^3,\ \Phi^4$ of anharmonicity vector equal zero.

In regard to the radial component Φ^1, it depends on the choice of the background connection. In the considered case it equals

$$\Phi^1 = \frac{1}{VFH^2}\ \left[\frac{d}{d\rho}(F^{-1}\,V\,H^2) - 2\,F\,V\rho\right]\ .$$

As a consequence of the Fock harmonicity condition

$$\frac{d}{d\rho}(F^{-1}\,V\,H^2) - 2\,F\,V\,\rho = 0\,,$$

the radial component Φ^1 equals zero. But the Fock condition does not follow from the Einstein's equations.

5. THE GENERAL CASE $(k < \infty,\ c < \infty)$

I had considered the general case on the occasion of the 200th anniversary of Lobachevsky's birthday. In [4] I have given the following solution of the new equations of gravity:

$$R_{11} = -\frac{2}{k^2}\,,\ R_{22} = -2\,\sinh^2\frac{\rho}{k},\ R_{33} = -2\sinh^2\frac{\rho}{k}\sin^2\theta,\ R_{44} = 0,$$

$$R_{mn} = 0\,,\quad \text{if}\quad m \neq n\,.$$

According to [4], in the case $(k < \infty,\ c < \infty)$ the gravitational metrics equals

$$k^2 e^{-2\beta}[\Xi^{-1}\,d\xi^2 + \sinh^2(\xi+\beta)(d\theta^2 + \sin^2\theta\, d\phi^2)] - c^2 e^{2\beta}\Xi\, dt^2,$$

where

$$\Xi = \frac{\sinh(\xi - \beta)}{\sinh(\xi + \beta)}, \quad \xi = \frac{\rho}{k}\,, \quad \frac{1}{2}\sinh 2\beta = \frac{\gamma M}{kc^2}$$

(See [8] for details).

In this case the background connection is a harmonic one unconditionally. Indeed, like in the previous case we have Φ^2, Φ^3, Φ^4 being equal to zero. But from new equations of gravity the theorem follows

$$\Phi^m \breve{R}_{mn} + \frac{1}{2}\, g^{am}(\breve{\nabla}_a \breve{R}_{mn} + \breve{\nabla}_m \breve{R}_{an} - \breve{\nabla}_n \breve{R}_{am}) = 0\,.$$

According to this theorem, in the given case we have $\Phi^1(-2k^{-2}) = 0$. If $k < \infty$, from the last equality follows the equality $\Phi^1 = 0$.

It is interesting that in the given case

$$\Phi^1 = \frac{1}{V\,F\,H^2}\,\left[\frac{d}{d\rho}(F^{-1}\,V\,H^2) - F\,V\,k\sinh\frac{2\rho}{k}\right]\,.$$

Consequently

$$\frac{d}{d\rho}(F^{-1}V\,H^2) - FVk\sinh\frac{2\rho}{k} = 0\,.$$

In the limit $k \to \infty$ this equality makes a transition to the Fock condition.

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VORTEX INSTABILITY OF THE CONTINUOUS MEDIUM MOVEMENTS

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Hydrodynamics equations are rewritten for the velocity deformation tensor $D_{ik} = (\partial v_i/\partial x_k + \partial v_k/\partial x_i)/2$ and for vorticity ($\Omega = \mathrm{curl}\ \mathbf{v}$) as observation variables. It ensues from the new written equations that there takes place a pendulum-like process of the energetic conversion between D_{ik} and Ω_i and intermittence of the two structures: tube-like and sheet-like («pancake»-like). It is formulated at the end the analogy of the Bernulli theorem for the vorticity case: the pressure in the area with developed vorticity becomes lower in the average.

It is well known that Halileo invariance dictates the existence of the term $(\mathbf{v}\nabla)\mathbf{v}$ in the continuous medium equations [1]. And vice versa, term $(\mathbf{v}\nabla)\mathbf{v}$ guarantees the Halileo invariance of the movements equations [1,2]. On the other hand, term $(\mathbf{v}\nabla)\mathbf{v}$ is connected closely with the medium vortex behavior due to the identity $(\mathbf{v}\nabla)\mathbf{v} = (1/2)\nabla v^2 - [\mathbf{v}\Omega]$, ($\Omega = \mathrm{curl}\ \mathbf{v}$). It means that the medium vortex behavior and Halileo invariance are mutually interconnected, i.e., the vorticity of the continuous medium is the geometrical property to some extent. Let us study the vorticity and its behavior for the hydrodynamics case.

It is convenient to use the generalized Helmholz equation [2] to study the vortex solutions of the Euler or Navie–Stokes hydrodynamic equations:

$$\frac{\partial \Omega_i}{\partial t} + (\mathbf{v}\nabla)\Omega_i = \frac{1}{2}(\partial v_i/\partial x_k + \partial v_k/\partial x_i)\Omega_k - \nu\ \mathrm{curl\ curl}\ \Omega, \qquad \mathrm{div}\ \mathbf{v} = 0. \tag{1}$$

If we can find some solution for the equations system (1) we can then find the pressure p, as we have an expression for ∇p. The system (1) is a compatibility condition for the initial hydrodynamical equations then.

The system (1) shows that the deformation and vorticity of the fluid are interconnected [3,4]. It is easier to see this if we multiply the system (1) by Ω:

$$\frac{\partial \Omega^2}{\partial t} = 2\Omega_i D_{ik}\Omega_k - \mathrm{div}(\Omega^2\mathbf{v} - 2\nu\ [\Omega\ \mathrm{curl}\ \Omega]) - 2\nu\ (\mathrm{curl}\ \Omega)^2, \qquad \mathrm{div}\ \mathbf{v} = 0. \tag{2}$$

If the vector Ω is parallel to the eigenvector of the velocity deformation matrix $D_{ik} = (\partial v_i/\partial x_k + \partial v_k/\partial x_i)/2$ corresponding to a positive (negative)

eigenvalue, then the first term on the right-hand side of (2) will be positive (negative). Then the local vorticity $|\Omega|$ of the fluid will increase (decrease) if the deformation rate is sufficiently large (large eigenvalues) in order that the first term on the right-hand side of (2) dominates the second and third ones together. A positive eigenvalue exists always due to the assumption of fluid incompressibility: $\mathrm{div}\ \mathbf{v} = 0$, i.e., sum of all eigenvalues is equal to zero. Consequently every enough intensive fluid flow selforganizes so that the vorticity $|\Omega|$ increases due to the deformation motion, determined by the symmetrical tensor D_{ik}, and consequently the spontaneous symmetry distortion takes place as a consequence of the vortex instability process when antisymmetrical part of the tensor $\partial v_i/\partial x_k$ (the vorticity) responds to the symmetrical one behavior. So, the first term on the right hand side of (1) or (2) describes the generation (distortion) of the vorticity $|\Omega|$ [3–5].

The second (divergent) term on the right-hand side of (2) describes the transfer of vorticity in (out of) the point under consideration from (into) the adjoined volume. If we consider the confined volume, then the integral of the second divergent term can be converted into a surface integral after integrating (2) over the volume. Due to zero boundary conditions for $\mathbf{v}$: $\mathbf{v}|_s = 0$ only surface integral remains: $2\nu \oint [\Omega\ \mathrm{curl}\ \Omega]_n dS_n$ and it will affect the integral growth of the vorticity as a result of the vorticity transferring from the volume boundary.

So, abstracting from an irreversible attenuation of the vorticity, described by the third term on the right-hand side of (2), we can represent the following scenario of the growth of the integral of vorticity in the volume studied: the vorticity in the volume increases due to the vorticity transfer from the boundary and due to the actual increasing of the vorticity directed along an eigenvector of the matrix D_{ik} corresponding to a positive eigenvalue. The illustration of both the growth mechanisms is presented in [3, 4] for some examples of the hydrodynamical equations exact solutions.

Here we would like to consider a simple exact solution of the hydrodynamical equations and to follow the actual vorticity growth phenomenon without the influence of the transfer process. Let us consider the following three-dimensional solution [6]:

$$\begin{aligned} v_x &= a_{11}(x - x_0) - a_{12}(y - y_0) + a_{13}(z - z_0), \\ v_y &= a_{12}(x - x_0) + a_{22}(y - y_0) - a_{23}(z - z_0), \\ v_z &= -a_{13}(x - x_0) + a_{23}(y - y_0) + a_{33}(z - z_0). \end{aligned} \tag{3}$$

Here $a_{ik}(t)$ are functions of time. The vorticity vector $\Omega = \mathrm{curl}\ \mathbf{v}$ depends only upon the time: $\Omega = 2(a_{23}, a_{13}, a_{12})$, i.e., $a_{ik} \quad (i \neq k)$ are components of the axial vorticity vector $\mathrm{curl}\ \mathbf{v}$ relative to the principal axes and the matrix D_{ik} has a diagonal form: $D_{ik} = 0$ at $i \neq k$, and $D_{11} = a_{11}$, $D_{22} = a_{22}$, $D_{33} = a_{33}$. Consequently a_{11}, a_{22}, a_{33} are eigenvalues and represent the principal extension–contraction of the fluid flow. Due to the assumption of incompressibility:

$a_{11} + a_{22} + a_{33} = 0$. The expression (3) for v_i is the solution of (1) if a_{ik} satisfies the system of the ordinary differential equations:

$$\mathrm{d}a_{23}/\mathrm{d}t = a_{11}a_{23}, \qquad \mathrm{d}a_{13}/\mathrm{d}t = a_{22}a_{13}, \qquad \mathrm{d}a_{12}/\mathrm{d}t = a_{33}a_{12}. \tag{4}$$

It is interesting to note that the time behavior of the vorticity component along any axis depends upon the extension (contraction) along the same axis. All three components satisfy the condition $a_{12}a_{13}a_{23} = \mathrm{const}$ that follows from (4) and $\mathrm{div}\ \mathbf{v} = 0$. Consequently our solution depends on two arbitrary functions of time. It is possible to combine the results (3),(4) as follows:

$$\begin{array}{l} v_x = (\tau_1'/\tau_1)(x - x_0) - \tau_3(y - y_0) + \tau_2(z - z_0) \\ v_y = \tau_3(x - x_0) + (\tau_2'/\tau_2)(y - y_0) - \tau_1(z - z_0) \qquad \tau_1(t)\tau_2(t)\tau_3(t) = \mathrm{const}, \\ v_z = -\tau_2(x - x_0) + \tau_1(y - y_0) + (\tau_3'/\tau_3)(z - z_0) \end{array} \tag{5}$$

where τ_i' denotes derivative of the time function $\tau_i(t)$: $\mathrm{d}\tau_i/\mathrm{d}t = \tau_i'$.

The solutions (3), (4) describe the increasing of the vorticity vector components directed along eigenvectors (one or two) corresponding to positive eigenvalues and decreasing in the other direction. It means that the vorticity vector turns with time towards the extension directions, whereas along contraction directions the corresponding components are diminishing to zero. The solutions (3) and (4), or (5) demonstrate the important intercorrelation of the deformational and vorticity parts of the flow: the vorticity responds to the deformational structure. The hydrodynamical equations connect two, generally speaking, independent parts of the tensor $\partial v_i/\partial x_k$, i.e., symmetrical (six components) part and antisymmetrical (three components) one. Moreover the presented solution is nonstationary: the vorticity depends on time exponentially even for the constant principal compression–extension. It is important that the solution (5) is essentially three-dimensional despite its simplicity.

It is possible to consider the solution in the form of (3) as a decomposition of every hydrodynamical solution in the vicinity of any point x_0, y_0, z_0 and the rotation of coordinate system up to principal axis. Then we can state: at every point the small vorticity disturbance grows in accordance with (4), as there is always one or two positive from the set a_{11}, a_{22}, a_{33} due to $a_{11} + a_{22} + a_{33} = 0$ (incompressibility). This means that the deformational flow of incompressible ideal fluids is unstable everywhere relative to the vorticity disturbances if the external force is represented by a gradient of some function.

The essential nonstationarity of the vortex behavior can be an important moment for the turbulence problem solution in case of continuous medium movements. But it is necessarily to study not only the vortex dependance of deformation but the influence of the vorticity on the deformation of the flow. Corre-

sponding equations for D_{ik} can be obtained from Navie–Stoks equations:

$$\frac{\partial D_{ik}}{\partial t} + (\mathbf{v}\nabla)D_{ik} = -D_{in}D_{nk} + \frac{1}{4}\Omega^2\delta_{ik} - \frac{1}{4}\Omega_i\Omega_k - \frac{1}{\rho}\frac{\partial^2 p}{\partial x_i \partial x_k} + \nu\frac{\partial}{\partial x_n}(\frac{\partial D_{in}}{\partial x_k} + \frac{\partial D_{kn}}{\partial x_i}) + \frac{\partial^2 \phi}{\partial x_i \partial x_k}, \qquad D_{kk} = 0, \tag{6}$$

where ϕ is a potential of the external force $\nabla\phi$. The equations (1) and (6) define mutual influence of the deformation D_{ik} and vortex Ω_i. In accordance with the Halileo principle we observe the gradients of velocity (but not velocity itself), i.e., nine values $\partial v_i/\partial x_k$. Tensor $\partial v_i/\partial x_k$ consists of symmetrical part D_{ik} (six components) and antisymmetrical part Ω_i (three components): $\partial v_i/\partial x_k = (\partial v_i/\partial x_k + \partial v_k/\partial x_i)/2 + (\partial v_i/\partial x_k - \partial v_k/\partial x_i)/2$. In the end, the formal conservation laws (1), (6) connect both parts D_{ik} and Ω_i so, that observable variables D_{ik} and Ω_i are not independent. For the better understanding of the hydrodynamical flow main characteristics it is convenient to have equation for $D^2 = D_{ik}D_{ik}$ multiplying (6) by D_{ik}:

$$4\frac{\partial D^2}{\partial t} = -2\Omega_i D_{ik}\Omega_k - 8D^3 - 16\nu(\frac{\partial D_{ik}}{\partial x_k})(\frac{\partial D_{in}}{\partial x_n}) + \frac{8}{\rho}\frac{\partial}{\partial x_i}[(\frac{\partial v_i}{\partial x_k})\frac{\partial(\rho\phi - p)}{\partial x_k}) + \frac{\rho}{2}v_i D^2 + 2\rho\nu D_{ik}(\frac{\partial D_{kn}}{\partial x_n})], \tag{7}$$

where $D^3 = D_{in}D_{nk}D_{ki}$. The first terms on the right-hands in (2) and (7) have the same absolute value but different signs. Consequently they are describing the channel of the energy exchange between vortex and deformation. The described above phenomenon of the local vortex instability everywhere is a stage of the general pendulum-like exchange process. **The nonlinear pendulum-like process of the energy exchange between vortex and deformations means substantial nonstationarity of the ideal incompressible fluid with chaotic elements of the behavior.** The role of the term D^3 could be clarified after volume integrating of the equation (7) and taking into account zero boundary conditions. D^2 and D^3 are invariants (scalars) and we can therefore express D^2 and D^3 via principal values of the fluid flow extension–contraction. Then:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\overline{\lambda_1^2} + \overline{\lambda_2^2} + \overline{\lambda_3^2} + \overline{\omega^2}/4) = -6\overline{\lambda_1\lambda_2\lambda_3} - 4\nu\left[\overline{\left(\frac{\partial D_{ik}}{\partial x_k}\right)\left(\frac{\partial D_{in}}{\partial x_n}\right)} + \overline{\frac{(\mathrm{curl}\Omega)^2}{8}}\right], \tag{8}$$

where the line above symbols means volume integrating. The value $\overline{\lambda_1\lambda_2\lambda_3}$ depends on the two characteristic elements population of the deform–vortex medium behavior. First element has one positive eigenvalue and two negative ones ($\lambda_1\lambda_2\lambda_3 > 0$) and gets the name tube-like vortex structure, and the second one under the name sheet-like structure or «pancake» has one negative eigenvalue and two positive ones ($\lambda_1\lambda_2\lambda_3 < 0$). Abstracting from dissipation we can

conclude: the behavior of the continuous media is organized so that both characteristic elements should alternate or intermit each other in space and time in such a way to convert $\overline{\lambda_1\lambda_2\lambda_3}$ into zero for the stationary case (for example the case of the isotropic turbulence). Consequently, the approach with observable variables D_{ik} and Ω_i reveals the fundamental intermittence low: **under the intermittence condition there takes place the conservation of the sum of the deformation square and vortex square.** This new intermittence low is very important for the theory of the developed, stationary, homogeneous turbulence. It brings the elements of the organized chaos together with the pendulum-like process into the continuous medium behavior.

It is useful to connect pressure p with D^2 and Ω^2. We can get such connection putting in (6) $i = k$, summing up and taking into account $D_{kk} = 0$. Then:

$$(\Omega^2/2) - D^2 = \Delta p. \tag{9}$$

Equation (9) is Laplace equation with volume sources presented by difference between vortex square and deformation square. Volume integration of (9) gives:

$$\overline{\Omega^2}/2 - \overline{D^2} = \oint \nabla_i p dS_i, \tag{10}$$

i.e., the average value of the pressure gradient on the surface, surrounding the considered volume, is equal to the difference of the integral vortex square and the integral deformation square. Then we can state: **the pressure averaged value in the volume becomes lower relative to the pressure averaged value on the boundary surrounding volume if the vorticity is enough intensive relative to deformation so that $\overline{\Omega^2}/2 > \overline{D^2}$.** This statement is an analogy of the Bernulli theorem.

It is interesting to give as an example two important applied consequences of the studied instabilities. First, there is a mathematical analogy between an equation for vorticity Ω and an equation for magnetic field in magnetohydrodynamics. The result concerning local vortex instability, everywhere we have studied above, can be reformulated in the magnetohydrodynamics as follow: magnetohydrodynamic flows are locally unstable everywhere. Such conclusion could follow from paper [9], too. Consequently it is possible to say that **the stationary magnetic restraint of plasma is impossible.** Second, it is supposed, that the movement of the interstellar or intergalactic medium is described by hydrodynamical equations [10]. Consequently we could appropriately apply our results to the study of the such medium behaviors. We can see the vortex structure everywhere in the Universe: for example spiral galaxies. And the streamlines are, generally speaking, spirals as is possible to see from characteristic equations $\mathrm{d}x_i/\mathrm{d}t = v_i$ with special choice of parameters a_{ik} in (3), for example. The questions appear in connection with the incompressibility condition, which is not valid, generally

speaking, for cosmical gas medium. But the study of the incompressible behavior of the gas medium will be correct if the relative movements in this medium have velocities smaller than sound speed. And such situation takes place [10] for the problem of the galaxies or galactic system vortex instability. Let us consider now the very important and very intriguing cosmological problem of dark matter using our result concerning the total instability of the hydrodynamical flow.

The dark-matter problem we speak about originates under the interpretation of the objects motion on the boundary of large-scale gravitating formations such as galaxies or galactic systems [10, 11]. The velocity of this objects is considered as an orbital motion due to the attractive force influence of the such formations gravity mass. It means that we assume stationary condition. Then the attracting mass, evaluated at observed velocities, is ten or more times larger than the visible mass [10, 11]. In this case people are speaking about dark matter, i.e., about latent, invisible, nonbaryon mass that is not observed yet. But if we consider the velocity of the boundary objects as a result of the vortex instability development due to the deformation of the gravitating formation, then the dark matter problem may be dismissed and considered as artifact of the stationary hypothesis. For example, the round motion of the air particles in tornado is a result of the vortex instability development but not due to the existence of the gravitating mass in the middle of tornado. Indeed the Navie–Stokes equations describe the deformational flow of the cosmic cloud due to the gravitational influence of the neighboring mass through $\nabla\phi$ in the right-hand side of the equations. The compatibility system (1) has the nonstationary vortex solutions as we have shown, i.e., a vorticity will develop due to the deformational collective flow of the cosmic medium. It means that the gravitational influence on the vortex behavior takes place through the process of deformation (the gravitational force $\nabla\phi$ disappears in the compatibility equations (1)). Consequently the large-scale movements of the interstellar or intergalactic medium are principally nonstationary when we can neglect the medium viscosity. So the dark matter paradox means indeed the nonstationarity and vortex instability of the large-scale cosmic formation flow under the indirect influence of the gravity. Such resolution of the paradox could give an evaluation of the instability rate.

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SYMMETRY AND ANALYTICITY

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On the basis of general space-time and crossing symmetry, a general analytic structure for amplitudes describing spin-particle binary reactions is considered. Using knowledge about the kinematic structure of helicity amplitudes in the dynamic amplitude approach we can get: dispersion relations for helicity amplitudes; low-energy theorems; sum rules; model-independent sum-rule type inequalities for observable quantities and some asymptotic relations between polarization parameters. In this short paper we will consider only dispersion relations for each individual helicity amplitudes describing any elastic processes.

1. INTRODUCTION

A nice analytic structure of the scattering amplitude can be seen from dispersion relations. Dispersion relations for pion-nuclon scattering for fixed t were first proved by Nikolai Nikolaevich Bogoliubov in axiomatic approach to quantum field theory. This famous work was presented at the Siettle conference in 1956 (see [1]). In the framework of the so-called S-matrix approach [2], dispersion relations are postulated — they are considered as basis of theory.

For real binary processes with particles of nonzero spins, analytic structures of amplitudes are defined by spin-kinematics (they give us kinematic singularities) and general properties defined by the unitarity condition (dynamic singularities).

On the basis of general space-time and crossing symmetry, a general analytic structure for amplitudes describing spin-particle binary reactions is considered. Using knowledge about the kinematic structure of helicity amplitudes in the dynamic amplitude approach we can get: dispersion relations for helicity amplitudes; low-energy theorems; sum rules; model-independent sum-rule type inequalities for observable quantities and some asymptotic relations between polarization parameters. In this short paper we will consider only dispersion relations for each individual helicity amplitudes describing any elastic processes.

2. SYMMETRY AND SPIN PARTICLES

Due to the symmetry in particle physics (quantum field theory), we have a Lagrangian of a definite form that depends on a certain number of masses and

interaction constants. This is in sharp contrast with quantum mechanics where interactions are considered as arbitrary functions (potentials) for every pair of particles. The symmetry does not admit arbitrary functions.

Today we have the following succession:

$$\text{Symmetry} \rightarrow \text{group} \rightarrow \text{particle interaction}.$$

Besides the Lagrangian approach, in particle physics there exists a problem that has its own history: the problem of direct investigation of processes with elementary particles, based on the general principles and independent of the explicit form of Lagrangian. This general principles are: symmetry, causality and unitarity.

Analytic properties of the amplitudes of certain particle reaction are connected with causality and unitarity, and properly defined amplitudes obey dispersion relations. Dispersion relations for invariant amplitudes of pion-nucleon interaction were given in [1].

In studying analytic properties of amplitudes, we have two types of singularities: dynamic singularities connected with unitarity and kinematic singularities connected with spin.

3. SPIN AND PARTICLE REACTIONS

Most of the particles have a nonzero spin. We are going to consider binary reactions with particles of arbitrary spins. If we consider reactions with particles with spin

$$s_1 + s_2 \rightarrow s_3 + s_4, \tag{1}$$

we have $N = (2s_1 + 1)(2s_2 + 1)(2s_3 + 1)(2s_4 + 1)$ functions to describe the process, and we must choose the optimal set of these functions. The spin-particle reactions are convenient to describe in the helicity amplitude formalism [3]. Helicity amplitudes $f_{\lambda_3,\lambda_4;\lambda_1,\lambda_2}(s,t)$ have a clear physical meaning, observables are expressed by them in a simple way. Helicity amplitudes contain all the information about the considered process. Helicity amplitudes have kinematic singularities independent of interactions.

Scattering of spinless particles is described by one amplitude. Considering this amplitude as a function of invariant variables, we have the function $A(s,t)$. This amplitude has some singularities. They are called the dynamic singularities.

For spin-particles, the process is described by several functions, several helicity amplitudes. And they have additional, so-called kinematic, singularities. So helicity amplitudes do not fulfil simple dispersion relations. It is necessary to find and separate kinematic singularities. So, helicity amplitudes are expressed via a

set of other amplitudes without kinematic singularities. For a lowest spin it is convenient to introduce invariant amplitudes.

Let us consider the simplest nontrivial reaction: π-N scattering, elastic scattering of a spin-zero particle with the mass μ on the spin-1/2 particle of mass m. Using the Dirac equation one can find the following connection between the helicity and invariant amplitudes (in the standard notation):

$$f^s_{0,\lambda_4;0,\lambda_2}(s,t) = \bar{u}^{\lambda 4}(p_4)\{A(s,t) + \hat{Q}B(s,t)\}u^{\lambda 2}(p_2). \tag{2}$$

Here $A(s,t)$ and $B(s,t)$ are invariant amplitudes. Properly defined invariant amplitudes have no kinematic singularities.

For the general case of scattering of particles with spins s_i we have relations of the following type [4]:

$$f_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t) = \sum_{n=1}^{N} a^n_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t)A_n(s,t). \tag{3}$$

Kinematic singularities of $f_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t)$ are contained in the coefficient functions $a^n(s,t)$.

This procedure is nice for low spins. It is difficult to construct such an expansion for high spins; for all $s_i = 3/2$, $N = 256$ and for $s_i = 11/2$, $N \simeq 20000$. Besides, the main difficulty is to find a decomposition of that type so that coefficients of invariant amplitudes do not contain «secret singularities» rather than in dimensions. So, in describing the Compton effect for several years people used a decomposition suggested in [5], but then it appeared that those invariant amplitudes had additional singularities, and later a more complicated decomposition [6] was suggested.

Besides technical difficulties for spins larger than 1, a nontrivial question of uniqueness of that decomposition arises, and since for higher spins the invariant amplitude decomposition is not unique, «secret» singularities, additional and noncontrollable kinematic constraints appear.

There exists another way based on symmetry principles, and it uses representations of a rotation group — Wigner's d-functions. If we use d-functions in the s-channel, then use d-functions in the t-channel, and finally connect channels also by d-functions, we can get a result much more convenient than (3).

4. ANALYTIC PROPERTIES OF AMPLITUDES: SEPARATION OF SPIN-KINEMATICS AND DYNAMICS

A lot of people worked in this direction by considering spin-kinematics and decomposition of helicity amplitudes in terms of other sets of amplitudes [4–6].

Combining some approaches and modifying others we suggest a new variant of the formalism that has all advantages of different approaches, differs from all of them, and is based on the symmetry and conservation laws, and is general and simple.

Symmetry imposes restrictions on amplitudes. When one has additional symmetries in definite directions, the number of independent amplitudes in such «symmetric directions» is reduced. Such situations occur for forward and backward scattering.

Consider the reaction in the s-channel described by the helicity amplitudes. Introduce the quantities $\lambda = \lambda_1 - \lambda_2$ and $\mu = \lambda_3 - \lambda_4$. Two particles in the centre-of-mass system are moving in the opposite directions, and thus, λ and μ are projections of the total spin in the directions of motion prior to and after collision. Owing to the conservation of the projection of the total angular momentum, the amplitudes in the forward direction, $\theta_s \to 0$, should vanish in all cases except for $\lambda = \mu$. Analogously, for backward scattering, $\theta_s \to \pi$, the amplitudes should vanish for the same reasons in all cases except for $\lambda = -\mu$.

For forward scattering we have

$$f^{\text{forward}}_{\lambda_3\lambda_4,\lambda_1,\lambda_2} = \begin{cases} f_{\lambda_3\lambda_4,\lambda_1,\lambda_2}, & \text{when} \quad \lambda = \mu, \\ 0, & \text{when} \quad \lambda \neq \mu, \end{cases} \tag{4}$$

whereas for backward scattering

$$f^{\text{backward}}_{\lambda_3\lambda_4,\lambda_1,\lambda_2} = \begin{cases} f_{\lambda_3\lambda_4,\lambda_1,\lambda_2}, & \text{when} \quad \lambda = -\mu, \\ 0, & \text{when} \quad \lambda \neq -\mu. \end{cases} \tag{5}$$

Two questions arise: Can the helicity amplitudes be parametrized so as to satisfy the conditions (4) and (5) automatically? Can kinematic singularities of helicity amplitudes be found and separated in a simple way? The answer to both questions is «yes».

For the spinless case we have the decomposition via the Legendre polynomials depending on $\cos\theta$. By definition, in the spinless case we have no kinematic singularities.

In the nonzero spin case, helicity amplitudes have decomposition via Wigner d-functions of rotation. Helicity amplitudes are splitted into two parts; one part is defined by the symmetry properties and enters into the functions $d^J_{\lambda\mu}(\cos\theta)$ [7] that make the conservation laws of the angular momentum valid, and the other part has a dynamic nature and enters into the partial helicity amplitudes $f^J_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s)$.

Kinematic singularities in d-functions do not depend on J, and we can separate the common singular factors. The rest sum in the decomposition contains the

decomposition over polynomials in the t-variable. So, we can defin the so-called dispersion amplitudes [8] for any binary processes:

$$f^s_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t) = A^{|\lambda-\mu|}B^{|\lambda+\mu|}\bar{f}^s_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t), \tag{6}$$

here

$$A = \frac{\sqrt{L^2-a^2}}{(m_1+m_2)(m_3+m_4)}, B = \frac{\sqrt{L^2+a^2}}{(m_1+m_2)(m_3+m_4)},$$

$$\begin{aligned} L^2 \quad = \quad & \{[s-(m_1+m_2)][s-(m_1+m_2)] \\ & [s-(m_3+m_4)][s-(m_3+m_4)]\}^{1/2}, \end{aligned}$$

$$a^2 = 2st + s^2 - s\sum m_k^2 + (m_1^2-m_2^2)(m_3^2-m_4^2).$$

The mass factors in the denominators make A and B dimensionless without introducing additional singularities in the variable s . Under this parametrization, the conditions (4) and (5) are fulfilled automatically. All kinematic singularities in variable t are separated explicitly, and no false singularities in s are introduced. The amplitudes $\bar{f}^s_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t)$ suit well for studying the analytic properties of the amplitudes at fixed s, because they obey dispersion relations. Therefore, we call them the dispersion amplitudes [12]. They still may have the kinematic singularities in the variable s.

Dispersion amplitudes remind reduced amplitudes [10], but they have no additional s-variable false singularities.

For t-channel processes the corresponding dispersion amplitudes are free from kinematic singularities in the variable s. Expressing the dispersion amplitudes of the s-channel in terms of the dispersion amplitudes on the annihilation channel, we obtain the connection between the amplitudes having kinematic singularities in s with the amplitudes that are free from them. So, kinematic singularities of the s-channel helicity amplitudes are in crossing coefficients in crossing relations between s- and t-channel amplitudes. The number of coefficients is restricted, and we do know the singularities of these coefficients; indeed these coefficients are Wigner's functions, and we do know their singularities!

So, using crossing symmetry we can find kinematic singularities of the s-channel dispersion amplitudes also in the variable s; separating these singularities we determine a new set of functions describing binary processes — dynamic amplitudes. Dynamic amplitudes for elastic processes ($m+\mu \longrightarrow m+\mu$) have the following relations with the helicity amplitudes [11]:

$$f_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t)=\left(\frac{\sqrt{-t}}{m+\mu}\right)^{-|\lambda-\mu|}\left(\frac{\sqrt{L^2+st}}{(m+\mu)^2}\right)^{-|\lambda+\mu|}\times$$
$$\times\left(\frac{L}{(m+\mu)^2}\right)^{-2(s_1+s_2)}D_{\lambda_3\lambda_4,\lambda_1,\lambda_2}(s,t). \qquad (7)$$

Dynamic amplitudes are in fact modified regularized helicity amplitudes, they differ from the reduced amplitudes by dimensions: all dynamic amplitudes have the same dimensions, whereas the dimensions of regularized amplitudes depend on spins and helicities [10].

5. ANALYTIC PROPERTIES AND DISPERSION RELATIONS FOR INDIVIDUAL HELICITY AMPLITUDES

Let us consider dispersion relations with fixed t, a certain number of them was strongly proved for definite regions of t, and which are used much more frequently, then relations with fixed s. For getting such dispersion relations one has to have amplitudes free of kinematic singularities in s and u variables. Such functions are: dynamic amplitudes, correctly defined invariant amplitudes, and t-channel dispersion amplitudes. Of course, considering process in the centre-of-mass system of s-channel it is convenient to use s-channel amplitudes.

Dynamic amplitudes when t is fixed fulfil the following dispersion relations:

$$D_h(s,t)=D_h^B(s,t)+\frac{1}{\pi}\int\limits_{s_0}^{\infty}\frac{ds^{'}}{s^{'}-s}\Big\{D_h(s^{'},t)\Big\}^s+\frac{1}{\pi}\int\limits_{u_0}^{\infty}\frac{du^{'}}{u^{'}-u}\Big\{D_h(u^{'},t)\Big\}^u. \qquad (8)$$

One can easily add corresponding subtraction terms, if they are necessary.

Taking into account a simple, one-to-one correspondence between dynamic and helicity amplitudes, we get dispersion relations for each individual helicity amplitudes for any spin-particle elastic scattering:

$$f_h(s,t)=f_h^B(s,t)+K_h(s,t)\times$$
$$\times\left\{\frac{1}{\pi}\int\limits_{s_0}^{\infty}\frac{ds^{'}}{s^{'}-s}\left\{\frac{f_h(s^{'},t)}{K_h(s^{'},t)}\right\}^s+\frac{1}{\pi}\int\limits_{u_0}^{\infty}\frac{du^{'}}{u^{'}-u}\left\{\frac{f_h(u^{'},t)}{K_h(u^{'},t)}\right\}^u\right\}. \qquad (9)$$

In invariant amplitudes it is possible to get dispersion relations for combinations of helicity amplitudes if the connection matrix between helicity and invariant

amplitudes is known. But they are known only for small values of spins, and even in this case they are very complicated.

6. OTHER APPLICATIONS OF DYNAMIC AMPLITUDES

The spin kinematics allows one to obtain the low-energy theorems for photon-hadron processes [12] and gravitino scattering on a spin-0 target. For the latter process at low energies, the helicity amplitudes up to $0(E^3)$ are determined by their t-channel Born terms with the photon exchange [13]. The dynamic amplitudes, or more simply the t-channel dispersion amplitudes, can be used to prove model-independent dispersion inequalities for the Compton effect on a pion and a nucleon target, including the case of the polarized photon scattering [14].

In the framework of the «dynamic amplitude» approach, obligatory kinematic factors arise in the expressions of observables. These spin structures for high energies give a small parameter that orders the contributions of helicity amplitudes to observables. Such a «kinematic hierarchy» predicts a simple connection between asymmetry parameters and even numerical values for them [15] for pp elastic scattering at high energies and a large fixed angle (90°).

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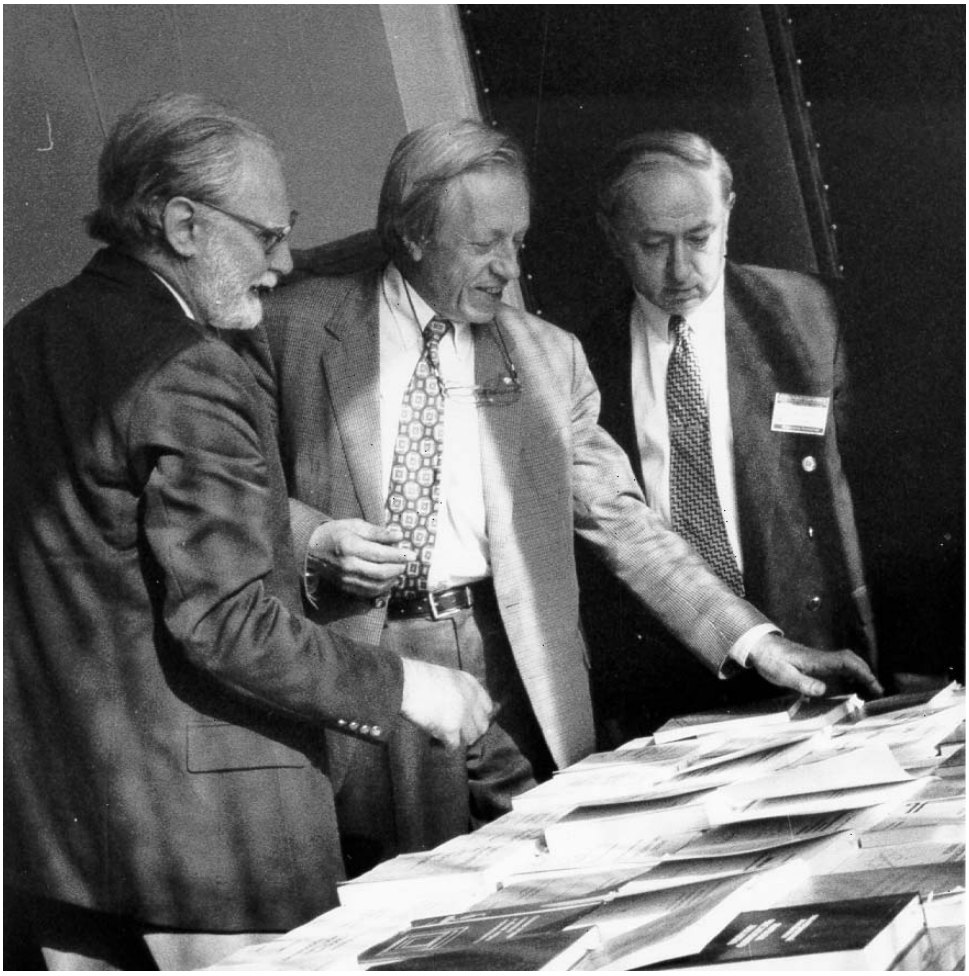

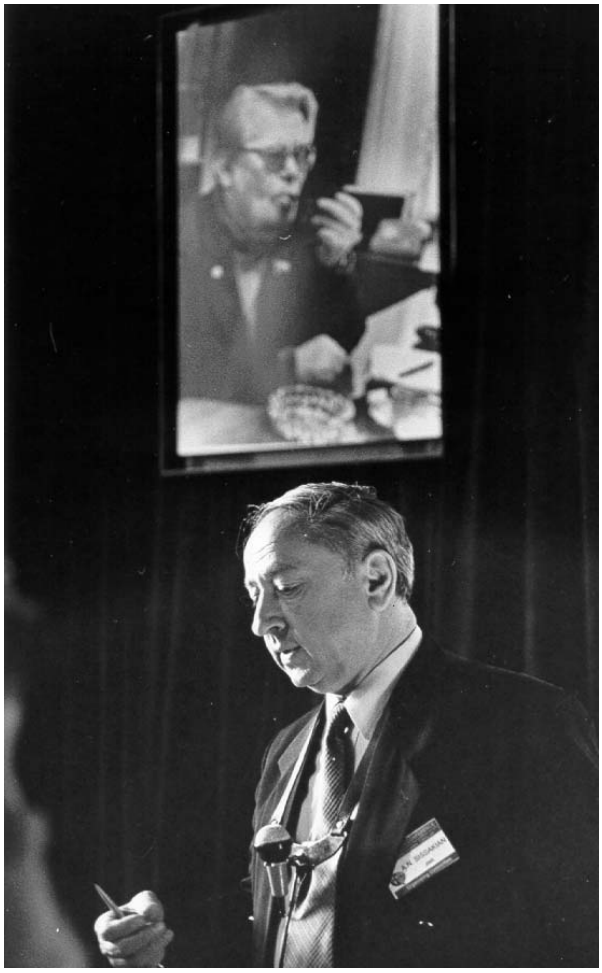


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СТАТИСТИЧЕСКАЯ ФИЗИКА

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PHASE TRANSITION ASSOCIATED WITH FORMATION OF SPATIALLY PERIODIC STRUCTURES IN A FERMI LIQUID

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The phase transition in a Fermi liquid, associated with translational symmetry breaking and the formation of periodic structures is considered. Special attention is paid to the formation of one-dimensional long-periodic structures in a three-dimensional Fermi liquid. The relation between the formation of such structures and kinetic and thermodynamic stability of the normal state of the Fermi liquid is analyzed.

The term «normal Fermi liquid» is traditionally applied to a degenerate (charged or neutral) Fermi liquid possessing main properties of a system of noninteracting fermions in the case of a quasiparticle description. Such a definition of a normal Fermi liquid presumes that the equilibrium state of the Fermi liquid is the most symmetric, i.e., the distribution function describing this state is invariant to spatial translations and rotations in the spin and momentum spaces.

In spite of differences in the behavior of charged and neutral Fermi liquids, basic concepts of the Landau–Silin theory of the normal Fermi liquid [1,2] studying low-lying excitations against the background of the equilibrium state make it possible to disregard the electric charge of quasiparticles in the description of some phenomena in charged and neutral systems of interacting fermions. Apart from the main condition of applicability of the theory of the normal Fermi liquid, i.e., the smallness of temperature T as compared to the Fermi energy ε_F ($T \ll \varepsilon_F$), the main postulate of the theory which is common for neutral and charged systems concerns the functional dependence of the energy of the system E on the fermion distribution function $f(\vec{p},\vec{r})$: $E = E(f)^*$.

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*We are using the system of units in which Boltzmann's constant k and Plank's constant $\hbar$ are equal to unity.

In this case, the quasiparticle energy which is a functional of the distribution function is defined as

$$\varepsilon(\vec{p},\vec{r}) = V\frac{\delta E(f)}{\delta f(\vec{p},\vec{r})},$$

$$\varepsilon(\vec{r},\vec{p}) = \varepsilon_p + \frac{2}{V}\sum_{\vec{p}'}\int d\vec{r}\,' F(\vec{r}-\vec{r}\,';\vec{p},\vec{p}\,')f(\vec{r}\,',\vec{p}\,'), \qquad S=1/2, \quad (1)$$

where $F(\vec{r}-\vec{r}\,';\vec{p},\vec{p}\,')$ is the Landau amplitude characterizing two-particle interactions, and $\varepsilon_p \equiv F(\vec{p})$ is the fermion energy in the absence of interaction between quasiparticles. In the absence of magnetic ordering, the existence of the fermion spin $S = 1/2$ is important only for the calculation of the fermion density of states, which is reflected in the factor $2S + 1 = 2$ in the second term of formula (1). The equilibrium state of the normal fermi liquid in a spatially inhomogeneous case is described by the Fermi–Dirac distribution function

$$f(\vec{p},\vec{r}) = \{\exp\beta(\varepsilon(\vec{p},\vec{r}) - \mu) + 1\}^{-1} \quad (2)$$

($\beta^{-1} = T$ is the inverse temperature and μ the chemical potential). Together with Eq. (1), this equation determines the dispersion relation for quasiparticles in the equilibrium state.

An important aspect of the theory is the determination of the stability conditions for an equilibrium state of a normal Fermi liquid. This problem was solved for the first time in the spatially homogeneous case by Pomeranchuk [3] who formulated the stability criterion for the normal state down to the temperature $T = 0$:

$$1 + \frac{\nu(\mu)F_l}{2l+1} > 0, \quad (3)$$

where F_l are the coefficients of the l-th harmonic in the expansion of the spatially homogeneous Landau amplitude

$$F(\vec{p},\vec{p}\,') = \int d\vec{r}\,' F(\vec{r}-\vec{r}\,';\vec{p},\vec{p}\,') \quad (4)$$

into a series in Legendre polynomials near the Fermi surface ($p \approx p' \approx p_F$).

$$F(\vec{p},\vec{p}\,') = \sum_{l=0}^{\infty} F_l(p,p')P_l(\cos\theta). \quad (4)$$

The quantity $\nu(\varepsilon)$ appearing in formula (3) is the density of energy states defined as

$$\nu(\varepsilon) = \frac{2}{(2\pi)^3}\int d^3p\,\delta(\varepsilon - \varepsilon(p)) \quad (5)$$

($\varepsilon(p)$ corresponds to the spatially homogeneous distribution function $f(p)$).

It should be noted that the violation of Pomeranchuk's criterion indicates that the stability of the normal state is broken at temperatures $T < T_0$ (T_0 is the transition temperature, $T \ll \varepsilon_F$).

The present work [4] is devoted to an analysis of such a phase transition, i.e., the transition involving the violation of the stability condition (3) for the zeroth harmonic ($l = 0$), for which the following relation holds:

$$\nu(\mu)F_0 \lesssim -1. \tag{6}$$

We shall prove that condition (6) characterizes a phase transition in a Fermi liquid, associated with translational symmetry breaking for the equilibrium state.

Let us seek the solution of self-consistent Eqs. (1), (2) in the form of functions periodic in x with the period $X = 2\pi/q$

$$\varepsilon(\vec{r}, \vec{p}) \equiv \varepsilon(x, p) = \varepsilon_0(p) + \widetilde{\varepsilon}(x), \tag{7}$$

where

$$\varepsilon_0(p) = \langle \varepsilon(x, p) \rangle, \qquad \langle \widetilde{\varepsilon}(x) \rangle = 0 \tag{8}$$

and the angle brackets $\langle ... \rangle$ denote the averaging over periods. Consequently, Eqs. (1), (2) can be written in the form:

$$\varepsilon_0(p) = \varepsilon_p + F_0 \langle n(\beta, \mu - \widetilde{\varepsilon}(x)) \rangle, \tag{9}$$

$$\widetilde{\varepsilon}(x) = \int dx' F(x - x') \{ n(\beta, \mu - \widetilde{\varepsilon}(x')) - \langle n(\beta, \mu - \widetilde{\varepsilon}(x'')) \rangle \}, \qquad \widetilde{\varepsilon}(\vec{p}, x) \equiv \widetilde{\varepsilon}(x), \tag{10}$$

where

$$F_0 = \int_{-\infty}^{\infty} dx F(x) \tag{11}$$

and the function $n(\beta, \mu)$ is defined by the expression:

$$n(\beta, \mu) = \frac{2}{V} \sum_{\vec{p}} \frac{1}{e^{\beta(\varepsilon_0(p) - \mu)} + 1}. \tag{12}$$

Let us now go over to the solution of Eq. (10) near the phase transition point (the transition to the states with spatially periodic structure), when the quantity $\widetilde{\varepsilon}(x)$ describing the order parameter is small. Noting that the quantity $F(x - x')$ has a sharp peak at $x = x'$ ($X \gg r_0; F(x - x') \approx 0$ at $x - x' \gtrsim r_0$) and also considering that the quantity $\widetilde{\varepsilon}(x)$ varies slowly on the account of the large lattice period, we can write Eq. (10) in the form

$$\widetilde{\varepsilon}(x) = F_0 \{ n(\beta, \mu - \widetilde{\varepsilon}(x)) - \langle n(\beta, \mu - \widetilde{\varepsilon}(x)) \rangle \} + F_2 \frac{\partial^2 n(\beta, \mu - \widetilde{\varepsilon}(x)}{\partial x^2}, \tag{13}$$

where

$$F_2 = \frac{1}{2}\int dx' F(x-x')(x-x')^2 \tag{14}$$

(while deriving Eq. (13), we assumed that the function $F(x-x')$ is even). Carrying out the power expansion in $\widetilde{\varepsilon}(x)$ and $(\beta-\beta_0)$ in Eq. (13) (β_0-corresponds to the transition temperature for $q=0$) and taking into account that in accordance with (8) $\langle\widetilde{\varepsilon}(x)\rangle = 0$ we have

$$\widetilde{\varepsilon}(x)\left(1 + F_0\frac{\partial n(\beta_0,\mu)}{\partial\mu}\right) = 0, \tag{15}$$

$$F_0\left\{-(\beta-\beta_0)\frac{\partial^2 n(\beta_0,\mu)}{\partial\beta\partial\mu}\widetilde{\varepsilon}(x) + \frac{1}{2}\frac{\partial^2 n(\beta_0,\mu)}{\partial\mu^2}(\widetilde{\varepsilon}^2(x) - \langle\widetilde{\varepsilon}^2(x)\rangle)\right\} - \tag{16}$$

$$-F_2\frac{\partial n(\beta_0,\mu)}{\partial\mu}\,\frac{\partial^2\widetilde{\varepsilon}(x)}{\partial x^2} = 0.$$

The Eq. (15) determines the transition temperature β_0. Carrying out in this equation the low-temperature expansion for the function $n(\beta_0,\mu)$ we obtain

$$T_0^2 = -\frac{6}{\pi^2}\frac{1+F_0\nu(\mu)}{F_0\nu''(\mu)}. \tag{17}$$

Since $\nu''(\mu) < 0$, it can be easily seen that the inequality $T_0^2 > 0$ holds only when the relation (6) reflecting the violation of the criterion of stability of the equilibrium state of a normal Fermi liquid is valid.

Equation (16) used for defining the quantity $\widetilde{\varepsilon}(x)$ can be written in another form more convenient for the subsequent analysis. For this purpose, we introduce the quantity $\varepsilon(x) = -\widetilde{\varepsilon}(x)$ that can be regarded as a correction to chemical potential (see (9) and (10)). Then Eq. (16) assumes the form

$$\frac{\partial^2\varepsilon(x)}{\partial x^2} + g(\varepsilon(x)) = 0, \qquad g(\varepsilon(x)) = A\varepsilon(x) + B(\varepsilon^2(x) - \langle\varepsilon^2(x)\rangle), \tag{18}$$

where

$$A = -\frac{F_0^2}{F_2}(\beta-\beta_0)\frac{\partial^2 n(\beta_0,\mu)}{\partial\beta_0\partial\mu}, \qquad B = -\frac{1}{2}\,\frac{F_0^2}{F_2}\,\frac{\partial^2 n(\beta_0,\mu)}{\partial\mu^2}. \tag{19}$$

We shall seek periodic solutions of Eq. (18) which gives

$$\varepsilon' = \pm\sqrt{2(E-U(\varepsilon))}, \qquad x = \pm\int^{\varepsilon}\frac{d\varepsilon}{\sqrt{2(E-U(\varepsilon))}}, \tag{20}$$

where

$$U(\varepsilon) = \int_0^{\varepsilon} g(\varepsilon)d\varepsilon = \frac{1}{3}B\varepsilon^3 + \frac{1}{2}A\varepsilon^2 - Bd^2\varepsilon, \qquad d^2 = \langle\varepsilon^2(x)\rangle$$

and E is the integration constant. The cubic polynomial $E-U(\varepsilon)$ can be written in the form

$$E-U(\varepsilon)=E-\frac{1}{3}B\varepsilon^3-\frac{1}{2}A\varepsilon^2+Bd^2\varepsilon=-\frac{1}{3}B(\varepsilon-\varepsilon_1)(\varepsilon-\varepsilon_2)(\varepsilon-\varepsilon_3)>0. \quad (21)$$

The points of extrema of the function $U(\varepsilon)$ are defined as

$$\varepsilon_\pm=-\frac{A}{2B}\pm\sqrt{\frac{A^2}{4B^2}+d^2}, \qquad \varepsilon_+>0,\ \varepsilon_-<0.$$

Since $E-U>0$, periodic solutions of Eq. (18) correspond to the region $\varepsilon_2<\varepsilon<\varepsilon_1$, and since $\langle\varepsilon\rangle=0$, we have $\varepsilon_2<0$, $\varepsilon_1>0$. Consequently we have

$$x(\varepsilon)=-\int_\varepsilon^{\varepsilon_1}\frac{d\varepsilon}{\sqrt{2(E-U(\varepsilon))}}, \qquad -\frac{X}{2}<x<0, \quad (22)$$

$$x(\varepsilon)=\int_\varepsilon^{\varepsilon_1}\frac{d\varepsilon}{\sqrt{2(E-U(\varepsilon))}}, \qquad \frac{X}{2}>x>0.$$

The period of the function $\varepsilon(x)$ is defined by the formula

$$X=2\int_{\varepsilon_2}^{\varepsilon_1}\frac{d\varepsilon}{\sqrt{2(E-U(\varepsilon))}}=2x(\varepsilon_2). \quad (23)$$

Substituting expression (21) for $E-U(\varepsilon)$ into the formula (22) for $x(\varepsilon)$ for $\frac{X}{2}>x>0$ and transforming the corresponding integral, we obtain

$$x(\varepsilon)=\sqrt{\frac{6}{B}}\frac{1}{\sqrt{\varepsilon_1-\varepsilon_3}}\int_0^\varphi\frac{d\varphi}{\sqrt{1-k^2\sin^2\varphi}}, \qquad k^2=\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1-\varepsilon_3},$$

$$\varphi=\arcsin\sqrt{\frac{\varepsilon_1-\varepsilon}{\varepsilon_1-\varepsilon_2}}.$$

Taking into account the definition of the first-order elliptical integral

$$\mathcal{F}(k,\varphi)=\int_0^\varphi\frac{d\varphi}{\sqrt{1-k^2\sin^2\varphi}}, \quad (24)$$

we can write $x(\varepsilon)$ in the form

$$x(\varepsilon)=\sqrt{\frac{6}{B}}\frac{1}{\sqrt{\varepsilon_1-\varepsilon_3}}\mathcal{F}(k,\varphi). \quad (25)$$

In accordance with (23), in this case we have

$$X=\sqrt{\frac{6}{B}}\frac{2}{\sqrt{\varepsilon_1-\varepsilon_3}}\mathcal{F}(k), \qquad \mathcal{F}(k)\equiv\mathcal{F}(k,\pi/2). \quad (26)$$

Let us now determine the quantities ε_1, ε_2, and ε_3. For this purpose, we note that

$$\langle\varepsilon(x)\rangle = \frac{1}{X}\int_0^{X/2}\varepsilon(x)dx + \frac{1}{X}\int_{X/2}^{X}\varepsilon(x)dx = \frac{2}{X}\int_0^{X/2}\varepsilon(x)dx,$$

or, going over to integration with respect to ε

$$\langle\varepsilon(x)\rangle = \frac{2}{X}\int_{\varepsilon_2}^{\varepsilon_1}\varepsilon\frac{d\varepsilon}{\sqrt{2(E-U)}}. \tag{27}$$

Equation (18) implies that $\langle\varepsilon\rangle = 0$. Transforming the integral appearing in (27) and taking into account (21), we obtain

$$\int_0^{\pi/2} d\varphi\,\frac{\varepsilon_1 - (\varepsilon_1-\varepsilon_2)\sin^2\varphi}{\sqrt{1-k^2\sin^2\varphi}} = 0, \qquad k^2 = \frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1-\varepsilon_3}.$$

Using the definition of the second-order elliptical integral

$$E(k) = \int_0^{\pi/2} d\varphi\sqrt{1-k^2\sin^2\varphi}, \tag{28}$$

we obtain

$$E(k) + \left(k^2\frac{\varepsilon_1}{\varepsilon_1-\varepsilon_2} - 1\right)\mathcal{F}(k) = 0.$$

This expression can also be written in the form

$$\frac{\varepsilon_1}{\varepsilon_1-\varepsilon_2} = \frac{\mathcal{F}(k)-E(k)}{k^2\mathcal{F}(k)}, \qquad \frac{\varepsilon_1}{\varepsilon_1-\varepsilon_3} = \frac{\mathcal{F}(k)-E(k)}{\mathcal{F}(k)}. \tag{29}$$

These formulas indicate that the ratios $\varepsilon_1/\varepsilon_2$, $\varepsilon_1/\varepsilon_3$, $\varepsilon_2/\varepsilon_3$ can be expressed only in terms of the parameter k. Let us now find the expression for the quantity ε_1 in terms of k. For this purpose, we note that, according to (20)

$$\varepsilon_1+\varepsilon_2+\varepsilon_3 = -\frac{3}{2}\frac{A}{B} \equiv \gamma(\beta-\beta_0), \tag{30}$$

where

$$\gamma = -3\frac{\partial^2 n(\beta_0,\mu)}{\partial\beta\partial\mu}\Big/\frac{\partial^2 n(\beta_0,\mu)}{\partial\mu^2}, \tag{31}$$

in accordance with (19). Using further formulas (29), we obtain the following expression for the quantity ε_1:

$$\varepsilon_1 = \frac{\gamma(\beta-\beta_0)}{3-(1+k^2)\dfrac{\mathcal{F}(k)}{\mathcal{F}(k)-E(k)}}. \tag{32}$$

Taking into account this relation and (29), we can easily determine the quantity $1/\sqrt{\varepsilon_1-\varepsilon_3}$ appearing in the expression (26) for the period:

$$\frac{1}{\sqrt{\varepsilon_1-\varepsilon_3}}=\left(\left(3\frac{\mathcal{F}(k)-E(k)}{\mathcal{F}(k)}-k^2-1\right)\Big/\gamma(\beta-\beta_0)\right)^{1/2}. \qquad (33)$$

Noting that $k^2=\dfrac{\varepsilon_1-\varepsilon_2}{\varepsilon_1-\varepsilon_3}$ and introducing the new variable $\varepsilon\equiv\varepsilon_1-\varepsilon_3$, we obtain

$$\varepsilon_1-\varepsilon_2=\varepsilon k^2, \qquad \varepsilon_1=\varepsilon\frac{\mathcal{F}(k)-E(k)}{\mathcal{F}(k)},$$

or

$$\varepsilon_1=\varepsilon\left(1-\frac{E(k)}{\mathcal{F}(k)}\right), \qquad \varepsilon_2=\varepsilon\left(1-k^2-\frac{E(k)}{\mathcal{F}(k)}\right), \qquad \varepsilon_3=-\varepsilon\frac{E(k)}{\mathcal{F}(k)}. \quad (34)$$

Since $\varepsilon>0$ and $\gamma(\beta-\beta_0)<0$ (see (30), (31)), the inequality $3\dfrac{\mathcal{F}-E}{\mathcal{F}}-k^2-1<0$, must hold in accordance with (33), which gives $k<k_0\approx 0.95$.

The period X of the function $\varepsilon(x)$ is connected with the quantity q through the formula

$$X=\frac{2\pi}{q}=2\sqrt{\frac{6}{B}}\,\frac{1}{\sqrt{\varepsilon}}\mathcal{F}(k). \qquad (35)$$

The variables k and ε can be taken as independent thermodynamic variables instead of β and q.

Expression for the $\varepsilon(x)$ can be expressed in the terms of Jacobi functions

$$\varepsilon(x)=\varepsilon\left(1-\frac{E(k)}{\mathcal{F}(k)}-k^2\mathrm{sn}^2\left(2\mathcal{F}(k)\frac{x}{X},k\right)\right), \qquad (36)$$

where the quantity X is defined by (35). Formula (36) determines the long-periodic structure of the system under investigation at temperatures close to the transition temperature T_0.

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BOSON FQHE STATE IN CUPRATE OXIDE INDUCED BY ZERO-POINT OSCILLATION AND MACROSCOPIC INTERFERENCE PHENOMENA DEMONSTRATING FRACTIONAL CHARGE

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It is pointed out that in cuprate high-temperature superconductor (HTS) with carriers with large //c zero-point energy, the fractional quantum Hall effect (FQHE) can appear even at room temperature when space charge and moderate localization are present. The experimental process for the infallible observation of the FQHE charge fractionality is described.

1. INTRODUCTION

A many-particle boson (or fermion pair) system in the ground state can assume two typical macroscopic quantum states (phase-definite state Ψ_Θ and particle-number definite state Ψ_N) satisfying $\Delta N \Delta\Theta = 1/2$, where they are connected with each other by transformation relationship. Ideal Ψ_Θ (Ψ_N) is realized when $t \gg U (t \ll U)$ where t is the energy of the particle transition between discretely quantized particle sites and U is the double occupancy energy in one site. Metal superconductivity in $t \gg U$ is a typical Ψ_Θ, where the materialization of Ψ_N durable for electrical measurement is very difficult. Concerning the study of HTS, the Hubbard energy ~ 10 eV is normally considered as U. In this study, however, we consider the situation where each quantum site includes several ($\geq$2) Cu ions with partial occupation (or occupied by fractional charges), and where $U \sim t$ in ideal bulk crystal. It is known experimentally that Ψ_Θ in HTS is very fragile against localization which tends to cause $t < U$. The fragility suggests the stability of Ψ_N in thin HTS crystal with localization where enough durability for electrical measurement is expected.

We note the following [1], [2] concerning the possible Ψ_N in the hole-carrier system in c-oriented $La_{2-x}Sr_x\ CuO_4$ film with localization:

(i) Being confined in a CuO_2 layer with $//c$ wave-function spreading $\Delta x(//c) < 0.66$ nm, a carrier in ground state has zero-point energy $\Delta E(//c) \sim \Delta p(//c)^2/2m \sim \hbar^2/2m\Delta x(//c)^2 \sim (0.1 - 1\mathrm{eV}) \sim E_F \gg 300 k_B$, where x axis is $//c$;

(ii) Singlet pairing is favorable even at 300K because $\Delta p(//\mathrm{c})^2/2m$ reduces to $\Delta p(//\mathrm{c})^2/4m$ in the replacement $(m \to 2m)$;

(iii) Supposing parabolic confining potential at a CuO_2 layer at $x = \zeta d(\zeta = 1, 2, 3, ...; d$, separation), the zero-point carrier wave function in the layer takes the same form as the lowest level solution in Landau-gauge $\mathbf{A}^*$ = $(0, B^*(x - \zeta d), 0)$ in //c magnetic field $B^* \sim 10^{3-4}$T, which is strong enough to cause FQHE (a typical Ψ_N in $\perp B$ 2D carrier system)[3] even at room temperature;

(iv) The «gauge» $\mathbf{A}^*$ varies from CuO_2 layer to layer through its ζ dependence, and hence is incapable of making an effective field $\mathbf{B}^* = (0, 0, B^*)$. It was shown [1] that the existence of space charge («ground charge») $\pm\rho_0$ helps to construct a regime, where the ζ-dependent «gauges» are unified, materializing the effective magnetic field $\mathbf{B}^*$;

(v) In the regime the combination of Landau-gauge solutions leads to symmetrical gauge solutions, and hence Laughlin function [4];

(vi) Reducing Coulomb-energy in total system, 2D FQHE appears under the strong $\mathbf{B}^*$ even at room temperature on xy plane (x //c and y //current $\mathbf{j}$) with $\pm$ charged regions, where $\pm\rho_0$ makes no chemical potential gradient;

(vii) The singlet pairing caused by $\Delta E(//\mathrm{c})$ reduction provides boson type ground FQHE states [1] at «filling factor» $\nu \to$ x = 1/2k $(k = 1, 2, 3, ...)$;

(viii) Equating the «flux-quantum-site» area $2\pi l_0^2$ to 2 Cu-site area (in ac or xy plane) $2 \times 0.38 \times 0.66$ nm^2, we find «magnetic length» $l_0 = 0.28$ nm, $\mathbf{B}^*$ = 4.1 $\times 10^3$T and $\Delta E(//\mathrm{c}) \equiv \hbar\omega_b/2$ = 0.24 eV;

(ix) The introduction of moderate localization not only makes $t \ll U$ stabilizing the FQHE state, but also facilitates the observation of FQHE by fixing charge;

(x) The FQHE planes $\perp$ $\mathbf{B}^*$ may make a multi-layer-stacked array with separation tentatively equated to $t \sim \xi_{\mathrm{ab}} = 3.7$ nm [1, 2];

(xi) Since the z-axis can be taken in parallel with either a- or b-axes, a 3D FQHE state may be materialized in «multi-parallel-cross» shape superposing a- and b-axis stacks;

(xii) The «ground charge» density $\pm\rho_0$ is embodied by quasiparticle charge array with separation $\lambda_{\mathrm{S}} \sim 100$ nm [2];

(xiii) In a 3D Ψ_N as the «multi-parallel-cross» FQHE regime, we expect the negative-capacitance relationship $\tilde{\rho}/\tilde{\phi} < 0$ with external charge expulsion [1, 2], just as London equation $\tilde{\mathbf{A}} + \mu_0\lambda_L^2\tilde{\mathbf{j}} = 0$ in Ψ_Θ leads to $\tilde{\mathbf{j}}/\tilde{\mathbf{A}} < 0$ and Meissner effect, where $\tilde{\mathbf{j}}$ and $\tilde{\rho}$ are field-induced current and charge, and $\tilde{\mathbf{A}}$ and $\tilde{\phi}$ are variations of vector and scaler potentials, respectively.

We reported studies on the above properties using c-axis-oriented $La_{2-x}Sr_xCuO_{4-y}$ film where localization is intentionally introduced [1, 2]. Concerning $La_{2-x}Sr_xCuO_{4-y}$, it is known that x makes hole-carrier doping, and that the deoxidization in cooling at temperature T <700°C gives rise to small y,

inducing carrier localization with slight doping effect less than 0.01. We show below the macroscopic quantum interference of the FQHE state observed in the $La_{2-x}Sr_xCuO_{4-y}$ film.

2. QUASIPARTICLE EXCITATION ENERGY

Consider a ground Laughlin state [4] for a $\perp\mathbf{B}^*$ 2D carrier system with particle charge Q_0 in field $\mathbf{B}^* = (0, 0, B^*)$ at filling factor $\nu = 1/m$ $(m = 2k + 1$ for fermion, and $m = 2k$ for boson (or fermion-pair) $(k = 1, 2, 3, ...))$. The quasiparticle excitation in FQHE system of spin-polarized ($\uparrow$) 2D fermion gas was studied by Halperin [5], where is used the initial (lebel $s = 0$) parameter set [filling factor $\nu_0 = 0$, charge $q_0 = 1$ (expressed in the ratio to Q_0), angular momentum quantum $m_0 = 1$]. In boson system, however, we use an initial parameters set $[\nu_0 = 0, q_0 = 1, m_0 = 1/2]$. With $\nu_0 = 0$ condition the nominal double occupation condition $m_0 = 1/2$ may cause no Coulomb energy increase. In real experimental condition, the filling factor of the samples is always $\nu \to x \ll 1$. Therefore we need not worry about Coulomb energy increase in the strong coupling system. Figure 1 shows the filling-factor ν dependence of the

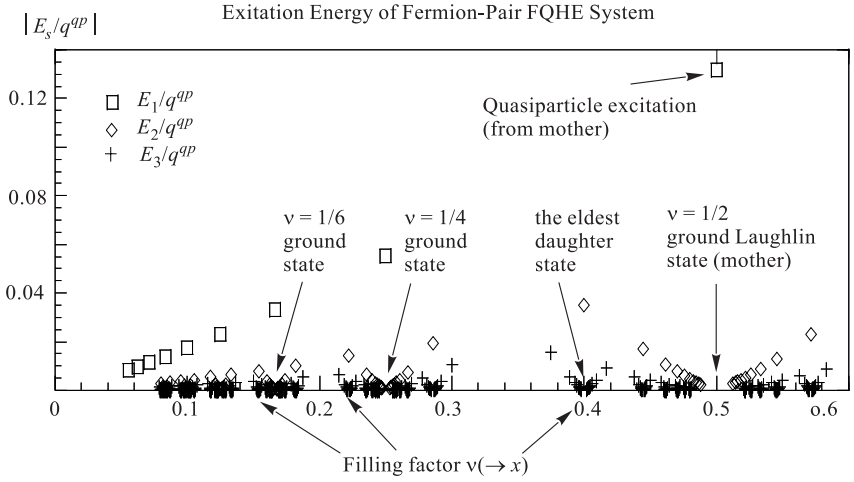

Fig. 1. The filling-factor ν dependence of the excitation energy E_s of singlet-hole-pair FQHE system. q^{qp} is the fraction of quasiparticle charge

calculated quasiparticle-excitation energy E_s (s, level) in the fermion-pair system, where $q_s^{\mathrm{qp}} \equiv Q_s^{\mathrm{qp}}/Q_0$ is the fraction of quasiparticle charge Q_s^{qp}. The ordinate

unit is $e/\pi\varepsilon l_0$ (e electron charge, ε crystal-lattice dielectric constant, l_0 magnetic length). In Ref. 5 an empirical factor Λ = 3 is used concerning the excitation-energy ratio between «particle» and «hole». This parameter is tentatively put Λ = 1 in our calculation.

In Fig. 1 the ν values 0.15, 0.22, and 0.4 are denoted by up-pointing arrows, where is expected the co-existence of both a ground Laughlin (mother) state and its eldest daughter Laughlin state (see the example at $\nu = 1/2$), and where ($\nu \to$ x) the dielectric interference experiment described in the following section is made to demonstrate the existence of FQHE fractional charge. Since FQHE states of more descendent order may be unstable due to the smaller particle-particle interaction, we restrict our consideration only to the ground states and the eldest daughter states.

3. DIELECTRIC INTERFERENCE BETWEEN TWO INTERACTING LAUGHLIN STATES

We study the «dielectric interference» of two Laughlin states (= «electrode» Laughlin states) formed in the doubly charged regions in c-oriented $La_{2-x}Sr_xCuO_4$ film. The «electrode» states are connected via a neutral interface with a FQHE character slightly different from «electrodes» (see Fig. 2) [1, 2, 6]. The study of the inter-«electrodes» interference is made after Josephson effect [7]. We suppose that the «ground charges» $Q_x = Q^g N_x$ composed of quasiparticles have passed $//x$ across the interface from one «electrode» region to the other, and that flux quanta $\Phi_y = N_y\Phi_s(\Phi_s = h/Q_s^{\mathrm{L}})$ in the level s Laughlin state have traversed $//y$ along the interface. The phase is written $\Theta(N_x, N_y) = \hbar^{-1}\int dt[Q_x(d\Phi_y/dt) + \Phi_y(dQ_x/dt)] = 2\pi(Q^g/Q_s^{\mathrm{L}})N_xN_y$. Using the Q_x-definiteness of «electrodes» and a Hamiltonian $H\Psi_{N_y} = E_0\Psi_{N_y} + J_0(\Psi_{N_y+1} + \Psi_{N_y-1})$ with constant E_0 and J_0, we get energy $E(N_x) = E_0 + 2J_0\cos[2\pi(Q^g/Q_s^{\mathrm{L}})N_x]$ and voltage

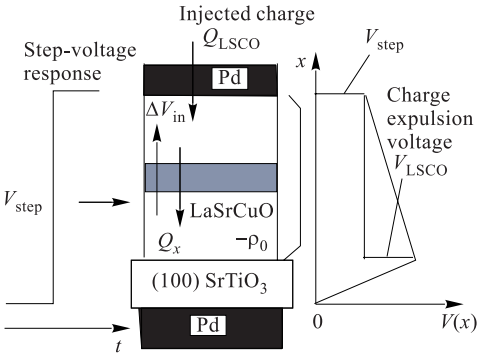

Fig. 2. Capactance element C_{t} having c-oriented $La_{2-x}Sr_xCuO_4$ film with naturally formed charge double layer

$$\Delta V_{\rm in} = \frac{d\Phi_y}{dt} = \Phi_s \frac{dN_y}{dt} = \frac{\Phi_s}{h}\frac{\partial E(N_x)}{\partial N_x} = -\frac{4\pi Q^g \Phi_s J_0}{h Q_s^{\rm L}} \sin(\frac{2\pi Q_x}{Q_s^{\rm L}}). \quad (1)$$

Physical meaning of Eq. (1) is as follows. Both «electrodes» are stabilized when they accept Q_x of integral multiple of the Laughlin-particle charge $Q_s^{\rm L}$ of level s. Therefore the system induces pulling-back voltage $\Delta V_{\rm in}$ at the beginning stage of the cycle of charge passage ($N' \leq Q_x/Q_s^{\rm L} < N' + \frac{1}{2}, N'$ integer) across the interface, and it induces an accelerating voltage $\Delta V_{\rm in}$ at the final stage ($N' + \frac{1}{2} < Q_x/Q_s^{\rm L} \leq N' + 1$).

In Fig. 2 is schematically shown the capacitance element C_t used to measure the dielectric interference in the c-oriented $La_{2-x}Sr_xCuO_4$ with stacked array of xy 2D FQHE planes each of which is composed of $\pm$ charged FQHE regions connected by neutral interface [1, 2]. When $Q_{\rm LSCO} > 0$ is injected downward into $La_{2-x}Sr_xCuO_4$, a $//x$ charge-expulsion voltage $V_{\rm LSCO}$ appears inside the film keeping the relationship $Q_{\rm LSCO} = C_{\rm LSCO} V_{\rm LSCO}$. With the $Q_{\rm LSCO}$ injection the displacement $Q_x = Q_{\rm LSCO}$ of «ground charge» takes place across the interface. Since the «ground charge» is supposed to form 3D lattice structure with lattice constant $\sim \lambda_{\rm S}$ [2], we may divide the capacitance $C_{\rm LSCO}$ with total areas S into many small «sub-capacitances» each of which has area $\sim \lambda_{\rm S}^2$ and with the induced voltage of Eq. (1). With charge $(\lambda_{\rm S}^2/S)Q_x$ passage through the interface of each «sub-capacitance», the resultant capacitance $C'_{\rm LSCO}$ over area S has the following $V_{\rm LSCO}$ dependence with a constant V_0.

$$C'_{\rm LSCO}(V_{\rm LSCO}) \equiv \frac{Q_{\rm LSCO}}{V_{\rm LSCO} + \Delta V_{\rm in}(Q_x)} \simeq$$

$$\simeq C_{\rm LSCO}\left(1 - \frac{V_0}{V_{\rm LSCO}} \sin\Big(\frac{2\pi V_{\rm LSCO}}{SQ_s^{\rm L}/\Big|C_{\rm LSCO}\Big|\lambda_{\rm S}^2}\Big)\right). \quad (2)$$

Thus a Fraunhofer pattern should appear in $C'_{\rm LSCO}(V_{\rm LSCO})$ with constant $C_{\rm LSCO} < 0$, where the pattern period $\Delta V = SQ_s^{\rm L}/\Big|C_{\rm LSCO}\Big|\lambda_{\rm S}^2 \propto Q_s^{\rm L}$.

The following must be noted for the infallible observation of charge fractionality: (i) On ideally *dielectric* (at $\omega < 10^5 {\rm s}^{-1}$) 1mm (100) $SrTiO_3$ substrate, make by sputtering good c-oriented $La_{2-x}Sr_xCuO_4$ films of x$\approx 0.15, 0.22, 0.40$ of special thickness $t_{\rm LSCO}$ (e.g., at x≈ 0.15, $t_{\rm LSCO} \approx 60, 100$nm) removing oxygen in cooling stage [1]; (ii) Make samples with $C_{\rm t}$ and $C_{\rm LSCO}$ elements with identical area; (iii) Select large $C_{\rm t}/C_{\rm LSCO}$ value samples ($C_{\rm t}/C_{\rm LSCO} \sim$ 1.2-1.5: 20-30% yield due to difficulty of uniform crystal formation) by ac measurement at 300K; (iv) Measure equilibrium charge $Q_{\rm t}$ and $Q_{\rm STO}$ stored in $C_{\rm t}$ and $C_{\rm STO}$

after several sec application of step voltage $V_{\rm step}$; (v) Considering the notable field dependence of $SrTiO_3$ dielectric property and the continuity of dielectric flux density **D**, find $C_{\rm LSCO} = Q/V_{\rm LSCO}$ at $Q = Q_{\rm t} = Q_{\rm STO}$ (see Fig. 3); (vi) Suppress the leakage current of $C_{\rm t}$ element less than 1 pA to obtain correct capacitance data.

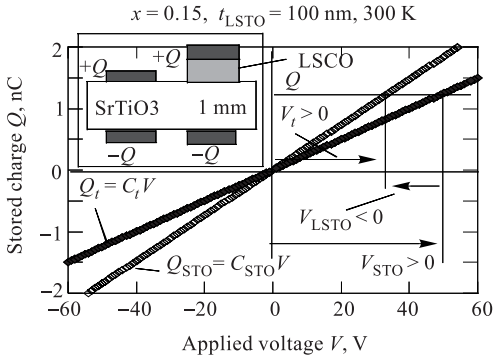

Fig. 3. The determination of $V_{\rm LSCO}$ and $V_{\rm STO}$ from charge-voltage-relationship data of $C_{\rm t}$ and $C_{\rm STO}$ elements

In Fig. 4 are exemplified the Fraunhofer patterns observed at room temperature when x = 0.15, 0.22, and 0.4. The following are noted: a) The superposed interference patterns are observed; b) The ratio of voltage-period ΔV of the superposed patterns just coincides with the expected ratio of $Q_s^{\rm L}$'s for coexisting mother (s=1) and the eldest daughter (s=2) state; c) Corresponding to FQHE theory where bulk current flows when $\left|Q_s^{\rm L} V_{\rm LSCO}\right| > \hbar\omega_{\rm b}$, the interference patterns suffer impairment in low $\left|V_{\rm LSCO}\right|$ region, which effect is intensified especially at lower temperature (77K, 4.2K); d) The centre peaks of the mother and daughter states appear in phase in the cases x = 0.15 and 0.4, and *out of phase* in x = 0.22 case, which may be related to the statistically different property at x $\simeq 1/4k$ and x $\simeq 1/2(2k+1)$; e) Using values $S = 7 \times 10^{-6}{\rm m}^2$, $\Delta V \approx 10$V (for $q_s^{\rm L} = 1$), $\left|C_{\rm LSCO}\right| \approx 10^{-10}$F, we find from Eq. (2) $\lambda_{\rm S} \approx 1.5 \times 10^{-7}$m, showing good agreement with theoretical estimation for $\lambda_{\rm S}$ [1, 2]; f) The fractionally charged particles can only survive in FQHE atmosphere, which prevents the observation of the charge fractionality in HTS using ordinary tunneling devices with insulator barrier [6].

4. CONCLUSION

The macroscopic interference in c-oriented $La_{2-x}Sr_xCuO_4$ film with localization is studied. The experimental process for the infallible observation of charge fractionality is described. The quasi-static measurement of capacitance of the $La_{2-x}Sr_xCuO_4$ film with localization reveals interference patterns with period proportional to Laughlin particle charges. The observation supports the model of HTS with localization in which boson-type FQHE is established under the strong effective magnetic field caused by the large //c zero-point energy and space charge.

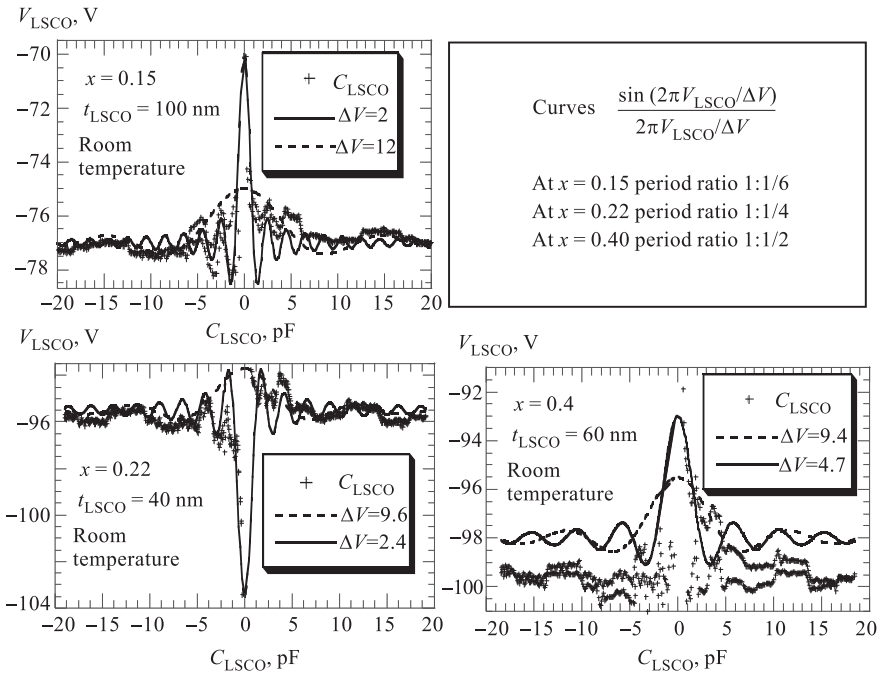

Fig. 4. The dielectric Fraunhofer patterns found in the capacitive devices in Fig. 2 when x=0.15, 0.22, and 0.4. The observed period ratios of the superposed patterns are shown in the inset table, which coincides with the ratios of the fraction of Laughlin charge $q_s^{\mathrm{L}} = Q_s^{\mathrm{L}}/Q_0$ expected from theory [4]

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«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
2000, ТОМ 31, ВЫП. 7Б

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ORDER-DISORDER TRANSITIONS IN AN ASYMMETRIC NEXT-TO-NEAREST NEIGHBOURS ISING-TYPE MODEL

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The distribution of Cu–O chains with respect to their length and orientation in YBCO–123 is studied by means of numerical simulations of the ASYNNNI model. It is found that the formation of Cu–O chains can be either anisotropic or isotropic, depending on the temperature and concentration. A suitable order parameter is introduced to study transitions between the isotropic and anisotropic phases of the model.

The topic of oxygen ordering in the basal Cu–O plane of $YBa_2Cu_3O_{6+x}$ (where $0 < x \leq 1$) has been studied in considerable detail [1]. From the theoretical point of view, the temperature-concentration phase diagram is well explained by the two-dimensional asymmetric next-to-nearest neighbours Ising model (the ASYNNNI model) [1]. In particular, the model contains as ground states two ordered orthorhombic structures consisting of Cu-O chains. Ortho I occurs (at appropriate temperatures) for x close to 1 (50% O concentration) and Ortho II for x close to 0.5 (25% O concentration). The Ortho I structure is shown for a 10 by 10 lattice in Fig. 1: in this structure, all the O sites in the Cu–O chains are occupied. The Ortho II phase is similar, except that all the O sites in alternate Cu–O chains are vacant.

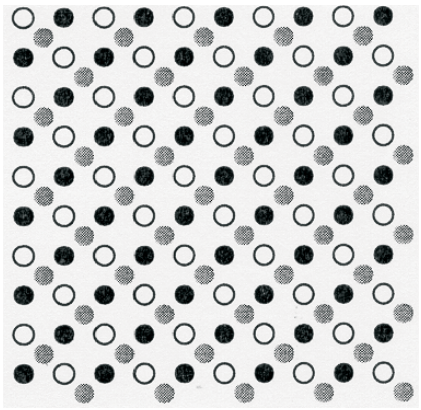

Fig. 1. The Ortho I structure in the basal plane of YBCO–123 for a 10×10 lattice

The orthorhombic structures are anisotropic in the sense that the Cu–O chains are all oriented in one direction (in Fig. 1, to the right). One can ask whether there are also isotropic structures which contain chains that are oriented in both possible directions. The purpose of

this paper is to use the ASYNNNI model to study this question and, in particular, to study transitions between the isotropic and anisotropic structures.

In the ASYNNNI model, only the interactions of an oxygen ion with its nearest-neighbour oxygen ions ($V_{NN} = V_1$) and its next-to-nearest neighbour oxygen ions are taken into account. For the latter there are two types of interaction: V_2 (or V_3), according to whether a Cu atom is (is not) present in the NNN bond (see Fig. 1). The Hamiltonian is

$$H = V_1 \sum_{NN} n_i n_j + V_2 \sum_{NNN} n_i n_j + V_3 \sum_{NNN}{}' n_i n_j, \tag{1}$$

where $n_i = 1$ if site i is occupied by an oxygen ion, otherwise $n_i = 0$. The site contribution to H has been omitted in Eq. (1) because it is irrelevant to the study of oxygen mobility in the context of the model. We have used the potentials [2] $V_1 = 0.190\text{eV}$, $V_2 = -0.136\text{eV}$, $V_3 = 0.054\text{eV}$. (Other values of these potentials are given in the literature; however, our results are not particularly sensitive to the precise values.)

We have used Monte Carlo simulations of the ASYNNNI model to study the isotropy of the ground state configurations for a large number of points in the temperature-concentration plane. For this purpose it is necessary to identify a suitable «order parameter» to distinguish between the isotropic and anisotropic phases of the model (see below). In this paper we present some preliminary results on the behaviour of this order parameter, more details are published elsewhere.

In our Monte Carlo simulations of the canonical ensemble, we have used the Metropolis algorithm. All simulations were on a lattice 64 by 64. A detailed analysis was performed of the Cu–O chains in the equilibrium configurations obtained from the numerical simulation. For this purpose, histograms revealing the frequency of formation of chains of particular lengths and orientations (either «left» or «right») were produced from large samples of equilibrium configurations. The analysis of such histograms led to the formulation of a quantity which depends on the Cu–O chain pattern and exhibits a dramatic change for certain values of the temperature and concentration, and can thus serve as an order parameter for studying the isotropy of the model.

Specifically, we define an order parameter

$$\Delta = |N_L - N_R|/N, \tag{2}$$

where N_L (N_R) is the number of oxygen ions in chains oriented to the left (right), and N is total number of oxygen ions. It is clear that for the Ortho I and Ortho II structures, either $N_R = N$ and $N_L = 0$ (as in Fig. 1) or $N_L = N$ and $N_R = 0$; in either case $\Delta = 1$.

Typical results for the temperature and concentration dependence of this order parameter are shown in Figs. 2 and 3. In Fig. 2 the temperature is fixed

at 0.05 eV and the order parameter is plotted for values of the concentration parameter between 0.2 and 1.4. (Note that in YBCO–123 $x \leq 1$; however, it is also of interest to study the ASYNNNI model for $x > 1$.) The first feature to notice in Fig. 2 is the lack of symmetry of the order parameter about $x = 1$: thus the order parameter (2) for the ground state does not possess the particle-hole symmetry of the Hamiltonian in Eq. (1).

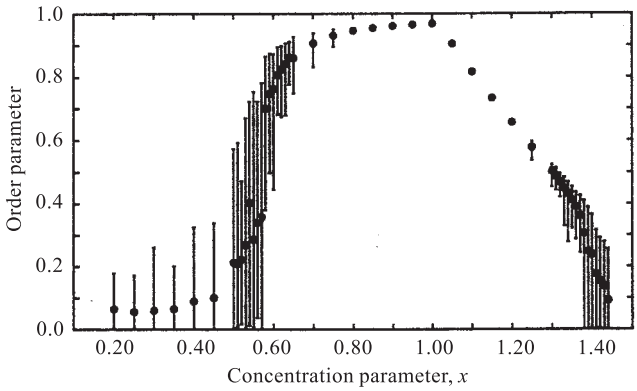

Fig. 2. Variation of the order parameter defined in Eq. (2) with concentration parameter for a temperature $T = 0.05$ eV

We also see that in Fig. 2 $\Delta \approx 1$ for $x = 1.0$: the structure corresponds to the Ortho I phase. The structure at the left-hand edge of the «plateau» in Fig. 2 (at $x \approx 0.6$) corresponds mainly to the Ortho II phase. We remark that for lower values of T the plateau in Fig. 2 broadens: the right-hand edge remains at $x = 1$, but the value of x at the left-hand edge decreases. Conversely, for higher values of T the plateau becomes narrower. The order parameter in Fig. 2 decreases to half its maximum value at $x_c = 0.55$ and $x_c = 1.28$. To clarify the behaviour of the model at these two points, many additional simulations were performed with a much smaller step in x and significantly increased number of Monte Carlo steps. The statistical analysis of the results clearly shows a dramatic increase of the variance, which is typical for the behaviour of any statistical system near a critical point, and is a direct consequence of what is often referred to as «critical slowing down» or «critical increase of the relaxation time».

Similar remarks apply to Fig. 3 where Δ is plotted as a function of temperature for fixed $x = 0.80$. The results indicate a critical temperature $T_c \approx 0.10$ eV for the transition from anisotropic to isotropic orientation of Cu–O chains at this concentration. We remark that the decrease in Δ for the lower temperatures ($T \lesssim 0.02$ eV) in Fig. 3 is associated with inhomogeneous configurations of the model which occur at these temperatures [3]. The critical values (x_c, T_c) obtained

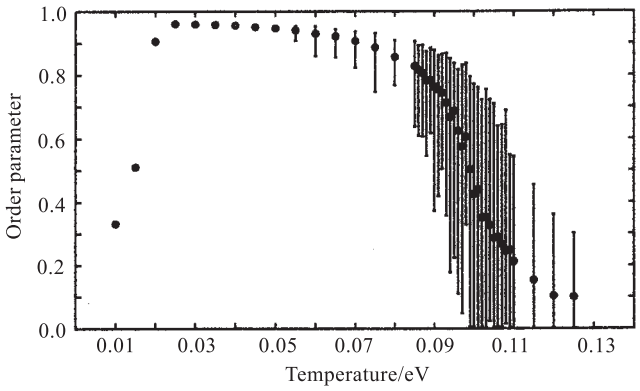

Fig. 3. Variation of the order parameter with temperature for a concentration parameter $x = 0.80$

from analysis of the order parameter can be used to determine a phase diagram for the isotropic and anisotropic phases of the model [4].

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UNCONVENTIONAL SUPERCONDUCTORS

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The problem of electronic spectrum and superconductivity in strongly correlated electronic liquids is discussed. A microscopical theory within the framework of the t-J model is considered. Constraint of no double occupancy for electron hopping results in the kinematical interaction that induces strong electron-electron coupling by spin and charge fluctuations. Rigorous treatment of the constraints is achieved by applying the Hubbard operator technique within the Green's function method of Bogoliubov.

1. INTRODUCTION

In developing a theory of superconductivity it is necessary to solve two problems which are of foremost importance and which are definitely interrelated: namely, what is the nature of the normal state for the electrons in the metal and what is the mechanism of the formation of the superconducting phase? While in conventional superconductors the picture of the Fermi liquid with a properly determined spectrum of quasiparticles (QP) near the Fermi surface is well established, in recently discovered unconventional metals, as heavy-fermion compounds and copper oxides we have many experimental evidences for anomalous behavior of low-energy electronic excitation spectra. These materials can be called marginal electronic liquids where strong electron correlations play an important role and the conventional Fermi-liquid description in terms of single-particle excitations may be violated. Therefore, the Bardeen–Cooper–Schrieffer (BCS) theory of pairing which works perfectly well for the system of weakly bounded QP in conventional metals, can be questioned for the system of electrons with strong Coulomb correlations.

In the present report we discuss the problem of high-temperature superconductivity in copper oxides. In spite of an unprecedented scientific activity we are still far from the solution of the problem and there is no consensus on theoretical explanation of unusual normal and superconducting behavior of high temperature superconductors (for a review of experiment and theory see, for example, Ref. 1). Experimental studies of high-temperature superconductors have provided strong support for a major role of strong electron correlations in copper-oxide materials as it first has been proposed by P.W. Anderson [2,3].

The simplest model allowing for the electron correlations is the one-band Hubbard model [4]:

$$H = -\sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where t_{ij} is an effective transfer integral and U is the Coulomb one-site energy. In the strong coupling limit, $U \gg |t_{ij}|$, we can reduce the Hubbard model (1) (or a more realistic for copper oxides p-d model [5]) to the t-J model [6]:

$$H_{t-J} = -\sum_{i,j\sigma} t_{ij} \tilde{c}^+_{i\sigma} \tilde{c}_{j\sigma} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j). \tag{2}$$

Here the electron operators $\tilde{c}^+_{i\sigma} = c^+_{i\sigma}(1 - n_{i-\sigma})$ act in the space without double occupancy. $n_i = \sum_\sigma \tilde{c}^+_{i\sigma} \tilde{c}_{i\sigma}$ is the number operator for electrons. The second term describes spin-1/2 Heisenberg antiferromagnet (AF) with exchange energy J for the nearest neighbors which is equal to $J = 4t^2/U$ for the Hubbard model (1) or can be considered as independent parameter in the case of the p-d model. In the model two main features of a doped hole motion in copper-oxides are properly taken into account: constraints on no double occupancy for holes on lattice sites due to strong electron correlations and interaction of holes with AF spin fluctuations that brings about strong renormalization of the QP spectrum. Exclusion of doubly occupied states in electronic hopping and strong coupling of charge carriers with spin fluctuations make it difficult to apply mean field type approximations or perturbation theory.

To deal with the strong coupling limit for the Hubbard model and the t-J model a number of numerical methods for finite clusters has been developed (for reviews see [7], [8]). These studies show strong antiferromagnetic correlations which lead to the formation of the $d_{x^2-y^2}$ pairing correlations. However, the finite cluster calculations due to known limitations (finite size effects, few filling fractions, etc.) can give only restricted information. For instance, as it was shown recently by applying the constrained-path Monte Carlo method [9] to the two-dimensional Hubbard model, small lattice sizes and weak interactions show $d_{x^2-y^2}$ pairing correlations while with increasing lattice size or interaction they vanish. So to prove superconducting pairing in the strong coupling limit an analytical treatment is highly demanded.

The main problem in studies of the t-J model is the so-called kinematical interaction imposed by the projected character of electron operators acting in the subspace of singly occupied lattice sites. To take into account the constraints of no double occupancy different types of slave-boson (-fermion) technique were proposed (see [10–13] and references therein). In the mean field approximation (MFA) the local constraints are approximated by a global one, that reduces the

problem to free fermions and bosons in the mean field [10]. To treat the constraints in a systematic way, in [11, 12] a large-N expansion, with N being a number of states (orbitals) at a lattice cite, was used. In that approach the local constraints are relaxed and a weak coupling approximation is possible. By using the $1/N$ expansion, the d-wave superconducting instability induced by the exchange interaction was obtained in the t-J model close to half filling [12].

Another method is based on the Baym-Kadanoff variational technique for Green's functions in terms of the Hubbard operators [14]. The method was used in [15, 16], also in the limit of large N, to consider superconducting pairing in the t-J model. It was shown that in the lowest order of $1/N$ there is a strong compensation of different contributions to the pairing interaction and for $J = 0$ the superconducting T_c is extremely small. For a finite J the d-wave superconducting instability mediated by exchange and charge fluctuations was obtained below $T_c \simeq 0.01t$. However, in the large-N expansion the kinematical interaction is suppressed and this approach, being rigorous in the limit $N \to \infty$, is difficult to extrapolate to real spin systems with $N = 2$.

A formally rigorous method to treat the unconventional commutation relations for the projected electron operators is based on the diagram technique for the Hubbard operators [17] since in this method the local constraints are rigorously implemented by the Hubbard operator algebra. A superconducting pairing due to the kinematical interaction in the Hubbard model in the limit of strong electron correlations ($U \to \infty$) was first obtained by Zaitsev and Ivanov [18] who studied the lowest order diagrams for a two-particle vertex equation. Their approximation, being equivalent to the MFA for a superconducting order parameter, gives only the s-wave pairing. Close results were obtained for the Hubbard model in [19,20] by applying the Bogoliubov equation of motion method for the thermodynamical Green's functions. However, as was shown later [21, 22], the s-wave pairing in the limit of strong correlations violates an exact requirement of no single-site pairs and should be rejected. In [21, 22] the BCS mean field theory for the t-J model was developed within the formally exact projection technique [23] for Green's functions in terms of the Hubbard operators. It was proved that the d-wave superconducting pairing mediated by the exchange interaction is thermodynamically stable and has high $T_c \simeq 0.1\ t$ for $J \simeq 0.4\ t$.

On the basis of the diagram technique, detailed studies of spin fluctuations and superconducting pairing in the t-J model were performed by Izyumov et al. [24]. Summation of the first order diagrams for the self-energy reproduced the results of the MFA in [21, 22]. In the second order diagrams only the exchange interaction J was taken into account while the corresponding contributions due to the kinematical interaction t_{ij} were disregarded. Estimations done in the weak coupling limit for the Dyson equation revealed quite a low superconducting T_c.

In the limit of small hole concentrations, one can consider a one-hole motion on the antiferromagnetic background within the spin-polaron representation for

the t-J model [25,26]. A number of studies of this model (see, e.g., [27,28] and references therein) predicts that a doped hole dressed by antiferromagnetic spin fluctuations can propagate coherently as a spin-polaron QP even for a finite hole doping [28]. It was suggested that the same spin fluctuations could mediate a superconducting pairing of the spin-polaron QP. This problem was treated in the framework of the weak coupling BCS formalism for a phenomenological model of QP with numerically evaluated spectrum [29, 30]. A self-consistent numerical solution of the Dyson equations for spin-polarons and magnons in the t-J model has been given in [31]. A strong renormalization of the hole spectrum due to spin-fluctuations and the d- wave pairing of spin-polaron QP with maximum $T_c \simeq 0.01t$ were obtained.

However, numerical studies [32] of the 2D t-J model at moderate doping have questioned the single spin-polaron QP picture for the paramagnetic regime. To elucidate the problem, in the recent paper [33] we propose a theory of electron spectrum and superconducting pairing for the t-J model in paramagnetic state by applying the projection technique [23] for the Green's function method of Bogoliubov [34]. Below we present the main results of this approach.

2. APPLICATION OF BOGOLIUBOV GREEN'S FUNCTION

By using the Hubbard operator (HO) representation for $\tilde{a}^+_{i\sigma} = X^{\sigma 0}_i$ and $\tilde{a}_{j\sigma} = X^{0\sigma}_j$ we write the Hamiltonian of the t-J model (2) in the form:

$$H_{t-J} = -\sum_{i\neq j,\sigma} t_{ij} X^{\sigma 0}_i X^{0\sigma}_j - \mu \sum_{i\sigma} X^{\sigma\sigma}_i + \frac{1}{4}\sum_{i\neq j,\sigma} J_{ij}\left(X^{\sigma\bar{\sigma}}_i X^{\bar{\sigma}\sigma}_j - X^{\sigma\sigma}_i X^{\bar{\sigma}\bar{\sigma}}_j\right), \tag{3}$$

where $\bar{\sigma} = -\sigma$. We introduced also the chemical potential μ which can be calculated from the equation for the average number of electrons $n = \sum_\sigma \langle X^{\sigma\sigma}_i\rangle = \sum_\sigma \langle X^{\sigma 0}_i X^{0\sigma}_i\rangle$.

To discuss the superconducting pairing within the model (3) we consider the thermodynamical GF introduced by Bogoliubov and Tyablikov [34]

$$\hat{G}_{ij,\sigma}(t-t') = \langle\langle \Psi_{i\sigma}(t) | \Psi^+_{j\sigma}(t')\rangle\rangle \tag{4}$$

in terms of the Nambu operators:

$$\Psi_{i\sigma} = \begin{pmatrix} X^{0\sigma}_i \\ X^{\bar{\sigma}0}_i \end{pmatrix}, \qquad \Psi^+_{i\sigma} = \begin{pmatrix} X^{\sigma 0}_i & X^{0\bar{\sigma}}_i \end{pmatrix}. \tag{5}$$

By differentiating the GF (4) over time t we get for the Fourier component the following equation

$$\omega \hat{G}_{ij\sigma}(\omega) = \delta_{ij}\hat{Q}_\sigma + \langle\langle [\Psi_{i\sigma}, H] \mid \Psi_{j\sigma}\rangle\rangle_\omega, \tag{6}$$

where $\hat{Q_\sigma} = \begin{pmatrix} Q_\sigma & 0 \\ 0 & Q_{\bar{\sigma}} \end{pmatrix}$ with $Q_\sigma = \langle X_i^{00} + X_i^{\sigma\sigma} \rangle$. By using the completeness relation for the HO

$$X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} = 1, \tag{7}$$

which rigorously preserves the constraint of no double occupancy we can write for the correlation function in a spin-singlet state $Q_\sigma = 1 - \langle X_i^{\bar{\sigma}\bar{\sigma}} \rangle = 1 - n/2 = Q$. To calculate the many-particle GF in the left-hand side of Eq. (6) we use the equation of motion for the HO:

$$\left(i\frac{d}{dt} + \mu \right) X_i^{0\sigma} = -\sum_l t_{il} B_{i\sigma\sigma'} X_l^{0\sigma'} + \frac{1}{2} \sum_l J_{il} (B_{l\sigma\sigma'} - \delta_{\sigma\sigma'}) X_i^{0\sigma'}, \tag{8}$$

where we have introduced the operator

$$B_{i\sigma\sigma'} = (X_i^{00} + X_i^{\sigma\sigma})\delta_{\sigma'\sigma} + X_i^{\bar{\sigma}\sigma}\delta_{\sigma'\bar{\sigma}} = (1 - \frac{1}{2}N_i + \sigma S_i^z)\delta_{\sigma'\sigma} + S_i^{\bar{\sigma}}\delta_{\sigma'\bar{\sigma}}. \tag{9}$$

The Bose-like operator (9) describes electron scattering on spin and charge fluctuations caused by the nonfermionic commutation relations for the HO (the first term in (8) – the kinematical interaction) and by the exchange spin-spin interaction (the second term in (8)).

By projecting out the linear part of the equation of motion (8) we introduce the zero-order GF in the generalized mean field approximation (MFA)

$$\hat{G}^0_{ij\sigma}(\omega) = Q\{\omega\hat{\tau}_0\delta_{ij} - \hat{E}_{ij\sigma}\}^{-1}, \tag{10}$$

with the frequency matrix $\hat{E}_{ij\sigma}$

$$\hat{E}_{ij\sigma} = \langle \{ [\Psi_{i\sigma}, H], \Psi^+_{j\sigma} \} \rangle \; Q^{-1} \; . \tag{11}$$

The nonlinear part of equation of motion (8) gives the irreducible GF in Eq. (6) which is essentially many-particle GF. By writing down an equation of motion for them with respect to the second time t' for the right-hand side operator $\Psi^+_{j\sigma}(t')$ and performing the same projection procedure we can obtain the Dyson equation for the GF (4) in the form (see [33]):

$$\hat{G}_{ij\sigma}(\omega) = \hat{G}^0_{ij\sigma}(\omega) + \sum_{kl} \hat{G}^0_{ik\sigma}(\omega) \; \hat{\Sigma}_{kl\sigma}(\omega) \; \hat{G}_{lj\sigma}(\omega), \tag{12}$$

where the self-energy operator $\hat{\Sigma}_{kj\sigma}(\omega)$ is defined by the equation

$$\hat{\Sigma}_{ij\sigma}(\omega) = Q^{-1} \langle\langle \hat{Z}^{(irr)}_{i\sigma} \mid \hat{Z}^{(irr)^+}_{j\sigma} \rangle\rangle^{(irr)}_\omega \; Q^{-1} \; , \tag{13}$$

with $\hat{Z}^{(irr)}_{i\sigma} = [\Psi_{i\sigma}, H] - \sum_l \hat{E}_{il\sigma}\Psi_{l\sigma}$, $\langle\{\hat{Z}^{(irr)}_{i\sigma}, \Psi^+_{j\sigma}\}\rangle = 0$. The self-energy operator (13) is given by the irreducible part, (irr), of the scattering matrix that has no parts connected by the single zero-order GF (10).

To calculate the self-energy operator (13) we employ the noncrossing approximation (or the self-consistent Born approximation) which is given by the two-time decoupling of the corresponding many-particle correlation functions [33]:

$$\langle X^{\sigma' 0}_{j'} B^+_{j\sigma\sigma'} X^{0\sigma'}_{i'}(t) B_{i\sigma\sigma'}(t)\rangle|_{j\neq j', i\neq i'} \simeq \langle X^{\sigma' 0}_{j'} X^{0\sigma'}_{i'}(t)\rangle\langle B^+_{j\sigma\sigma'} B_{i\sigma\sigma'}(t)\rangle \ . \quad (14)$$

Using the spectral representation for the GF, we obtain in the noncrossing approximation the following expression for the normal (diagonal) and anomalous (nondiagonal) components of the self-energy, $\tilde{\Sigma}_{\alpha\beta}(k,\omega) = Q\hat{\Sigma}_{\alpha\beta}(k,\omega)$, in the $\mathbf{k}$-space:

$$\tilde{\Sigma}^{\sigma}_{11(12)}(k,\omega) = \frac{1}{N}\sum_q \int\!\!\!\int_{-\infty}^{+\infty} dz d\Omega N(\omega, z, \Omega)\lambda_{11(12)}(q, k-q \mid \Omega) A^{\sigma}_{11(12)}(q,z), \quad (15)$$

where $N(\omega, z, \Omega) = [\tanh(z/2T) + \coth(\Omega/2T)]/2(\omega - z - \Omega)$. Here we introduce for the GF $\tilde{G}_{\alpha\beta}(k,\omega) = (1/Q)\hat{G}_{\alpha\beta}(k,\omega)$ the spectral density:

$$A^{\sigma}_{11(12)}(q,z) = -\frac{1}{\pi}\mathrm{Im}\ \tilde{G}^{\sigma}_{11(12)}(q, z + i\delta). \quad (16)$$

The electron-electron interaction functions caused by spin-charge fluctuations are given by

$$\lambda_{11(12)}(q, k-q \mid \Omega) = g^2(q, k-q)[-\frac{1}{\pi}\mathrm{Im}\ D^{+(-)}(k-q, \Omega + i\delta)], \quad (17)$$

where $g(q, k-q) = t(q) - \frac{1}{2}J(k-q)$. The spectral density for the spin-charge fluctuations is defined by the boson-like commutator GF

$$D^{\pm}(q,\Omega) = \langle\langle \mathbf{S}_q \mid \mathbf{S}_{-q}\rangle\rangle_{\Omega} \pm \frac{1}{4}\langle\langle n_q \mid n^+_q\rangle\rangle_{\Omega}, \quad (18)$$

for the spin $\mathbf{S}_q$ and number density n_q operators.

The resulting Dyson equation (12) can be written in the form

$$\tilde{G}^{\sigma}(k,\omega) = \{\omega\hat{\tau}_0 - (E^{\sigma}_k - \mu + \delta\mu)\hat{\tau}_3 - \Delta^{\sigma}_k\hat{\tau}_1 - \tilde{\Sigma}(k,\omega)\}^{-1}, \quad (19)$$

where $\hat{\tau}_0$, $\hat{\tau}_1$, $\hat{\tau}_3$ are the Pauli matrices. The energy of the quasiparticles E^{σ}_k, the renormalization of the chemical potential $\delta\mu$, and the gap function Δ^{σ}_k in the MFA are given by $\mathbf{k}$-representation of Eq.(11).

The equation for the anomalous self-energy in Eq. (15) in comparison with the diagram technique [24] has an additional contribution proportional to $t^2(q)$ due to the kinematical interaction in (17) which enhances the d-wave pairing.

By using the imaginary frequency technique a numerical study of the linearized system of the Dyson equations (19),(15) was performed in [33]. The electron spectral density Eq.(16) shows QP excitations at the FS crossing and a dispersive incoherent band. For small hole concentration the QP dispersion is small while the intensity of the incoherent band is quite large. With doping the QP band width strongly increases and the incoherent band is suppressed. The results for single-electron spectral functions are in general agreement with the studies within exact-diagonalization technique [32]. The occupation numbers $N(\mathbf{k})$ have the characteristic behavior for strongly correlated systems. Being large throughout the BZ, due to the incoherent contribution, they show only a small drop at the FS. The volume of the FS at small doping is proportional to the hole concentration δ that does not obey the Luttinger theorem. The superconducting pairing due to the exchange and the kinematic interactions (in the second order) has the d-wave symmetry and high $T_c \simeq 0.04t \simeq 200$ K. The calculations confirm the results of the d-wave superconducting pairing obtained within the spin-polaron $t-J$ model [31].

The advantage of the proposed microscopical theory of the d-wave spin-fluctuation superconducting pairing, in comparison with phenomenological approaches based on the Fermi liquid models close to AFM instability, is that we rigorously take into account local constraints of no double occupancy due to strong correlations that result in electron–spin-fluctuation interaction. Therefore in our approach we used only two basic parameters for the model, the hopping energy, t_{ij}, and the (super)exchange energy, J, which are characteristic of strongly correlated systems and no artificial parameters for electron scattering on antiferromagnetic spin-fluctuation were introduced as in phenomenological theories [35].

Generalization of the calculations for the asymmetric (p-d) Hubbard model [36] is presented in [37]. A possibility of $s+d$ mixing of the order parameter (the gap function) in orthorhombic phase is discussed in [38].

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ASYMPTOTIC BEHAVIOUR OF CORRELATION FUNCTIONS IN THE TRAPPED BOSE GAS

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The functional integral method was applied for the calculation of the asymptotic behaviour of the correlation functions for the repulsive Bose gas in a paraboloidal trap. Results are reported here for the two-point correlation functions below the critical temperatures in $d = 3, 2$ and 1 dimensions. Only for $d = 3$ correlations are long range. The two-dimensional condensate is marginally stable in the sense that correlations decay by a power law.

The observation of Bose condensation in vapours of alkali atoms [1–3] held in magneto-optical traps, and recently [4] in atomic hydrogen, has stimulated enormous interest, both experimentally and theoretically, in this phenomenon. The natural starting point for studying the behaviour of such systems is the theory of the dilute weakly interacting Bose gas which was originated by Bogoliubov's 1947 paper [5]. Much of the theoretical work has been concerned with solutions of the Gross–Pitaevskii (GP) equation in the presence of the paraboloidal potential describing the trap [6–8]. Without the trap this equation is also called the Nonlinear Schrödinger (NLS) equation [9] which, in one space dimension ($d = 1$), can be solved exactly at both classical and quantum level including [10, 11] calculation of the finite-temperature correlation functions for the repulsive case (coupling constant $g > 0$). For $d = 1$ as well as for the higher dimensions, the finite-temperature properties of the quantum NLS equation have otherwise been extensively analyzed [12] by functional integral methods. This way it is established, e.g., that without any trap no long-range correlations arise for $d < 3$.

Thus far it has remained an open question whether the presence of a trap potential will induce long-range order for $d < 3$. We'll establish here that, even in the presence of a paraboloidal trap, there is long-range order only for $d = 3$. To this end we have applied the previous [12, 13] functional integral methods to the case when a trap is included. An important new aspect is then that the trap breaks translational invariance; and this introduces wholly new many-body theoretical problems. Thus, rather than using periodic boundary conditions (b.c.s), we must expect to impose vanishing b.c.s at infinity, and so to work at «zero density» [14].

The functional integral method provides a framework within which, in principle, all thermodynamic properties of the trapped bose gas can be determined. The main result reported here is the calculation of the asymptotic behaviour of the two-point correlation functions for trapped Bose gases at finite temperature for each of $d = 1, 2, 3$. Because there is no translational invariance these correlation functions no longer depend solely on the difference of two position vectors. It can still be concluded that long-range order arises, for $T < T_c$, in $d = 3$, and the first-order coherence function asymptotically approaches unity. In $d = 2$ and for $T < T_c$ the condensate is *marginally* stable for correlations decay algebraically, namely as a power law. In $d = 1$ correlations decay exponentially for $T < T_c$, and we have not yet analyzed any $T = 0$ limit. For $T > T_c$ there is a Gaussian decay in all dimensions.

One can write the finite-temperature correlation function $G(\mathbf{r}_1, \mathbf{r}_2) \equiv \langle \mathbf{T}_\tau \hat{\psi}(\mathbf{r}_1, \tau_1) \hat{\psi}^\dagger(\mathbf{r}_2, \tau_2) \rangle$ (where $\mathbf{T}_\tau$ means a thermal ordering in τ) as the ratio of two functional integrals,

$$G(\mathbf{r}_1, \mathbf{r}_2) = Z^{-1} \int e^S \psi(\mathbf{r}_1, \tau_1) \bar{\psi}(\mathbf{r}_2, \tau_2) D\psi D\bar{\psi}, \tag{1}$$

in which Z is a partition function $Z = \int e^S D\psi D\bar{\psi}$. The action S is

$$S = \int_0^\beta d\tau \int d^d r \left\{ \bar{\psi}(\mathbf{r}, \tau) K \psi(\mathbf{r}, \tau) - \frac{g}{2} \bar{\psi}(\mathbf{r}, \tau) \bar{\psi}(\mathbf{r}, \tau) \psi(\mathbf{r}, \tau) \psi(\mathbf{r}, \tau) \right\}. \tag{2}$$

The boundary conditions are vanishing at infinity for $\mathbf{r}$ and periodic, period $\beta = (k_B T)^{-1}$, for τ. The action S yields the quantum many-body problem at $T > 0$ for a gas with repulsive pairwise δ-function interactions of strength g in $\mathbf{R}^d$. The differential operator $K = \partial_\tau - H$, and $H = -\dfrac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) - \mu$; μ is the chemical potential and $V(\mathbf{r}) = \dfrac{m}{2} \Omega^2 \mathbf{r}^2$ is the paraboloidal trap potential, taken with spherical symmetry for simplicity.

For $T < T_c$ we shall put $\psi(\mathbf{r}, \tau) = \psi_o(\mathbf{r}) + \psi_1(\mathbf{r}, \tau)$ [7, 12, 15] and likewise for $\bar{\psi}$: where the condensate variable $\psi_o(\mathbf{r})$ will not depend on τ, and ψ_1 is

that due to thermal fluctuations. In this Letter we shall only consider terms in S up to quadratic (bilinear) in ψ_1, $\bar{\psi}_1$ and can therefore explicitly integrate out the thermal fluctuations. This way we arrive at $S_{\rm eff}[\psi_o, \bar{\psi}_o] = \ln \int e^S D\psi_1 D\bar{\psi}_1$, and

$$\begin{aligned} &S_{\rm eff}[\psi_o, \bar{\psi}_o] + \beta F_{nc}(\mu) \\ &= \beta \int d^d r \{\bar{\psi}_o(\mathbf{r})[\frac{\hbar^2}{2m}\nabla^2 + \mu - \tilde{V}(\mathbf{r})]\psi_o(\mathbf{r}) - \frac{g}{2}\bar{\psi}_o(\mathbf{r})\bar{\psi}_o(\mathbf{r})\psi_o(\mathbf{r})\psi_o(\mathbf{r})\}. \end{aligned} \tag{3}$$

In $S_{\rm eff}$, $\tilde{V}(\mathbf{r}) = V(\mathbf{r}) + 2g\rho_{nc}(\mathbf{r})$ is a renormalized trap potential, while $\rho_{nc}(\mathbf{r})$ is the density profile of the thermal particles in the ideal gas approximation — as is consistent with terms only quadratic in $\psi_1, \bar{\psi}_1$ retained. More precisely, at this level of approximation (Hartree–Fock–Bogoliubov) this density profile derives from the fundamental solution of the $d+1$-dimensional operator K: $K\mathcal{G}(\mathbf{r}, \tau; \mathbf{r}', \tau') = -\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau')$, and Green's function $\mathcal{G}$ can be expressed in the form

$$\mathcal{G}(\mathbf{r}, \tau; \mathbf{r}', \tau') = \sum_{\mathbf{n}} \frac{u_{\mathbf{n}}(\mathbf{r}) u_{\mathbf{n}}(\mathbf{r}')}{e^{\beta \mathrm{E}_{\mathbf{n}}} - 1} e^{\mathrm{E}_{\mathbf{n}}(\tau - \tau')}, \tau > \tau'. \tag{4}$$

For $d = 3$ the vectors $\mathbf{n} = (n_1, n_2, n_3)$, and the $u_{\mathbf{n}}(\mathbf{r})$ and $\mathrm{E}_{\mathbf{n}}$ are the eigenfunctions and eigenenergies, respectively, of the $d = 3$ harmonic oscillator Hamiltonian H; and similarly for $d = 1, 2$. Then $\rho_{nc}(\mathbf{r}) = \mathcal{G}'(\mathbf{r}, \tau; \mathbf{r}, \tau)$, where prime means $\mathbf{n} = (0, 0, 0)$ is omitted. The free energy of the thermal particles $F_{nc}(\mu)$ is simply $F_{nc}(\mu) = \beta^{-1} \sum_{\mathbf{n}}{}' \ln(1 - e^{-\beta \mathrm{E}_{\mathbf{n}}})$.

At this point it is possible to calculate the actual temperatures T_c. The leading, i.e., zeroth order term is found by replacing $\rho_{nc}(\mathbf{r})$ by a constant $\rho_{nc}(0)$: this defines the renormalized chemical potential $\Lambda = \mu - 2g\rho_{nc}(0)$, and $\Lambda = 0$ determines T_c [6]. At first order in g we can add the appropriate terms arising in $S_{\rm eff}$. Beyond this we also need to include fluctuations ψ_1 to an order higher than quadratic.

The free energy F of the trapped Bose gas is calculated from $-\beta F(\mu) = \ln \int e^{S_{\rm eff}} D\psi_0 D\bar{\psi}_0$. By the steepest descents for large β (low T) we find that

$$F(\mu) = F_{nc}(\mu) - \frac{g}{2} \int d^d r \mid \Phi(\mathbf{r}) \mid^4 . \tag{5}$$

In Eq.(5) the fields $\Phi, \bar{\Phi}$ are the quasi-classical fields satisfying the extremum condition $\delta(S_{\rm eff}[\Phi, \bar{\Phi}]) = 0$. This condition is equivalent to the stationary Gross–Pitaevskii equations

$$\frac{\hbar^2}{2m}\nabla^2 \Phi(\mathbf{r}) + (\mu - \tilde{V}(\mathbf{r}))\Phi(\mathbf{r}) - g \mid \Phi(\mathbf{r}) \mid^2 \Phi(\mathbf{r}) = 0, \tag{6}$$

and the similar equation for $\bar{\Phi}$. At this quasi-classical approximation we already find through the presence of $\tilde{V}(\mathbf{r})$ the Hartree–Fock–Bogoliubov (HFB) corrections to the Gross–Pitaevskii equation introduced earlier [6].

We turn next to the calculation of the finite-temperature correlation function, Eq. (1). By integrating out the thermal fluctuations included up to terms quadratic in ψ_1,$\bar{\psi}_1$ we find that

$$G(\mathbf{r}_1,\mathbf{r}_2) \simeq \frac{\int e^{S_{\rm eff}}\psi_o(\mathbf{r}_1)\bar{\psi}_o(\mathbf{r}_2)D\psi_o D\bar{\psi}_o}{\int e^{S_{\rm eff}}D\psi_o D\bar{\psi}_o} \equiv C(\mathbf{r}_1,\mathbf{r}_2). \tag{7}$$

At low enough temperatures these remaining functional integrals can be evaluated by the steepest descents where again we work consistently at the HFB level. At this level the correlation functions can be expressed in the form

$$C(\mathbf{r}_1,\mathbf{r}_2) \simeq e^{-S_{\rm eff}[\Phi_0,\bar{\Phi}_0]+S_{\rm eff}[\Phi_1,\bar{\Phi}_1]+\ln\Phi_1(\mathbf{r}_1)\bar{\Phi}_1(\mathbf{r}_2)}, \tag{8}$$

and the fields $\Phi_0,\bar{\Phi}_0$ satisfy Eq. (6). Evidently the fields $\Phi_1,\bar{\Phi}_1$ are determined by $\delta(S_{\rm eff}[\Phi_1,\bar{\Phi}_1]+\ln\Phi_1(\mathbf{r}_1)\bar{\Phi}_1(\mathbf{r}_2))=0$, and this variational equation also leads to a pair of equations with additional sources from the $\ln(\Phi_1\bar{\Phi}_1)$. This pair of equations is

$$\begin{aligned}
-\frac{\hbar^2}{2m}\nabla^2\Phi_1(\mathbf{r}) - (\mu-\tilde{V}(\mathbf{r}))\Phi_1(\mathbf{r}) + g\Phi_1^2(\mathbf{r})\bar{\Phi}_1(\mathbf{r}) &= \frac{\delta(\mathbf{r}-\mathbf{r}_2)}{\beta\bar{\Phi}_1(\mathbf{r}_2)},\\
-\frac{\hbar^2}{2m}\nabla^2\bar{\Phi}_1(\mathbf{r}) - (\mu-\tilde{V}(\mathbf{r}))\bar{\Phi}_1(\mathbf{r}) + g\bar{\Phi}_1^2(\mathbf{r})\Phi_1(\mathbf{r}) &= \frac{\delta(\mathbf{r}-\mathbf{r}_1)}{\beta\Phi_1(\mathbf{r}_1)}.
\end{aligned} \tag{9}$$

For simplicity, we shall solve them only at the Thomas-Fermi approximation: this is expected to be valid at low enough temperatures [6–8]. The stationary Gross–Pitaevskii equation Eq. (6) is now reduced to a simple algebraic equation and we then easily find the expected inverted paraboloidal density profile which is

$$\rho_0(\mathbf{r}) \equiv \Phi_0(\mathbf{r})\bar{\Phi}_0(\mathbf{r}) = \frac{1}{g}(\mu-\tilde{V}(\mathbf{r}))\Theta(\mu-\tilde{V}(\mathbf{r})), \tag{10}$$

in which Θ is the Heaviside step function. Evidently $\rho_0(\mathbf{r})$ can be interpreted as the condensate density expressed in terms of order parameters $\Phi_0,\bar{\Phi}_0$. The radius of the condensate R_c can now be determined from the condition $\mu-\tilde{V}(R_c)=0$.

The solution of Eqs. (9) is more complicated. Notice first that the fields $\Phi_1,\bar{\Phi}_1$, appearing in these equations will be complex valued fields in general. But they are two independent fields with independent variations. We can therefore seek first of all solutions in the form

$$\Phi_1(\mathbf{r}) = \sqrt{\rho(\mathbf{r})}e^{\phi(\mathbf{r})},\ \bar{\Phi}_1(\mathbf{r}) = \sqrt{\rho(\mathbf{r})}e^{-\phi(\mathbf{r})},$$

where $\phi(\mathbf{r})$ can be complex valued, but will be found bellow to describe the real contribution to the correlation functions of the complex phases of the wave functions. We can furthermore assume that, away from the boundaries, $\rho(\mathbf{r})$ is a slowly varying function of position $\mathbf{r}$ so that $\nabla^2\sqrt{\rho}$ and $\nabla\sqrt{\rho}$ are both small and can be neglected. This will not be true of $(\nabla\phi)^2$ or $\rho\nabla^2\phi$, so that Eqs. (9) become

$$g\rho(\mathbf{r}) - (\mu - \tilde{V}(\mathbf{r})) - \frac{\hbar^2}{2m}(\nabla\phi(\mathbf{r}))^2 = 0, \tag{11}$$

$$\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) = \frac{1}{2\beta\rho(\mathbf{r}_1)}\delta(\mathbf{r}-\mathbf{r}_1) - \frac{1}{2\beta\rho(\mathbf{r}_2)}\delta(\mathbf{r}-\mathbf{r}_2). \tag{12}$$

The first of these equations Eq. (11) has the solution $\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \dfrac{\hbar^2}{2mg}(\nabla\phi)^2$. Within the Thomas–Fermi approximation, $\rho(\mathbf{r})$ in Eq. (12) is then $\rho_0(\mathbf{r})$. We then express the solution of this equation in terms of a function $f(\mathbf{r},\mathbf{r}')$:

$$\phi(\mathbf{r};\mathbf{r}_1,\mathbf{r}_2) = f(\mathbf{r},\mathbf{r}_1) - f(\mathbf{r},\mathbf{r}_2).$$

The functional form of $f(\mathbf{r},\mathbf{r}')$ depends on the dimensionality of the system. We find that

$$f(\mathbf{r},\mathbf{r}') = -\frac{a}{2\pi\beta\rho_0(\mathbf{r}')}\ \frac{1}{R}\quad (d=3), \tag{13}$$

$$f(\mathbf{r},\mathbf{r}') = \frac{a}{\pi\beta\rho_0(\mathbf{r}')}\ln R\quad (d=2), \tag{14}$$

$$f(\mathbf{r},\mathbf{r}') = \frac{a}{\beta\rho_0(\mathbf{r}')}R\quad (d=1) \tag{15}$$

with $a \equiv \dfrac{m}{2\hbar^2}$ and $R \equiv \mid \mathbf{r}-\mathbf{r}' \mid$. It is already clear that the correlation functions can no longer depend on $R = \mid \mathbf{r}-\mathbf{r}' \mid$ alone: they depend also on both $\mathbf{r}_1$ and $\mathbf{r}_2$ separately, consistent with the breakdown of translational invariance induced by the trap.

We consider first the correlation function in $d=3$. In this case the points $\mathbf{r}=\mathbf{r}_1$ and $\mathbf{r}=\mathbf{r}_2$ in $\phi(\mathbf{r};\mathbf{r}_1,\mathbf{r}_2)$ are singular and introduce a divergence problem. This difficulty can be avoided first of all by considering a first-order «coherence function» $G^{(1)}(\mathbf{r}_1,\mathbf{r}_2)$ (compare, e.g., [16, 17]) which we define here as

$$G^{(1)}(\mathbf{r}_1,\mathbf{r}_2) = \frac{G(\mathbf{r}_1,\mathbf{r}_2)}{\langle\psi(\mathbf{r}_1,\tau_1)\rangle\langle\psi^\dagger(\mathbf{r}_2,\tau_2)\rangle} \simeq \frac{C(\mathbf{r}_1,\mathbf{r}_2)}{\langle\psi_o(\mathbf{r}_1)\rangle\langle\bar{\psi}_o(\mathbf{r}_2)\rangle}, \tag{16}$$

for identically the same singularities appear [12] in the direct calculation of the order parameters $\langle\psi(\mathbf{r},\tau)\rangle, \langle\psi^{\dagger}(\mathbf{r},\tau)\rangle$. Notice that in Eq. (16) we have already replaced $\langle\psi\rangle$, the order parameter of the trapped Bose gas, by $\langle\psi_o\rangle$ since average over thermal fluctuations vanishes: $\langle\psi_1\rangle = 0$. For $T < T_c$, when the order parameter is nonzero, we find that

$$\begin{aligned} G^{(1)}(\mathbf{r}_1,\mathbf{r}_2) &\simeq e^{-\frac{1}{2}(f(\mathbf{r}_1,\mathbf{r}_2)+f(\mathbf{r}_2,\mathbf{r}_1))} \\ &= \exp\{\frac{a}{4\pi\beta\rho_0(\mathbf{r}_1,\mathbf{r}_2)}\frac{1}{R}\}, \end{aligned} \tag{17}$$

where $\rho_0^{-1}(\mathbf{r}_1,\mathbf{r}_2) \equiv \rho_0^{-1}(\mathbf{r}_1) + \rho_0^{-1}(\mathbf{r}_2)$. Evidently that $G^{(1)}(\mathbf{r}_1,\mathbf{r}_2) \to 1$ for large R, thus indicating long-range order and long-range coherence, and there are thus features of a coherent state in this sense. The coherence length is given by $\dfrac{a}{4\pi\beta\rho_0(\mathbf{r}_1,\mathbf{r}_2)}$ and depends on both $\mathbf{r}_1$ and $\mathbf{r}_2$ separately. Notice that we have assumed $\mathbf{r}_1$ and $\mathbf{r}_2$ are not close to the boundaries of the condensate so that always $\rho_0(\mathbf{r}) > 0$ in the above expression.

Let us consider the *uniform* Bose gas ($V(\mathbf{r}) = 0$) and study the long distance ($R \to \infty$) behaviour of the correlation function:

$$G^{(1)}(\mathbf{r}_1,\mathbf{r}_2) - 1 \simeq \frac{m}{4\pi\hbar^2\beta}\frac{1}{\mid \mathbf{r}_1 - \mathbf{r}_2 \mid}.$$

Going over to the momentum representation one can see that for the small temperatures the Fourier transform of this function is divergent at small momenta as $\mid \mathbf{k} \mid^{-2}$ thus forbidding transitions for a lower symmetry phase at $d = 1, 2$ which is the famous Bogoliubov's result [18].

For $d = 2$ the singularity in $f(\mathbf{r},\mathbf{r}')$ is logarithmic and the divergence is renormalizable. For $d = 1$ the function f is nonsingular. Thus we can directly evaluate the correlation functions, and find that

$$G(\mathbf{r}_1,\mathbf{r}_2) \simeq \sqrt{\rho_0(\mathbf{r}_1)\rho_0(\mathbf{r}_2)}\exp\{-\frac{a}{2\pi\beta\rho_0(\mathbf{r}_1,\mathbf{r}_2)}\ln R\}\ ,\ (d=2); \tag{18}$$

$$G(\mathbf{r}_1,\mathbf{r}_2) \simeq \sqrt{\rho_0(\mathbf{r}_1)\rho_0(\mathbf{r}_2)}\exp\{-\frac{a}{2\beta\rho_0(\mathbf{r}_1,\mathbf{r}_2)}R\}\ \ ,\ (d=1). \tag{19}$$

It is obvious that these correlation functions both vanish for large R and that there is no long-range order in $d = 1$ or in $d = 2$. In the case $d = 2$ the condensate is marginally stable in that correlations decay algebraically, namely by a power law. The exponent of this power-law is proportional to T so that at very low temperatures, correlations may thus prevail over almost macroscopic distances. In real magneto-optical traps for $d = 3$ we still expect the condensate to be stable

even for extremely anisotropic trap potentials, as in, e.g., the experiments [4] on atomic hydrogen. The three correlation functions (Eqs. (17–19)) coincide with those obtained under translational invariance without the trap to the extent that for $\Omega \to 0, V(\mathbf{r}) \to 0$, and we can expect $2g\rho_{nc}(\mathbf{r}) \to \text{Const} = 2g\rho_{nc}$.

Thus in summary we have demonstrated that the functional integration techniques can be extended to Bose gases in a confining trap potential, and form a convenient framework in which to consider the thermal properties of the condensate. We have shown in particular that true long-range order only arises in $d = 3$. In $d = 2$ the condensate is only marginally stable, but the related power-law decay of correlations becomes increasingly weak as temperature decreases. We expect to define multipoint correlation functions similarly to Eq. (16) and find these ~ 1 for large separations of points.

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RIGOROUS RESULTS IN A NONIDEAL BOSE GAS THEORY

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A method of approach to the problem of the Bose condensation in a nonideal Bose gas based on Bogoliubov's theory of quasi-averages is examined. It is shown that the proof of the existence of a phase transition in this system can be reduced to the proof of some trace-inequality, gaussian domination condition, which is linked with some break of the continuous symmetry group. To prove this condition a special functional integral technique over Bogoliubov's measure defined on some space of continuous functions with a uniform metric is proposed.

1. PHASE TRANSITION IN A NONIDEAL BOSE GAS

In 1961 Bogoliubov proposed a universal method of approach to the phase transitions theory based on the study of a degeneracy of a thermodynamic equilibrium state [1]. This phenomenon arises for a temperature below some critical one $\theta \leq \theta_c$. For $\theta = \theta_c$ a phase transition to a regular nondegenerate state takes place.

In many systems with a continuous symmetry group a phase transition is linked with a break of the law of conservation of total particles number. A typical feature of such system is an emergence of some type of the condensation.

Consider a nonideal Bose gas model. Let in a ν-dimensional cube $V \in R^\nu$ with coordinates $x = (x^1, x^2, \ldots, x^\nu), x^j \in (-L/2, L/2), j = 1, 2, \ldots, \nu$ and with the volume $|V| = L^\nu$ be N identical spinless particles. The Hamiltonian of the system is

$$\hat{H} = -\frac{1}{2m}\sum_{n=1}^{N} \triangle_{x_n} + \sum_{n<m} \Phi(x_n - x_m), \tag{1}$$

where $\triangle_x$ is a Laplacian operator over x and a potential energy is defined by a real-valued symmetric function $\Phi(x) = \Phi(-x)$.

A superfluidity is a phase transition in a system of bosons accompanied by a long-range order in a coordinate space or by a Bose condensation in a momentum space.

Let $F(x_1, x_2) = \langle \hat{\psi}^+(x_1)\hat{\psi}(x_2)\rangle_V$ be a one-particle density matrix. The average is a Gibbs equilibrium average with the Hamiltonian $\hat{H}$ in the cube V.

An existence of a long-range order in a system means, that

$$\lim_{|x_1-x_2|\to\infty}\lim_{V\uparrow R^\nu} F(x_1,x_2)\equiv n_0>0. \tag{2}$$

Passing to the Fourier transformation $w(k)=(2\pi)^{-3}\int F(x)e^{ikx}dx$, one obtains from (2) that $w(k)=n_0\delta(k)+w_1(k)$, where $w_1(k)$ defines a continuous distribution of particles over nonzero momenta and n_0 is a Bose condensate density, i.e.,

$$n_0=\lim_{V\uparrow R^\nu}\frac{\langle\hat a_0^+\hat a_0\rangle_V}{|V|}=\lim_{|V|\to\infty}\frac{1}{|V|^2}\iint\langle\hat\psi^+(x_1)\hat\psi(x_2)\rangle_V\,dx_1dx_2>0. \tag{3}$$

So an appearance of a phase transition in a model of a nonideal Bose gas, which is connected with the existence in the system of the long-range order in relation to (2), is determined by an appearance of a nonzero Bose condensate density n_0.

2. GAUSSIAN DOMINATION AND BOSE CONDENSATION

To prove the condition (3) it is necessary to obtain an upper bound for the correlation function $\langle\hat a_p^+\hat a_p\rangle_V$ for $p\neq 0$. Really we have the sum rule

$$n=\frac{1}{|V|}\sum_p\langle\hat a_p^+\hat a_p\rangle_V, \tag{4}$$

where n is the average density of the number of particles in the system. Therefore the inequality (3) will take place if from the estimate

$$\langle\hat a_p^+\hat a_p\rangle_V\le G_p^{(V)}(\theta),\quad p\neq 0 \tag{5}$$

will result that in the thermodynamic limit $n>|V|^{-1}\sum_{p\neq0}G_p^{(V)}(\theta)$. In this way the condition $n=\lim_{V\uparrow R^\nu}|V|^{-1}\sum_{p\neq0}G_p^{(V)}(\theta)$ gives a lower bound for the critical temperature $\theta_c^{(0)}$ of the phase transition.

Thus the main thing in our approach is to obtain the estimate (5), which is connected with Bogoliubov's quasi-averages theory. Let the Hamiltonian of a system takes the form $\hat H=\hat H_0+\hat H_1$, where $\hat H_0=\sum\omega_p\hat a_p^+\hat a_p,\omega_p>0(p\neq0),\omega_0=0$ be a free Hamiltonian, $\hat H_1$ be an interaction. Consider a one-parameter family of the Hamiltonians $\hat H(h)=\hat H_0(h)+\hat H_1$, where $\hat H_0(h)=\sum\omega_p(\hat a_p^++h_p^*)(\hat a_p+h_p)$ and $h_p\in C$ are arbitrary complex numbers. Define the functional (a statistical sum) $Z(h)=\mathrm{Tr}\exp[-\beta\hat H(h)]$, where $\beta=\theta^{-1}$ is an inverse temperature. We shall say that the gaussian domination condition [2] takes place if for any $h_p\in C$

$$Z(h)\le Z(0). \tag{6}$$

If the functional $Z(h)$ has for $h = 0$ a local maximum we shall say that the local gaussian domination condition takes place [3]. The condition of the maximum of $Z(h)$ at zero leads to an inequality [4] for Bogoliubov's inner product (two-point Duhamel function) $(\hat{a}_p^+, \hat{a}_p) \leq (\beta\omega_p)^{-1}$.

It is possible to show, that if the gaussian domination condition (or the more weak local gaussian domination condition) is fulfilled, then in the nonideal Bose gas with the repulsion $\Phi(x) \geq 0$ for $\nu \geq 3$ and $\theta \leq \theta_c^{(0)}$ the Bose condensate is arisen [5], i.e., the phase transition condition (3) is accomplished. In this way we have $\theta_c^{(0)} = \theta_0$, where θ_0 is a temperature of the Bose condensation in an ideal Bose gas. So the London's assumption that the repulsive-type interaction favoured to Bose condensation finds the rigorous substantiation.

To prove the condition (6) in the model (1) use the functional integrals technique [6].

3. GAUSSIAN FUNCTIONAL INTEGRALS OVER BOGOLIUBOV'S MEASURE

Consider a case of the one degree of freedom, the Hamiltonian of a one-dimensional harmonic oscillator

$$\hat{\Gamma} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2,$$

and the chronological average

$$\left\langle T \exp\left[i \sum_{j=1}^{N+1} \nu_j \hat{Q}(s_j)\right] \right\rangle, \tag{7}$$

with the Hamiltonian $\hat{\Gamma}$. The operator $\hat{Q}(s)$ is given by $\hat{Q}(s) = e^{s\Gamma}\hat{q}e^{-s\Gamma}$, where ν_j are real numbers and $0 = s_1 < s_2 < \cdots < s_N < s_{N+1} = \beta$. It is possible to show, that the average (7) in this case takes the form

$$\left\langle T \exp\left[i \sum_{j=1}^{N+1} \nu_j \hat{Q}(s_j)\right] \right\rangle = \exp\left(-\frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} A_{jk}\eta_j\eta_k \right), \tag{8}$$

where the covariance matrix A entries are

$$A_{jk} = \frac{1}{2m\omega \operatorname{sh} \frac{\beta\omega}{2}} \operatorname{ch}\left(\frac{\beta\omega}{2} - \frac{\beta\omega}{N}|j-k| \right)$$

and we used the uniform separation of the interval $(0, \beta)$. Taking into account the formula (8), the complex Fourier formula and the fact, that operators commute

under the T-product sign, it is possible to show that for an arbitrary T-product average the following formula takes place

$$\left\langle T\left[f\left(\hat{Q}(s_1),\ldots,\hat{Q}(s_{N+1})\right)\right]\right\rangle =$$

$$= \int f(q_1,\ldots,q_{N+1})\rho(q_1,\ldots,q_{N+1})dq_1\ldots dq_{N+1},$$

where

$$\rho(q_1,q_2,\ldots,q_{N+1}) = \frac{1}{(2\pi)^{\frac{N}{2}}}\frac{\delta(q_1-q_{N+1})}{(\det A)^{\frac{1}{2}}}\exp\left[-\frac{1}{2}\sum_{j,k=1}^{N}(A^{-1})_{jk}q_jq_k\right]. \quad (9)$$

It follows from (9) that $\rho \geq 0$, $\int \rho\, dq_1\ldots dq_{N+1} = 1$.

Consider the space $X \equiv C^{\circ}[0,\beta]$ of continuous functions $q(s)$, defined on the segment $[0,\beta]$, that satisfy the condition $q(0) = q(\beta)$. This is the metric space with respect to the uniform metric $\rho(q,p) = \sup_{s\in[0,\beta]}|q(s)-p(s)|$. In the space X we can introduce a σ-algebra generated by cylindrical sets. This σ-algebra is the same as the σ-algebra generated by the sets that are open in the metric ρ. Extending the gaussian measure from the cylindrical sets to their Borel closure, we obtain a gaussian measure μ in the space X [7] with the average value equal to zero and with the correlation function

$$B(t,s) = \frac{1}{2m\omega\,\mathrm{sh}\,\frac{\beta\omega}{2}}\,\mathrm{ch}\left(\omega|t-s|-\frac{\beta\omega}{2}\right). \quad (10)$$

An integral corresponding to the measure μ can be defined as an abstract Daniell integral [8]. By means of this integral the Gibbs T-product average for an arbitrary measurable functional can be represented as

$$\left\langle T\left(f(\hat{Q})\right)\right\rangle = \int_X f(x)d\mu(x). \quad (11)$$

4. GAUSSIAN DOMINATION AND FUNCTIONAL INTEGRALS

Consider a system with the Hamiltonian $\hat{H} = \hat{\Gamma} + \hat{V}$, where $\hat{V} = V(\hat{q})$ is an interaction, as well a one-parameter family of the Hamiltonians $\hat{H}(h) = \hat{\Gamma}(h) + \hat{V}, h \in R$ with

$$\hat{\Gamma}(h) = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}(\hat{q}-h)^2.$$

The statistical sum of the system is $Z(h) = \operatorname{Tr} e^{-\beta \hat{H}(h)}$. Let the potential of interaction be the nonnegative and symmetric function, i.e., $V(x) \geq 0,\ V(x) = V(-x)$. Using the above-mentioned functional integral (11), we have

$$R(h) = \int_X d\mu(x) \exp\left[-\int_0^\beta ds V\left(x(s) + h\right) \right].$$

Use now the theorem of linear substitution of a variable in an integral over gaussian measure [9], which gives for an integrable functional $F(x)$ and for a function $a \in H$, that

$$\int_X F(x) d\mu(x) = e^{-\frac{1}{2}||a||_H^2} \int_X F(x+a) e^{-(a,x)} d\mu(x).$$

The space H is a linear covering of the eigenfunctions of the kernel (10) that is closed relative to an appropriate norm [7]. Apply this formula for a case of the considered measure and for the constant functions a, which belong to H. We obtain, that

$$R(h) = \exp\left[-\frac{\beta m \omega^2 h^2}{2} \right] \int_X d\mu(x) \exp\left[-\int_0^\beta V(x(t)) dt \right] \cdot \exp\left[mh\omega^2 \int_0^\beta x(t) dt \right].$$

Consider the Fourier–Gauss transformation

$$\tilde{f}(y) \equiv F(f; y) = \int_X d\mu(x) f(x + iy)$$

of the functional $f(x)$ and the Parseval equality

$$\int_X f\left(\frac{x}{\sqrt{2}}\right) g^*\left(\frac{x}{\sqrt{2}}\right) d\mu(x) = \int_X F\left(f; \frac{y}{\sqrt{2}}\right) F^*\left(g; \frac{y}{\sqrt{2}}\right) d\mu(y) \qquad (12)$$

for the case of functionals

$$f(x) = F(x) \equiv \exp\left[-\int_0^\beta dt V(x(t)) \right], \quad g(x) = \exp\left[mh\omega^2 \int_0^\beta x(t) dt \right].$$

The equality (12) takes the form

$$\exp\left[-\frac{\beta m h^2 \omega^2}{2} \right] \int_X F\left(\frac{x}{\sqrt{2}}\right) \exp\left[\frac{1}{\sqrt{2}} hm\omega^2 \int_0^\beta x(t) dt \right] d\mu(x)$$
$$= \int_X \tilde{F}\left(\frac{y}{\sqrt{2}}\right) \exp\left[\frac{i}{\sqrt{2}} hm\omega^2 \int_0^\beta y(t) dt \right] d\mu(y)$$

and we see that if for any y

$$\tilde{F}(y) \geq 0, \tag{13}$$

then $R(h) = \tilde{F}(-ih) \leq R(0) = \tilde{F}(0)$. The condition (13) in our case can be proved for symmetric, nonnegative potentials by the Iensen inequality.

Up to here we considered a case of one degree of freedom. For situation which is interesting in the nonideal Bose gas theory there is a system of N spinless particles of the mass m everyone of which interact with each other by means of the pairwise symmetric potential $\hat{H} = \hat{\Gamma} + \hat{V}$, where

$$\hat{\Gamma} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2, \quad \hat{V} = V(\hat{q}) = \sum_{i<j=1}^{N} \Phi(\hat{q}_i - \hat{q}_j) = V(-\hat{q})$$

and by now $\hat{p} = (\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_N), \hat{q} = (\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_N)$. Let us assume also, that $\hat{V} \geq 0$.

In this case all our arguments and proofs are true. In this situation the multiple integral over a gaussian measure is defined on the direct product of N copies of the space $X^N \equiv X \times X \times \cdots \times X$. An appropriate measure $\mu^N = \bigotimes_{k=1}^{N} \mu$ is a Cartesian product of the gaussian measures μ and as well as the measure μ is σ-additive [10]. The functional integral in this case is

$$\int_{X^N} F(x) d\mu^N(x),$$

where $x = (x_1, x_2, \ldots, x_N)$ is a function on $\bigotimes_1^N C^\circ[0, \beta]$. The gaussian domination condition takes the form $R(h) \leq R(0)$, where $h = (h_1, h_2, \ldots, h_N)$ is an arbitrary vector in R^N.

Consider construction of a functional integral over Bogoliubov's measure when an integrand function depends not only on coordinates but on momenta also. In this case instead of the expression (7) let us consider the average

$$\left\langle T \exp\left[i \sum_{j=1}^{N+1} \left(\sqrt{2m\omega}\, x_j \hat{Q}(s_j) + \sqrt{\frac{2}{m\omega}}\, y_j \hat{P}(s_j) \right) \right] \right\rangle,$$

with the Hamiltonian $\hat{\Gamma}$ again. This average is $\exp\left[-\Omega\left(\{x_j, y_j\}\right)\right]$, where the quadratic form on the variables x_j, y_j is

$$\Omega\left(\{x_j, y_j\}\right) = \sum_{j,k=1}^{N+1} S_{jk}(x_j x_k + y_j y_k) + \sum_{j,k=1}^{N+1} R_{jk} x_j y_k$$

and matrices are

$$S_{jk} = \frac{\omega}{\beta} \sum_{n=-\infty}^{\infty} \frac{e^{2\pi i n \beta^{-1}(s_j - s_k)}}{\omega^2 + (2\pi n \beta^{-1})^2} = S_{kj},$$

$$R_{jk} = \frac{4\pi}{\beta^2} \sum_{n=-\infty}^{\infty} \frac{n e^{2\pi i n \beta^{-1}(s_j - s_k)}}{\omega^2 + (2\pi n \beta^{-1})^2} = -R_{kj}.$$

The Gibbs T-product average for an arbitrary measurable functional can be written down as $\langle T(f(\hat{Q}, \hat{P}))\rangle = \int_X f(\xi) d\mu(\xi)$ with the gaussian measure defined on the space X of continuous functions of two variables that satisfy the conditions $x(0) = x(\beta), y(0) = y(\beta)$. The correlation function takes the form

$$M(t,s) = \left[\operatorname{ch}\left(\frac{\beta\omega}{2} - \omega|t-s|\right) + i\epsilon(t-s)\operatorname{sh}\left(\frac{\beta\omega}{2} - \omega|t-s|\right)\right] / \operatorname{sh}\frac{\beta\omega}{2},$$

where

$$\epsilon(x) = \begin{array}{rl} 1, & x > 0; \\ 0, & x = 0; \\ -1, & x < 0. \end{array}$$

The formula of linear substitution of a variable in integral over gaussian measure in this case takes the form

$$\int_X F(\xi) d\mu(\xi) = e^{-\frac{1}{2}(a,a)} \int_X F(\xi + a) e^{-(a,\xi)} d\mu(\xi),$$

where the linear measurable functional is defined as $(a, \xi) = \tilde{a} M \xi$.

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EXCITONS AND POLARONS IN QUANTUM WELLS

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We study properties of polarons and excitons confined to a potential generated in a planar semiconductor heterostructure of the $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ type. In contrast with results of other authors, peaks are found for the exciton energy and the polaron effective mass as functions of the potential width while the polaron energy reveals rather monotonous behavior.

1. GENERAL DISCUSSION

The purpose of this article is to analyze the dependence of the energy of an elementary excitation on the strength of the confinement potential, which exists in a planar semiconductor heterostructure. Due to the fascinating technological progress in the field of man-made structures, it has become possible to fabricate, e.g., quantum wells of a widely varying shape. It is an interesting theoretical task to discuss the excitation spectrum of such semiconductor structures as function of the tunable parameters, such as well width, well height, etc.. Concerning the excitations of interest, we concentrate on particle-phonon systems, the particles being electrons or holes. The simplest example is that of a single polaron, that is an electron, coupled to a certain branch of lattice vibrations. Another example is that of a polaronic exciton, that is an electron-hole pair, coupled to phonons. Whereas the latter one is important to characterize optical properties, the former one has direct implications for the transport behavior of the materials of interest.

We assume that the interface(s)-induced confinement can be mimicked by a simple potential $V_n(z_n)$, n being the particle number; z_n, the corresponding coordinate (the growth direction of the heterostructure will always be assumed as z-direction). Explicit forms of $V_n(z_n)$ may be rectangular wells, parabolas, etc. In addition, we suppose translation invariance to hold within the xy-plane. We remark that effects as surface roughness would destroy this property and could lead to the appearance of new phenomena (e.g., localized states).

In the following equation, we define the class of models under discussion:

$$\begin{aligned} H: &= \frac{1}{2}\sum_{n=1}^{N} \mathbf{p}_n {m_n}^{-1} \mathbf{p}_n + U(\mathbf{r}_1,..,\mathbf{r}_N) + \\ &\quad \sum_{\mathbf{k}} \hbar\,\omega_{\mathbf{k}}\, a^{+}_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{\sqrt{V}} \sum_{n=1}^{N}\sum_{\mathbf{k}} \left(g_{\mathbf{k},\mathbf{n}}\, e^{\,i\,\mathbf{k}\mathbf{r}_\mathbf{n}}\, a_{\mathbf{k}} + h.c. \right) \\ &= : H_{el} + H_{ph} + H_{int}. \end{aligned} \tag{1}$$

The nomenclature is self-explaining. The quantity $U(\mathbf{r_1}, \mathbf{r_2})$ is to contain the confinement potentials as well as the particle interaction:

$$U(\mathbf{r}_1,..,\mathbf{r}_N) := \sum_{n=1}^{N} V_n(z_n) + \frac{1}{2} \sum_{\substack{n,n'=1 \\ n\neq n'}}^{N} V_{n,n'}(\mathbf{r}_n, \mathbf{r}_{n'}), \tag{2}$$

where $V_{n,n'}$ has to be calculated as potential energy of particle n, exposed to the electrostatic potential of particle n'. Because of the boundary conditions, $V_{n,n'}(\mathbf{r}_n, \mathbf{r}_{n'})$ itself is not translation invariant (see, e.g., Ref. 1). The particle-phonon coupling is of Fröhlich type. The most prominent example to be used here is that of a coupling to (LO)-phonons.

The model has two relevant limiting cases, which should be reproduced by any theory. Let the maximum of the well widths be L and the minimum L'. If L' tends to infinity, the confinement is irrelevant and the energy spectrum of H is that of a three-dimensional well-material excitation. If L tends to zero, the (finite height) well is irrelevant, leaving us with the spectrum of a three-dimensional barrier-material excitation. The behaviour for intermediate values of the well widths can qualitatively be discussed as follows. Varying L, L' from sufficiently large values to smaller ones, the binding energy should increase due to the higher Coulomb correlation (for instance, the reader should recall that the energy of the two-dimensional hydrogen ground state is four times larger than that of a three-dimensional one). When L, L' become smaller and smaller, the ground-state wave function will more and more effectively tunnel into the barrier material — the energy approaches the barrier limit.

Thus, we might expect a maximum of the binding energy to appear at intermediate values of L, L'. It was a controversely discussed question whether or not this maximum appears at relevant (that is not too small) values of L. The answer to this question might be not the same for different systems.

2. POLARONS

The physics of polarons, confined to quantum wells, passed a few stages, and it is not possible to present here even a brief list of references. In particu-

lar, it was found that different phonon modes contribute to the polaron binding energy — confined bulk 2 phonons inside the well, interface phonon mode and half-space bulk phonon mode in the barrier. We cite only papers [2, 3] concerning polarons confined to a finite rectangular potential (one layer heterostructure) where contributions of all phonon modes were taken into account. Anyway, there are problems to be addressed while dealing with multilayered heterostructures. Namely, we have to answer the following questions:

1) How to deal with multilayered heterostructures? The total number of phonon modes becomes too large to make numerical calculations even with modern computers. Besides, a multilayered heterostructure can generate a confining potential of rather complicated form, not only the rectangular one.

2) How to deal with mass- and dielectric mismatches in different layers? The polaron effective mass $m(z)$, the electron-phonon coupling constant $\alpha(z)$ and the phonon dispersion law do depend on a layer, that is, on the electron position. To glue solutions in different layers seems to be a cumbersome job.

To tackle these problems we suggest specific approximations, which will briefly be indicated here.

- A multilayered $GaAs/Al_xGa_{1-x}As$ heterostructure is considered as an *effective medium*. Its mean parameters are to be defined by averaging over different layers according to the way they enter the Hamiltonian.
- The bulk phonon mode only inhabits an effective medium with mean characteristics.

We specify the electronic part of the Hamiltonian:

$$H_{el} = H_{el,\parallel} + H_{el,\perp} = \frac{\vec{p}_\parallel^{\,2}}{2m} + \frac{p_z^2}{2m} + V(z), \tag{3}$$

The mean electron band mass m is defined by the equation

$$H_{el,\perp}\psi_1 = E_1\psi_1, \qquad \frac{1}{m} = \int\limits_{-\infty}^{\infty} dz\, \frac{|\psi_1(z)|^2}{m(z)}, \tag{4}$$

where $\psi_1(z), E_1$ are the ground state wave function and the energy for the electron motion in z direction. As ψ_1 and E_1 depend on m, we actually have the system of two equations (4) to calculate the mean band mass m.

The free LO-phonon Hamiltonian reads as follows:

$$H_{ph} = \hbar\omega_{\text{LO}} \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} \ , \qquad \omega_{\text{LO}} = \int\limits_{-\infty}^{\infty} dz\, \omega(z)\, |\psi_1(z)|^2. \tag{5}$$

As m is found already, we define here the mean phonon frequency $\omega_{\rm LO}$. Note that in this paper we are not interested in processes of emission, absorption or scattering of phonons. Instead we concentrate on virtual phonons in a cloud around an electron. Subsequently, the properties of the *effective* phonons do depend on the position of the electron as it follows from Eq. (5).

In the same way we define the effective electron-phonon interaction Hamiltonian in the standard Fröhlich form with the mean Fröhlich coupling constant α:

$$\sqrt{\alpha} = \int\limits_{-\infty}^{\infty} dz\, |\psi_1(z)|^2\, \frac{\omega(z)}{\omega_{\rm LO}} \left(\alpha(z) \sqrt{\frac{m\omega_{\rm LO}}{m(z)\omega(z)}} \right)^{1/2}. \tag{6}$$

Evidently, this model belongs to the class defined in Eq. (1). As examples we studied 1) a one-layer heterostructure described by a rectangular confining potential

$$V(z) = \begin{cases} 0, & |z| \le L/2 \\ V_0, & |z| > L/2 \end{cases} \tag{7}$$

(the z-dependence of the masses and dielectric parameters is completely analogous) and 2) a multilayered heterostructure corresponding to the Rosen–Morse potential

$$V(z) \quad = \quad V_0 \tanh^2 \left(\frac{z}{L_{RM}} \right). \tag{8}$$

We use perturbation theory in powers of α for both potentials, but in the first case we perform the summation over all virtual states while in the case of the Rosen–Morse potential the Green function (see [4, 5]) can be used. To compare results for the Rosen–Morse and the rectangular potentials, an effective width L of the Rosen–Morse potential has to be found. We define it as the width of a rectangular potential of the same height V_0 with the same ground-state energy. The dependence $L(L_{RM})$ can then be calculated. The parametrization for experimental data concerning $GaAs/Al_xGa_{1-x}As$ heterostructure is based on the results reported in Ref. 6 with some modifications, which are discussed in our paper [7]. Actually we use the dependence of the parameters on the Al mole fraction x which depends in turn on the coordinate z via the relation $V(z) = 600 \cdot (1.155x + 0.37x^2)$ meV. The confining potential $V(z)$ being given, we know the dependence $x(z)$ and, subsequently, the values of the parameters α, m, ω at each point of the heterostructure which are averaged then following Eqs. (4), (5), and (6).

The polaron energy and effective mass are calculated for $x = 0.3$. Peaks are found for the effective mass at some potential widths, while the energy

demonstrates rather a smooth behavior between the correct 3D-limits as is seen in Fig. 1. As to the Rosen–Morse potential, the results are presented in Fig. 2 together with those for the rectangular potential of the corresponding effective width. One can see an excellent coincidence of the results obtained within the different techniques; clearly, this fact increases their reliability. A comparison is also made with the results of the papers [2, 3], and the details are discussed in our paper [7].

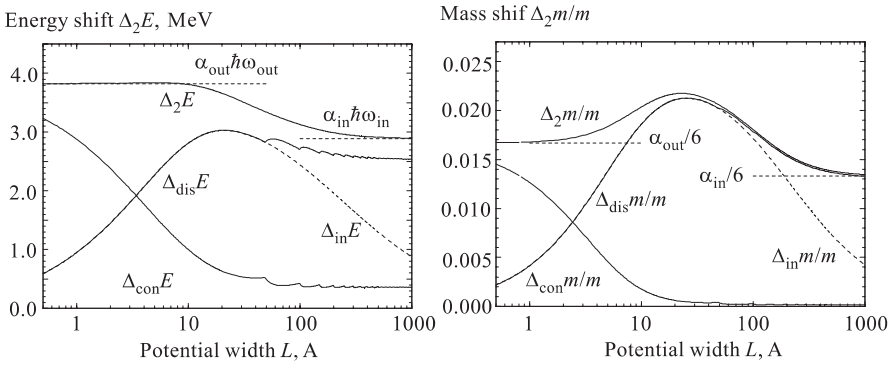

Fig. 1. The polaron binding energy and the effective mass in the rectangular potential. Contributions of the discrete $\Delta_{\rm dis}E$ $(\Delta_{\rm dis}m/m)$ and continuous $\Delta_{\rm con}E$ $(\Delta_{\rm con}m/m)$ spectrum are shown as well as the so-called leading term approximation $\Delta_{lt}E$ $(\Delta_{lt}m/m)$ when only the ground state is taken into account as an intermediate virtual state (dashed line)

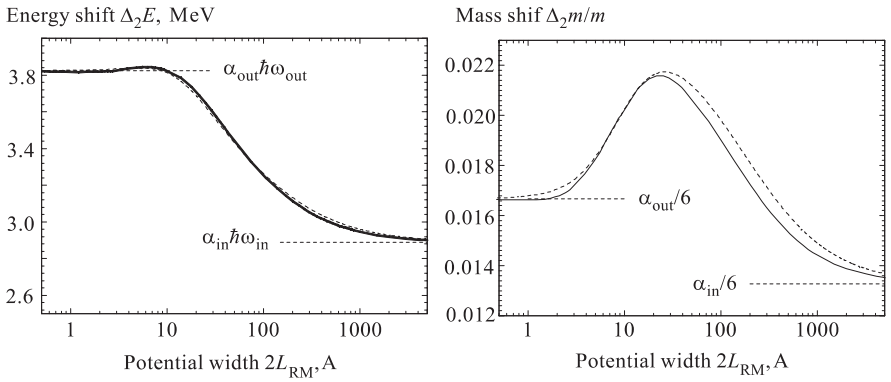

Fig. 2. Our results for the Rosen–Morse potential in comparison with these for the rectangular potential (dashed line) of the same effective width $L(L_{\rm RM})$

3. EXCITONS

Sampling the previous literature, most work has been done on rectangular quantum wells with confinement potentials of type (7). The electron-hole potential can be calculated as indicated above and was given, e.g., in Ref. 1.

To treat eigenvalue problems as the present one, we use tractable decompositions of the Hamiltonian to generate lower bounds for the ground-state energy. The basic idea is as follows: Assume we study the Hamiltonian $H = p_z^2/2m + V_1(z) + V_2(z)$ to find its ground-state energy E. Then we use the decomposition

$$H_1 = x\frac{p_z^2}{2m} + V_1(z), \quad H_2 = (1-x)\frac{p_z^2}{2m} + V_2(z), \qquad 0 \le x \le 1. \tag{9}$$

If $E_1(x), E_2(x)$ are the corresponding ground-state energies of H_1, H_2, then a lower bound for E is: $E \ge \max_x(E_1(x) + E_2(x))$.

Upper bounds are produced by variational methods: The trial wave-function used in our calculations had the form:

$$\Psi(\vec{r}_\perp, z_1, z_2) = \Phi_1(z_1)\Phi_2(z_2)e^{-a\sqrt{r_\perp^2 + b(z_1-z_2)^2}}, \tag{10}$$

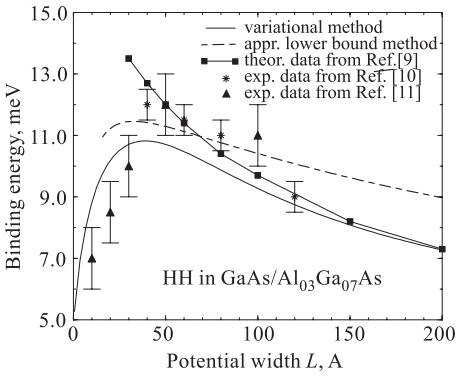

Fig. 3. Comparison of results for the binding energy of an exciton in a rectangular quantum well as function of the well width

where $\Phi_i(z_i)$ are the ground-state eigenfunctions of the free electron ($i = 1$) or the hole ($i = 2$) in the confining potentials of the type (7). Evidently, the variational parameters a, b can be used to fit 3D and 2D limiting cases. If the masses can be assumed as constant over the heterostructure, these methods can profitably be combined with functional-integral techniques. Figure 3 shows our result [8] for $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ in comparison with experimental [10, 11] and previous theoretical results [9]. Clearly, the maximum appears at a relevant width.

A second class of confinement potentials is of parabolic type, that is,

$$V_i(z) = \frac{m_i R_\infty^2 \lambda_i^2}{2\hbar^2} z_i^2, \tag{11}$$

where λ_i denotes the dimensionless confinement strength, R_∞ is the Rydberg unit, which was extracted for reasons of convenience. To study the confinement-induced effects on the spectrum as accurately as possible, we disregarded any parameter mismatch. The quantity of interest is the diagonal element of the reduced density operator, namely

$$P_\beta(\mathbf{C}) := < \mathbf{C}|tr_{Ph}e^{-\beta H}|\mathbf{C} > . \tag{12}$$

In this formula $\mathbf{C}$ is an abbreviation for an arbitrary (but fixed) set of the position coordinates of the particles involved. The right-hand side of Eq. (12) can be represented as a functional integral

$$P_\beta(\mathbf{C}) = Z_{Ph} \int \delta^6 R \; e^{-S[\mathbf{R}]}. \tag{13}$$

In Eq. (13) Z_{Ph} is the free-phonon partition function, and S reads as follows:

$$S[\mathbf{R}] := \int_0^\beta d\tau \left(\sum_{n=1}^{2} \frac{m_n}{2} \dot{\mathbf{R}}_n^2(\tau) + U(\mathbf{R}_1(\tau), \mathbf{R}_2(\tau)) \right)$$

$$- \sum_{n,n'=1}^{2} \sum_{\mathbf{k}} \frac{g_{\mathbf{k},n} g_{\mathbf{k},n'}}{V} \int_0^\beta \int_0^\beta d\tau \, d\tau' \, G(\tau - \tau') \, e^{i\mathbf{k}[\mathbf{R}_n(\tau) - \mathbf{R}_{n'}(\tau')]}. \tag{14}$$

Within the functional integral (13), $\int \delta^6 R....$ is to indicate integration over all real, 6-dimensional paths $\mathbf{R}(\tau)$, which start and end at the point $\mathbf{C}$. The kernel function $G(\tau - \tau')$ is defined as

$$G(\tau) := \frac{e^{\hbar\omega(\beta - |\tau|)} + e^{\hbar\omega|\tau|}}{2[e^{\beta\hbar\omega} - 1]}. \tag{15}$$

It is well known that functional integrals of type (13) with an action (14) cannot be evaluated in analytical form. Starting from the exact expression, we use variational procedures as in Feynman's famous paper on polarons to find upper bounds on the ground-state energy. The necessary input is a trial action, which is accessible to a numerical treatment.

The trial companions of the exact action (14) were combinations of oscillator trial actions for the centre-of-mass and the z-coordinate and three-dimensional (two-dimensional) Coulomb potentials for the three-dimensional (two-dimensional in-plane) relative coordinates. The corresponding results (see Ref. 12) can be found in the following figures and are denoted as quasi three-dimensional (Q3D) and quasi two-dimensional (Q2D or Q2Dalt) ansatz. In Fig. 4 we neglect any phonon influence to demonstrate the smooth interpolation of the limiting values

$1R_\infty$ and $4R_\infty$ of the binding energy (actually we plotted there the ground-state energy with the continuum edge being subtracted, that is, the quantity $-E_B$). Figure 5 shows results for the general case; we present data for the ground-state energy as well as the continuum edge, which is the reference for the binding energy and has to be calculated separately.

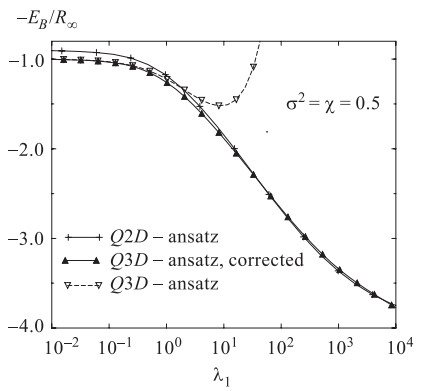

Fig. 4. Binding energy of an exciton in a parabolic quantum well as function of the electron confinement strength λ_1. The comparison is made for different approaches described in Ref. 12. The parameters $\sigma^2 = m_1/m_2$ and $\chi = \lambda_2/\lambda_1$ are fixed as indicated

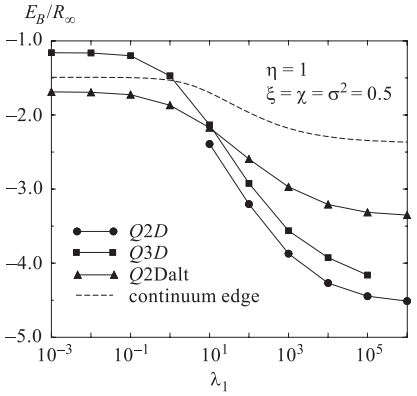

Fig. 5. Ground-state energy of an exciton-phonon system in a parabolic quantum well as function of the confinement electron strength λ_1. The remaining parameters $\eta = \sqrt{R_\infty/\hbar\omega}$ and $\xi = 1 - \varepsilon_\infty/\varepsilon_0$ are fixed as indicated. In addition, an upper bound for the energy of the continuum edge is shown

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«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
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GENERALIZATION OF THE PEIERLS–BOGOLIUBOV INEQUALITY BY MEANS OF A QUANTUM-MECHANICAL VARIATIONAL PRINCIPLE

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The Peierls–Bogoliubov inequality was generalized and a set of inequalities was derived instead, so that every subsequent inequality in this set approximates the quantity in question with better precision than the preceding one. These inequalities lead to a sequence of improving upper bounds to the free energy of a quantum system if this system allows representation in terms of coherent states.

1. INTRODUCTION

It is well known that the following inequality

$$\langle\Psi|e^{-t\hat{H}}|\Psi\rangle \geq e^{-t\langle\Psi|\hat{H}|\Psi\rangle} \tag{1}$$

holds for any normalized quantum state $|\Psi\rangle$, self-adjoint Hamiltonian of a quantum system $\hat{H}$, and nonnegative parameter t. As a rule, this inequality is referred to in the theoretical physics as the Peierls–Bogoliubov inequality. It has been widely used as an intermediate step in numerous schemes of mathematical reasoning and in proofs of various theorems. For instance, it plays an important role in the proof of the left-hand side of the Lieb–Berezin inequality [1–3],

$$\int \exp\left(-tQ(\alpha,\bar{\alpha})\right) d\mu(\alpha) \leq \mathrm{Sp}\left(\exp(-t\hat{H})\right) \leq \int \exp\left(-tP(\alpha,\bar{\alpha})\right) d\mu(\alpha) \tag{2}$$

which, in its turn, provides two-side bounds to the free energy of a quantum system in case the Hamiltonian of the system allows representation in terms of the set of coherent states $|\alpha\rangle$. Here $Q(\alpha,\bar{\alpha})$ and $P(\alpha,\bar{\alpha})$ are the so-called Wick and anti-Wick symbols of the Hamiltonian $\hat{H}$, such that

$$\hat{H}=\int P(\alpha,\bar{\alpha})\,|\alpha\rangle\langle\alpha|\,d\mu(\alpha), \quad Q(\alpha,\bar{\alpha})=\langle\alpha|\hat{H}|\alpha\rangle=\int e^{-|\alpha-\beta|^2}P(\beta,\bar{\beta})d\mu(\beta),$$

$$\langle\alpha|\alpha\rangle=1, \langle\alpha|\beta\rangle=\exp\left(-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2+\bar{\alpha}\beta\right),$$

$$d\mu(\alpha) = \frac{1}{\pi} d\mathrm{Re}(\alpha) d\mathrm{Im}(\alpha),$$

and the integration in (2) is carried out over the whole complex plane α. The left-hand side of the inequality (2) is a direct consequence of the Peierls–Bogoliubov inequality:

$$\mathrm{Sp}\left(e^{-t\hat{H}}\right) = \int \langle\alpha|e^{-t\hat{H}}|\alpha\rangle d\mu(\alpha) \geq \int e^{-t\langle\alpha|\hat{H}|\alpha\rangle} d\mu(\alpha) = \int e^{-tQ(\alpha,\bar{\alpha})} d\mu(\alpha).$$

At the same time the inequality (1) is of considerable value itself because it can be used to derive an upper bound to the ground state energy of a quantum system:

$$E_{\mathrm{g}} \leq -\lim_{t\to+\infty} \frac{1}{t} \ln\langle\Psi|e^{-t\hat{H}}|\Psi\rangle \leq \langle\Psi|\hat{H}|\Psi\rangle. \tag{3}$$

Thus it is worthy to find a regular algorithm allowing to strengthen the inequality (1) so as to improve existing upper bounds obtained by the conventional variational method.

2. VARIATIONAL SCHEME

Assume that the Hamiltonian $\hat{H}$ is of the form

$$\hat{H} = \sum_{n=1}^{\infty} E_n |E_n\rangle\langle E_n| + \int_{E_1'}^{E_{\max}} dE E|E\rangle\langle E|,$$

where $E_1' \leq E_{\max} \leq +\infty$ and $\langle E|E_n\rangle = 0$. Energy levels may be degenerate in general case. Consider the Laplace transformation

$$f(s) = \int_0^{+\infty} dt e^{-st} \langle\Psi|e^{-t\hat{H}}|\Psi\rangle = \left\langle \Psi \left| \frac{1}{s+\hat{H}} \right| \Psi \right\rangle, \tag{4}$$

where $\mathrm{Re}(s) > -\min(E_1, E_1')$. An identity transformation made of two subsequent steps

$$\left\langle \Psi \left| \frac{1}{s+\hat{H}} \right| \Psi \right\rangle = \frac{1}{s+a_1} - \left\langle \Psi \left| \frac{\hat{H}-a_1}{(\hat{H}+s)(s+a_1)} \right| \Psi \right\rangle$$

and

$$\left\langle \Psi \left| \frac{1}{s+\hat{H}} \right| \Psi \right\rangle = \frac{1}{s+a_1} - \left\langle \Psi \left| \left[\frac{\hat{H}-a_1}{(s+a_1)^2} + \frac{(\hat{H}-a_1)^2}{(\hat{H}+s)(s+a_1)^2} \right] \right| \Psi \right\rangle \tag{5}$$

can be applied n times to the right-hand side of Eq.(4) leading to the identity

$$f(s) \equiv W_n(s, a_1, ..., a_n) + R_n(s, a_1, ..., a_n),$$

$$W_n(s, a_1, ..., a_n) = \left\langle \Psi \left| \sum_{k=1}^{n} \left[\frac{1}{s + a_k} - \frac{\hat{H} - a_k}{(s + a_k)^2} \right] \prod_{j=1}^{k-1} \frac{(\hat{H} - a_j)^2}{(s + a_j)^2} \right| \Psi \right\rangle,$$

$$R_n(s, a_1, ..., a_n) = \left\langle \Psi \left| \frac{1}{s + \hat{H}} \prod_{j=1}^{n} \frac{(\hat{H} - a_j)^2}{(s + a_j)^2} \right| \Psi \right\rangle,$$

where $a_1, ..., a_n$ is a set of arbitrary variational parameters chosen in such a way that both, W_n and R_n exist. To my knowledge, similar identity transformation was introduced firstly in [4]. The inverse Laplace transformation $\mathcal{L}^{-1} f(s)$ results in the identity

$$F(t) = \langle \Psi | e^{-t\hat{H}} | \Psi \rangle \equiv \rho_n(t, a_1, ..., a_n) + \Omega_n(t, a_1, ..., a_n), \tag{6}$$

where

$$\rho_n(t, a_1, ..., a_n) = \mathcal{L}^{-1} R_n(t, a_1, ..., a_n),\ \Omega_n(t, a_1, ..., a_n) = \mathcal{L}^{-1} W_n(t, a_1, ..., a_n).$$

In case of real parameters $a_1, ..., a_n$ the following statements regarding the properties of $\rho_n(t, a_1, ..., a_n)$ can be proved [5].

(1.) $\rho_n(t, a_1, ..., a_n) \geq 0$.

(2.) $\rho_n(t, a_1, ..., a_n)$ always has $n!$ absolute minima as a function of real parameters $a_1, ..., a_n$ and the location of these minima does not depend on t. All these minima are equivalent up to the permutation of parameters.

(3.) The absolute minimum of $\rho_n(t, a_1, ..., a_n)$ is provided by the solution to a system of equations

$$\frac{\partial}{\partial a_k} \rho_n(t, a_1, ..., a_n) = 0$$

which can be effectively reduced to a polynomial equation of the nth order

$$P_n(x) = 0, \qquad \text{where} \qquad P_n(x) = \sum_{i=0}^{n} A_i x^{n-i}. \tag{7}$$

Here, $A_0 \equiv 1$ and the other n coefficients are given by the solution to a system of n linear equations

$$\mathcal{M}\vec{A} + \vec{Y} = 0,$$

where $Y_i = M_{2n-i}$, $\mathcal{M}_{ij} = M_{2n-(i+j)}$, $i, j = 1, 2, ..., n$, and $M_n = \langle \Psi | (\hat{H})^n | \Psi \rangle$ are the moments of the Hamiltonian $\hat{H}$. Roots $(a_1^{(n)}, a_2^{(n)}, ..., a_n^{(n)})$ of the polynomial $P_n(x)$ provide the absolute minimum for $\rho_n(t, a_1, ..., a_n)$.

(4.) All roots $(a_1^{(n)}, a_2^{(n)}, ..., a_n^{(n)})$ are real, mutually disjoint, i.e., $a_i^{(n)} \neq a_j^{(n)}$ if $i \neq j$, $(i, j = 1, 2, ..., n)$, and independent of the parameter t.

(5.) For any order n of approximation an inequality holds:

$$\rho_{n+1}(t, a_1^{(n+1)}, ..., a_{n+1}^{(n+1)}) \leq \rho_n(t, a_1^{(n)}, ..., a_n^{(n)}).$$

Moreover, if to take the statement (1.) into account, the limit

$$\lim_{n\to\infty} \rho_n(t, a_1^{(n)}, ..., a_n^{(n)}) = \rho(t)$$

exists for any $t \geq 0$.

(6.) If $\hat{H}$ is a bounded operator or if it possesses a discrete spectrum only, or the state $|\Psi\rangle$ can be expanded in the eigenstates corresponding to the discrete spectrum of $\hat{H}$ exclusively, then $\rho(t) = 0$ for any $t \geq 0$. The same strict equality also holds if $|\Psi\rangle$ can be expanded in a set of eigenstates with bounded energies.

(7.) The following sequence of the upper bounds to the ground state energy of the Hamiltonian $\hat{H}$ takes place

$$E_g \leq \min(a_1^{(n+1)}, ..., a_{n+1}^{(n+1)}) \leq \min(a_1^{(n)}, ..., a_n^{(n)}) \leq a_1^{(1)}, \tag{8}$$

and the limit exists $\mathcal{E}_0 = \lim_{n\to\infty} \min(a_1^{(n)}, ..., a_n^{(n)})$, so that if the function $|\Psi\rangle$ is expanded in the eigenstates of $\hat{H}$ as

$$|\Psi\rangle = \sum_{i=1}^{\infty} C_i |\tilde{E}_i\rangle + \int_{\tilde{E}_1'}^{+\infty} dE C(E) |E\rangle,$$

then

$$E_g \leq \min(\tilde{E}_1, \tilde{E}_1') \leq \mathcal{E}_0,$$

and $\mathcal{E}_0 = \min(\tilde{E}_1, \tilde{E}_1')$ in case of the bounded $\hat{H}$. The same strict equality also holds if $|\Psi\rangle$ can be expanded in a set of eigenstates with bounded energies.

In case when $|\Psi\rangle$ is only expanded in a set of eigenstates belonging to the discrete spectrum of $\hat{H}$, i.e.,

$$|\Psi\rangle = \sum_{i-1}^{\infty} C_i |E_i\rangle, \tag{9}$$

then the set of roots $(a_1^{(n)}, ..., a_n^{(n)})$ converges to the set of eigenvalues $\{E_i\}$ which are present in the expansion (9):

$$(a_1^{(n)}, ..., a_n^{(n)}) \underset{n\to\infty}{\longrightarrow} \{E_i\}.$$

The same situation takes place in case of $\hat{H}$ possessing discrete eigenvalues only. In case when the expansion (9) includes only the finite number N of different eigenvalues E_i, the proposed approximation algorithm stops at the order $n = N$. At this point $a_1^{(N)} = E_1,\ a_2^{(N)} = E_2,\ ...,\ a_N^{(N)} = E_N$ and the inequality (10) becomes an equality. Of course, it is formally possible to apply the identity transformation (5) several times more, thus introducing p additional parameters $a_{N+1},\ a_{N+2}, ..., a_{N+p}$. In this case the function $\rho(t, a_1, a_2,...,\ a_N,\ a_{N+1},...,\ a_{N+p})$, which is symmetric in its arguments $\{a_i\}$ by construction, has infinitely degenerate equivalent absolute minima at points $(E_1, ...,\ E_N,\ a_{N+1},...,\ a_{N+p})$ and the corresponding points obtained by the permutation of arguments, where this function is equal to zero. In effect, these minima are provided by only N out of total $N + p$ parameters $\{a_i\}$, those which are equal to the eigenvalues $E_1, ..., E_N$. Only these parameters will make sense and enter the right-hand side of the inequality (10) transforming it into equality. The values of the remainder p parameters are totally irrelevant and drop out of the final results automatically.

3. GENERALIZED PEIERLS–BOGOLIUBOV INEQUALITY

As a consequence of statements (1.)–(5.), the following inequality holds

$$\langle\Psi|e^{-t\hat{H}}|\Psi\rangle \geq \Omega_n(t, a_1^{(n)}, ..., a_n^{(n)}) \geq e^{-t\langle\Psi|\hat{H}|\Psi\rangle}, \tag{10}$$

and the middle part of this inequality can be calculated explicitly at the point $(a_1^{(n)}, ..., a_n^{(n)})$:

$$\Omega\left(t, a_1^{(n)}, ..., a_n^{(n)}\right) = \sum_{k=1}^{n}\langle\Psi|\left[\prod_{\substack{j=1\\ j\neq k}}^{n}\frac{\left(\hat{H} - a_j^{(n)}\right)^2}{\left(a_j^{(n)} - a_k^{(n)}\right)^2}\right]|\Psi\rangle e^{-a_k^{(n)}t}.$$

The case $n = 1$ with the only variational parameter $a_1^{(1)} = \langle\Psi|\hat{H}|\Psi\rangle$ corresponds to the original Peierls–Bogoliubov inequality (1) which can be written in the form

$$\langle\Psi|e^{-t\hat{H}}|\Psi\rangle \geq \Omega_1(t, a_1^{(1)}) = e^{-ta_1^{(1)}}. \tag{11}$$

It follows from Eqs. (6), (11) and the statements (1.) and (5.) that

$$\Omega_1(0, a_1^{(1)}) = \Omega_1(0, a_1^{(2)}, a_2^{(2)}) = ... = \Omega\left(0, a_1^{(n)}, ..., a_n^{(n)}\right) = 1,$$

$$\rho_1(0, a_1^{(1)}) = \rho_1(0, a_1^{(2)}, a_2^{(2)}) = ... = \rho\left(0, a_1^{(n)}, ..., a_n^{(n)}\right) = 0.$$

Therefore, good approximation is guaranteed for small t in all orders n.

4. GENERALIZED LIEB–BEREZIN INEQUALITY

The Lieb–Berezin inequality can also be generalized straightforward if one considers the coherent states $|\alpha\rangle$ in Eq.(2) as the $|\Psi\rangle$ state and is able to calculate explicitly the corresponding moments of $\hat{H}$ as functions of complex variables $\alpha, \bar{\alpha}$. This results in the inequality

$$\mathrm{Sp}\left(e^{-t\hat{H}}\right) \geq$$

$$\geq \int d\mu(\alpha) \sum_{k=1}^{n} \langle\alpha| \left[\prod_{\substack{j=1 \\ j\neq k}}^{n} \frac{\left(\hat{H} - a_j^{(n)}(\alpha,\bar{\alpha})\right)^2}{\left(a_j^{(n)}(\alpha,\bar{\alpha}) - a_k^{(n)}(\alpha,\bar{\alpha})\right)^2} \right] |\alpha\rangle e^{-a_k^{(n)}(\alpha,\bar{\alpha})t} \geq$$

$$\geq \int e^{-tQ(\alpha,\bar{\alpha})} d\mu(\alpha)$$

which can be constructed explicitly up to $n = 4$. For $n > 4$ the polynomial equation (7) cannot be solved analytically in general case.

5. CONCLUSION

It follows from Eqs.(3), (8), (11) that nearly any upper bound to the ground state energy obtained by the conventional variational principle can be improved by means of the proposed method. This can be done in two steps. First of all, one should construct a trial state $|\Phi(\{\xi\})\rangle$ as a function of variational parameters $\{\xi\}$ and choose these parameters to minimize the average $\langle\Phi(\{\xi\})|\hat{H}|\Phi(\{\xi\})\rangle$ as usual. In terms of the outlined above scheme, this step provides one with the first-order bound $a_1^{(1)}$. Then the subsequent better bounds (8) can be derived as it was shown if one takes the state $|\Phi(\{\xi\})\rangle$ with the optimal set of parameters $\{\xi\}$, defined at the first step, as the $|\Psi\rangle$ state throughout all computations.

What is more, the roots $(a_1^{(n)}, ..., a_n^{(n)})$ of Eq.(7) provide not only the upper bound to the ground state energy but may also be used as estimations for the excited energy levels at least in the case of Hamiltonians with purely discrete spectrum.

It is worth noticing in conclusion that the proposed method of approximation has nothing to do with any kind of perturbation approach because the whole set of roots $(a_1^{(n)}, ..., a_n^{(n)})$ of Eq. (7) is to be recalculated once again at any subsequent order of approximation n.

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COMBINED BCS AND VAN HOVE SCENARIOS: A SOLVABLE THERMODYNAMICS IN HALF-FILLED SYMMETRIC BANDS

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The subcritical and low-temperature thermodynamics is obtained for half-filled symmetric bands with the logarithmic peak of DOS in the centre. The ratio of the zero temperature order parameter to the critical temperature coincides with the BCS value for S-pairing but is slightly different for D-pairing. Moreover, the relative jumps of the critical specific heat coincide with conventional BCS results for S- and D-pairing as well.

We are going to consider the S-, [1] and D-paired electrons in the band with the following DOS, per unit volume and spin

$$N(\varepsilon) = N(0)[a - \ln|\varepsilon|], \quad |\varepsilon| \leq 1, \;\; a \geq 0, \tag{1}$$

with ε being the particle energy in the units of the half-width of the band. Because of the bilateral symmetry, the chemical potential is equal to zero and temperature-independent in the symmetric bands at their half-filling, [2], for both normal and BCS-superconducting systems. For an appropriate choice of $N(0)$ and a, the DOS (1) is a quite good approximation to the real DOS in the square lattice when the tight binding overlap integrals are restricted to the nearest neighbours [3]. Similar DOS has been used in the thermodynamic calculations in HTSC [4–6], for S-pairing in the BCS approach [4,5] and for S- and D-pairing in the charge transfer model [6].

In the papers [4,5] the main topic was restricted to the calculation of the ratio $\Delta(0)/T_c$ and to the penetration depth [5]. Note that this problem has recently attracted a lot of attention in the context of the planar electron motion in HTSC, c.f. the review article [7].

The BCS-like gap equation [1], for our system reads

$$\frac{1}{\kappa} = \int\limits_0^1 d\varepsilon(a - \ln\varepsilon) \left\langle d^2(\hat{\mathbf{p}}) \frac{\tanh(E_\varepsilon/2T)}{E_\varepsilon} \right\rangle_{\mathbf{p}}, \tag{2}$$

where $E_\varepsilon^2 = \varepsilon^2 + d^2(\hat{\mathbf{p}})\Delta^2$, Δ is the order parameter, $\kappa \equiv \lambda N(0)$ with λ being S or D the coupling constant. The function $d^2(\hat{\mathbf{p}})$ is equal to 1 for S-pairing and to $\sqrt{2}(\hat{p}_x^2 - \hat{p}_y^2)$, $\hat{\mathbf{p}} = \mathbf{p}/p$, for D-pairing in the plane. The bracket $\langle \dots \rangle_{\mathbf{p}}$ denotes the angular average. Herein we consider only the weak coupling, $\kappa \ll 1$.

Calculating the integral (2) in the limiting cases $\Delta = 0$ or $T = 0$, with the accuracy up to the big logarithms $|\ln T_c|$ or $|\ln \Delta(0)|$, we find

$$T_c = \frac{2}{\pi} \exp(a + c - 1/x)\,[1 + O(x^2)], \quad (S, D), \tag{3}$$

$$\Delta(0) = 2 \exp(a - 1/x)\,[1 + O(x^2)], \quad (S),$$

$$\Delta(0) = \frac{1}{\sqrt{2}} \exp(a + 1 - 1/x)\,[1 + O(x^2)], \quad (D), \tag{4}$$

where $x \equiv \sqrt{\kappa/2}$ and c is the Euler constant. To accomplish the integral (2) at T_c we need only the integration by parts, whereas at $T = 0$, the integration by parts after the substitution $\varepsilon = \Delta |d(\hat{\mathbf{p}})| \mathrm{sh} u$. The angular integrals for D-pairing are well known. As we see, the ratio $\Delta_s(0)/T_c$ attains its BCS value, [1,4,5]. On the other hand, the ratio $\Delta_D(0)/T_c$ is the product of the BCS value and $e/2\sqrt{2} \approx 0.961$. It is note worthy that this factor for D-pairing at energy-independent DOS, i.e., D-superconductors of the BCS type is $\sqrt{2/e} \approx 0.858$.

In all further calculations, we will apply the conventional methods of the theory, cf., e.g., [8,9], substituting the DOS (1) into the appropriate integrals determining thermodynamic functions. Let us discuss the subcritical properties first. For the order parameter we have

$$\Delta(T) = \Delta_{\mathrm{BCS}}(T)(1 - 0.121x) + O(\tau^{3/2}), \quad (S),$$

$$\Delta(T) = \sqrt{\frac{2}{3}} \Delta_{\mathrm{BCS}}(T)(1 - 0.121x) + O(\tau^{3/2}), \quad (D), \tag{5}$$

where $\tau \equiv 1 - T/T_c$. The sub or supercritical specific heat, per unit volume, is given by

$$C = 2\pi^2 N(0) \left\{ \left[\frac{4T_c}{7\zeta(3)x}(1 + O(\tau)) + O(1) \right] \Theta(\tau) - \frac{1}{3} T(\ln T + O(1)) \right\}, \tag{6}$$

for the S-pairing, where Θ is the Heaviside step function. For the D-pairing, the term proportional to Θ should be multiplied by $4/9$. Hence, the critical jump of the specific heat in the main term coincides with the BCS value divided by x or $9/4\,x$, for S or D pairing, respectively. On the other hand, the relative jump coincides with the BCS results because of the term $O(T \ln T)$ for S pairing and with $4/9$ of the BCS value for D pairing.

Let us pass to the compressibility, $(\partial\varrho/\partial\mu)_{V,T}\varrho^{-2}$, where ϱ is the density of the system. We have the general formula, valid for half-filled symmetric bands

$$\left(\frac{\partial\varrho}{\partial\mu}\right)_{V,T} = 2N(0)\left\langle \frac{a}{E_1} + \int\limits_0^1 d\varepsilon \frac{\tanh(E_\xi/2T)}{E_\varepsilon}\right\rangle_{\mathbf{p}}. \tag{7}$$

For the normal system, from (7) we get

$$\left(\frac{\partial\varrho}{\partial\mu}\right)_{V,T} = 2N(0)[a + c + \ln(2/\pi T)], \tag{8}$$

and the compressibility is logarithmically divergent if $T \to 0$. Note that in the normal systems, the spin susceptibility χ equals $\mu_B^2(\partial\varrho/\partial\mu)_{V,T}$, with μ_B being Bohr's magneton. For S and D paired systems we have

$$\left(\frac{\partial\varrho}{\partial\mu}\right)_{V,T} = 2N(0)\left[\frac{1}{x} + \tau - \tau\left(1 + \frac{4\pi^2T_c^2}{7\zeta(3)}\right)\Theta(\tau)\right], \tag{9}$$

with the accuracy $O(\tau^2)$. Note that the difference between S and D paired systems is of the same order. Let us add that the difference between the normal and superconducting phases is equal to the term proportional to Θ. The spin susceptibility is equal to, cf. [10]

$$\begin{aligned} \chi &= \frac{2}{x}\mu_B^2 N(0)[1 - 2\tau + O(\tau x)], \quad (S), \\ \chi &= \frac{2}{x}\mu_B^2 N(0)\left[1 - \frac{4}{3}\tau + O(\tau x)\right], \quad (D). \end{aligned} \tag{10}$$

Note that the simplicity of the coefficients at τ in Eqs. (10) are the result of analytic calculation of some integral not appearing in usual sources [11].

Considering low-temperature properties, let us start from the energy difference between S or D and the normal system. Almost repeating the calculations of Ref. 1 (cf. also the comments after the formula (4)) we find

$$\frac{1}{V}(E_{\sup} - E_n) = -\frac{1}{2}N(0)\Delta^2(0)\begin{cases} 1/x + 1/2, & (S), \\ 1/x + 1 - 3/2\,\ln 2, & (D). \end{cases} \tag{11}$$

For the low-temperature order parameter we find

$$\frac{\Delta(T)}{\Delta(0)} = 1 - \begin{cases} (\pi T/\Delta)^{1/2}\ \exp(-\Delta/T)\,(1 - x\ln T + O(x)), & (S), \\ \sqrt{2}\,x\,(\ln T + O(1))(T/\Delta)^3 \sum\limits_{n=1}^{\infty}(-1)^n n^{-3}, & (D). \end{cases} \tag{12}$$

Note that $\sqrt{2}\sum\limits_{n=1}^{\infty}(-1)^n n^{-3} \approx -1.2750$. The specific heat, per unit volume, is given by

$$C = N(0)T \begin{cases} (2\pi\Delta^5/T^5)^{1/2}\ \exp(-\Delta/T)\ (1/x - \ln T + O(1)), & (S), \\ 12\sqrt{2}(T/\Delta)(\ln T + O(1))\ \sum\limits_{n=1}^{\infty}(-1)^n\, n^{-3}, & (D). \end{cases} \tag{13}$$

Determining the compressibility, one can write

$$\left(\frac{\partial \varrho}{\partial \mu}\right)_{V,T} = 2N(0)\left(\frac{1}{x} - \frac{\Delta(T)-\Delta(0)}{\Delta(0)}\right) + 2N(0)\begin{cases} 0, & (S), \\ 1 - 1/2\ \ln 2, & (D). \end{cases} \tag{14}$$

As we see, the infinite limit value of $(\partial\varrho/\partial\mu)_{V,T}$ in the normal state is replaced here by the large value $2N(0)/x + O(1)$, as a result of a quasiparticle distribution functions smeared out in the superconducting state. For the spin susceptibility we have

$$\chi = \mu_B^2 N(0) \begin{cases} (2\pi\Delta/T)^{1/2}\ \exp(-\Delta/T)\ (1/x + a + c - \ln T + O(x)), & (S), \\ -2\sqrt{2}\ \ln 2\ (T/\Delta)\ (\ln T + O(1)), & (D). \end{cases} \tag{15}$$

It is interesting to note that the temperature derivative of χ is logarithmically divergent for the D-pairing.

In calculations of subcritical thermodynamic functions we applied their series expansions with respect to Δ^2 and used the typical integral of the BCS theory [1,8,9]. In the low-temperature limit, the asymptotic form of the integral was obtained, according to the ideas of Ref. 12. For D-pairing, it was done in a more sophisticated way. The validity of these results for this model is firm through the general theorem proved by Bogoliubov [13].

Note that for the chemical potential, μ, such that $0 < |\mu| \ll 1$, even for the normal systems we have two low-temperature regimes, $|\mu| \ll T \ll 1$ and $T \ll |\mu| \ll 1$. For the superconductivity systems we have 3! regimes obtained by the permutations of $\Delta(T)$, $|\mu|$ and T. Moreover, because the particle-hole symmetry is broken and, hence, $\mu_s - \mu_n = O(\Delta^2)$ we deal with the first-order phase transition, because the subcritical $\Omega_s - \Omega_n$ is $O(\Delta^4)$ and the character of Δ still remains unchanged [2].

Note that treating our system as a gas we find that the relative jump of the critical specific heat is equal to

$$1.43\ \varrho^2/p\ \left(\frac{\partial \varrho}{\partial \mu}\right)\Big|_{T_c} = 1.43\ x\ \frac{(a+1)^2}{(a+\frac{3}{4})} + O(x^2(1+a^2)), \tag{16}$$

for S-pairing and $\frac{2}{3}$ of this value for D-pairing.

The details of calculations and some formulae calculated to higher orders will be published elsewhere. In addition, the normal system will be considered also at filling close to the particle-hole symmetric case.

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2000, ТОМ 31, ВЫП. 7Б

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NOISE INDUCED PHASE TRANSITIONS IN SPATIALLY EXTENDED SYSTEMS

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We consider systems of spatially distributed and harmonically coupled nonlinear constituents driven by a Gaussian white noise. In contrast to the single constituent one finds noise-induced nonequilibrium *phase transitions* connected with a breaking of ergodicity in the coupled infinite array depending on the control parameter and the strength of the noise and the spatial coupling. We compare the results for global coupling with those for nearest neighbor coupling on cubic lattices. The globally coupled case allows for analytical results and can be considered as a mean-field approximation for the case of nearest neighbor coupling. We discuss first a model which exhibits both continuous and discontinuous phase transitions, the latter one is connected with a hard onset of the order parameter. In a second model we consider a coupling which favours a coherent behaviour of the individual systems (ferromagnetic coupling) and also an antiferromagnetic coupling.

1. INTRODUCTION

Nonlinear systems exposed to external noise are investigated in the two past decades with growing interest both theoretically and in experiments [1].

Zero-dimensional models described by stochastic ordinary differential equations may exhibit bifurcations of the maximum of the stationary probability density for a spatially homogeneous order parameter. Models with spatially distributed nonlinear constituents subject to external noise may show noise induced nonequilibrium *phase transitions*.

In this paper we deal with systems of identical nonlinear constituents where each one is coupled in a harmonic way to any other one (global coupling) or, alternatively, to the nearest neighbors on a cubic lattice which are described by ordinary stochastic differential equations. The case of global coupling is by far easier to investigate and allows even for explicit analytical results [2–4] which may be considered as mean field approximation for the case of nearest neighbor coupling. Shiino [2] extended the concept of phase transitions to nonequilibrium phenomena in systems of globally coupled nonlinear oscillators subject to additive noise. More recently, Van den Broeck et al. [4] demonstrated the appearance of a *second* order noise induced phase transition in a model with multiplicative and additive noise which shows no transitions in the absence of noise. In [5] we constructed a model which exhibits a *first* order noise induced phase transition

connected with a hard onset of the coexisting ergodic components of the system. Varying parameters of the system the order of the phase transition may be changed similar to changes from supercritical to subcritical bifurcations observed previously in zero dimensional models [6].

We consider a class of models where the dynamics of the individual constituents x_i at the lattice sites i is governed by a system of stochastic ordinary differential equations in the Stratonovich sense

$$\dot{x}_i = f(x_i) + g(x_i)\,\xi_i - \frac{D}{N}\sum_{j\in\mathcal{N}(i)}(x_i - x_j)\;, \tag{1}$$

where $\mathcal{N}(i)$ denotes the set of involved neighbors of site i and $N = \#\mathcal{N}(i)$ is equal to $L-1$ in the case of global coupling and to $2d$ in the case of nearest neighbor coupling. The parameter D is the strength of the spatial interactions. $\xi_i(t)$ is a zero mean spatially uncorrelated Gaussian white noise with autocorrelation function

$$\left\langle\, \xi_i(t)\,\xi_j(t')\,\right\rangle = \sigma^2\delta_{ij}\delta(t-t')\;, \tag{2}$$

and σ^2 is the noise strength.

The (reduced) stationary probability density $P_s(x_i)$ fulfills the Fokker–Planck equation [4]

$$0=\frac{\partial}{\partial x_i}\left(-f(x_i)+\frac{D}{N}\sum_{j\in\mathcal{N}(i)}(x_i-\langle x_j|x_i\rangle)+\frac{\sigma^2}{2}g(x_i)\frac{\partial}{\partial x_i}g(x_i)\right)P_s(x_i)\;, \tag{3}$$

where $\langle x_j|x_i\rangle = \int dx_j x_j P_s(x_j|x_i)$ denotes the steady state conditional average of x_j, $j\in\mathcal{N}(i)$, given x_i at site i. For the case of global coupling, fluctuations disappear in the average $1/(L-1)\sum_{j\in\mathcal{N}(i)}\langle x_j|x_i\rangle$ if $L\to\infty$, and $\langle x_j|x_i\rangle$ may be determined self-consistently.

In Section 2 we discuss the appearance of first order vs. second order phase transitions for a special model and in Section 3 we extend the method to treat spatially inhomogeneous solutions which are favoured by an antiferromagnetic coupling of the constituents.

2. FIRST VS. SECOND ORDER PHASE TRANSITIONS

Here we consider the case $D>0$ which favours a «ferromagnetic» behaviour of the constituents. Restricting to spatially homogeneous solutions for which $\langle x_j|x_i\rangle$ is independent of lattice site i, $\langle x_j|x_i\rangle$ can be replaced by the steady state mean value $\langle x\rangle$ to be determined self-consistently from

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\, x P_s\left(x,\langle x\rangle\right) \equiv F\left(\langle x\rangle\right)\;, \tag{4}$$

where $P_s\left(x, \langle x \rangle\right)$ is the formal solution of (3) considering $\langle x \rangle$ as a parameter,

$$P_s(x, \langle x \rangle) \propto \exp\left\{ \frac{2}{\sigma^2} \int_0^x dy \frac{f(y) - \frac{\sigma^2}{2} g(y) g'(y) - D(y - \langle x \rangle)}{g^2(y)} \right\}. \qquad (5)$$

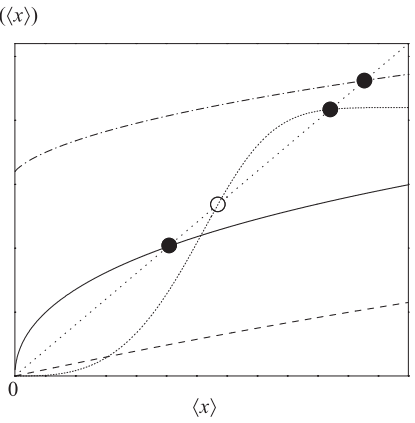

Fig. 1. Solution of the self-consistency equation (4) in typical cases

The solution of the self-consistency equation 4 is visualized in Figure 1 in different situations typically for continuous and discontinuous phase transitions, respectively. In the case of the dashed line the only solution is $\langle x \rangle = 0$. Typical for a continuous transition (solid line) are two stable solutions $\langle x \rangle = \pm x_s$ (full circle), $\langle x \rangle = 0$ is unstable. In the discontinuous case (tightly dotted line) we have a pair of unstable solutions $\langle x \rangle = \pm x_u$ (empty circle) and a pair of stable solutions $\langle x \rangle = \pm x_s$ (full circle) besides the stable solution $\langle x \rangle = 0$. In the latter case the nontrivial solutions appear with nonzero value at the critical value of the control parameter which indicates a *first* order nonequilibrium phase transition. The dash-dotted line shows a typical situation for the system of coupled Stratonovich models considered in Section 3.

A simple model [5] displaying both continuous and discontinuous phase transitions is given by

$$f(x) = ax + x^3 - x^5\,, \qquad g(x) = 1 + x^2\,. \qquad (6)$$

In the case of global coupling the stationary probability density can be obtained explicitly.

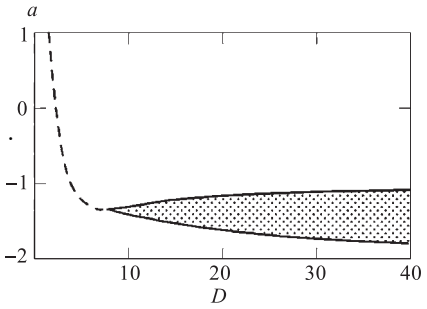

Fig. 2. Phase diagram of model (6) in the case of global coupling, cf. text

Figure 2 shows the phase diagram in the *a*-*D* plane for a given strength of the noise, $\sigma^2 = 1$. For small D we have a second order transition (dashed line). The spatial coupling favours a coherent behaviour of the constituents, acting thus opposite to the noise. With increasing coupling strength D the critical value of a is reduced and above a critical strength of D the first order transition (solid line) of the model without noise and spatial

coupling is «restored». The number of ergodic components is three in the shadowed region, two in the region above and one in the region below. Hysteresis appears in the shadowed region.

3. FERROMAGNETIC VS. ANTIFERROMAGNETIC COUPLING

The analytic results for infinite systems with global coupling give a very good idea of the behaviour of finite systems or systems with nearest neighbor coupling. Figure 3 compares the order parameter obtained by simulation for a 2-dimensional square lattice of size $L = 100 \times 100$ with the results for the globally coupled model for $D = 30$. The diamonds denote the average of $x_i(t)$ over all lattice sites and over a time span of order 100 during which no jumps between the ergodic components occur. The error bars indicate the time average of the standard deviation. Figures 3,*a* and *b* show the order parameter as a function of the control parameter a ($\sigma^2 = 1$) and the noise strength σ^2 ($a = -1.5$), respectively.

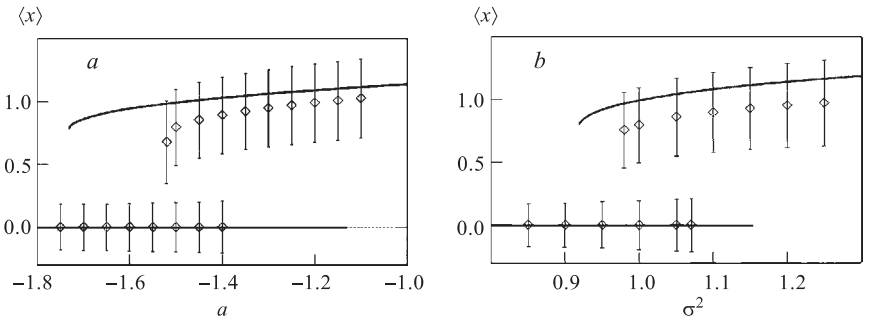

Fig. 3. Order parameter $\langle x \rangle$ as a function of a and σ^2 for a 2-dimensional square lattice (diamonds) and the globally coupled case (thick solid line)

In this Section we consider a system of coupled Stratonovich models specified by

$$f(x) = ax - x^3 \ , \qquad g(x) = x \ . \tag{7}$$

The stationary probability density in the globally coupled case is easily obtained from (5) as

$$P_s(x, \langle x \rangle_s) \propto |x|^{2(a-D)/\sigma^2 - 1} \exp\left\{ - \left(x^2 + 2D\langle x \rangle_s / x \right) / \sigma^2 \right\}, \tag{8}$$

provided $D\langle x \rangle_s / x \geq 0$, otherwise P_s is zero because the above expression is not normalizable then. Note that $\langle x \rangle_s$ is the *spatial* average over all involved sites.

For $D > 0$ a solution is found where all constituents have the same (statistical or temporal) average $\langle x \rangle$ as it is typical for ferromagnets; in this case we have $\langle x \rangle = \langle x \rangle_s$. Depending on the parameters a, σ, and D one finds continuous transitions from zero to nonzero values of $\langle x \rangle$ determined as solutions of Equation (4).

For $D < 0$ an 'antiferromagnetic' solution is preferred. We find two subsystems labeled by $+$ and $-$ respectively, for which the averages $\langle x \rangle$ have opposite sign. In the globally coupled case they are given by

$$\langle x_+ \rangle = \int_0^\infty dx\, x P_s(x, \langle x \rangle_s) = -\int_{-\infty}^0 dx\, x P_s(x, \langle x \rangle_s) = -\langle x_- \rangle, \qquad (9)$$

where P_s is obtained from (8) by inserting $\langle x \rangle_s = (\langle x_+ \rangle + \langle x_- \rangle)/2 = 0$. For nearest neighbor coupling on a cubic lattice, the subsystems correspond just to the two Néel sublattices.

An antiferromagnetic solution exists also for $D > 0$. It is less stable than the ferromagnetic solution in the following sense. For the model with global coupling we prepared such initial conditions that a fraction λ of the constituents has, say, positive initial values; and a fraction $1 - \lambda$, negative ones. We then simulated the dynamics of the system and determined the first time for which one of the constituents changed the sign (first passage time), cf. Figure 4.

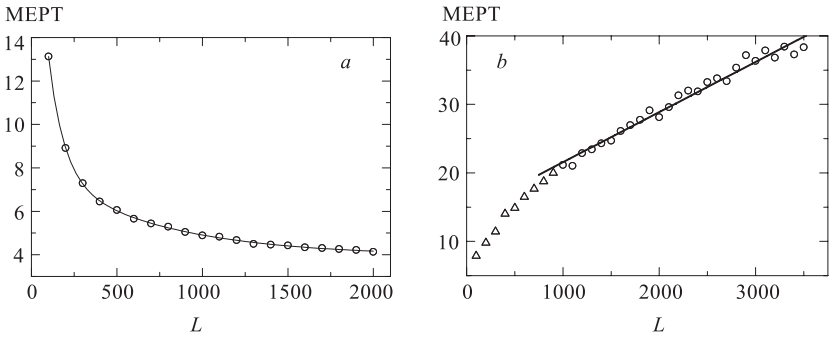

Fig. 4. Mean first passage time as a function of the system size L for globally, ferromagnetically coupled Stratonovich models. The initial conditions are characterized by $\lambda \neq 1/2$ in (a) and $\lambda = 1/2$ in (b). The lines indicate exponential and linear fits, respectively. For other parameters and discussion see text

We found that for $\lambda \neq 1/2$, the mean first passage time (MFPT) decreases exponentially and the system reaches very fast the ferromagnetic state. For $\lambda = 1/2$ the MFPT increases with the system size L and one expects that it diverges in the limit $N \to \infty$. However, the antiferromagnetic state is only

metastable since an additive noise can easily lead to $\lambda \neq 1/2$ and finally to a ferromagnetic state.

Figure 4,*a* shows the MFPT for a system with initial conditions characterized by $\lambda = 0.4$ (parameter values $a = 1.5$, $D = 0.5$, $\sigma^2 = 0.3$) and Figure 4,*b* the same for $\lambda = 1/2$ (parameter values $a = 4$, $D = 2.5$, $\sigma^2 = 0.4$). The average is over 10^3 samples.

A more detailed account on the model discussed in this Section will be published elsewhere, cf. also [7].

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HYPERSPHERICAL ADIABATIC FORMALISM OF THE BOLTZMANN THIRD VIRIAL

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First, we show that, if there are no bound states, we can express the q.m. third cluster — involving 3 and fewer particles in Statistical Mechanics — as a formula involving adiabatic eigenphase shifts. This is for Boltzmann statistics.

From this q.m. formulation, in the case of purely repulsive forces, we recover, as $\hbar$ goes to 0, the classical expressions for the cluster.

We then discuss difficulties which arise in the presence of 2-body bound states and present a tentative formula involving eigenphase shifts and the 2- and 3-body bound state energies. We emphasize that important difficulties have not been resolved.

STATISTICAL MECHANICS

In equilibrium Statistical Mechanics ALL wisdom derives from the partition function! Here, we need the logarithm of the Grand Partition function $\mathcal{Q}$:

$$\begin{aligned}\ln \mathcal{Q} &= z\ Tr(e^{-\beta T_1}) \\ &+ z^2\,[Tr(e^{-\beta H_2}) - \frac{1}{2}(Tr(e^{-\beta T_1}))^2] \\ &+ z^3\,[Tr(e^{-\beta H_3}) - Tr(e^{-\beta T_1})Tr(e^{-\beta H_2}) + \frac{1}{3}(Tr(e^{-\beta T_1})^3] \\ &+ \cdots\end{aligned}$$

which, when divided by V, gives coefficients which are independent of the volume, when the latter becomes large; we call them b_l. The fugacity z equals $\exp(\mu/\kappa T)$, where μ is the Gibbs function per particle, κ is Boltzmann's constant and T is the temperature; $\beta = 1/\kappa T$. We can then write for the pressure and the density

$$p/\kappa T = (1/V)\ln \mathcal{Q} = \sum_l b_l\, z^l$$

$$N/V = \rho = \sum_l l\, b_l\, z^l.$$

The fugacity can then be eliminated to give the pressure in terms of the density.

$$p/kT = \rho + \cdots$$

The coefficients of the second and higher powers are called the virial coefficients.

Crucial Step. For this work we extract the Boltzmann part of the traces: we write

$$Tr(e^{-\beta H_n}) = \frac{1}{n!}\,\mathrm{Trace}^B(e^{-\beta H_n}) + \text{Exchange Terms.}$$

We can then write for the Boltzmann b_3:

$$b_3 = (3!V)^{-1}\,\mathrm{Trace}^B[(e^{-\beta H_3} - e^{-\beta T_3}) - 3\,(e^{-\beta(H_2+T_1)} - e^{-\beta T_3})],$$

where I have made use of the Boltzmann statistics to express the answer in terms of 3-body traces.

ADIABATIC PRELIMINARIES

For 3 particles of equal masses, in three dimensions, we first introduce centre-of-mass and Jacobi coordinates. We define

$$\vec{\eta} = \left(\frac{1}{2}\right)^{1/2}(\vec{r}_1 - \vec{r}_2)\,,\ \vec{\xi} = \left(\frac{2}{3}\right)^{1/2}\left(\frac{\vec{r}_1 + \vec{r}_2}{2} - \vec{r}_3\right),\ \vec{R} = \frac{1}{3}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3)$$

where, of course, the $\vec{r}_i$ give us the locations of the 3 particles. This is a canonical transformation and insures that in the kinetic energy there are no cross terms.

The variables $\vec{\xi}$ and $\vec{\eta}$ are involved separately in the Laplacians and we may consider them as acting in different spaces. We introduce a higher dimensional vector $\vec{\rho} = \begin{pmatrix} \vec{\xi} \\ \vec{\eta} \end{pmatrix}$ and express it in a hyperspherical coordinate system (ρ and the set of angles Ω). If we factor a term of $\rho^{5/2}$ from the solution of the relative Schrödinger equation, i.e., we let $\psi = \phi/\rho^{5/2}$, we are led to:

$$\left[-\frac{\partial^2}{\partial\rho^2} + H_\rho - \frac{2mE}{\hbar^2}\right]\phi(\rho,\Omega) = 0,$$

where

$$H_\rho = -\frac{1}{\rho^2}\left[\nabla^2_\Omega - \frac{15}{4}\right] + \frac{2m}{\hbar^2}V(\rho,\Omega)$$

and m is the mass of each particle, E is the relative energy in the centre of mass. ∇^2_Ω is the purely angular part of the Laplacian. We now introduce the adiabatic

basis, which consists of the eigenfunctions of part of the Hamiltonian: the angular part of the kinetic energy and the potential.

$$H_\rho B_\ell(\rho,\Omega) = \Lambda_\ell(\rho) B_\ell(\rho,\Omega),$$

where ℓ enumerates the solutions.

Using this adiabatic basis, we can now rewrite the Schrödinger equation as a system of coupled ordinary differential equations. We write

$$\phi(\rho,\Omega) = \sum_{\ell'} B_{\ell'}(\rho,\Omega)\tilde{\phi}_{\ell'}(\rho)$$

and obtain the set of coupled equations

$$\begin{aligned}(\frac{d^2}{d\rho^2} - \Lambda_\ell(\rho) \quad &+ \quad k^2)\tilde{\phi}_\ell(\rho) + 2\sum_{\ell'} C_{\ell,\ell'}\,\frac{d}{d\rho}\tilde{\phi}_{\ell'}(\rho) \\ &+ \quad \sum_{\ell'} D_{\ell,\ell'}\,\tilde{\phi}_{\ell'}(\rho) = 0,\end{aligned}$$

where k^2 is the relative energy multiplied by $2m/\hbar^2$ and we defined:

$$\begin{aligned}C_{\ell,\ell'}(\rho) &= \int d\Omega\, B^*_\ell(\Omega,\rho)\frac{\partial}{\partial\rho}B_{\ell'}(\Omega,\rho), \\ D_{\ell,\ell'}(\rho) &= \int d\Omega\, B^*_\ell(\Omega,\rho)\frac{\partial^2}{\partial\rho^2}B_{\ell'}(\Omega,\rho).\end{aligned}$$

We note that

$$D_{\ell,\ell'} = \frac{d}{d\rho}\left(C_{\ell,\ell'}\right) + \left(C^2\right)_{\ell,\ell'}.$$

THE PHASE SHIFT FORMULA

When there are no bound states, we may write

$$Tr^B(e^{-\beta H_3}) = \int d\vec{\rho}\int dk \sum_i \psi^i(k,\vec{\rho})(\psi^i(k,\vec{\rho}))^*\; e^{-\beta\left(\frac{\hbar^2}{2m}k^2\right)},$$

where we have introduced a complete set of continuum eigenfunctions. Expanding in the adiabatic basis, we obtain

$$Tr^B(e^{-\beta H_3}) = \int d\rho\int dk \sum_{i,\ell} |\tilde{\phi}^i_\ell(k,\rho)|^2\; e^{-\beta(\frac{\hbar^2}{2m}k^2)},$$

where we note that we have integrated over the angles and taken advantage of the orthogonality of our B_l's. We integrate from 0 to ∞.

We now return to our expression for b_3 and proceed as above, but drop the tildas, to obtain:

$$\frac{3^{1/2}}{2\lambda_T^3}\int dk\, e^{-\beta E_k}\int d\rho \sum_{i,\ell}[(|\phi_\ell^i|^2-|\phi_{\ell,0}^i|^2)-3(|\bar{\phi}_\ell^i|^2-|\bar{\phi}_{\ell,0}^i|^2)],$$

where we have evaluated the trace corresponding to the centre of mass. The amplitudes ϕ_ℓ^i correspond to H_3, $\bar{\phi}_\ell^i$ to H_2+T_1 and amplitudes with a zero belong to the free particles. The thermal wavelength λ_T is defined as $h/\sqrt{2\pi m\kappa T}$.
We now make use of a trick to evaluate the ρ integrals. We first write

$$\int_0^{\rho_{\max}}\sum_\ell |\phi_\ell^i(k,\rho)|^2\, d\rho = \lim_{k'\to k}\int_0^{\rho_{\max}}\sum_\ell \phi_\ell^i(k,\rho)\phi_\ell^i(k',\rho)\, d\rho$$

and then, and there is the trick,

$$\int_0^{\rho_{\max}}\sum_\ell (\ \phi_\ell^i(k,\rho)\ \ \phi_\ell^i(k',\rho))d\rho =$$
$$\frac{1}{k^2-(k')^2}\sum_\ell [\ \phi_\ell^i(k,\rho)\ \ \frac{d}{d\rho}\phi_\ell^i(k',\rho)-\phi_\ell^i(k',\rho)\frac{d}{d\rho}\phi_\ell^i(k,\rho)],$$

evaluated at $\rho=\rho_{\max}$.

That is, our identity is:

$$\sum_\ell \frac{d}{d\rho}\left[\phi_\ell(k')\frac{d}{d\rho}\phi_\ell(k)-\phi_\ell(k)\frac{d}{d\rho}\phi_\ell(k')\right]$$
$$+\left(k^2-(k')^2\right)\sum_\ell \phi_\ell(k)\ \phi_\ell(k')$$
$$+2\ \sum_{\ell,\ell'}\frac{d}{d\rho}\left[\phi_\ell(k')\ C_{\ell,\ell'}\ \phi_{\ell'}(k)\right]=0$$

and we integrate with respect to ρ. Using then the fact that ϕ goes to zero, as ρ itself goes to zero, and that C decreases fast enough for ρ large, we are left with the expression displayed earlier (that of our «trick»).

We now put in the asymptotic form of our solutions, oscillatory solutions valid for $\rho_{\max}$ large, and use l'Hospital's rule to take the limit as $k'\to k$. The solutions are:

$$\phi_\ell^i \to (k\rho)^{1/2}\mathcal{C}_{\ell,i}\,[\cos\delta_i\ J_{K+2}(k\rho)-\sin\delta_i\ N_{K+2}(k\rho)],$$

where the order K is one of the quantities specified by ℓ. Inserting this into our integrals we find that

$$\sum_{\ell} \int_0^{\rho_{\max}} |\phi_\ell^i(k)|^2 \, d\rho \to \frac{1}{\pi} \frac{d}{dk} \delta^i(k) + \frac{1}{\pi} \rho_{\max} \; + \; \text{osc. terms}$$

and, thus, that

$$\int_0^{\rho_{\max}} (|\phi_\ell^i(k)|^2 - |\phi_{\ell,0}^i(k)|^2) \, d\rho \to \frac{1}{\pi} \frac{d}{dk} \delta^i(k) \; + \; \text{osc. terms.}$$

We let $\rho_{\max}$ go to infinity, and the oscillating terms — of the form $\sin(2k\rho_{\max} + \cdots)$ — will not contribute to the subsequent integration over k. A partial integration now gives us our basic formula

$$b_3^{\text{Boltz}} = \frac{3^{1/2}}{(2\pi)^2 \lambda_T} \int_0^\infty dk \; k \, G(k) \; e^{-\beta \frac{\hbar^2}{2m} k^2},$$

where

$$G(k) = \sum_i [\delta_i(k) - 3 \, \bar{\delta}_i(k)].$$

The first δ arises from comparing three interacting particles with three free particles. The second $\bar{\delta}$ arises when a 3-body system, where only two particles are interacting (one particle being a spectator), is compared to three free particles.

CLASSICAL LIMIT

The idea behind our WKB treatment of our equations, is to argue that when the potentials change slowly — within oscillations of the solutions — then the adiabatic eigenfunctions will also change slowly and we can neglect their derivatives. Thus we will obtain **uncoupled** equations with effective potentials (the eigenpotentials $\Lambda_\ell(\rho)$). We then proceed with these in a more or less conventional WKB fashion. Let us assume, here, one turning point ρ_0.

The phases can now be obtained by considering simplified forms of the asymptotic solutions for the $\phi' s$. Let us denote them as ϕ_ν. The phases will then be

$$\delta_\nu \sim (K+2)\frac{\pi}{2} - k\rho_0 + \int_{\rho_0}^\infty \left[\sqrt{k^2 - \Lambda_\nu - \frac{1}{4\rho^2}} - k \right] d\rho.$$

Inserting our expression for δ_ν into $\int_0^\infty dk\, k\, \delta_\nu(k)\, \exp\left(-\lambda_T^2 k^2/4\pi\right)$ and interchanging the order of integration (ρ and k) we obtain:

$$\frac{2(\pi^2)}{\lambda_T^3}\int_0^\infty d\rho \left\{\exp\left[-\frac{\lambda_T^2}{4\pi}(\Lambda_\nu+\frac{1}{4\rho^2})\right]-\exp\left[-\frac{\lambda_T^2}{4\pi}\frac{(K+2)^2}{\rho^2}\right]\right\}.$$

Summing now over ν, we can rewrite the exponentials as traces:

$$\sum_\nu \{\ \exp\left[-\frac{\lambda_T^2}{4\pi}\ \left(\Lambda_\nu+\frac{1}{4\rho^2}\right)\right]-\exp\left[-\frac{\lambda_T^2}{4\pi}\ \frac{(K+2)^2}{\rho^2}\right]\}$$
$$= \ \text{Trace}^R\left\{\exp\left[-\frac{\lambda_T^2}{4\pi}\ \left(\Lambda(\rho)+\frac{1}{4\rho^2}\right)\right]-\exp\left[-\frac{\lambda_T^2}{4\pi}\ \frac{\mathcal{K}^2+\frac{1}{4}}{\rho^2}\right]\right\},$$

where Λ is the operator (matrix) which yields the diagonal elements Λ_ν and $\mathcal{K}^2$ the operator which yields the eigenvalue when the interaction is turned off (and therefore takes on the diagonal values $(K+2)^2-\frac{1}{4}$, associated with the hyperspherical harmonic of order K). The trace is restricted so as not to involve ρ.

In another key step, we switch to a hyperspherical basis. We note that Λ is related to $(2m/\hbar^2)\,V+\mathcal{K}^2/\rho^2$ by a similarity transformation and an orthogonal matrix U. Substituting in the trace, we lose the U and obtain

$$\text{Tr}^R\left[\exp\left(-\beta V-\frac{\lambda_T^2}{4\pi}\ \frac{\mathcal{K}^2+\frac{1}{4}}{\rho^2}\right)-\exp(-\frac{\lambda_T^2}{4\pi}\ \frac{\mathcal{K}^2+\frac{1}{4}}{\rho^2})\right].$$

We write the exponential as a product of 2 exponentials, disregarding higher order terms in $\hbar$. Introducing eigenkets and eigenbras which depend on the hyperspherical angles, we write the trace as:

$$\int d\Omega <\Omega|\exp(-\frac{\lambda_T^2}{4\pi}\ \frac{\mathcal{K}^2+\frac{1}{4}}{\rho^2})|\Omega>\{\exp[-\beta V(\vec{\rho})]-1\}.$$

The matrix element above can be evaluated and, to leading order in a Euler McLaurin expansion, yields ρ^5/λ_T^5. For the phase shifts of type δ_ν, associated with the fully interacting 3 particles, V equals $V(12)+V(13)+V(23)$ and we obtain as its contribution to b_3^{Boltz}:

$$\frac{3^{1/2}}{2\lambda_T^9}\int d\vec{\xi}\, d\vec{\eta}\,(\exp[-\beta(V(12)+V(13)+V(23))]-1).$$

The expression above, derived solely from the contribution of the δ's, diverges for infinite volume. However, including the terms in $\bar{\delta}$, associated with the pairs 12, 13 and 23, provides a convergent answer. The complete result for b_3^{Boltz} divided by b_1^3, where $b_1=\lambda_T$, equals

$$\frac{1}{3!V}\int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\,\{\exp[-\beta(V(12)+V(13)+V(23))]$$
$$-\exp[-\beta V(12)]-\exp[-\beta V(13)]-\exp[-\beta V(23)]+2\},$$

where I have integrated over $\vec{R}$ the center of mass coordinate, divided by V, and changed to the coordinates $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$. The result is the classical expression with all the correct factors.

BOUND STATES

If there are bound states, the major change in the eigenpotentials is that for some of these potentials, instead of going to zero at large distances (large ρ), there appears a negative «plateau», i.e., the eigenpotential (up to some contribution in $1/\rho^2$), becomes flat and negative. This is the indication that asymptotically the physical system consists of a 2-body bound state and a free particle. The eigenpotential may also «support» one or more 3-body bound states.
The eigenfunction expansion of the trace associated with H_3, will read:

$$\sum_m \exp(-\beta E_{3,m}) + \sum_i \int_0^\infty dk \int d\vec{\rho}\, \psi^i(k,\vec{\rho})\,(\psi^i(k,\vec{\rho}))^*\ \exp\left\{-\beta\left(\frac{\hbar^2}{2m}k^2\right)\right\}$$
$$+ \sum_i \int_0^{q_i} dq \int d\vec{\rho}\, \psi^i(q,\vec{\rho})\,(\psi^i(q,\vec{\rho}))^*\ \exp\left\{-\beta\left(\frac{\hbar^2}{2m}q^2 - \epsilon_{2,i}\right)\right\}.$$

The q's are defined by $k^2 = q^2 - \epsilon_{2,i}$, where $\epsilon_{2,i}$ is the binding energy of the corresponding bound state. The limit q_i equals $\sqrt{\frac{2m}{\hbar^2}\epsilon_{2,i}}$. The new continuum term represents solutions which are still oscillatory for negative energies (above that of the respective bound states).

Assume, now, that we have 1 bound state, and introduce amplitudes. The asymptotic behaviour will be as follows.
For $E > 0$.

$$\phi^i_\ell(\rho) \to (k\rho)^{1/2}\mathcal{C}_{\ell,i}\left[\cos\delta_i\, J_{K_\ell+2}(k\rho) - \sin\delta_i\, N_{K_\ell+2}(k\rho)\right]$$

$$\phi^i_{\ell_0}(\rho) \to (k\rho)^{1/2}\mathcal{C}_{\ell_0,i}\left[\cos\delta_i\, J_{K_{\ell_0}+2}(q\rho) - \sin\delta_i\, N_{K_{\ell_0}+2}(q\rho)\right].$$

Using our procedure as before we obtain for the integral over ρ:

$$\frac{1}{\pi}\frac{d}{dk}\delta_i + \frac{\rho_{\max}}{\pi}\Big(\sum_{\ell\neq\ell_0}|\mathcal{C}_{\ell,i}|^2 + |\mathcal{C}_{\ell_0,i}|^2\frac{k}{q}\Big).$$

For $E < 0$,

$$\phi^i_{\ell_0}(\rho) \to (q\rho)^{1/2}[\cos\delta_i\, J_{K_{\ell_0}+2}(q\rho) - \sin\delta_i\, N_{K_{\ell_0}+2}(q\rho)]$$

which then yields

$$\frac{1}{\pi}\frac{d}{dk}\delta_i + \frac{\rho_{\max}}{\pi}.$$

The problem is that I can no longer eliminate the $\rho_{\max}$ term by subtracting the contribution of the free particle term, i.e., using the $\rho_{\max}$ from T_3 to cancel the $\rho_{\max}$ from H_3. **All is not lost** however, as we saw (for example in the terms arising in the classical limit) that all the terms of the cluster (b_3) are needed to obtain a volume-independent and convergent result. The obvious terms to examine are the ones associated with $H_2 + T_1$, which also have amplitudes that correspond to (2-body) bound states. I have not been able, to date, to prove that all the coefficients are such that the final coefficient of $\rho_{\max}$ is zero.

If we were ... to assume that the terms in $\rho_{\max}$ **do** indeed cancel, then we can write the following formula for the complete trace.

$$\begin{aligned}
&\mathrm{Trace}^B[(e^{-\beta H_3} - e^{-\beta T_3}) - 3\,(e^{-\beta(H_2+T_1)} - e^{-\beta T_3})] \\
&= \sum_m e^{-\beta E_{3,m}} + \frac{1}{\pi}\sum_i \int_0^\infty dk \frac{d}{dk}[\delta_i(k) - 3\bar{\delta}_i(k)]e^{-\beta(\frac{\hbar^2}{2m}k^2)} \\
&\qquad + \frac{1}{\pi}\sum_i e^{\beta\epsilon_i}\int_0^{q_i} dq \frac{d}{dq}[\delta_i(q) - 3\bar{\delta}_i(q)]e^{-\beta(\frac{\hbar^2}{2m}q^2)}.
\end{aligned}$$

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EXACT RESULTS FOR 1D SIMPLE-EXCLUSION PROCESS WITH ORDERED-SEQUENTIAL DYNAMICS AND OPEN BOUNDARIES

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An exact and rigorous calculation of the current and density profile in the steady state of the one-dimensional fully asymmetric simple-exclusion process (FASEP) with open boundaries and forward-ordered sequential dynamics is presented. An interpretation of the phase transitions between the different phases is given in terms of eigenvalue splitting from a bounded quasi-continuous spectrum.

1. INTRODUCTION

One-dimensional (1D) systems of particles, hopping stochastically to the nearest neighbors (with hard-core exclusion), provide examples of systems far from thermal equilibrium, which exhibit boundary-induced phase transitions and steady state phases with long-range correlations. Here we consider the current and density profile in the steady state of a 1D fully asymmetric simple-exclusion process (FASEP) on a chain of L sites, with open boundaries and forward-ordered sequential dynamics. Each site can be empty or occupied by exactly one particle. At each time step a particle is injected with probability α at the left end. Then each pair of nearest-neighbor sites is updated sequentially from the left to the right: a particle hops with probability p one site to the right, provided that site is empty. Finally, a particle is removed with probability β at the right end.

In the case of random-sequential dynamics, a matrix-product representation of the steady state probability distribution has been found by Derrida, Evans, Hakim, and Pasquier [1]. The representation involves two infinite-dimensional square matrices D and E, which act on the vectors of an auxiliary vector space $\mathcal{S}$, and satisfy a quadratic algebra known as the DEHP algebra. The open boundary conditions are taken into account by the action of the above matrices on two vectors, $|V\rangle \in \mathcal{S}$ and $\langle W| \in \mathcal{S}^{\dagger}$, the dual of $\mathcal{S}$. We make use of the mapping of the algebra for the ordered-sequential dynamics onto the DEHP algebra, suggested in [2]. Starting from one of the matrix representations of the DEHP algebra given in [1], we obtain matrices D and E with nonzero elements only on the main and the upper (for D), or lower (for E) next-to-the-main diagonal. These matrices solve the bulk algebra for the ordered-sequential update, $pDE = D+(1-p)E$, and

satisfy the left, $\langle W|E = \alpha^{-1}\langle W|$, and right, $D|V\rangle = (\beta^{-1} - 1)|V\rangle$, boundary conditions. Crucial points for our method are: (i) the choice of the vectors $\langle W| = |V\rangle^T = (1,\ 0,\ 0,\ \dots)$, and (ii) the representation of the 'lattice translation operator' $C \equiv E + D$ as a symmetric tri-diagonal matrix. By standard arguments, the expressions for the stationary current J_L and particle density $\rho_L(i)$ at site i are

$$J_L = Z_{L-1}/Z_L, \qquad \rho_L(i) = Z_L^{-1}\langle W|C^{i-1}DC^{L-i}|V\rangle, \tag{1}$$

where $Z_L = \langle W|C^L|V\rangle$. In our representation J_L and $\rho_L(i)$ depend on the elements of the matrices D and C only in the first $[L/2]+1$ rows and columns ($[x]$ denotes the entire part of $x \geq 0$). Therefore, for any finite L and a sufficiently large integer $M \geq [L/2]+1$, we can use a truncated M-dimensional representation of the matrices and vectors involved. The truncated lattice propagator C_M is

$$C_M(\xi,\eta) = \frac{d}{p}\begin{pmatrix} a+\xi+\eta & \sqrt{1-\xi\eta} & 0 & 0 & \dots & \dots \\ \sqrt{1-\xi\eta} & a & 1 & 0 & \dots & \dots \\ 0 & 1 & a & 1 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & a & 1 \\ \dots & \dots & \dots & \dots & 1 & a \end{pmatrix}, \tag{2}$$

where

$$d = \sqrt{1-p}, \quad a = d + d^{-1}, \quad \xi = \frac{p-\alpha}{\alpha d}, \quad \eta = \frac{p-\beta}{\beta d}. \tag{3}$$

In the limit $M \to \infty$ the results become exact for any size of the chain. Since the matrix C_M is (real or complex) symmetric, and has, as we have shown, a real nondegenerate spectrum, it can be diagonalized by a similarity transformation with an orthogonal matrix U_M. This makes possible the explicit calculation of the relevant scalar products. For details we refer the reader to [3].

2. SPECTRAL PROPERTIES OF C_M

Let $\lambda_M(k)$, $k = 1, \dots, M$, be the eigenvalues of $C_M(\xi,\eta)$. For $p \neq 0, 1$ we set $\lambda = (d/p)(a + 2x)$ and write the secular equation in the form

$$(1-\xi\eta)U_M(x) + (2x\,\xi\eta - \xi - \eta)U_{M-1}(x) = 0, \tag{4}$$

where $U_n(x)$ is the Chebyshev polynomial of the second kind. After the substitution: $x = \cos\phi$, if $|x| \leq 1$, and $x = \cosh\phi$, if $|x| \geq 1$, by assuming first $|x| \leq 1$ and $\xi\eta \neq 1$, we rewrite (4) as an equation for ϕ

$$\sin[(M+1)\phi]/\sin(M\phi) = (\xi + \eta - 2\xi\eta\cos\phi)/(1-\xi\eta). \tag{5}$$

We need to consider only the roots $\phi \in [0, \pi]$. The case of $|x| \geq 1$ is obtained by analytical continuation to imaginary ϕ. The condition $\xi\eta = 1$, or $(1-\alpha)(1-\beta) = 1-p$, defines a line on which the mean-field approximation is exact. The analysis of Eq. (5) shows that there are four regions in the square $\alpha, \beta \in [0,1]^2$ with different spectral properties of C_M. Their boundaries involve the mean-field line, as well as the lines $\xi = 1$ ($\alpha = \alpha_c \equiv 1 - d$) and $\eta = 1$ ($\beta = \beta_c \equiv 1 - d$).

Region A: $\alpha_c < \alpha \leq 1$ and $\beta_c < \beta \leq 1$. For sufficiently large M Eq. (5) has exactly M simple real roots $\phi_M(k)$, $k = 1, \ldots, M$, in the interval $(0, \pi)$. The eigenvalues of the matrix C_M are

$$\lambda_M(k) = (d/p)[a + 2\cos\phi_M(k)], \qquad k = 1, \ldots, M. \tag{6}$$

A complete set of orthonormal eigenvectors of C_M is given by the column-vectors $|u_M(k)\rangle$, $k = 1, \ldots, M$, with components

$$|u_M(k)\rangle_1 \equiv u_M(1,k) = b_M(k)\frac{\sin[M\phi_M(k)]}{\sqrt{1-\xi\eta}},$$

$$|u_M(k)\rangle_l \equiv u_M(l,k) = b_M(k)\sin[(M+1-l)\phi_M(k)], \text{ for } l = 2, \ldots, M, \tag{7}$$

where $b_M(k)$ is the normalization constant.

Region B: $(1-\alpha)(1-\beta) < 1-p$ and $\alpha < \alpha_c$ or $\beta < \beta_c$. For sufficiently large M Eq. (5) has $M-1$ simple real roots $\phi_M(k)$, $k = 2, \ldots, M$, in the interval $(0, \pi)$. The missing eigenvalue of C_M is provided by the pair of complex conjugate imaginary solutions $\phi = \pm \mathrm{i}\phi_M(1)$ which yield the largest eigenvalue

$$\lambda_M(1) = (d/p)[a + 2\cosh\phi_M(1)]. \tag{8}$$

The remaining $M-1$ eigenvalues have the form (6).

Region C: $(1-\alpha)(1-\beta) > 1-p$ and $\alpha > \alpha_c$ or $\beta > \beta_c$. Now the off-diagonal elements $(C_M)_{1,2} = (C_M)_{1,2} = \mathrm{i}\sqrt{\xi\eta - 1}$, see Eq. (2), are imaginary. The largest eigenvalue of C_M has the same analytical form (8) as in regin B; the remaining $M-1$ eigenvalues have the form (6). The diagonalization problem in regions C and D (see below) differs from the one in regions A and B in that the matrix C_M is complex symmetric, and not Hermitian (or real symmetric).

Region D: $\alpha < \alpha_c$ and $\beta < \beta_c$. The essential difference from the previous case is that for sufficiently large M there are two large eigenvalues of the matrix C_M, which have the form (8) and map onto one another under the transformation $\xi \leftrightarrow \eta$. The remaining $M-2$ eigenvalues have the form (6). The case $\xi = \eta > 1$ is a special one, since then the two large eigenvalues $\lambda_M(1,2) = (d/p)(a + 2\cosh\xi) \pm O(\xi^{-M})$ become degenerate in the limit $M \to \infty$.

In the thermodynamic limit region A corresponds to the *maximum current phase*; regions B, C and D for $\xi > \eta$ ($\alpha < \beta$) belong to the *low-density phase*,

and for $\xi < \eta$ ($\alpha > \beta$) belong to the *high-density phase*. The distinction between the latter three regions within a single phase is expeced to affect more subtle characteristics like density profile, correlation functions, rate of approach to the thermodynamic limit.

3. CALCULATION OF THE CURRENT

In region A we obtain in the limit $M \to \infty$ the exact result ($\xi \neq \eta$)

$$Z_L^{\mathrm{A}}(\xi,\eta) = \left(\frac{d}{p}\right)^L \left[\frac{\xi}{\xi-\eta} I_L(\xi) + \frac{\eta}{\eta-\xi} I_L(\eta)\right], \tag{9}$$

where

$$I_L(\xi) = \frac{2}{\pi} \int_0^\pi \mathrm{d}\phi \frac{(a+2\cos\phi)^L \sin^2\phi}{1-2\xi\cos\phi+\xi^2}. \tag{10}$$

The expression for $Z_L^{\mathrm{A}}(\xi,\xi)$ can be obtained by taking the limit $\eta \to \xi$ in (9).

In regions B and C there is a contribution from the single largest eigenvalue:

$$Z_L^{\mathrm{B,C}}(\xi,\eta) = \left(\frac{d}{p}\right)^L \frac{\xi-\xi^{-1}}{\xi-\eta}(a+\xi+\xi^{-1})^L + Z_L^{\mathrm{A}}(\xi,\eta) \quad (\xi > \eta). \tag{11}$$

The case $\eta > \xi$ follows from the above by exchanging places of ξ and η. In region D ($\xi \neq \eta$) there are separate contributions from the two large eigenvalues:

$$Z_L^{\mathrm{D}}(\xi,\eta) = \left(\frac{d}{p}\right)^L \left[\frac{\xi-\xi^{-1}}{\xi-\eta}(a+\xi+\xi^{-1})^L + \frac{\eta-\eta^{-1}}{\eta-\xi}(a+\eta+\eta^{-1})^L\right] + Z_L^{\mathrm{A}}(\xi,\eta). \tag{12}$$

On the line $\xi = \eta$ in region D Eq. (12) yields

$$Z_L^{\mathrm{D}}(\xi,\xi) = \left(\frac{p}{d}\right)^L \left[\frac{L(\xi-\xi^{-1})^2}{\xi(a+\xi+\xi^{-1})} + 1 + \xi^{-2}\right](a+\xi+\xi^{-1})^L + Z_L^{\mathrm{A}}(\xi,\xi). \tag{13}$$

The exact results for the current follow from Eq. (1) and the above expressions.

Current in the Maximum-Current Phase. By substituting the leading-order asymptotic form of the Laplace integral (10) in the expression for $Z_L^{\mathrm{A}}(\xi,\eta)$, we obtain the large-$L$ asymptotic form of the current

$$J_L^{\mathrm{m.c.}} = \frac{1-\sqrt{1-p}}{1+\sqrt{1-p}}[1+O(L^{-1})] \tag{14}$$

independently of the parameters α and β.

Current in the Low- and High-Density Phases. Due to the dominant contribution of the largest eigenvalue, we obtain that up to exponentially small in L corrections

$$J_L^{\mathrm{l.d.}}(\xi,\eta) \simeq (p/d)(a+\xi+\xi^{-1})^{-1} = \frac{\alpha(p-\alpha)}{p(1-\alpha)}. \tag{15}$$

The result for the high-density phase follows under the replacement $\xi \leftrightarrow \eta$ ($\alpha \leftrightarrow \beta$):

$$J_L^{\mathrm{h.d.}}(\xi,\eta) \simeq (p/d)(a+\eta+\eta^{-1})^{-1} = \frac{\beta(p-\beta)}{p(1-\beta)}. \tag{16}$$

Only on the line $\xi = \eta > 1$ in region D the current $J_L^{\mathrm{D}}(\xi,\xi)$ has $O(L^{-1})$ corrections to the thermodynamic limit, see Eq. (13). The limiting expressions for the current coincide with the mean-field results [4].

4. CALCULATION OF THE LOCAL DENSITY PROFILE

Here we present the large-L asymptotic forms only (for the exact results see [3]).

Local Density in the Maximum-Current Phase. To obtain the particle density profile on the *macroscopic scale* $r = i/L$, as $L \to \infty$, we assume that $i \gg 1$ and $L - i \gg 1$. Then, by using the assymptotic form of $Z_n(\xi,\eta)$ for $n \gg 1$, we obtain the density profile

$$\rho_L^{\mathrm{m.c.}}(rL) \simeq \frac{\sqrt{1-p}}{1+\sqrt{1-p}} + \frac{L^{-1/2}\sqrt{d}}{\sqrt{\pi}(1+d)} \frac{1-2r}{\sqrt{r(1-r)}} \quad (0<r<1) \tag{17}$$

independently of the parameters α and β; it has the same shape as in the case of random-sequential dynamics, see Eq. (53) in [5].

Local Density in the Low-Density Phase. By neglecting terms which are uniformly in $i = 1,\ldots,L$ exponentially small as $L \to \infty$, we obtain that the local density of the low-density phase in regions B and C is given by

$$\rho_L^{\mathrm{B,C}}(i) \simeq \frac{\alpha(1-p)}{p(1-\alpha)} - \frac{\xi I_{L-i}(\xi) - \eta I_{L-i}(\eta)}{(a+\xi+\xi^{-1})^{L-i+1}}. \tag{18}$$

One clearly sees that the shape of the density profile drastically changes on crossing the phase boundary. In the low-density phase the profile is constant (up to exponentially small in L terms) near the left end of the chain, and changes exponentially fast near the right end. The bending of the profile near the right

end is downward in region B and upward in region C. In the part of region D occupied by the low-density phase ($\xi > \eta > 1$) we obtain

$$\rho_L^{\mathrm{D}}(i) \simeq \frac{\alpha(1-p)}{p(1-\alpha)} + \frac{\eta - \eta^{-1}}{a+\xi+\xi^{-1}} \left(\frac{a+\eta+\eta^{-1}}{a+\xi+\xi^{-1}} \right)^{L-i} -$$

$$- \frac{\xi I_{L-i}(\xi) - \eta I_{L-i}(\eta)}{(a+\xi+\xi^{-1})^{L-i+1}}. \tag{19}$$

A comparison with Eq. (18) reveals a *new feature:* the leading-order asymptotic form of the density profile changes on passing from region C to region D *within* the low-density phase.

Local Density in the High-Density Phase. By ignoring the uniformly in $i = 1, \ldots, L$ exponentially small as $L \to \infty$ corrections, we obtain that the local density of the high-density phase in regions B and C is

$$\rho_L^{\mathrm{B,C}}(i) \simeq 1 - \frac{\beta}{p} + \frac{\eta I_{i-1}(\eta) - \xi I_{i-1}(\xi)}{(a+\eta+\eta^{-1})^i}. \tag{20}$$

The profile bends near the left end of the chain: upward in region B and downward in region C. In the part of region D occupied by the high-density phase ($\eta > \xi > 1$)

$$\rho_L^{\mathrm{D}}(i) \simeq 1 - \frac{\beta}{p} - \frac{\xi - \xi^{-1}}{a+\eta+\eta^{-1}} \left(\frac{a+\xi+\xi^{-1}}{a+\eta+\eta^{-1}} \right)^{i-1} + \frac{\eta I_{i-1}(\eta) - \xi I_{i-1}(\xi)}{(a+\eta+\eta^{-1})^i}. \tag{21}$$

As in region C, the profile bends downward near the left end of the chain. Its asymptotic form changes on passing from region C to region D *within* the high-density phase.

The above asymptotic expressions are in excellent agreement with the results of computer simulations. The bulk densities coincide with the mean-field results [4].

Local Density on the Coexistence Line. The condition $\xi = \eta > 1$ defines the coexistence line between the low- and high-density phases in region D. On the *macroscopic scale* of distance, i.e., when $r \equiv i/L = O(1)$ as $L \to \infty$, by ignoring the $O(L^{-1})$ corrections, we obtain

$$\rho_L^{\mathrm{coex}}(rL; \xi, \xi) \simeq \frac{1}{a+\xi+\xi^{-1}} \left[d + \xi^{-1} + (\xi - \xi^{-1}) r \right]. \tag{22}$$

The local density changes linearly between the bulk densities of the low- ($r = 0$) and high-density ($r = 1$) phase.

5. CONCLUSIONS

For the FASEP with ordered-sequential dynamics open boundary conditions we have calculated rigorously the current and the local particle density, both for finite chains and in the thermodynamic limit. For any finite L these quantities are real-analytic functions of the parameters; only in the thermodynamic limit different asymptotic forms appear. We have shown that the asymptotic form of the profile changes when α or β crosses the value $1-\sqrt{1-p}$ within the high- or low-density phase, respectively. This reflects the appearance of a second correlation length, related to the next-to-the-largest eigenvalue of the lattice propagator. A similar fact has been found in the case of random-sequential dynamics [6].

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SOME NEW EXACT CRITICAL-POINT AMPLITUDES

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The scaling properties of the free energy and some of universal amplitudes of a group of models belonging to the universality class of the quantum nonlinear sigma model and the $O(n)$ quantum ϕ^4 model in the limit $n \to \infty$ as well as the quantum spherical model, with nearest-neighbor and long-range interactions (decreasing at long distances r as $1/r^{d+\sigma}$) are presented.

For temperature driven phase transitions quantum effects are unimportant near critical points with $T_c > 0$. However, if the system depends on another «nonthermal critical parameter» g, at rather low (as compared to characteristic excitations in the system) temperatures, the leading T dependence of all observables is specified by the properties of the zero-temperature (or quantum) critical point, say at g_c. The *dimensional crossover rule* asserts that the critical singularities with respect to g of a d-dimensional quantum system at $T = 0$ and around g_c are *formally* equivalent to those of a classical system with dimensionality $d + z$ (z is the dynamical critical exponent) and critical temperature $T_c > 0$. This makes it possible to investigate low-temperature effects (considering an effective system with d infinite spatial and z finite temporal dimensions) in the framework of the theory of finite-size scaling. A compendium of some universal quantities concerning $O(n)$-models at $n \to \infty$ in the context of the finite-size scaling is presented.

Casimir Amplitudes in Critical Quantum Systems. Let us consider a critical quantum system with a film geometry $L \times \infty^{d-1} \times L_\tau$, where $L_\tau = \hbar/(k_B T)$ is the «finite-size» in the temporal (imaginary time) direction and let us suppose that *periodic boundary conditions* are imposed across the finite space dimensionality L (in the remainder we will set $\hbar = k_B = 1$).

The confinement of *critical fluctuations* of an order parameter field induces long-ranged force between the boundary of the plates [1, 2]. This is known as «statistical-mechanical Casimir force». The Casimir force in statistical-mechanical systems is characterized by the excess free energy due to the *finite-size contribu-*

tions to the free energy of the bulk system. In the case it is defined as

$$F_{\rm Casimir}(T,g,L|d) = -\frac{\partial f^{\rm ex}(T,g,L|d)}{\partial L}, \tag{1}$$

where $f^{\rm ex}(T,g,L|d)$ is the excess free energy

$$f^{\rm ex}(T,g,L|d) = f(T,g,L|d) - Lf(T,g,\infty|d). \tag{2}$$

Here $f(T,g,L|d)$ is the full free energy per unit area and per k_BT, and $f(T,g,\infty|d)$ is the corresponding bulk free energy density.

Then, near the quantum critical point g_c, where the phase transition is governed by the nonthermal parameter g, one could state that (see, [3])

$$\frac{1}{L} f^{\rm ex}(T,g,L|d) = (TL_\tau)\, L^{-(d+z)} X^{\rm u}_{\rm ex}(x_1,\rho|d), \tag{3}$$

with scaling variables

$$x_1 = L^{1/\nu}\delta g, \text{ and } \rho = L^z/L_\tau. \tag{4}$$

Here ν is the usual critical exponent of the bulk model, $\delta g \sim g - g_c$, and $X^{\rm u}_{\rm ex}$ is the universal scaling function of the excess free energy. According to the definition (1), one gets

$$F^d_{\rm Casimir}(T,g,L) = (TL_\tau)\, L^{-(d+z)} X^{\rm u}_{\rm Casimir}(x_1,\rho|d), \tag{5}$$

where $X^{\rm u}_{\rm Casimir}(x_1,\rho|d)$ is the *universal* scaling function of the Casimir force.

It follows from Eq. (5) that depending on the scaling variable ρ one can define Casimir amplitudes

$$\Delta^{\rm u}_{\rm Casimir}(\rho|d) := X^{\rm u}_{\rm Casimir}(0,\rho|d)\,. \tag{6}$$

In addition to the «usual» excess free energy and Casimir amplitudes, denoted by the superscript «u», one can define, in a full analogy with what it has been done above, «*temporal excess free energy density*» $f^{\rm ex}_{\rm t}$,

$$f^{\rm ex}_{\rm t}(T,g,|d) = f(T,g,\infty|d) - f(0,g,\infty|d). \tag{7}$$

If the quantum parameter g is in the vicinity of g_c, then one expects

$$f^{\rm ex}_{\rm t}(T,g|d) = TL_\tau^{-d/z} X^{\rm t}_{\rm ex}\left(x_1^t|d\right), \tag{8}$$

i.e., instead of $X^{\rm u}_{\rm ex}(x_1,\rho|d)$ one has a scaling function $X^{\rm t}_{\rm ex}\left(x_1^t|d\right)$ which is the corresponding analog with scaling variables

$$x_1^t = L^{1/\nu z}\delta g. \tag{9}$$

Obviously one can define the «temporal Casimir amplitude»

$$\Delta^{\mathrm{t}}_{\mathrm{Casimir}}\,(d) := X^{\mathrm{t}}_{\mathrm{ex}}\,(0|d)\,. \tag{10}$$

Whereas the «usual» amplitudes characterize the leading L corrections of a finite size system to the bulk free energy density at the critical point, the «temporal amplitudes» characterize the leading temperature-dependent corrections to the ground state energy of an *infinite* system at its quantum critical point g_c. For the universality class under consideration the following exact results are obtained:

(i) For the «usual» Casimir amplitudes

$$\Delta^{\mathrm{u}}_{\mathrm{Casimir}}\,(0|2,2) = -\frac{2\zeta(3)}{5\pi} \approx -0.1530, \tag{11}$$

here $\zeta(x)$ is the Riemann zeta function, and

$$\Delta^{u}_{\mathrm{Casimir}}(0|1,1) = -0.3157. \tag{12}$$

(ii) For the «temporal» Casimir amplitudes in the case $(0 < \sigma \leq 2)$

$$\Delta^{\mathrm{t}}_{\mathrm{Casimir}}(\sigma,\sigma) = -\frac{16}{5\sigma}\frac{\zeta(3)}{(4\pi)^{\sigma/2}}\frac{1}{\Gamma(\sigma/2)}. \tag{13}$$

Note that the defined «temporal Casimir amplitude» $\Delta^{\mathrm{t}}_{\mathrm{Casimir}}(\sigma,\sigma)$ reduces for $\sigma = 2$ to the «normal» Casimir amplitude $\Delta^{\mathrm{u}}_{\mathrm{Casimir}}\,(0|2,2)$, given by Eq. (11). This reflects the existence of a special symmetry in that case between the «temporal» and the space dimensionalities of the system.

When $\sigma \neq 2$, it is easy to verify that the following general relation

$$\frac{\Delta^{\mathrm{t}}_{\mathrm{Casimir}}(\sigma,\sigma)}{\Delta^{\mathrm{t}}_{\mathrm{Casimir}}(2,2)} = \frac{8\pi}{\sigma(4\pi)^{\sigma/2}\Gamma(\sigma/2)} \tag{14}$$

between the temporal amplitudes holds. The r.h.s. of (14) is a decreasing function of σ.

Relation with the Zamolodchikov's C-Function. Let us note that if $z = 1$ the temporal excess free energy introduced above coincides, up to a (negative) normalization factor, with the proposed by Neto and Fradkin definition of the nonzero temperature generalization of the C-function of Zamolodchikov (see, e.g., Ref. 4).

For $z \neq 1$ a straightforward generalization of this definition can be proposed at least in the case of long-range power-low decaying interaction

$$C(T,g|d,z) = -T^{-(1+d/z)}\frac{v^{d/z}}{n(d,z)}f^{\mathrm{t}}_{\mathrm{ex}}(T,g|d), \tag{15}$$

where $z = \sigma/2$, $v = TL_\tau$ and

$$n^{t}(d,\sigma) = \frac{4}{\sigma}\frac{\zeta\,(1+2d/\sigma)}{(4\pi)^{d/2}}\frac{\Gamma(2d/\sigma)}{\Gamma(d/2)}. \tag{16}$$

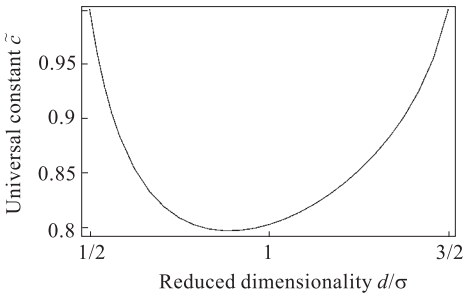

Fig. 1. Behaviour of the universal constant $\tilde{c}$ as a function of d/σ

The quantity $\tilde{c}_0(d,\sigma) := C(T, g_c|d, z)$ is an important universal characteristic of the theory. The behavior of $\tilde{c}_0(d,\sigma)$ is calculated numerically for dimensions between the lower critical dimension $\sigma/2$ and upper critical dimension $3\sigma/2$ for arbitrary values of $0 < \sigma \leq 2$. The results are universal as function of d/σ as it is presented in Fig. 1. In the particular case $d/\sigma = 1$, one can obtain analytically [3]

$$\tilde{c}_0(\sigma,\sigma) = 4/5. \qquad (17)$$

This generalizes the result obtained for $d = \sigma = 2$ [5] to the case of long-range interaction.

To shed some light to what extent the amplitudes presented above are close to that one of more realistic models we present a comparison of the scaling functions of the excess free energy of the Ising, XY, Heisenberg and spherical model (limit $n \to \infty$) in Fig. 2. The results for the spherical model are exact while that ones for the Ising, XY, and Heisenberg models are obtained by ϵ-expansion technique up to the first order in ϵ. The Monte Carlo results for the 3d Ising model give -0.1526 ± 0.0010 [6], which is *surprisingly close* to the exact value (11). This makes difficult to resolve the question how $X^{\rm ex}/n$ approaches the corresponding result for the spherical model when $n \to \infty$. Note that all the curves practically overlap for $L > 2\xi$, where ξ is the correlation length.

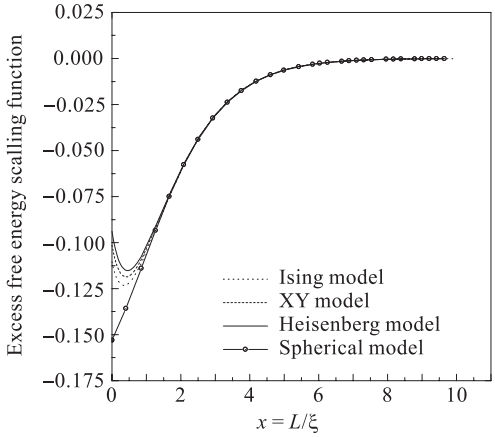

Fig. 2. The *universal* zero-field finite-size scaling functions $X^{\rm ex}$ of the excess free energy as a function of the scaling variable $x = L/\xi(T > T_c)$ for Ising, XY, Heisenberg, Spherical models

Other Amplitudes. Other important universal critical amplitudes, in finite-size scaling, depend upon the geometry $L_{d-d'} \times \infty^{d'} \times \mathrm{L}_\tau^x$ as well as the range of the

interaction. One of the most important quantities for a numerical analysis is the Binder's cumulant ratio. For the quantum 2d spherical model with $\sigma = 2$ at the critical point it is [7]

$$B = \frac{2\pi}{\sqrt{5}\ln^3\tau} \approx 25.21657, \tag{18}$$

where $\tau = (1+\sqrt{5})/2$ is the «golden mean» value.

In what follows we will list a number of results obtained in the framework of the quantum spherical model [8] and the $\mathcal{O}(n)$ quantum φ^4 model [9].
(**i**) Finite system at zero temperature:

$$d = \sigma = 1: \qquad \frac{L}{\xi} = 0.624798 \quad \text{for} \quad d' = 0. \tag{19}$$

$$d = \sigma = 2: \qquad \frac{L}{\xi} = \begin{cases} 1.511955 & \text{for} \quad d' = 0, \\ 0.962424 & \text{for} \quad d' = 1. \end{cases} \tag{20}$$

(**ii**) Bulk system at finite temperature:

$$d = \sigma: \qquad \frac{L_\tau}{\xi} = 0.962424. \tag{21}$$

This result is just a point in graph presented in Fig. 3, where we show the behaviour of L_τ/ξ as a universal function of the ratio d/σ. The point corresponding to $(\frac{d}{\sigma} = 1, y_0 = 0.962424)$ can be obtained analytically [9].

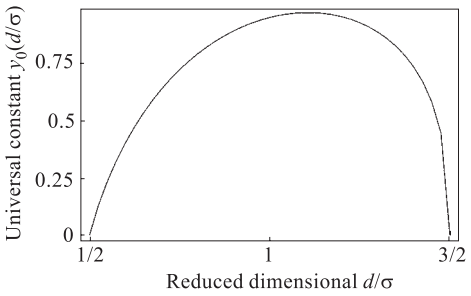

Fig. 3. Behaviour of the scaling variable $y_0 = L_\tau/\xi$ at the quantum critical point as a function of d/σ

The above results are obtained for the case when the quantum parameter controlling the phase transition is fixed at its critical value. Now we will present results obtained when the quantum parameter is fixed by «running» values corresponding to the shifted critical quantum parameter. We are limited to the case $d = \sigma = 2$

$$\frac{L}{\xi} = \begin{cases} 7.061132 & \text{for} \quad d' = 1, \\ 4.317795 & \text{for} \quad d' = 0 \end{cases} \tag{22}$$

for finite system at zero temperature and

$$\frac{L_\tau}{\xi} = \begin{cases} 7.061132 & \text{for} \quad d' = 1, \\ 6.028966 & \text{for} \quad d' = 0 \end{cases} \tag{23}$$

for the bulk system at finite temperature [8].

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MAGNETIC TRANSPORT ALONG ONE-DIMENSIONAL PERTURBATIONS IN THE PLANE

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We review several recent results concerning two-dimensional systems which exhibit a transport induced by a «one-dimensional» perturbation of a homogeneous magnetic field. The first concerns the «local» Iwatsuka model, where a charged particle interacts with a field which is homogeneous outside a finite strip and translationally invariant along it: we present two new sufficient conditions for absolute continuity of the spectrum and show that in most cases the number of open spectral gaps is finite. In the second model the perturbation is a periodic array of point obstacles. In this case the Landau levels remain to be infinitely degenerate eigenvalues, and between them the system has bands of absolutely continuous spectrum.

1. INTRODUCTION

The purpose of this talk is to present results of two recent papers [7, 8] investigating transport of a charged particle in the plane due to a perturbation of a homogeneous magnetic field. We give a short overview referring to the said papers for more details, proofs, references, as well as for numerical analysis of examples.

Magnetic transport and the edge states are since the eighties a standard object of solid-state physics [11–13]. Recently the subject attracted new «theoretical» interest: it was shown that current-carrying states in a halfplane or a more general domain survive a weak disorder [4, 9, 10, 14] and new sufficient conditions were found for existence of transport induced by a variation of the field alone [15].

Our aim here is to contribute to this development in two directions. First we shall present a pair of new sufficient conditions for the absolute continuity in the Iwatsuka model. Of them the second one is important being a rather weak *local* requirement; this represents a step towards the proof of a conjecture put forth in [5, Sec. 6.5] which states that *any* nonzero (translationally invariant) field variation spreads the Landau levels into a purely absolutely continuous spectrum. In addition, we shall show that the number of open gaps is finite here provided the field variation has a nonzero mean and we conjecture that this claim holds generally.

The second topic to address are the edge states: we shall show that they can exist even if there is no edge. This is illustrated by a simple model in which the magnetic transport is a purely quantum effect (in the sense that a quantum particle propagates while its classical counterpart moves on localized circular trajectories, apart of a zero-measure family of the initial conditions): a charged quantum particle in the plane exposed to a homogeneous magnetic field and interacting with a periodic array of point obstacles described by δ potentials.

2. LOCAL IWATSUKA MODEL

Consider a two-dimensional charged particle interacting with a magnetic field perpendicular to the plane. We assume that field is translationally invariant in the y-direction, nonzero and constant away of a strip of a width $2a$:

(a) the functional form of the field is $B(x,y) = B(x) = B + b(x)$, where $B > 0$ and b is bounded and piecewise continuous with $\operatorname{supp} b = [-a, a]$. With an abuse of notation, we employ the same symbol for functions on $\mathbb{R}$ and R^2 if they are independent of one variable.

We use the Landau gauge, $A_x = 0$, $A_y(x) = Bx + a(x)$, with $a(x) := \int_0^x b(t)\,\mathrm{d}t$. We also adopt the natural system of units, $2m = \hbar = c = |e| = 1$; then the Hamiltonian $H \equiv H(B, b)$ of our system is

$$H = (\mathbf{p} + \mathbf{A})^2$$

with the appropriate domain in $L^2(\mathbb{R}^2)$. Since it commutes with y-translations, it allows for a standard decomposition [12, Sec. 2] being unitarily equivalent $\int^{\oplus} H(p)\mathrm{d}p$ with the fiber space $L^2(\mathbb{R})$ and fiber operator

$$H(p) = -\partial_x^2 + (p + xB + a(x))^2. \tag{1}$$

The function a is bounded, so the spectrum of $H(p)$ is purely discrete and consists of a sequence of eigenvalues $\epsilon_n(p)$. In the absence of the perturbation b they are the Landau levels, $\{(2n+1)B : n \in \mathbb{N}_0\}$. In the perturbed case they belong to the spectrum too, at least as its accumulation points.

Lemma 2.1 *$\epsilon_n(p) \to (2n+1)B$ as $|p| \to \infty$ for any $n \in \mathbb{N}_0$.*

To proceed, let us observe first the following analyticity property.

Lemma 2.2 *$\{H(p) : p \in \mathbb{R} \cup \{\infty\}\}$ is an analytic family of type (A). In particular, each $\epsilon_n(\cdot)$ is an analytic function.*

Let $\psi_n(\cdot, p)$ be the eigenfunctions of (1), i.e., $H(p)\psi_n(x,p) = \epsilon_n(p)\psi_n(x,p)$, and denote $f_n(x,p) := (p+xB+a(x))\psi_n(x,p)^2$. Using then a standard semiclassical technique [16], we can derive the following estimates.

Lemma 2.3 *For any p large enough there is $c(p) > 0$ such that*

$$5c(p)\,\mathrm{e}^{-p(x-x_0)} \geq f_n(x,p) \geq \frac{c(p)}{7}\,\mathrm{e}^{-3p(x-x_0)}$$

holds for all $-a \leq x_0 \leq x \leq a$.

With these preliminaries, we were able to prove in [8] the desired result under one of the following additional assumptions:

(b) $b(\cdot)$ is nonzero and does not change sign in $[-a, a]$,

(c) let $a_\ell < a_r$, where we have put $a_\ell := \sup\{x : b(x) = 0 \text{ in } (-\infty, x)\}$ and $a_r := \inf\{x : b(x) = 0 \text{ in } (x, \infty)\}$. There exist $c_0, \delta > 0$ and $m \in \mathbb{N}$ such that one of the following conditions holds:

$$|b(x)| \geq c_0(x - a_\ell)^m \qquad \text{for} \quad x \in [a_\ell, a_\ell + \delta),$$
$$|b(x)| \geq c_0(a_r - x)^m \qquad \text{for} \quad x \in (a_r - \delta, a_r].$$

Theorem 2.4 *Assume (a) and (b), or (a) and (c); then $|\epsilon_n'(p)| > 0$ for each $n \in \mathbb{N}_0$ and all $|p|$ large enough. In particular, the spectrum of H is absolutely continuous.*

We also want to know how the spectrum of H looks like as a set. It follows from direct-integral decomposition that $\sigma(H)$ consists of a union of spectral bands I_n:

$$I_n = \Big[\inf_{p \in \mathbb{R}} \epsilon_n(p),\ \sup_{p \in \mathbb{R}} \epsilon_n(p) \Big] ;$$

the question is how many gaps between them remain open. We shall distinguish two cases depending on whether the functional $A[b] := \int_{-a}^{a} b(x)\,\mathrm{d}x$ vanishes or not. In the latter situation the Bohr–Sommerfeld quantization condition yields:

Proposition 2.5 *Assume $\int_{-a}^{a} b(x)\,\mathrm{d}x \neq 0$. Let $n(E,p)$ and $n_0(E)$ be the numbers of eigenstates of $H(p)$ and H_0, respectively, with the eigenenergy smaller than E. Then for any $m \in \mathbb{N}_0$ there exist p_0 and $E(m, p_0)$ such that*

$$(n_0(E) - n(E, p_0))\ \operatorname{sgn} A[b] > m$$

holds for all $E > E(m, p_0)$.

Corollary 2.6 *If $A[b] \neq 0$ the number of open gaps in the spectrum of H is finite.*

If $A[b] = 0$ the situation is more complicated since the perturbed and unperturbed potentials on (1) differ only in a subset of the interval $(-a, a)$. In [8] we gave an example showing that also in this case the number of open gaps may be finite, and conjectured that this is true generally. However, to prove it one obviously needs a more sophisticated technique.

3. ARRAY OF POINT PERTURBATION

Let us turn now to the second model mentioned in the introduction. The Hamiltonian can be formally written as

$$H_{\alpha,\ell} = (-i\partial_x + By)^2 - \partial_y^2 + \sum_j \tilde{\alpha}\delta(x - x_0 - j\ell)\,, \tag{2}$$

where $\ell > 0$ is the array spacing. To introduce the interaction term in a rigorous way, we follow the usual definition [1] which employs the boundary conditions

$$L_1(\psi, \vec{a}_j) + 2\pi\alpha L_0(\psi, \vec{a}_j) = 0\,, \quad j = 0, \pm 1, \pm 2, \ldots$$

with $\vec{a}_j := (x_0 + j\ell, 0)$, where L_k are the generalized boundary values

$$L_0(\psi, \vec{a}) := \lim_{|\vec{x}-\vec{a}|\to 0} \frac{\psi(\vec{x})}{\ln|\vec{x}-\vec{a}|}\,,\ L_1(\psi, \vec{a}) := \lim_{|\vec{x}-\vec{a}|\to 0} \Big[\psi(\vec{x}) - L_0(\psi, \vec{a})\,\ln|\vec{x}-\vec{a}|\Big]\,,$$

and α is the (rescaled) coupling constant; the free (Landau) Hamiltonian corresponds to $\alpha = \infty$. Using the periodicity, we can write the Bloch decomposition in the x direction, $H_{\alpha,\ell} = \frac{\ell}{2\pi} \int_{|\theta\ell|\le\pi}^{\oplus} H_{\alpha,\ell}(\theta)\, d\theta$, where the fiber operator $H_{\alpha,\ell}(\theta)$ is of the form (2) on the strip $0 \le x \le \ell$ with the boundary conditions

$$\partial_x^i \psi(\ell-, y) = e^{i\theta\ell}\partial_x^i \psi(0+, y)\,, \quad i = 0, 1\,,$$

and its Green's function is given by means of the Krein formula

$$\begin{aligned}(H_{\alpha,\ell}(\theta) - z)^{-1}(\vec{x}, \vec{x}') &= G_0(\vec{x}, \vec{x}'; \theta, z) \\ &\quad + (\alpha - \xi(\vec{a}_0; \theta, z))^{-1} G_0(\vec{x}, \vec{a}_0; \theta, z) G_0(\vec{a}_0, \vec{x}'; \theta, z)\,,\end{aligned}$$

where

$$\xi(\vec{a}; \theta, z) := \lim_{|\vec{x}-\vec{a}|\to 0} \left(G_0(\vec{a}, \vec{x}; \theta, z) - \frac{1}{2\pi}\,\ln|\vec{x}-\vec{a}| \right)$$

and G_0 is the free Green's function,

$$G_0(\vec{x}, \vec{x}'; \theta, z) = -\sum_{m=-\infty}^{\infty} \frac{u_m^\theta(y_<) v_m^\theta(y_>)}{W(u_m^\theta, v_m^\theta)}\, \eta_m^\theta(x) \overline{\eta_m^\theta}(x')\,,$$

where $\eta_m^\theta(x) = \frac{1}{\sqrt{\ell}}\,\mathrm{e}^{i(2\pi m+\theta\ell)x/\ell}$, m runs through integers, $y_<, y_>$ is the smaller and the larger value, respectively, of y, y', and u_m^θ, v_m^θ are solutions to the equation

$$-u''(y) + \left(By + \frac{2\pi m}{\ell} + \theta\right)^2 u(y) = zu(y)$$

such that u_m^θ is L^2 at $-\infty$ and v_m^θ is L^2 at $+\infty$; in the denominator we have their Wronskian. We have $u_m^\theta(y) = u\left(y + \frac{2\pi m+\theta\ell}{B\ell}\right)$ and the analogous relation for v_m^θ, where

$$\left\{ \begin{array}{c} u \\ v \end{array} \right\}(y) = \sqrt{\pi}\, e^{-By^2/2}\left[\frac{M\left(\frac{B-z}{4B}, \frac{1}{2}; By^2\right)}{\Gamma\left(\frac{3B-z}{4B}\right)} \pm 2\sqrt{B}y\,\frac{M\left(\frac{3B-z}{4B}, \frac{3}{2}; By^2\right)}{\Gamma\left(\frac{B-z}{4B}\right)}\right].$$

An explicit computation then leads to the formula

$$G_0(\vec{x}, \vec{x}'; \theta, z) = -\frac{2^{(z/2B)-(3/2)}}{\sqrt{\pi B}\ell}\,\Gamma\left(\frac{B-z}{2B}\right)\,\mathrm{e}^{i\theta(x-x')} \times \sum_{m=-\infty}^{\infty} u\left(y_< + \frac{2\pi m+\theta\ell}{B\ell}\right) v\left(y_> + \frac{2\pi m+\theta\ell}{B\ell}\right)\,\mathrm{e}^{2\pi i m(x-x')/\ell}.$$

As expected the function has singularities which are independent of θ and coincide with the Landau levels, $z_n = B(2n+1),\ n = 0, 1, 2, \ldots$. Using an argument modified from [3, 6] one can check that these points are preserved in the spectrum of the «full» fiber operator $H_{\alpha,\ell}(\theta)$. On the other hand, $H_{\alpha,\ell}(\theta)$ has also eigenvalues away of z_n which we denote as $\epsilon_n(\theta) \equiv \epsilon_n^{(\alpha,\ell)}(\theta)$; they are given by the implicit equation

$$\alpha = \xi(\vec{a}_0; \theta, \epsilon) \tag{3}$$

and the corresponding eigenfunctions are

$$\psi_n^{(\alpha,\ell)}(\vec{x}; \theta) = G_0(\vec{x}, \vec{a}_0; \theta, \epsilon_n(\theta))\,. \tag{4}$$

The regularized Green's function appearing in (3) can be computed to be

$$\xi(\vec{x}; \theta, z) = \sum_{m=-\infty}^{\infty}\left\{\frac{1-\delta_{m,0}}{4\pi|m|} - \frac{2^{-2\zeta-1}}{\sqrt{\pi B}\ell}\,\Gamma(2\zeta)\,(uv)\left(y + \frac{2\pi m+\theta\ell}{B\ell}\right)\right\}, \tag{5}$$

where $\zeta := \frac{B-z}{4B}$. Spectral bands of the model are given by the ranges of the functions $\epsilon_n(\cdot)$. Solutions of the condition (3) do not cross the Landau levels, because $\xi(\vec{a}_0; \theta, \cdot)$ is increasing in the intervals $(-\infty, B)$ and $(B(2n-1), B(2n+1))$ and diverges at the endpoints. It is easy to see that $\xi(\vec{x}; \cdot, z)$ is real-analytic,

hence the spectral bands will be absolutely continuous if the function is non-constant in the whole Brillouin zone $[-\pi/\ell, \pi/\ell)$. Using the explicit expression (5) together with properties of the Fourier transformation, we have arrived in [7] at the following conclusion:

Theorem 3.1 *For any real α the spectrum of $H_{\alpha,\ell}$ consists of the Landau levels $B(2n+1),\ n = 0, 1, 2, \ldots$, and absolutely continuous spectral bands situated between adjacent Landau levels and below B.*

Let us mention for comparison that a chain of point scatterers in a three-dimensional space with a homogeneous magnetic field was discussed recently in [2]. Due to the higher dimensionality, the spectrum is purely a.c. in that case and has at most finitely many gaps.

The band function for different values of the parameters are computed in [7]. When α runs from $+\infty$ to $-\infty$ a band splits from each Landau level and moves down being finally absorbed by the neighbouring LL (with the exception of the lowest one). To characterize the transport associated with the bands, one can also use the probability current, $\vec{j}_n(\vec{x};\theta) = 2\,\mathrm{Im}\left(\bar{\psi}_n^{(\alpha,\ell)}(\vec{\nabla} - i\vec{A})\psi_n^{(\alpha,\ell)}\right)(\vec{x};\theta)$, which is in general nonzero because the Bloch functions (4) are complex-valued. The current pattern changes with θ oscillating between a symmetric «two-way» picture and the situations where one direction clearly prevails; examples are worked out in [7]. They show in particular that the probability current may exhibit vortices in some regions.

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CLASSICAL MANY-PARTICLE DISTRIBUTION FUNCTIONS: SOME NEW APPLICATIONS

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We present a new purely equilibrium microscopic approach to the description of liquid-glass transition in terms of space symmetry breaking of three- and four-particle distribution functions in the cases of two and three dimensions, respectively. The approach has some features of spin glass theories as well as of density-functional theories of freezing.

The main purpose of the report is to present a new purely equilibrium microscopic approach to the description of liquid-glass transition in terms of space symmetry breaking of three- and four-particle distribution functions in the cases of two and three dimensions, respectively. The approach has some features of the spin glass theories as well as of the density-functional theories (DFT) of freezing.

It is usually believed that there are two essential differences between spin glasses and real structural glasses: 1) in the Hamiltonian of spin glasses there is explicit randomness from the very beginning, while in the case of real glasses there is no such randomness. 2) In experiments with spin glasses there is always the range of the concentration of magnetic impurities where nothing else that a spin glass phase appears while in the case of space glass there exists a crystalline ground state. However, in real systems one can consider these differences simply as time scales differences for the freezing of corresponding degrees of freedom with respect to the time scale of the real or computer experiments. In fact, there are now some indications that two possible candidates for equilibrium glasses do exist: some polydisperce hard-sphere systems and some binary mixtures of hard spheres. Even if it is not so, it seems to us that one needs an «underlying» equilibrium theory of liquid-glass transition to understand what really glasses present as space symmetry breaking problem. We should mention that beautiful and fruitful time-dependent mode-coupling theory [1] which describes a number of subtle experimental facts does not consider the problem of space symmetry breaking. Some other arguments can be found in the recent papers by Parisi (see, e.g., [2] and references therein).

To describe different kinds of space symmetry breaking we use the formalism of classical many particle conditional distribution functions

$$F_{s+1}(\mathbf{r}_1|\mathbf{r}_1^0...\mathbf{r}_s^0) = \frac{F_{s+1}(\mathbf{r}_1,\mathbf{r}_1^0,...,\mathbf{r}_s^0)}{F_s(\mathbf{r}_1^0,...,\mathbf{r}_s^0)}.$$

Here $F_s(\mathbf{r}_1,...,\mathbf{r}_s)$ is the s-particle distribution function. The functions $F_{s+1}(\mathbf{r}_1|\mathbf{r}_1^0...\mathbf{r}_s^0)$ satisfy the equation [3]

$$\begin{aligned}\frac{\rho F_{s+1}(\mathbf{r}_1|\mathbf{r}_1^0...\mathbf{r}_s^0)}{z} &= \exp\Big\{-\beta\sum_{k=1}^{s}\Phi(\mathbf{r}_1-\mathbf{r}_k^0)+\sum_{k\geq 1}\frac{\rho^k}{k!}\int S_{k+1}(\mathbf{r}_1,...,\mathbf{r}_{k+1})\\ &\times F_{s+1}(\mathbf{r}_2|\mathbf{r}_1^0...\mathbf{r}_s^0)...F_{s+1}(\mathbf{r}_{k+1}|\mathbf{r}_1^0...\mathbf{r}_s^0)d\mathbf{r}_2...d\mathbf{r}_{k+1}\Big\}. \quad (1)\end{aligned}$$

Here z is the activity, ρ is the mean number density, $S_{k+1}(\mathbf{r}_1,...,\mathbf{r}_{k+1})$ is the irreducible cluster sum of Mayer functions connecting (at least doubly) $k+1$ particles, $\beta = 1/k_BT$ and T is the temperature.

If one takes the derivative of (1) relative to $\mathbf{r}_1$, one obtains the equilibrium Bogoliubov hierarchy [4] along with the explicit expression for F_{s+2} as the functional on F_{s+1} which gives the formally exact closure. However it contains infinite series and integrals and one has to use some approximations to exploit it. The same can be said about the Eq.(1) itself.

Let us now consider the symmetry breaking of the one-particle distribution function and formulate briefly DFT of freezing (see [6] and the reviews [7]). The equation (1) for $s=0$ is the extremum condition for the free energy functional of the inhomogeneous system with the density $\rho(\mathbf{r}) = \rho F_1(\mathbf{r})$ and has the form:

$$\begin{aligned}&\mathcal{F}/k_BT = \int d\mathbf{r}_1\,\rho(\mathbf{r}_1)[\ln(\lambda^d\rho(\mathbf{r}_1)-1]-\\ &-\sum_{k\geq 1}\tfrac{1}{(k+1)!}\int\cdots\int S_{k+1}(\mathbf{r}_1...\mathbf{r}_{k+1})\rho(\mathbf{r}_1)\cdots\rho(\mathbf{r}_{k+1})\,d\mathbf{r}_1\cdots d\mathbf{r}_{k+1}\end{aligned} \quad (2)$$

or

$$\mathcal{F}/k_BT = \int d\mathbf{r}_1\,\rho(\mathbf{r}_1)[\ln(\lambda^d\rho(\mathbf{r}_1)-1] - \mathcal{F}_{ex}[\rho(\mathbf{r})]/k_BT. \quad (3)$$

The excess free energy $\mathcal{F}_{ex}[\rho(\mathbf{r})]/k_BT$ is just the generating functional for direct correlation functions

$$c_n(\mathbf{r}_1...\mathbf{r}_n) = \frac{\delta^n\mathcal{F}_{ex}[\rho(\mathbf{r})]/k_BT}{\delta\rho(\mathbf{r}_1)\cdots\rho(\mathbf{r}_n)}, \quad (4)$$

so that Taylor expansion around the liquid can be written in the following form:

$$\beta\Delta F = \int d\mathbf{r}\varrho(\mathbf{r})\ln\frac{\varrho(\mathbf{r})}{\varrho_0} - \sum_{k\geq 2}\frac{1}{k!}\int c^{(n)}(\mathbf{r}_1,...,\mathbf{r}_k)\Delta\varrho(\mathbf{r}_1)...\Delta\varrho(\mathbf{r}_k)d\mathbf{r}_1...d\mathbf{r}_k, \quad (5)$$

where

$$\Delta\varrho(\mathbf{r}) = \varrho(\mathbf{r}) - \varrho_l$$

is the local density difference between solid and liquid phases.

The full system of equations to be solved in DFT contains the nonlinear integral equation for the function $\rho(\mathbf{r})$, obtained as the extremum condition for the free energy and the equilibrium conditions for the chemical potential and the pressure written in terms of the same functions as in (5). To proceed constructively in the frame of DFT we must choose a concrete form of the free energy functional — a kind of closure or truncating — and we must make an ansatz for the average density of the crystal. The importance of such an ansatz follows from the fact that we are dealing with a theory which is equivalent to Gibbs distribution and one has to break symmetry following the Bogoliubov concept of quasiaverages [5]. Now it is necessary to specify the crystal symmetry (e.g., lattice type) and to locate the freezing transition for that particular lattice type

$$\begin{aligned} \Delta\rho(\mathbf{r}) &= \rho_l \textstyle\sum_{\mathbf{k}} \varphi_{\mathbf{k}} e^{i\mathbf{kr}} = \rho_l\varphi_0 + \rho_l\varphi(\mathbf{r}), \\ \varphi_{\mathbf{k}} &= \frac{1}{\Delta}\int_{\Delta} \frac{\Delta\rho(\mathbf{r})}{\rho_l} e^{-i\mathbf{kr}} d\mathbf{r}. \end{aligned} \tag{6}$$

The sum is over reciprocal lattice vectors and the integral is taken over the elementary lattice cell Δ. $\varphi_{\mathbf{k}}$ are the order parameters of the problem. The DFT approach occurs to be very fruitful and was used to calculate a lot of melting curves for different systems.

The 3D DFT scenario of freezing is valid for some 2D systems. However, there is a number of 2D systems which melts through two continuous phase transition including intermedeate (so-called hexatic) anisotropic liquid phase. The scenario for such a case of 2D melting is the well-known KTNHY [8] phenomenological scenario. We develop a microscopic approach to 2D melting [9, 10] in the spirit of 3D DFT. Our approach differs from the standard DFT theory of freezing in two main points: First, we allow the Fourier coefficients $\rho_{\mathbf{G}}(\mathbf{r})$ of the one-particle distribution function expanded in a Fourier series in reciprocal-lattice vectors $\{\mathbf{G}\}$: $\rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}}(\mathbf{r}) e^{i\mathbf{Gr}}$ to fluctuate and to have amplitude and phase. Second, we allow the liquid to be anisotropic: we consider as possible the existence of a phase with constant density but angular dependent two-particle distribution function $F_2(\mathbf{r}_1 - \mathbf{r}_0) \neq g(r_{10})$.

These two points of generalization define two new order parameters: the fluctuating $\rho_{\mathbf{G}}(\mathbf{r})$ and the Fourier coefficients characteristic for the broken symmetry of the function $F_2(\mathbf{r}_1 - \mathbf{r}_0)$. Our approach again is based on the Eq.(1) but now, considering hexatic phase, we are dealing with the bifurcation of the solution for the two-particle distribution function. The relative spatial distribution of pairs of particles is characterized by the function $F_2(\mathbf{r}_1|\mathbf{r}_0) = F_2(\mathbf{r}_1 - \mathbf{r}_0)$. The vector $\mathbf{r}_1 - \mathbf{r}_0$ defines the direction of the bond between the molecules at the points $\mathbf{r}_1$ and $\mathbf{r}_0$. In the ordinary isotropic liquid the nearest neighbouring of a given

molecule (the first coordination sphere) has a definite local symmetry, which can be characterized by the set of bond directions. The local structure of the liquid in the neighbourhood of a molecule at the point $\mathbf{r}_0'$ is characterized by the bond directions $\mathbf{r}' = \mathbf{r}_2 - \mathbf{r}_0'$. It occurs that if the point $\mathbf{r}_0'$ is at sufficiently large distance from $\mathbf{r}_0$ then there is no correlation between the directions $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_0$ and $\mathbf{r}' = \mathbf{r}_2 - \mathbf{r}_0'$. In this case after the averaging over the system as a whole the pair distribution function transforms into the RDF and the equation (1) for $s = 1$ has the solution $F_2(\mathbf{r}_1 - \mathbf{r}_0) = g(|\mathbf{r}_1 - \mathbf{r}_0|)$, which corresponds to ordinary isotropic liquid. When we approach the anisotropic liquid phase the long-ranged correlations between the bond directions $\mathbf{r}$ and $\mathbf{r}'$ do appear and the averaged two-particle distribution function depends on the bond direction now.

In the vicinity of the transition one can write

$$F_2(\mathbf{r}_1, \mathbf{r}_0) = g(|\mathbf{r}_1 - \mathbf{r}_0|)(1 + f(\mathbf{r}_1 - \mathbf{r}_0)), \tag{7}$$

where $f(\mathbf{r}_1 - \mathbf{r}_0)$ has the symmetry of the local neighbourhood of the particle at $\mathbf{r}_0$. The bifurcation point is given by the linearized equation (1) for $s = 1$, namely,

$$f(\mathbf{r}_1 - \mathbf{r}_0) = \int \Gamma(\mathbf{r}_1, \mathbf{r}_0, \mathbf{r}_2) f(\mathbf{r}_2 - \mathbf{r}_0)\, g(|\mathbf{r}_2 - \mathbf{r}_0|) d\mathbf{r}_2, \tag{8}$$

where

$$\Gamma(\mathbf{r}_1, \mathbf{r}_0, \mathbf{r}_2) = \sum_{k \geq 1} \frac{\rho^k}{(k-1)!} \int S_{k+1}(\mathbf{r}_1, ..., \mathbf{r}_{k+1}) \times g(|\mathbf{r}_3 - \mathbf{r}_0|)...g(|\mathbf{r}_{k+1} - \mathbf{r}_0|)\, d\mathbf{r}_3 ... d\mathbf{r}_{k+1}. \tag{9}$$

At the same time, when one approaches the line defined by the bifurcation condition, the correlation radius for the orientation fluctuations of the pair distribution function diverges. This fact can be shown with the use of the gradient expansion technique in the case of the equation (1) for $s = 3$, if we write the long range part of the correlator using the principle of vanishing correlations ([4]) as:

$$F_4(\mathbf{r}_1, ..., \mathbf{r}_4) = g(|\mathbf{r}_1 - \mathbf{r}_2|) g(|\mathbf{r}_3 - \mathbf{r}_4|)(1 + f_4(\mathbf{r}_1, ..., \mathbf{r}_4)) \tag{10}$$

$$f_4(\mathbf{r}_1, ..., \mathbf{r}_4) = f_4(r, R, \rho, \varphi_1, \varphi_2).$$

Here φ_1 is the angle between the vector $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the axis $\mathbf{R} = \mathbf{r}_2 - \mathbf{r}_3$, φ_2 is the angle between the vector $\rho = \mathbf{r}_3 - \mathbf{r}_4$ and the same axis. We have $f_4(r, R, \rho, \varphi_1, \varphi_2) \to 0$ when $R \to \infty$.

The microscopic expressions for the elastic moduli and Frank constant [10] enable us to understand on the microscopic level whether the 2D melting for any given potential is 3D like or whether it follows the KTHNY scenario.

Let us consider now a possible description of the liquid-glass transition in terms of space symmetry breaking for three- (four) particle distribution function in 2D (3D) systems. At high temperature the nearest neighbours of a molecule can take different relative positions and there is no short-range order (SRO). At lower temperature a SRO appears which can be of different kinds at different densities (for phase transitions in liquids see [11]). The rotation and the translation of the clusters of prefered symmetry give rise to the fact that one-particle and two-particle distribution functions remain isotropic. If a kind of bond orientational order (BOO) appears the clusters are oriented in similar way and the two-particle distribution function becomes to be anisotropic (as in 2D hexatic phase). However, we can imagine another situation — freezing of the symmetry axes of the clusters in different position. The isotropic phase can be considered as analogous to the paramagnetic phase (of cluster symmetry axes), the BOO phase — to the ferromagnetic phase, and the mentioned freezed phase — to a spin glass phase.

Let us consider for simlicity a 2D system. In the vicinity of the transition one can write (in the superposition approximation for the liquid)

$$F_3(\mathbf{r}_1|\mathbf{r}_1^0,\mathbf{r}_2^0) = g(|\mathbf{r}_1-\mathbf{r}_1^0|)g(|\mathbf{r}_1-\mathbf{r}_2^0|)(1+f_3(\mathbf{r}_1|\mathbf{r}_1^0,\mathbf{r}_2^0). \tag{11}$$

In 2D case $f_3(\mathbf{r}_1|\mathbf{r}_1^0,\mathbf{r}_2^0)$ depends in fact on two distances and two angles

$$f_3(\mathbf{r}_1|\mathbf{r}_1^0,\mathbf{r}_2^0) = f_3(R_0,\phi_0;R_1,\Theta_1), \tag{12}$$

where $\mathbf{R}_0 = \mathbf{r}_2^0 - \mathbf{r}_1^0$, $\mathbf{R}_1 = \mathbf{r}_1 - \mathbf{r}_1^0$, $\mathbf{R}_2 = \mathbf{r}_2 - \mathbf{r}_1^0$ and ϕ_0 is the angle of the vector $\mathbf{R}_0$ with the z axis, Θ_1 – the angle between $\mathbf{R}_1$ and $\mathbf{R}_0$ and Θ_2 – the angle between $\mathbf{R}_2$ and $\mathbf{R}_0$.

The linearization of (1) for $s=2$ gives:

$$f_3(R_0,\phi_0;R_1,\Theta_1) =$$

$$= \int \Gamma'(R_0,\phi_0;\mathbf{r}_2;R_1,\Theta_1) f_3(R_0,\phi_0;R_2,\Theta_2) g(|\mathbf{R}_2-\mathbf{R}_0|) g(R_2) d\mathbf{r}_2, \tag{13}$$

where

$$\Gamma'(R_0,\phi_0;\mathbf{r}_2;R_1,\Theta_1) = \sum_{k\geq 1} \frac{\rho^k}{(k-1)!} \int S_{k+1}(\mathbf{r}_1,...,\mathbf{r}_{k+1}) g(|\mathbf{r}_3-\mathbf{r}_1^0|)$$
$$\times g(|\mathbf{r}_3-\mathbf{r}_2^0|)...g(|\mathbf{r}_{k+1}-\mathbf{r}_1^0|) g(|\mathbf{r}_{k+1}-\mathbf{r}_2^0|)\, d\mathbf{r}_3...d\mathbf{r}_{k+1}. \tag{14}$$

There are two kinds of angles entering the equations and two kinds of order parameters, consequently. One angle (ϕ_0) fixes the position of one pair of particles of the cluster, and the other (Θ_i) — the position of the third particle in the coordinate frame defined by ϕ_0. The order parameter connected with Θ_i is the generalization of intracluster hexatic parameter for the case of different coordinate

frames. The order parameter connected with ϕ_0 is an analogue of magnetic moment and in glass-like phase one can consider an Edwards-Anderson parameter $< \cos\phi_0(t) \cos\phi_0(0) >$. In such a way we come to the concept of a «conditional» long range order: if we consider two pairs of particles at infinite distance from one another then there exists a preferable possibility for the relative position of the third particle near each pair. The directions of the bonds in the pairs of particles themselves are subjects to spin-glass-like order. In 3D case the rotation of clusters is given by matrices $D^{l'm'}_{lm}(\vec{\omega}_{0i})$ so that we obtain a kind of orientational multipole glass for the clusters.

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FREE ENERGY AND NON-LINEAR SUSCEPTIBILITIES OF $O(n)$-SYMMETRIC SYSTEMS AT CRITICALITY

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Renormalized coupling constants g_6 and g_8 entering the small-field expansion of the free energy and determining the system non-linear susceptibilities are calculated for the 3D n-vector model in the four-loop and three-loop approximations, respectively. Four-loop expansion for g_6 of the 2D Ising model is also found. The Padé–Borel–Leroy technique is used for resummation of these renormalization-group series, and numerical estimates for universal critical values of g_6 and g_8 are obtained.

Higher-order renormalized coupling constants g_{2k} for the basic models of phase transitions became the target of intensive theoretical studies in recent years (see, e.g., [1, 2] and references therein). These constants enter the small-field expansion of the free energy and scaling equation of state, determine the system nonlinear susceptibilities and thus play a key role at criticality. Along with critical exponents, they are universal, i.e., possess, under $T \to T_c$, numerical values which depend only on the space dimensionality and the symmetry of the order parameter. Calculation of the universal critical values of g_6, g_8, etc., for the 3D Ising model by various methods showed that the field-theoretical renormalization-group (RG) approach in fixed dimensions yields the most accurate numerical estimates. It is a consequence of a rapid convergence of the iteration schemes originating from RG expansions [3,4]. It is natural, therefore, to use the field theory for calculation of renormalized higher-order coupling constants for more general, $O(n)$-symmetric model and for the Ising model in two dimensions. In the report, the 3D RG expansions of the renormalized coupling constants g_6 and g_8 for arbitrary n will be presented along with the 2D RG series for g_6 at $n = 1$ and numerical estimates for their universal critical values will be obtained.

The 3D $O(n)$-symmetric model is described at criticality by Euclidean field theory with the Hamiltonian

$$H = \int d^3x \left[\frac{1}{2}(m_0^2 \varphi_\alpha^2 + (\nabla \varphi_\alpha)^2) + \lambda (\varphi_\alpha^2)^2 \right], \tag{1}$$

where m_0^2 is proportional to $T - T_c^{(0)}$, $T_c^{(0)}$ being the phase transition temperature in the absence of the order parameter fluctuations. The fluctuations give rise to

many-point correlations $\langle\varphi(x_1)\varphi(x_2)...\varphi(x_{2k})\rangle$ and, correspondingly, to higher-order terms in the expansion of the free energy in powers of the magnetization M:

$$F(M,m) = F(0,m) + \sum_{k=1}^{\infty} g_{2k} m^{3-k(1+\eta)} M^{2k}, \tag{2}$$

where m is a renormalized mass, η is a Fisher exponent, and g_{2k} are dimensionless coupling constants. Let, as usually, $g_2 = 1/2$. Then g_4, g_6, g_8,... will acquire, under $T \to T_c$, the universal values.

The asymptotic critical values of g_4, $g_4^*(n)$, determining critical exponents and other universal quantities, have been found from the 6-loop expansion for RG β-function [1,5–7]; they are known with rather high accuracy. To estimate the universal values g_6^* and g_8^* of the higher-order couplings, we calculate corresponding RG series and perform their resummation by means of the Padé–Borel–Leroy technique. The RG series for g_6 and g_8 are obtained from conventional Feynman graph expansions for the 6-point and 8-point vertices in terms of the bare coupling constant λ. In its turn, λ is expressed perturbatively via the renormalized coupling constant g_4. Substituting then the series for λ into the «bare» expansions, we obtain the RG expansions for g_6 and g_8.

As was earlier shown [3,8], the 1-, 2-, 3-, and 4-loop contributions to g_6 are formed by 1, 3, 16, and 94 one-particle irreducible Feynman graphs, respectively. In this case, the calculations just described give [9]:

$$g_6 = \frac{9}{\pi} g_4^3 \left[\frac{n+26}{27} - \frac{17\ n + 226}{81\pi} g_4 + (0.000999164\ n^2 + 0.14768927\ n + 1.24127452) g_4^2 - (-0.00000949\ n^3 + 0.00783129\ n^2 + 0.34565683\ n + 2.14825455) g_4^3 \right]. \tag{3}$$

In the case of g_8, the 1-, 2-, and 3-loop contributions are given by 1, 5, and 36 graphs, respectively [8]. Corresponding RG expansion is found to be [9]:

$$g_8 = -\frac{81}{2\pi} g_4^4 \left[\frac{n+80}{81} - \frac{81\ n^2 + 7114\ n + 134960}{13122\pi} g_4 + (0.00943497\ n^2 + 0.60941312\ n + 7.15615323) g_4^2 \right]. \tag{4}$$

Being a field-theoretical perturbative expansions these series are divergent (asymptotic). To get reasonable numerical estimates for g_6^* and g_8^* some procedure

of making them convergent should be applied. The Borel–Leroy transformation

$$f(x) = \sum_{i=0}^{\infty} c_i x^i = \int_0^{\infty} t^b e^{-t} F(xt) dt, \qquad F(y) = \sum_{i=0}^{\infty} \frac{c_i}{(i+b)!} y^i. \tag{5}$$

can play a role of such a procedure. Since the RG series considered turns out to be alternating, the analytical continuation of the Borel–Leroy transform may be then performed by using Padé approximants [L/M].

For g_6 we have the 4-loop RG expansion and can construct, in principle, three different Padé approximants: [2/1], [1/2], and [0/3]. To obtain proper approximation schemes, however, only diagonal [L/L] and near-diagonal Padé approximants should be employed. That's why further we limit ourselves with approximants [2/1] and [1/2]. Moreover, the diagonal Padé approximant [1/1] will be also dealt with although this corresponds to the usage of the lower-order, 3-loop approximation.

The algorithm of estimating g_6^* we use here is as follows. Since the Taylor expansion for the free energy contains as coefficients the ratios $R_{2k} = g_{2k}/g_4^{k-1}$ we work with the RG series for R_6. It is resummed in three different ways based on the Padé approximants just mentioned. The Borel–Leroy integral is evaluated as a function of the parameter b under $g_4 = g_4^*(n)$. For the fixed point coordinate $g_4^*(n)$ the values extracted from the six-loop RG expansion are adopted [1, 5]. The optimal value of b providing the fastest convergence of the iteration scheme is then determined. It is deduced from the condition that the Padé approximants employed should give, for $b = b_{opt}$, the values of R_6^* which are as close as possible to each other. Finally, the average over three estimates for R_6^* is found and claimed to be a numerical value of this universal ratio.

The results of our calculations of g_6^* are presented in the Table. It contains numerical estimates resulting from the 4-loop RG expansion (column 3) and their analogs given by the Padé–Borel resummed 3-loop RG series [1] (column 4). As is seen, with increasing n the difference between the 4-loop and 3-loop estimates rapidly diminishes: being small (0.9 %) even for $n = 1$, it becomes negligible at $n = 10$ and practically disappears for $n \geq 14$. Such a behaviour is quite natural since with increasing n the approximating properties of RG series for g_6 become better [1, 9].

How close to the exact values of g_6^* may the numbers in column 3 be? To clear up this point, let us compare our 4-loop estimate for R_6^* at $n = 1$ with those obtained recently by an analysis of the 5-loop scaling equation of state for the 3D Ising model [4, 10]. R. Guida and J. Zinn-Justin have obtained $R_6^* = 1.644$ and, taking into account some additional information, $R_6^* = 1.643$, while our estimate is $R_6^* = 1.648$. Keeping in mind that the exact value of R_6^* should lie between the 4-loop and 5-loop estimates (the RG series is alternating), our estimate can differ from the exact number by no more than 0.3 %. Since for $n > 1$ the RG

Table. Our estimates of universal critical values of the renormalized sextic coupling constant for the 3D n-vector model (column 3). The fixed point coordinates g^* are taken from [5] ($1 \le n \le 3$) and [1] ($4 \le n \le 40$). The g_6^* estimates extracted from the Pade–Borel resummed 3-loop RG expansion (column 4), from the exact RG equations (column 5), obtained by the lattice calculations (column 6), resulting from a constrained analysis of the ϵ-expansions (column 7), and given by the $1/n$-expansion (column 8) are presented for comparison

n	g^*	g_6^*	$g_6^*[1]$	$g_6^*[11]$	$g_6^*[12]$	$g_6^*[2]$	g_6^* $(1/n)$
	2	3	4	5	6	7	8
1	1.415	1.608	1.622	1.52	1.92(24)	1.609(9)	
2	1.406	1.228	1.236	1.14	1.27(25)	1.21(7)	
3	1.392	0.951	0.956	0.88	0.93(20)	0.931(46)	
4	1.3745	0.747	0.751	0.68	0.62(15)	0.725(29)	1.6449
5	1.3565	0.596	0.599				1.0528
6	1.3385	0.483	0.485				0.7311
8	1.3045	0.329	0.331			0.319(4)	0.4112
10	1.2745	0.235	0.236				0.2632
12	1.2487	0.174	0.175				0.1828
16	1.2077	0.105	0.105			0.1032(4)	0.1028
20	1.1773	0.0693	0.0694				0.0658
24	1.1542	0.0487	0.0488				0.0457
32	1.1218	0.0276	0.0276			0.0275(1)	0.0257
40	1.1003	0.0176	0.0176				0.0164

expansion (3) should provide better numerical estimates than in the Ising case, this value (0.3 %) represents an upper bound for the deviation of the numbers in column 3 of the Table from their exact counterparts.

It is interesting to compare our estimates with those obtained by other methods. Since 1994, the universal values of the sextic coupling constant for the 3D $O(n)$-symmetric model were estimated by solving the exact RG equations [11], by lattice calculations [12], and by a constrained analysis of the ϵ-expansion [2]; corresponding results are collected in columns 5, 6, and 7 of the Table respectively. As is seen, they are, in general, in accord with ours. For large n, our estimates are consistent also with those given by the $1/n$-expansion which are presented in column 8.

The RG expansion for the octic coupling constant g_8 turns out to be worse than the series (3) from the point of view of their summability. Indeed, the series (4) diverges considerably stronger and is one term shorter than that for g_6. It implies that the only Pade approximant — [1/1] — may be really used

in a course of the resummation of this series. In the Ising case $n = 1$, such a simple Pade–Borel procedure, when applied to the 3-loop RG expansion for g_8, was found to lead to rather crude numerical estimates [8]. As our analysis shows, with increasing n the situation becomes better but, nevertheless, the RG estimates for $g_8^*(n)$ remain much less accurate than those obtained for the sextic coupling constant. Corresponding numerical results are presented elsewhere [9].

For the 2D Ising model the four-loop calculations lead to the following RG expansion for the renormalized sextic coupling constant [13]:

$$g_6 = \frac{36}{\pi}\, g_4^3 \left(1 - 3.2234882\, g_4 + 14.957539\, g_4^2 - 85.7810\, g_4^3\right). \qquad (6)$$

This series is resummed in a manner quite similar to that used in three dimensions. For the fixed point coordinate the value $g_4^* = 0.6125$ [14–16] is accepted which was extracted from lengthy high-temperature expansions and is believed to be the most accurate estimate for g_4^* available nowadays. As our calculations show, for $b = b_{opt}$ all three working Pad$\acute{e}$ approximants yield practically the same value of g_6^*. It is as follows:

$$g_6^* = 1.10. \qquad (7)$$

To estimate an (apparent) accuracy of this number we analyze the sensitivity of estimates given by RG expansion (6) to the type of resummation. The results produced by Pad$\acute{e}$ approximant $[2/1]$ turn out to be most strongly dependent on the parameter b. This situation resembles that for 3D $O(n)$-symmetric model where Pad$\acute{e}$ approximants of $[L-1/1]$ type for β-function and critical exponents lead to numerical estimates demonstrating appreciable variation with b while for diagonal and near-diagonal approximants the dependence of the results on the shift parameter is practically absent [1, 5]. In our case, Pad$\acute{e}$ approximants $[1/1]$ and $[1/2]$ generate such «stable» approximations for g_6^*. For b varying from 0 to 15 (i.e., for any reasonable b) the magnitude of g_6^* averaged over these two approximations is found to remain within the segment (1.044, 1.142) [13]. Hence, the value (7) is believed to differ from the exact one by no more than 5%. Very good agreement between our estimate and those obtained recently from the high-temperature expansions [14] ($g_6^* = 1.104$) and by matching of corresponding ϵ-expansion with the exact results known for $D = 1$ and $D = 0$ [2] may be considered as an argument in favor of this belief.

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BETHE-ANSATZ EQUATIONS FOR QUANTUM HEISENBERG CHAINS WITH ELLIPTIC EXCHANGE

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The eigenvectors of the Hamiltonian $\mathcal{H}_N$ of N-sites quantum spin chains with elliptic exchange are connected with the double Bloch meromorphic solutions of the quantum continuous elliptic Calogero-Moser problem. This fact allows one to find the eigenvectors via the solutions to the system of highly transcendental equations of Bethe-ansatz type which is presented in explicit form.

It is known [1] that for a one-parameter set $\mathcal{H}_N$ of linear combinations of $N(N-1)/2$ elementary transpositions $\{P_{jk}\}$, $\mathcal{H}_N = \frac{J}{2}\sum_{1\le j\ne k}^{N} \wp(j-k)P_{jk}$ at arbitrary natural $N \ge 3$, one can construct a variety $\{I_m\}$ $(3 \le m \le N)$ of operators which commute with $\mathcal{H}_N$. Being applied to $SU(2)$ spin representations of the permutation group, this proves the integrability of 1D periodic spin chains with elliptic short-range interaction and the Hamiltonian

$$\mathcal{H}^{(s)} = \frac{J}{4}\sum_{1\le j\ne k\le N} h(j-k)(\vec{\sigma}_j\vec{\sigma}_k - 1), \tag{1}$$

where

$$h(j) = \left(\frac{\omega}{\pi}\sin\frac{\pi}{\omega}\right)^2\left[\wp_N(j) + \frac{2}{\omega}\zeta_N\left(\frac{\omega}{2}\right)\right], \tag{2}$$

where $\wp_N(x)$, $\zeta_N(x)$ are the Weierstrass functions defined on the torus $T_N = \mathbf{C}/\mathbf{Z}N + \mathbf{Z}\omega$, $\omega = i\alpha$, $\alpha \in \mathbf{R}_+$ is a free parameter.

The symmetry of two limiting cases of this one-parameter model, i.e., the Bethe lattice with nearest-neighbor interaction [2] ($\alpha \to 0$) and long-range $\left(\frac{N}{\pi}\sin\frac{\pi j}{N}\right)^{-2}$ exchange [3] ($\alpha \to \infty$), is now well understood, and regular procedures of finding eigenvectors are described in the literature [4–7]. At present, a number of impressive results are known for both these models. In particular, they include the additivity of the spectrum under proper choice of «rapidity» variables [2,3], the description of underlying symmetry [4,5], construction of thermodynamics in the limit $N \to \infty$ [9,10]. However, all that still cannot be applied to the general elliptic case.

In the paper [8], I have shown that there is a remarkable connection between the eigenvectors of the Hamiltonian of the above model with M down

spins and double Bloch meromorphic solutions to the quantum continuous elliptic Calogero-Moser problem at the special value of the coupling constant, i.e., the eigenfunctions of the *differential* operator

$$H = -\frac{1}{2}\sum_{j=1}^{M}\frac{\partial^2}{\partial x_j^2} + \sum_{j\neq k}^{M}\wp_N(x_j - x_k). \tag{3}$$

This allows one in principle to find an ansatz for the eigenvectors and even try to describe them completely if the solutions to (3) are known. This has been done in the simplest nontrivial case $M = 3$ in [11], where I have used the result for three-particle elliptic Calogero-Moser problem [12].

At that time, the explicit form of the eigenfunctions of (3) at $M > 3$ has not been known. The situation has been changed after publishing the seminal paper [13] where these eigenfunctions have been obtained in the process of constructing solutions to the elliptic Knizhnik–Zamolodchikov–Bernard equations. It has been a main motivation for this paper in which I shall describe the complete set of the Bethe-ansatz-type equations for the eigenvectors of (1) at *arbitrary* $M \leq N/2$.

The Hamiltonian (1) commutes with the operator of total spin $\vec{\mathbf{S}} = \frac{1}{2}\sum_{j=1}^{N}\vec{\sigma}_j$. Then the eigenproblem for it is decomposed into the problems in the subspaces formed by the common eigenvectors of $\mathbf{S}_3$ and $\vec{\mathbf{S}}^2$ such that $S = S_3 = N/2 - M$, $0 \leq M \leq [N/2]$,

$$\mathcal{H}^{(s)}|\psi^{(M)}> = E_M|\psi^{(M)}> . \tag{4}$$

The eigenvectors $|\psi^{(M)}>$ are written in the usual form

$$|\psi^{(M)}> = \sum_{n_1..n_M}^{N}\psi_M(n_1..n_M)\prod_{\beta=1}^{M}s_{n_\beta}^{-}|0>, \tag{5}$$

where $|0> = |\uparrow\uparrow ... \uparrow>$ is the ferromagnetic ground state with all spins up and the summation is taken over all combinations of integers $\{n\} \leq N$ such that $\prod_{\mu<\nu}^{M}(n_\mu - n_\nu) \neq 0$. The substitution of (5) into (4) results in the *lattice* Schrödinger equation for completely symmetric wave function ψ_M

$$\sum_{s\neq n_1,..n_M}^{N}\sum_{\beta=1}^{M}\wp_N(n_\beta - s)\psi_M(n_1,..n_{\beta-1},s,n_{\beta+1},..n_M)$$
$$+\left[\sum_{\beta\neq\gamma}^{M}\wp_N(n_\beta - n_\gamma) - \mathcal{E}_M\right]\psi_M(n_1,..n_M) = 0. \tag{6}$$

The eigenvalues $\{E_M\}$ are given by

$$E_M = J\left(\frac{\omega}{\pi}\sin\frac{\pi}{\omega}\right)^2\left\{\mathcal{E}_M + \frac{2}{\omega}\left[\frac{2M(2M-1)-N}{4}\zeta_N\left(\frac{\omega}{2}\right) - M\zeta_1\left(\frac{\omega}{2}\right)\right]\right\}, \tag{7}$$

where $\zeta_1(x)$ is the Weierstrass zeta function defined on the torus $T_1 = \mathbf{C}/\mathbf{Z}+\mathbf{Z}\omega$.

The solutions to (6) can be found with the use of the following ansatz for ψ_M:

$$\psi_M(n_1,..n_M) = \sum_{P\in\pi_M} \varphi_M^{(p)}(n_{P1},..n_{PM}), \tag{8}$$

$$\varphi_M^{(p)}(n_1,..n_M) = \exp\left(-i\sum_{\nu=1}^{M}\tilde{p}_\nu n_\nu\right)\chi_M^{(p)}(n_1,..n_M), \tag{9}$$

where

$$\tilde{p}_\nu = p_\nu - 2\pi N^{-1}l_\nu, \qquad l_\nu \in \mathbf{Z}, \tag{10}$$

π_M is the group of all permutations $\{P\}$ of the numbers from 1 to M and $\chi_M^{(p)}$ is some special solution to the *continuum* quantum many-particle problem

$$\left[-\frac{1}{2}\sum_{\beta=1}^{M}\frac{\partial^2}{\partial x_\beta^2} + \sum_{\beta\neq\lambda}^{M}\wp_N(x_\beta - x_\lambda) - \mathsf{E}_M(p)\right]\chi_M^{(p)}(x_1,..x_M) = 0. \tag{11}$$

It is specified up to a normalization factor by the particle pseudomomenta $(p_1,..p_M)$. The standard argumentation of the Floquet–Bloch theory shows that due to periodicity of the potential term in (49) $\chi_M^{(p)}$ obeys the quasi-periodicity conditions

$$\chi_M^{(p)}(x_1,..x_\beta+N,..x_M) = \exp(ip_\beta N)\chi_M^{(p)}(x_1,..x_M), \tag{12}$$

$$\chi_M^{(p)}(x_1,..x_\beta+\omega,..x_M) = \exp(2\pi i q_\beta(p)+ip_\beta\omega)\chi_M^{(p)}(x_1,..x_M), \quad 0\le \Re e(q_\beta) < 1, \tag{13}$$

$$1\le\beta\le M.$$

The eigenvalue $\mathsf{E}_M(p)$ is some symmetric function of $(p_1,..p_M)$. As will be seen later, the set $\{q_\beta(p)\}$ is also completely determined by $\{p\}$.

It turns out [8] that the equation (6) with the use of (8),(9) can be recast in the form

$$\sum_{P\in\pi_M}\left[-\frac{1}{2}\sum_{\beta=1}^{M}\left(\frac{\partial}{\partial n_{P\beta}} - f_\beta(p)\right)^2 + \sum_{\beta\neq\gamma}^{M}\wp_N(n_{P\beta}-n_{P\gamma}) - \right.$$

$$\left.\mathcal{E}_M + \sum_{\beta=1}^{M}\varepsilon_\beta(p)\right]\varphi^{(p)}(n_{P1},..n_{PM}) = 0, \tag{14}$$

where

$$f_\beta(p) = 2\tilde{q}_\beta(p)\zeta_1(1/2) - \zeta_1(\tilde{q}_\beta(p)), \tag{15}$$

$$\varepsilon_\beta(p) = \frac{1}{2}\wp_1(\tilde{q}_\beta(p)), \tag{16}$$

$$\tilde{q}_\beta(p) = q_\beta(p) + \frac{l_\beta}{N}\omega. \tag{17}$$

where $\wp_1(x), \zeta_1(x)$ are the Weierstrass functions defined on the torus $T_1 = \mathbf{C}/\mathbf{Z} + \mathbf{Z}\omega$.

Turning to the definition (9) of $\varphi^{(p)}$, one observes that each term of the left-hand side of (14) has the same structure as the left-hand side of the many-particle Schrödinger equation (11) and vanishes if $\mathcal{E}_M$ and $f_\beta(p)$ are chosen as

$$f_\beta(p) = -i\tilde{p}_\beta, \qquad \beta = 1, ..M, \tag{18}$$

$$\mathcal{E}_M = \mathsf{E}_M(p) + \sum_{\beta=1}^{M} \varepsilon_\beta(p). \tag{19}$$

One can see from (15-19) that it remains now to find the explicit dependence of $\{q\}$ and E_M on $\{p\}$. It can be done by using the results given in [13] where the explicit form of $\chi_M^{(p)}(x)$ has been indicated. In suitable notations, it reads

$$\chi_M^{(p)}(x) \sim \exp(i\sum_{\beta=1}^{M} p_\beta x_\beta) \sum_{s\in\pi_m} l(s) \prod_{j=1}^{m} \tilde{\sigma}_{\sum_{k=1}^{j}(x_{c(s(k))} - x_{c(s(k))+1})}(t_{s(j)} - t_{s(j+1)}), \tag{20}$$

where $m = M(M-1)/2$, c is nondecreasing function $c : \{1, .., m\} \to \{1, .., M-1\}$ such that $|c^{-1}\{j\}| = M - j$, $l(s)$ is an integer which is defined for the permutation s by the relation $x_{c(s(1))+1}\partial/\partial x_{c(s(1))}...x_{c(s(m))+1}\partial/\partial x_{c(s(m))}x_1^M = l(s)(x_1...x_M)$, $\{t\}$ is a set of m complex parameters obeying m relations [13]

$$\sum_{l:|c(l)-c(j)|=1} \rho(t_j - t_l) - 2 \sum_{l:l\neq j, c(l)=c(j)} \rho(t_j - t_l) + M\delta_{cj,1}\rho(t_j) = i(p_{c(j)} - p_{c(j)+1}), \tag{21}$$

$$\rho(t) = \zeta_N(t) - \frac{2}{N}\zeta_N(N/2)t,$$

and

$$\tilde{\sigma}_w(t) = \exp((2/N)\zeta_N(N/2)wt)\frac{\sigma_N(w-t)}{\sigma_N(w)\sigma_N(t)},$$

σ_N being the Weierstrass sigma function on $\mathbf{T}_N$. The elementary building blocks of the χ function obey the useful quasi-periodicity relations

$$\tilde{\sigma}_{w+N}(t) = \tilde{\sigma}_w(t), \qquad \tilde{\sigma}_{w+\omega}(t) = e^{2\pi i t/N}\tilde{\sigma}_w(t). \tag{22}$$

One can see that in this construction the color function $c(j)$ is of crucial role. It is useful to write it explicitly. Namely, define for every k=1,..$M-1$ the segment S_k

$$\frac{(k-1)(2M-k)}{2}+1 \le j \le \frac{k(2M-k-1)}{2}. \tag{23}$$

Then some calculation shows that

$$c(j)=k \qquad \text{if} \quad j \in S_k. \tag{24}$$

The main advantage of the explicit form of χ function is that it allows one to find the second set of relations between the Bloch factors $\{p\},\{q\}$. It is easy to see from (21) that $\{p\}'s$ in the definitions (12) and (20) are the same. The problem consists in calculation of $\{q\}$. To do this, it is not necessary to analyze each term in the sum over permutations in (20) since all of them must have the same Bloch factors. It is convenient to choose the term which corresponds to the permutation

$$s_0: \quad s_0(j)=m+1-j, \quad j=1,..m.$$

After some algebra, one finds that this permutation gives nontrivial contribution to the sum (20) with $l(s_0)=M!(M-1)!...2!$. Moreover, with the use of explicit form of the color function (23-24) one finds

$$c(s_0(l))=M-q \quad \text{if} \quad q(q-1)/2+1 \le l \le q(q+1)/2.$$

Now the problem of calculation of the second Bloch factors reduces, due to second relation (21), to some long and tedious, but in fact simple calculations of the product of factors which various $\tilde{\sigma}$ functions acquire under changing arguments of χ function to the quasi-period ω. The final result is surprisingly simple,

$$q_\beta(p)=N^{-1}\left(\sum_{l:c(l)=\beta} t_l - \sum_{l:c(l)=\beta-1} t_l\right), \qquad 1<\beta<M-1, \tag{25}$$

with the first and second term being omitted for $\beta=M$ and $\beta=1$.

The equations (25), together with (18) and (21), form a closed set for finding Bloch factors $\{p\},\{q\}$ at given integers $\{l_\beta\} \in \mathbf{Z}/M\mathbf{Z}$ and determining the eigenvalues of the spin Hamiltonian (1,2) completely. The corresponding eigenvalue of the continuum M-particle operator (11) is given by [13]

$$\mathsf{E}_M(p)=\frac{2M(M-1)}{N}\zeta\left(\frac{N}{2}\right)+\sum_{\beta=1}^{M} p_\beta^2/2$$

$$-\frac{1}{2}\left[\sum_{k<l}^{m}(2\delta_{c(k),c(l)}F(t_k-t_l)-\delta_{|c(k)-c(l)|,1}F(t_k-t_l))-M\sum_{c(k)=1}F(t_k)\right], \tag{26}$$

where

$$F(t) = -\wp_N(t) + (\zeta_N(t) - 2/N\zeta_N(N/2))^2 + 4/N\zeta_N(N/2).$$

This allows one to find, via (7) and (19), the explicit form of the eigenvalues of spin Hamiltonian (1,2). It is worth noting that for their real calculation one has to solve the Bethe-type equations (18), (21), (25) at first.

In conclusion, it is demonstrated that the procedure of the exact diagonalization of the lattice Hamiltonian with the nonnearest-neighbor elliptic exchange can be reduced in each sector of the Hilbert space with given magnetization to the construction of the special double quasi-periodic eigenfunctions of the many-particle Calogero-Moser problem on a continuous line. The equations of the Bethe-ansatz form appear very naturally as a set of restrictions to the particle pseudomomenta. The proof of this correspodence between lattice and continuum integrable models is based only on analytic properties of the eigenfunctions. One can expect that the set of spin lattice states constructed by this way is complete. This is supported by exact analytic proof in the two-magnon case.

The analysis of explicit form of the equations (21) available for $M = 2, 3$ shows that the spectrum of the lattice Hamiltonian with the exchange (1) is *not* additive being given in terms of pseudomomenta $\{p\}$ or phases which parametrize the sets $\{p, q\}$ [11]. For arbitrary M, this can be seen directly from (26). The problem of finding appropriate set of parameters which gives the «separation» of the spectrum remains open. It would be also of interest to consider various limits $(N \to \infty, \alpha \to 0, \infty)$ so as to recover the results of the papers [2,3] and prove the validity of the approximate methods of asymptotic Bethe ansatz.

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HEITLER–LONDON INSULATORS IN NEW OXIDE SYSTEMS

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The tight-binding band structure of AV_2O_5 systems (A is alkali element) is studied by taking into account the electron correlations in the framework of the Hubbard-like model. The evaluated band gaps, energy dispersion relations and density of electronic states are in good agreement with available experimental data. The correlated band gap provides the insulating state of the high-temperature phase. For the best studied α'–NaV_2O_5 the low-temperature phase earlier misinterpreted as the spin-Peierls state, is governed, in fact, by an opening of the Coulomb gap. Due to the nature of the correlated energy the story supports the idea to give the name *Heitler–London insulators* to $A^+V_2O_5$ compounds.

Since the discovery of a spin-Peierls behavior in quasi-1D $CuGeO_3$ there were a lot of efforts to find out similar effects in other inorganic materials. The AV_nO_{2n+1} family (A $\equiv$ alkali or alkali earth element) has been quite perspective in that respect. In the best studied $\alpha'-$ phase of NaV_2O_5 the opening of a spin gap $\Delta_0 \sim 80{-}100$ K at $T_c \sim 34{-}36$ K was attributed firstly to a spin-Peierls transition [1, 2]. At present it has become evident, that this scenario is not adequate for the description of the available experimental data (e.g., [3–5]).

The presented approach is based on the hypothesis that the $\alpha'{-}NaV_2O_5$ properties are governed by the electron correlations $U \gg t_a$ (intra-rung/dimer electron hopping integral) $> t_b$ (an electron hopping along legs in crystall b-direction) $> t_d$ (the hopping along ladder diagonals) $> t_{xy}^{bc,bm,qm}$ (interdimer hoppings between vanadium ions on the nearest ladders) (Fig. 1). According to the standard tight-binding method $(U = 0)$ in solids for solving the Schrödinger

equation the eigenfunctions of the problem are constructed on the basis of the electron eigenfunctions of the isolated atoms, i.e., a conventional tight-binding method is the more suitable the greater interatomic distances in the crystal. But in this case the prevailing term in the Hamiltonian is strong electron-electron repulsion, U, which cannot be reduced to the mean field and then the problem is beyond the scope of the conventional Slater–Koster scheme at all.

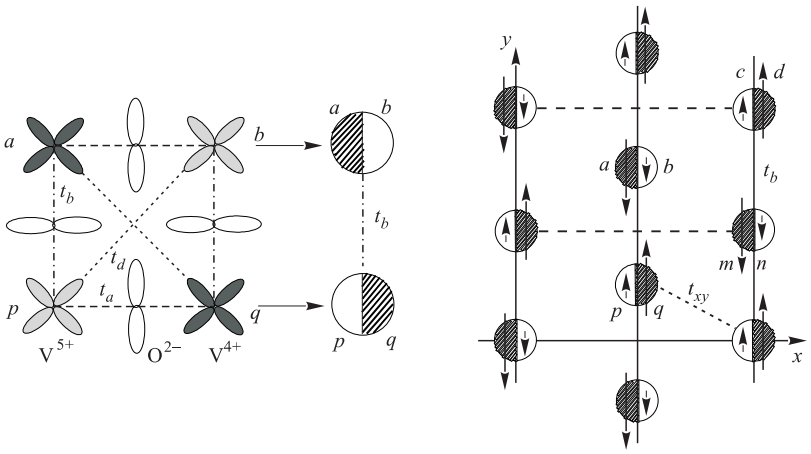

Fig. 1. The schematic view of $\alpha'-NaV_2O_5$. Each dimer/rung is replaced by a circle. The inter(intra)dimer hopping t_b (t_a) in the $b(a)$-direction is set along the $y(x)$ -axis. The distances at room temperature between the nearest V-ions on neighboring dimers/rungs are 3.04 Å and the leg constant is 3.61 Å. The dimer size is 3.44 Å. Oxygen p-wave functions (opened) enhance the hopping t_d along ladder diagonals. For $T > T_c$: the orthorhombic unit cell with two dimers is shown in lower panel. For $T < T_c$: the size of arrows (lower panel) reflects the charge disproportionation $\Delta n = n_{a,d,m,q} - n_{b,c,n,p}$ in the monoclinic unit cell; the shaded portions have a zigzag order

Reasonable simulation of the many-body effects is impossible in terms of the Fermi operators which are c-numbers. The necessity to introduce in this case the operators with more complicated permutation relations was indicated by Bogoliubov when developing the polar theory of metals already in 1949 year [6]. The applied technique [7] for the generalized Okubo-Hubbard X-operators in the superalgebra approach considers the tunneling part of any correlated Hamiltonian as perturbation with respect to strong electron correlations included in eigenvalues of the unperturbed part of Hamiltonian. The Hamiltonians with correlated electrons are rewritten in terms of basis and only basis vectors of corresponding superalgebra. The perturbation theory is based on the generalized Wick's theorem as an iteration procedure reducing the time-ordered product of n of X-operators to the product of $n - 1$ of thereof. The first order self-energy is the tunneling matrix itself from the perturbation Hamiltonian.

Here in the framework of the $su\,(2,2)$ superalgebra approach for $A^{+}V_2O_5$ systems we will neglect the effects of the scattering of correlated electrons at the spin and charge fluctuations, aiming at comparing the correlated electron spectra with the conventional tight-binding results which are done in the first order of the transfer energy. In the considered order of the perturbation theory we will concentrate on the influence of band structure effects which are of significance for multicomponent systems such as AV_2O_5.

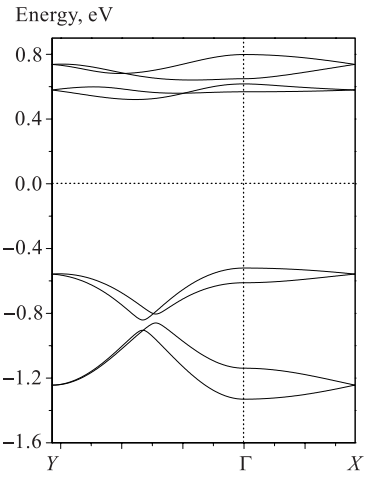

Fig. 2. The high-temperature ($T > T_c$) electron density of states in $\alpha' - NaV_2O_5$ for parameters $t_a = 0.35$ eV, $t_b = 0.15$ eV, $t_d = 0.1$ eV, $t_{xy} = 0.06$ eV, $U = 4$ eV (i.e., the effective value $I \simeq 0.6$ eV) as a function of dimensionless energies $\xi\ /(t_b + t_d)$, $E_F = 0$ (main panel). The inset shows the density of states for noninteracting bonding electrons

Angular part of d_{xy}-wave functions provides the layerness of $\alpha^{'}-NaV_2O_5$ and the small ratio r_B/a (a is a lattice constant and r_B is the V-ion Bohr radii) enables to calculate transfer integrals as power series of $(r_B/a)^2$. Their estimates show the strong influence of a V-ion core on an electron hopping and we will distinguish the t_{xy} magnitudes at $T < T_c$: $t_{xy}^{bc} = t + \delta$, $t_{xy}^{bm} = t$, $t_{xy}^{qm} = t - \delta$. Our main strategy is developed starting from the assumption that the quarter-filled dimers V_2 form an ideal triangular lattice in the layer of VO_5 pyramides (Fig. 1). *Below* T_c $\alpha' - NaV_2^{4+/5+}O_5$ is in an *ordered valence phase* whereas *above* T_c it is in a *mixed valence state*. Phase transition seems to be similar to the Verwey transition at $T_V \sim 120$ K in magnetite $FeFe_2^{2+/3+}O_4$ [8] with the charge ordered $Fe^{2+/3+}\left(3d^{6/5}\right)$ octahedral sites at $T < T_V$.

Below T_c the $d_{xy}-$electrons acquire the on-site energies in a monoclinic unit cell, $\varepsilon_{a,d,q,m}$=$-\varepsilon_{b,c,n,p} \equiv -\varepsilon$, influenced by neighboring Coulomb repulsion $V^{4+\Delta n/5-\Delta n}$: $\varepsilon = -V\Delta n$. Sites a, b, m, n and p, q, c, d have spin projections $down$ and up, respectively. This situation, in parallel with $U \gg t_{a,b,xy}$, allows one to consider spinless electrons. The energy dispersions are plotted in Fig. 2. The Coulomb gap Δ_C is provided by the zigzag order $\mp\varepsilon$ (Fig. 1), parameters $t_{a,d}$ and competing interdimer hops $t_{b,xy}$. The critical value $V_c \sim 0.02$ eV [9] corresponds to our threshold ε_c ($t_{xy} = 0.06$ eV, $\delta = 0.01$ eV) to trigger the phase transition. For realistic $t_{a,b,d,xy}$ and ε the so-called «spin-Peierls» phase transition occurs at $T_c = 35$ K (Fig.2). At small interladder hoppings the Coulomb gap is

$$\Delta_C = \sqrt{\varepsilon^2 + (t_a + 2t_b)^2} + \sqrt{\varepsilon^2 + (t_a - 2t_b)^2} - 4t_d. \tag{1}$$

Its estimated magnitude $\Delta_C \approx 1$ eV (see Fig. 2) for disproportionation $\Delta n = 0.8$, $V = 0.8$ eV [10], $t_a = 0.35$ eV, $t_b = 0.15$ eV, $t_d = 0.1$ eV corresponds to the observed strong absorption of the light [11]. Eq.(1) is the extension of the splitting in terms of the «charged-magnon» scenario used in Refs. 11, 12 for a single $V^{4+} - V^{5+}$ rung ($t_{b,d} = 0$).

Above T_c the tight-binding energy bands are split due to the electron correlations as

$$\begin{aligned} \frac{\xi_p^+}{t_b + t_d} &= \varepsilon_p^{\pm} + \frac{1}{2}\sqrt{\left(\frac{I}{t_b + t_d}\right)^2 + 4\left(\varepsilon_p^{\pm}\right)^2}, \\ \frac{\xi_p^-}{t_b + t_d} &= \varepsilon_p^{\pm} - \frac{1}{2}\sqrt{\left(\frac{I}{t_b + t_d}\right)^2 + 4\left(\varepsilon_p^{\pm}\right)^2}, \end{aligned} \tag{2}$$

where dimensionless tight-binding noncorrelated energies are

$$\varepsilon_p^{\pm} = -\cos p_y \pm 2t \cos\frac{p_y}{2} \cos\frac{p_x\sqrt{3}}{2} \left(t = \frac{t_{xy}}{2\left(t_b + t_d\right)}\right). \tag{3}$$

The correlated band gap

$$\Delta_g = \frac{1}{2}\left[\sqrt{I^2 + 4t_b^2} + \sqrt{I^2 + 4\left(t_b + t_{xy}\right)^2}\right] - 2t_b - t_{xy}, \tag{4}$$

is governed by the on-dimer repulsion for bonding electrons

$$I = 2t_a + U/2\left[1 - \sqrt{1 + \left(4t_a/U\right)^2}\right].$$

If it were metallic carriers, the ε_p^- and ε_p^+ would have provided the quasi-2D saddle and the quasi-1D saddleless portions of the Fermi surface. Therefore it would be quite interesting to investigate the doped oxides, e.g., $Na_{1-x}Ca_xV_2O_5$, $Na_{1-x}V_2O_5$. For noncorrelated energies the partial densities of electronic states

$\rho(\varepsilon)$ have an explicit form

$$\begin{aligned}
\rho\left(-1-2t\le\varepsilon^{-}\le-1\right) &= \frac{4}{\pi^2\sqrt{kt}}K(q),\\
\rho\left(-1\le\varepsilon^{-}\le-1+2t\right) &= \frac{4}{\pi^2\sqrt{kt}}F\left(\arcsin a\sqrt{\frac{2t}{(1+\varepsilon)k}};q\right),\\
\rho\left(-1+2t\le\varepsilon^{-}\le 1\right) &= \frac{4}{\pi^2 q\sqrt{kt}}K\left(\frac{1}{q}\right);\\
\rho\left(-1\le\varepsilon^{+}\le-1+2t\right) &= \frac{4}{\pi^2\sqrt{kt}}F(\arcsin a;q),\\
\rho\left(-1+2t\le\varepsilon^{+}\le\frac{1}{2}+t\right) &= \frac{4}{\pi^2 q\sqrt{kt}}F\left(\arcsin\frac{1}{a};\frac{1}{q}\right) \qquad (5)
\end{aligned}$$

via elliptic integrals F and K of the first kind with $q{=}\sqrt{[2t\,(t{+}k)+1{-}\varepsilon^2]\,/kt}/2$, $a=\sqrt{(1+\varepsilon)\,(t+k)\,k/\left[2t\,(t+k)+1-\varepsilon^2\right]}$, where $k=\sqrt{t^2+2\,(1-\varepsilon)}$. The main panel of Fig. 3 displays the density of correlated electron states, $\rho(\xi)$, with a gap Δ_g. In a limiting noncorrelated case, the $\rho(\varepsilon)$ (inset) reproduces the essentials of the first principle computations [13]. Logarithmic divergencies inside the band are clear manifestations of the 2D electronic structure. We would like to emphasize that in the 1D case ($t_{xy}\to 0$) the divergencies are square-root like and they are located at the band edges $\varepsilon=\pm 1$ (noncorrelated case).

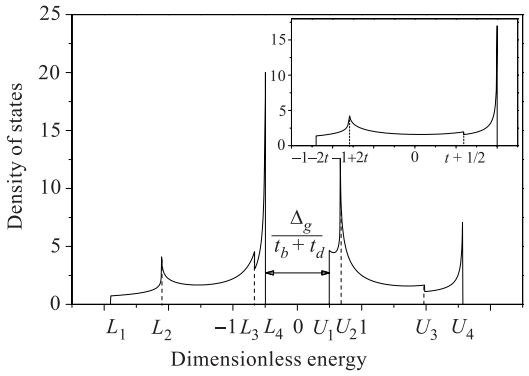

Fig. 3. The tight-binding energy dispersions for correlated d_{xy}-electrons in $\alpha'-NaV_2O_5$ below T_c for parameters $t_a=0.35$ eV, $t_b=0.15$ eV, $t_d=0.1$ eV, $t_{xy}^{bm}=0.06$ eV, $t_{xy}^{bc,qm}=t_{xy}^{bm}\pm\delta$ ($\delta=0.01$ eV) and $\varepsilon=V\Delta n$ ($V=0.8$ eV, $\Delta n=0.8$). Momenta are given in units $\left|p_x\sqrt{3}\right|=|p_y|=\pi$ of the Brillouine zone boundaries, the Fermi energy, $E_F=0$, is inside the Coulomb gap $\Delta_C=1$ eV

In summary, the analysis of the $\alpha^{'} - NaV_2O_5$ band structure leads to the conclusion about its pronounced 2D features. *The phase transition at T_c is shown to be not a spin-Peierls type but rather it is connected with the opening of the Coulomb gap in the electronic spectrum.* At $T > T_c$ the character of the insulating phase has been identified with a correlated band gap.

By virtue of the fact, that nature of the correlated energy (see Eq. (4)) is connected with the Heitler–London valence band state, our study supports the earlier proposal [5] to give the name *the Heitler–London insulators* to such systems as $A^{+}V_2O_5$, whereas the $A^{2+}V_2O_5$ materials are the Mott–Hubbard insulators. The presented description (also [14]) of the dimerized quarter-filled compounds, namely first members of AV_nO_{2n+1} oxides, in terms of the Hubbard-like model opens new possibilities to study a variety of their properties in terms of strongly correlated electron picture.

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A MIXED MEAN-FIELD/BCS-PHASE WITH AN ENERGY GAP AT HIGH T_c

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We construct a Hamiltonian which in a scaling limit becomes equivalent to one that can be diagonalized by a Bogoliubov transformation. There may appear simultaneously a mean-field and a superconducting phase. For instance, an attractive mean field may stimulate the superconducting phase even at high temperatures.

INTRODUCTION

In quantum mechanics a mean field theory means that the particle density $\rho(x) = \psi^*(x)\psi(x)$ (in second quantization) tends to a *c*-number in a suitable scaling limit. Of course, $\rho(x)$ is only an operator-valued distribution, and the smeared densities $\rho_f = \int dx\, \rho(x) f(x)$ are (at best) unbounded operators, so norm convergence is not possible. The best one can hope for is strong resolvent convergence in a representation where the macroscopic density is built in. The BCS-theory of superconductivity is of a different type where pairs of creation operators with opposite momentum $\tilde{\psi}^*(k)\,\tilde{\psi}^*(-k)$ ($\tilde{\psi}$ the Fourier transform and with the same provisio) tend to *c*-numbers. This requires different types of correlations and one might think that the two possibilities are mutually exclusive. We shall show that this is not so by constructing a pair potential where both phenomena occur simultaneously. On purpose we shall use only one type of fermions as one might think that the spin-up electrons have one type of correlation and the spin-down — the other. Also the state which carries both correlations is not an artificial construction but it is the KMS-state of the corresponding Bogoliubov Hamiltonian. Whether the phenomenon occurs or not depends on whether the emerging two coupled «gap equations» have a solution or not, which happens to be the case in certain regions of the parameter space (temperature, chemical potential, relative values of the two coupling constants). Moreover, in

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the new phases with $\lambda_B, \lambda_M < 0$ transition temperature T_c may become arbitrarily high. Our considerations hold for arbitrary space dimension.

1. QUADRATIC FLUCTUATIONS IN A KMS-STATE

The solvability of the BCS-model [1] rests upon the observation [2] that in an irreducible representation the space average of a quasi-local quantity is a *c*-number and is equal to its ground state expectation value. This allows one to replace the model Hamiltonian by an equivalent approximating one [3]. Remember that two Hamiltonians are considered to be equivalent when they lead to the same time evolution of the local observables [4].

The same property holds on also in a temperature state (the KMS-state) and under conditions to be specified later it makes the co-existence of other types of phases possible.

To make this apparent, consider the approximating (Bogoliubov) Hamiltonian

$$\begin{aligned} H'_B &= \int dp \left\{ \omega(p) a^*(p) a(p) + \frac{1}{2} \Delta_B(p) \left[a^*(p) a^*(-p) + a(-p) a(p) \right] \right\} \\ &= \int W(p) b^*(p) b(p) \,, \end{aligned} \tag{1.1}$$

which has been diagonalized by means of a standard Bogoliubov transformation with real coefficients (the irrelevant infinite constant in H'_B has been omitted)

$$b(p) = c(p) a(p) + s(p) a^*(-p) \,, \qquad a(p) = c(p) b(p) - s(p) b^*(-p)$$

with

$$c(p) = c(-p) \,, \qquad s(p) = -s(-p) \,, \qquad c^2(p) + s^2(p) = 1 \,, \tag{1.2}$$

so that the following relations hold (keeping in mind that Δ, W, s, c will be β-dependent)

$$W(p) = \sqrt{\omega^2(p) + \Delta_B^2(p)} = W(-p),$$

$$c^2(p) - s^2(p) = \omega(p)/W(p) \,, \qquad 2c(p)s(p) = \Delta_B(p)/W(p). \tag{1.3}$$

Hamiltonian (1.1) generates a well defined time evolution and a KMS-state for the b-operators. For the original creation and annihilation operators a, a^* this gives the following evolution

$$a(p) \to a(p) \left(c^2(p) e^{-iW(p)t} + s^2(p) e^{iW(p)t} \right) - 2i a^*(-p) c(p) s(p) \sin W(p) t$$

and nonvanishing termal expectations

$$\begin{aligned}\langle a^*(p)a(p')\rangle &= \delta(p-p')\left\{\frac{c^2(p)}{1+e^{\beta(W(p)-\mu)}}+\frac{s^2(p)}{1+e^{-\beta(W(p)-\mu)}}\right\}\\ &:= \delta(p-p')\{p\}, \qquad (1.4)\\ \langle a(p)a(-p')\rangle &= \delta(p-p')c(p)s(p)\tanh\frac{\beta(W(p)-\mu)}{2}:=\delta(p-p')[p], \qquad (1.5)\end{aligned}$$

$$\{p\}=\{-p\}, \qquad [p]=-[-p]$$

c and s are multiplication operators and are never Hilbert–Schmidt. Thus different c and s lead to inequivalent representations and should be considered as different phases of the system.

The expectation value of a biquadratic (in creation and annihilation operators) quantity is expressed through (1.4,5)

$$\begin{aligned}\langle a^*(q)a^*(q')a(p)a(p')\rangle = \delta(q+q')\delta(p+p')[q][p]-\\ -\delta(p-q)\delta(p'-q')\{p\}\{p'\}+\delta(p-q')\delta(p'-q)\{p\}\{p'\}. \qquad (1.6)\end{aligned}$$

So far we have written everything in terms of the operator valued distributions $a(p)$. They can be easily converted into operators in the Hilbert space generated by the KMS-state by smearing with suitable test functions. Thus, by smearing with, e.g.,

$$e^{-\kappa(p+p')^2-\kappa(q+q')^2}v(p)v(q), \qquad v\in L_2(\mathbf{R}^d) \qquad (1.7)$$

one observes that in the limit $\kappa\to\infty$ the first term in (1.6) remains finite

$$0<\int dp\,dq\,v(p)\,v(q)[p][q]<\infty\,,$$

while the two others vanish

$$\lim_{\kappa\to\infty}\int dp\,dp'e^{-2\kappa(p+p')^2}\,v(p)\,v(p')\{p\}\{p'\}=\lim_{\kappa\to\infty}\kappa^{-3/2}\int dpv^2(p)\{p\}^2=0.$$

Since we are in the situation of *Lemma 1* in [5], we have thus proved the following statement

$$\text{s-}\lim_{\kappa\to\infty}\int dp\,dp'\mathcal{V}(q,q',p,p')e^{-\kappa(p+p')^2}a(p)a(p')=\int dp\mathcal{V}(q,q',p,-p)[p] \qquad (1.8)$$

for kernels $\mathcal{V}$ such that the integrals are finite.

With this observation in mind, a potential which acts for $\kappa \to \infty$ like (1.1) might be written as

$$V_B{=}\kappa^{3/2} \int dp\, dp'\, dq\, dq'\, a^*(q)a^*(q')a(p)a(p')\mathcal{V}_B(q,q',p,p')\, e^{-\kappa(p+p')^2-\kappa(q+q')^2} \tag{1.9}$$

with $\mathcal{V}_B(q,q',p,p') = -\mathcal{V}_B(q',q,p,p')$, etc., in order to respect the Fermi-nature of a's. This potential has the property

$$\begin{aligned} \|V\| &< \infty \qquad \text{for } \kappa < \infty, \\ \|V\| &\to \infty \qquad \text{for } \kappa \to \infty. \end{aligned}$$

Despite this divergence, potential (1.9) may still generate a well-defined time evolution. The strong resolvent convergence in (1.8) is essential, weak convergence would not be enough since it does not guarantee the automorphism property

$$\tau^t_\kappa(ab) = \tau^t_\kappa(a)\tau^t_\kappa(b) \;\to\; \tau^t_\infty(ab) = \tau^t_\infty(a)\tau^t_\infty(b)\,.$$

Note that the parameter κ plays in this construction the role of the volume from the considerations in [2].

In the mean-field regime we want an effective Hamiltonian

$$H''_B = \int dp\, [\omega(p)a^*(p)a(p) + \Delta_M(p)a^*(p)a(p)]\ . \tag{1.10}$$

Here the KMS-state is defined for the operators a, a^* themselves and one should rather smear by means of

$$e^{-\kappa(q-p)^2-\kappa(q'-p')^2} v(p)v(p') \tag{1.11}$$

instead of (1.7), thus concluding that

$$\text{s-}\lim_{\kappa\to\infty} \int dp\, dq e^{-\kappa(q-p)^2} a^*(q)a(p)\mathcal{V}_M(q,q',p,p') = -\int dp \frac{\mathcal{V}_M(p,q',p,p')}{1+e^{\beta(\varepsilon(p)-\mu)}}\,, \tag{1.12}$$

with $\varepsilon(p) = \omega(p) + \Delta_M(p)$. Relation (1.12) then suggests another starting potential

$$V_M{=}\kappa^{3/2}\int dp\, dp'\, dq\, dq'\, a^*(q)a^*(q')a(p)a(p')\mathcal{V}_M(q,q',p,p')\, e^{-\kappa(q-p)^2-\kappa(q'-p')^2} \tag{1.13}$$

with the same symmetry for the density $\mathcal{V}_M$ as in (1.9). However, in both cases a Gaussian form factor in the smearing functions (1.7),(1.11) has been chosen just for simplicity. In principle, this might be C^∞_o functions which have the δ-function as a limit.

2. THE MODEL

Consider the following Hamiltonian

$$H = H_{\rm kin} + V_B + V_M\,, \tag{2.1}$$

where $H_{\rm kin}$ is the kinetic term and V_B, V_M are given by (1.9),(1.13). The solvability of the model for $\kappa \to \infty$ depends on whether or not it would be possible to replace (2.1) by an equivalent Hamiltonian that might be readily diagonalized. The object of interest is the commutator of, say, a creation operator with the potential. With (1.8), (1.12) taken into account, it reads

$$[a(k), V]{=}2\int dp\,\{c(p)s(p)\,[p]\,\mathcal{V}_B(k,-k,p,-p)a^*(-k){+}\mathcal{V}_M(p,k,p,k)\,\{p\}\,a(k)\}\,. \tag{2.2}$$

The Bogoliubov-type Hamiltonian for our problem should be a combination of (1.1) and (1.10), that is of the form

$$H_B{=}\int dp\left\{a^*(p)a(p)[\omega(p)+\Delta_M(p)] + \frac{1}{2}\Delta_B(p)[a^*(p)a^*(-p)+a(-p)a(p)]\right\}. \tag{2.3}$$

This Hamiltonian becomes equivalent to the model Hamiltonian (2.1), provided the commutator $[a(k), H_B - H_{\rm kin}]$ equals (2.2). Thus we are led to a system of two coupled «gap equations»

$$\frac{1}{2}\Delta_M(k) \;=\; \int \mathcal{V}_M(k,p)\left\{\frac{c^2(p)}{1{+}e^{\beta(\overline{W}(p)-\mu)}}{+}\frac{s^2(p)}{1{+}e^{-\beta(\overline{W}(p)-\mu)}}\right\}dp, \tag{2.4}$$

$$\Delta_B(k) \;=\; \int \mathcal{V}_B(k,p)\,\frac{\Delta_B(p)}{\overline{W}(p)}\,\tanh\frac{\beta(\overline{W}(p)-\mu)}{2}\,dp\,, \tag{2.5}$$

with

$$\overline{W}(p) = \sqrt{[\omega(p)+\Delta_M(p)]^2 + \Delta_B^2(p)}\,. \tag{2.6}$$

c (and thus s, Eq.(1.2)) are determined by either of the following conditions

$$c^2(p) - s^2(p) = [\omega(p)+\Delta_M(p)]/\overline{W}(p)\,, \qquad 2c(p)s(p) = \Delta_B(p)/\overline{W}(p)\,. \tag{2.7}$$

The temperature and the interaction-strength dependence of the system (2.4–7) encode the solvability of the model [6].

3. HIGH T_c CASE

We are now looking for a mechanism for high temperature superconductivity, i.e., a high T_c where Δ_B starts to vanish. If we make the ansatz

$$\mathcal{V}_B(k,p) = \lambda_B v(k) v(p)\,, \qquad \int v^2(p)dp = 1\,, \qquad v(p) = -v(-p)\,,$$

then (2.5) becomes

$$\Delta_B(k) = \lambda_B v(k) \int dp \frac{v(p)\Delta_B(p)}{\overline{W}(p)} \tanh \frac{\beta(\overline{W}(p)-\mu)}{2}\,.$$

For $\lambda_B < 0$ we must have $\overline{W} < \mu$ and since $\tanh x < x\,, \forall x > 0$, we conclude that

$$T < \frac{|\lambda_B|}{2} \int dp v^2(p) \left(\frac{\mu}{\overline{W}(p)} - 1\right)\,.$$

If Δ_B starts to vanish, $\overline{W}(p) = |\omega(p) + \Delta_M(p)|$, so if $\Delta_M < 0$ and near $\omega(p)$, T_c can become arbitrarily high

$$T_c < \frac{|\lambda_B|}{2} \left(-1 + \mu \int \frac{dp v^2(p)}{|\omega(p) + \Delta_M(p)|}\right)\,.$$

Thus a negative mean field which almost cancels the kinetic energy ω gives the electrons so much mobility to respond to $\lambda_B < 0$ that even at high temperatures a gap Δ_B can develope. There is a small problem since $\Delta_B(-k) = -\Delta_B(k)$. However $v(k)$ need not be continuous and since only Δ_B^2 enters in $\overline{W}$ the gap parameter $\Delta_B^2(0)$ can effectively be $\neq 0$. This problem disappears if we include spin and thus have $a_\uparrow(p)a_\downarrow(-p)$ in V_B.

4. CONCLUSION

Our model has four parameters, $\lambda_M, \lambda_B, \mu, T$, but by scaling only their ratios are essential. For infinite temperature $\beta = 0$ Eqs. (3.1–3) admit only the mean field solution $\Delta_B = 0$, $\Delta_M = \lambda_M$, $\overline{W} = \mu + \lambda_M$. By lowering the temperature one meets also the BCS-type solution but in a rather complicated region in the 3-dimensional parameter space.

Whenever λ_B is positive, it must be also $> \mu$. Also for negative λ_B, λ_M and $\lambda_M > -\mu$ there exists a finite gap for λ_B. A perturbation theory with respect to λ_B is in general doomed to failure since for no point on the $\lambda_B = 0$ axis there is a neighbourhood full of the $\Delta_B \neq 0$ phase.

It is interesting that without a mean field (the $\lambda_M = 0$ axis) there are superconducting solutions only for $\lambda_B > \mu$. An attractive mean field ($\lambda_M < 0$)

stimulates superconductivity since then it also appears for negative λ_B. However, too strong mean field attraction destroyes it again.

The most remarkable fact is that whilst for $\lambda > 0$ the temperature for a superconducting phase is limited as in the BCS theory by $T \ll (\lambda_B - \mu)/2$, in the new phases for $\lambda_B < 0$, $\lambda_M < 0$ we only get $T < |\lambda_B||\lambda_M|/2(\mu - |\lambda_M|)$ and thus for $\lambda_M \to -\mu$, T can become arbitrarily big.

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DUALITY SUMMETRY OF THE 2D Φ^4 FIELD MODEL

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We show that the exact beta-function $\beta(g)$ of the continuous 2D $g\Phi^4$ model in the strong coupling regime $g > g_+^*$ possesses the Kramers–Wannier duality symmetry. The duality symmetry transformation $\tilde{g} = d(g)$ such that $\beta(d(g)) = d'(g)\beta(g)$ is constructed. The approximate values of the fixed point g_+^* computed from the duality equation $d(g_+^*) = g_+^*$ are shown to agree with those obtained from the strong coupling expansion and with available numerical results.

1. INTRODUCTION

The 2D Ising model and some other lattice spin models are known to possess the remarkable Kramers–Wannier(KW) duality symmetry, playing an important role both in statistical mechanics and in quantum field theory [1–3]. The self-duality of the isotropic 2D Ising model means that there exists an exact mapping between the high-T and low-T expansions of the partition function [3]. In the transfer-matrix language this implies that the transfer-matrix of the model under discussion is covariant under the duality transformation. If we assume that the critical point is unique, the KW self-duality would yield the exact Curie temperature of the model. This holds for a large set of lattice spin models including systems with quenched disorder (for a review see [3, 4]).

In this paper we study mainly the symmetry properties of the beta-function $\beta(g)$ for the 2D $g\Phi^4$ theory, regarded as a continuum limit of the exactly solvable 2D Ising model. In contrast to the latter, the 2D $g\Phi^4$ theory is known not to be an integrable quantum field theory.

The beta-function $\beta(g)$ of the continuum limit theory is known to date only in the four-loop approximation within the framework of conventional perturbation theory at fixed dimension $d = 2$ [5]. (Five-loop RG calculations have also been recently completed [6]). Calculations of beta-functions are of great interest in statistical mechanics and quantum field theory. The beta-function contains the essential information on the renormalized coupling constant g_+^*, this being

important for constructing the equation of state of the 2D Ising model. Duality is known to impose some important constraints on the exact beta-function [7].

The paper is organized as follows. In Sect. II we set up basic notations and define both the correlation length and the beta-function $\beta(g)$. In Sect.III the duality symmetry transformation $\tilde{g} = d(g)$ is derived. Then it is proved that $\beta(d(g)) = d'(g)\beta(g)$. An approximate expression for $d(g)$ is also found. Sect. IV contains some concluding remarks.

2. CORRELATION LENGTH AND COUPLING CONSTANT

We begin by considering the standard Hamiltonian of the 2D Ising model (in the absence of an external magnetic field), defined on a square lattice with periodic boundary conditions; as usual:

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j, \tag{2.1}$$

where $< i, j >$ indicates that the summation is over all nearest-neighboring sites; $\sigma_i = \pm 1$ are spin variables and J is the spin coupling. The standard definition of the spin-pair correlation function reads:

$$G(R) =< \sigma_{\mathbf{R}} \sigma_{\mathbf{0}} >, \tag{2.2}$$

where $< ... >$ stands for the thermal average.

The statistical mechanics definition of the correlation length is given by [8]

$$\xi^2 = \frac{d \ln G(p)}{dp^2}|_{p=0}. \tag{2.3}$$

The quantity ξ^2 is known to be conveniently expressed in terms of the spherical moments of the spin correlation function itself, namely

$$\mu_l = \sum_{\mathbf{R}} (R/a)^l G(\mathbf{R}) \tag{2.4}$$

with a being some lattice spacing. It is easy to see that

$$\xi^2 = \frac{\mu_2}{2d\mu_0} \tag{2.5}$$

where d is the spatial dimension (in our case $d = 2$).

In order to extend the KW duality symmetry to the continuous field theory we have need for a «lattice» model definition of the coupling constant g, equivalent

to the conventional one exploited in the RG approach. The renormalization coupling constant g of the $g\Phi^4$ theory is closely related to the fourth derivative of the «Helmholtz free energy», namely $\partial^4 F(T,m)/\partial m^4$, with respect to the order parameter $m = \langle\Phi\rangle$. It may be defined as follows (see [8])

$$g(T,h) = -\frac{(\partial^2\chi/\partial h^2)}{\chi^2\xi^d} + 3\frac{(\partial\chi/\partial h)^2}{\chi^3\xi^d}, \tag{2.6}$$

where χ is the homogeneous magnetic susceptibility

$$\chi = \int d^2x G(x). \tag{2.7}$$

It is in fact easy to show that $g(T,h)$ in Eq.(2.6) is merely the standard four-spin correlation function taken at zero external momenta. The renormalized coupling constant of the critical theory is defined by the double limit

$$g^* = \lim_{h\to 0}\lim_{T\to T_c} g(T,h) \tag{2.8}$$

and it is well known that these limits do not commute with each other. As a result, g^* is a path-dependent quantity in the thermodynamic (T,h) plane [8].

Here we are mainly concerned with the coupling constant on the isochore line $g(T > T_c, h = 0)$ in the disordered phase and with its critical value

$$g_+^* = \lim_{T\to T_c^+} g(T, h=0) = -\frac{\partial^2\chi/\partial h^2}{\chi^2\xi^d}|_{h=0}. \tag{2.9}$$

The «lattice» coupling constant g_+^* defined in Eq. (2.9) is of course some given function of the temperature T_c.

3. DUALITY SYMMETRY OF THE BETA-FUNCTION

The standard KW duality tranformation is known to be as follows [1–3]

$$\sinh(2\tilde{K}) = \frac{1}{\sinh(2K)}. \tag{3.1}$$

We shall see that it will be more convenient to deal with a new variable $s = \exp(2K)\tanh(K)$, where $K = J/T$.

It follows from the definition that s transforms as $\tilde{s} = 1/s$; this implies that the correlation length of the 2D Ising model given by $\xi^2 = \frac{s}{(1-s)^2}$ is a self-dual quantity [9]. Now, on the one hand, we have the formal relation

$$\xi\frac{ds(g)}{d\xi} = \frac{ds(g)}{dg}\beta(g), \tag{3.2}$$

where $s(g)$ is defined as the inverse function of $g(s)$, i.e., $g(s(g)) = g$ and the beta-function is given, as usual, by

$$\xi \frac{dg}{d\xi} = \beta(g). \tag{3.3}$$

On the other hand, it is known from [9] that

$$\xi \frac{ds}{d\xi} = \frac{2s(1-s)}{(1+s)}. \tag{3.4}$$

From Eqs. (3.2)–(3.4), a useful representation of the beta-function in terms of the $s(g)$ function thus follows

$$\beta(g) = \frac{2s(g)(1-s(g))}{(1+s(g))\,(ds(g)/dg)}. \tag{3.5}$$

Let us define the dual coupling constant $\tilde{g}$ and the duality transformation function $d(g)$ as

$$s(\tilde{g}) = \frac{1}{s(g)}; \qquad \tilde{g} \equiv d(g) = s^{-1}(\frac{1}{s(g)}), \tag{3.6}$$

where $s^{-1}(x)$ stands for the inverse function of $x = s(g)$. It is easy to check that a further application of the duality map $d(g)$ gives back the original coupling constant, i.e., $d(d(g)) = g$, as it should be. Notice also that the definition of the duality transformation given by Eq. (3.6) has a form similiar to the standard KW duality equation, Eq. (3.1).

Consider now the symmetry properties of $\beta(g)$. We shall see that the KW duality symmetry property, Eq. (3.1), results in the beta-function being covariant under the operation $g \to d(g)$:

$$\beta(d(g)) = d'(g)\beta(g). \tag{3.7}$$

To prove it let us evaluate $\beta(d(g))$. Then Eq.(3.5) yields

$$\beta(d(g)) = \frac{2s(\tilde{g})(1-s(\tilde{g}))}{(1+s(\tilde{g}))\,(ds(\tilde{g})/d\tilde{g})}. \tag{3.8}$$

Bearing in mind Eq. (3.6) one is led to

$$\beta(d(g)) = \frac{2s(g)-2}{s(g)(1+s(g))\,(ds(\tilde{g})/d\tilde{g})}. \tag{3.9}$$

The derivative in the r.h.s. of Eq. (3.9) should be rewritten in terms of $s(g)$ and $d(g)$. It may be easily done by applying Eq. (3.6):

$$\frac{ds(\tilde{g})}{d\tilde{g}} = \frac{d}{d\tilde{g}}\frac{1}{s(g)} = -\frac{s'(g)}{s^2(g)}\frac{1}{d'(g)}. \tag{3.10}$$

Substituting the r.h.s. of Eq. (3.10) into Eq. (3.9) one obtains the desired symmetry relation, Eq. (3.7).

Therefore, the self-duality of the model allows us to determine the fixed point value in another way, namely from the duality equation $d(g^*) = g^*$.

Making use of a rough approximation for $s(g)$, one gets [9]

$$s(g) \simeq \frac{2}{g} + \frac{24}{g^2} \simeq \frac{2}{g}\frac{1}{1-12/g} = \frac{2}{g-12}. \tag{3.11}$$

Combining this Padé-approximant with the definition of $d(g)$, Eq. (3.6), one is led to

$$d(g) = 4\frac{3g-35}{g-12}. \tag{3.12}$$

The fixed point of this function, $d(g^*) = g^*$, is easily seen to be $g^*_+ = 14$. The recent numerical and analytical estimates yield $g^*_+ = 14.69$ (see [9–11] and references therein).

It is worth mentioning that the above-described approach may be regarded as another method for evaluating g^*_+, fully equivalent to the standard beta-function method.

4. CONCLUDING REMARKS

We have proved the existence of the duality symmetry transformation $d(g)$ in the $2D$ $g\Phi^4$ theory such that $\beta(d(g)) = d'(g)\beta(g)$. Actually, this symmetry property was shown to result from the KW duality of the 2D lattice Ising model.

It would be tempting but wrong to regard $d(g)$ as a function connecting the weak-coupling and strong coupling regimes. As a matter of fact, our proof is based on the properties of $g(s), s(g)$ defined only for $0 \le s < \infty, g^*_+ \le g < \infty$ and therefore does not cover the weak-coupling region, $0 \le g \le g^*$. The main statement is that the beta-function $\beta(g)$ does have the dual symmetry only in the strong-coupling region, in contrast to the weak-coupling regime where that symmetry is dynamically broken.

In contrast to widely held views, the duality symmetry imposes only mild restrictions on $\beta(g)$. It means that this symmetry property fixes only even derivatives of the beta-function, $\beta^{(2k)}(g^*_+)(k = 0, 1, ...)$, at the fixed point, leaving the odd derivatives free. The duality equation $d(g) = g$ provides yet another method for determining the fixed point, independently of the approach based on the equation $\beta(g) = 0$. Another open problem is also that of finding a systematic approach for calculating $d(g)$.

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«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
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QUASIAVERAGES IN MICROSCOPIC THEORY OF LIQUID CRYSTALS

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Currently, the theoretical substantiation of statistical physics of condensed media with spontaneously broken symmetry is a quasi-average concept by N.Bogoliubov [1]. Said concept extends Gibbs distribution to degenerate condensed media. Within liquid crystals, there occurs a spontaneous breaking of rotational and in some cases of translational invariance within a configuration space. Dynamic features of such media have been previously investigated mainly by phenomenology methods [2,3].

There in report is introduced an order-parameter operator for liquid crystals, which is expressed in terms of field operators. Thermodynamics and ideal hydrodynamics for uniaxial nematic was built. There is reviewed a connection between presently-proposed and phenomenological Hamiltonian approaches. A quasi-average of physical value is defined by relation

$$\begin{array}{c} \langle a(\mathbf{x})\rangle \equiv \lim_{\nu\to 0}\lim_{V\to\infty}\mathrm{Sp}w_\nu\hat{a}(\mathbf{x}), \\ \hat{w}_\nu \equiv \exp(\Omega_\nu - Y_a\hat{\gamma}_a - \nu\hat{F}). \end{array} \tag{1}$$

Here $\hat{\gamma}_a \equiv \int d^3x\hat{\gamma}_a(\mathbf{x})$ are operators of additive motion integrals ($\hat{H} = \int d^3x\hat{\varepsilon}(\mathbf{x})$ is Hamiltonian, $\hat{P}_k = \int d^3x\hat{\pi}_k(\mathbf{x})$ is a momentum operator, $\hat{N} = \int d^3x\hat{n}(\mathbf{x})$ is a particle number operator), ($Y_a \equiv Y_0,\ Y_k,\ Y_4$) are thermodynamic forces, (for simply we allow $Y_k = 0$). Thermodynamic potential Ω_ν should be defined from the normalization condition of $\mathrm{Sp}w_\nu = 1$. Operator $\hat{F}$ possesses the symmetry of the investigated phase and eliminates the degeneration of equilibrium state of statistical equilibrium. Let us define the liquid crystals order parameter by formula:

$$\hat{Q}_{uv} \equiv \nabla_u\hat{\psi}^+(\mathbf{x})\ \nabla_v\hat{\psi}(\mathbf{x}) + \nabla_v\hat{\psi}^+(\mathbf{x})\ \nabla_u\hat{\psi}(\mathbf{x}) - \frac{2}{3}\delta_{uv}\nabla_j\hat{\psi}^+(\mathbf{x})\ \nabla_j\hat{\psi}(\mathbf{x}). \tag{2}$$

The source $\hat{F}$ is a linear functional of the order parameter operator $\hat{Q}_{uv}$:

$$\hat{F} = \int d^3x\ f_{ik}(\mathbf{x},t)\hat{Q}_{ik}(\mathbf{x}). \tag{3}$$

Here $f_{ik}(\mathbf{x},t)$ are the c-number functions of coordinates and time respectively, which characterize equilibrium state values $Q_{ik}(\mathbf{x}) = \langle\hat{Q}_{ik}(\mathbf{x})\rangle$. Structure of functions $f_{ik}(\mathbf{x},t)$ is determined by the symmetry properties of the equilibrium phases. Taking into account definition (2) and form of additive integrals of motion one can obtain the following algebra:

$$\begin{gathered}[\,\hat{N},\hat{Q}_{uv}(\mathbf{x})\,]=0,\quad i[\,\hat{P}_k,\hat{Q}_{uv}(\mathbf{x})\,]=-\nabla_k\hat{Q}_{uv}(\mathbf{x}),\\ i[\,\hat{L}_i,\hat{Q}_{uv}(\mathbf{x})\,]=-\varepsilon_{iuj}\hat{Q}_{jv}(\mathbf{x})-\varepsilon_{ivj}\hat{Q}_{ju}(\mathbf{x})-\varepsilon_{ikl}x_k\nabla_l\hat{Q}_{uv}(\mathbf{x}),\end{gathered}\tag{4}$$

where $\hat{L}_i$ orbital momentum. The quasi-average of order parameter $Q_{ik}(\mathbf{x},\hat{\rho}) = \mathrm{Sp}\,\hat{\rho}\,\hat{Q}_{ik}(\mathbf{x})$, where $\hat{\rho}$ is an arbitrary statistical operator, possesses the properties: $Q_{uv}(\mathbf{x},\hat{\rho}) = Q_{vu}(\mathbf{x},\hat{\rho})$, $Q_{uu}(\mathbf{x},\hat{\rho}) = 0$, and, therefore, contains five independent values. Let us parametrize said values by relation

$$\begin{aligned}Q_{ik}(\mathbf{x},\hat{\rho}) = Q(\mathbf{x},\hat{\rho})\left(l_i(\mathbf{x},\hat{\rho})l_k(\mathbf{x},\hat{\rho})-\frac{1}{3}\delta_{ik}\right)+\\ +Q'(\mathbf{x},\hat{\rho})\left(m_i(\mathbf{x},\hat{\rho})m_k(\mathbf{x},\hat{\rho})-\frac{1}{3}\delta_{ik}\right).\end{aligned}\tag{5}$$

Here Q, Q' are modules of order parameter, $\mathbf{l},\mathbf{m}$ are vectors of spatial anisotropy and there are real and orthonormalized vectors (directors) $\mathbf{l}^2 = \mathbf{m}^2 = 1$, $\mathbf{lm} = 0$. In general case the order parameter (5) describes biaxial liquid crystals. Individual cases with uniaxial liquid crystals are reproduced from this factor by limit transition $Q \to 0$, or $Q' \to 0$.

Symmetry of equilibrium state of uniaxial nematics with respect to rotation in real space has the form:

$$[\,\hat{w},\hat{P}_k\,]=0,\quad [\,\hat{w},l_i\hat{L}_i\,]=0,\tag{6}$$

where l_i — vector of spatial anisotropy. Taking into account formulae (6) and operator algebra (4) we come to the equations determining equilibrium structure of order parameter:

$$\begin{gathered}i\mathrm{Sp}[\,\hat{w},l_i\hat{L}_i\,]=-l_i(\varepsilon_{iuj}Q_{jv}(\mathbf{x},Y,\mathbf{l})+\varepsilon_{ivj}Q_{ju}(\mathbf{x},Y,\mathbf{l}))=0,\\ i\mathrm{Sp}[\,\hat{w},\hat{P}_k\,]=-\nabla_kQ_{ju}(\mathbf{x},Y,\mathbf{l})=0,\end{gathered}$$

whereby the solution hereof is formed as

$$Q_{uv}(\mathbf{x},Y,\mathbf{l})\equiv Q_{uv}(Y,\mathbf{l})=Q(Y)(l_ul_v-\frac{1}{3}\delta_{ik}),\quad Q(Y)=Q(Y_0,Y_4).$$

It is not a problem to find, in similar way, that function f_{uv} has the form $f_{uv} = l_ul_v - \frac{1}{3}\delta_{uv}$. Such liquid crystal is described by statistical operator $\hat{w} = \hat{w}(Y,\mathbf{l})$,

which depends on thermodynamic forces and director, whereby dependence of averages from last argument is kept the same after limits $V \to \infty,\ \nu \to 0$.

Let's introduce into consideration densities and flux densities of additive integral of motion. According to [4]

$$\dot{\hat{n}}(\mathbf{x}) = -\nabla_k \hat{g}_k(\mathbf{x}), \quad \hat{g}_k(\mathbf{x}) = i \int d^3x'\, x'_k \int_0^1 d\lambda [\, \hat{\varepsilon}(\mathbf{x}-(1-\lambda)\mathbf{x}'), \hat{n}(\mathbf{x}+\lambda\mathbf{x}')\,] \tag{7}$$

is flux density operator of particle number,

$$\begin{gathered} \dot{\hat{\pi}}_i(\mathbf{x}) = -\nabla_k \hat{t}_{ik}(\mathbf{x}), \\ \hat{t}_{ik}(\mathbf{x}) = -\hat{\varepsilon}(\mathbf{x})\delta_{ik} + i \int d^3x'\, x'_k \int_0^1 d\lambda [\, \hat{\varepsilon}(\mathbf{x}-(1-\lambda)\mathbf{x}'), \hat{\pi}_i(\mathbf{x}+\lambda\mathbf{x}')\,] \end{gathered} \tag{8}$$

is flux density operator of momentum,

$$\dot{\hat{\varepsilon}}(\mathbf{x}) = -\nabla_k \hat{q}_k(\mathbf{x}), \quad \hat{q}_k(\mathbf{x}) = \frac{i}{2} \int d^3x'\, x'_k \int_0^1 d\lambda [\, \hat{\varepsilon}(\mathbf{x}-(1-\lambda)\mathbf{x}'), \hat{\varepsilon}(\mathbf{x}+\lambda\mathbf{x}')\,] \tag{9}$$

is flux density operator of energy. According to (5), relation

$$Q_{ik}(\mathbf{x}, \hat{\rho}) \equiv \frac{3}{2} l_j(\mathbf{x}, \hat{\rho}) Q_{jp}(\mathbf{x}, \hat{\rho}) l_p(\mathbf{x}, \hat{\rho}) (l_i(\mathbf{x}, \hat{\rho}) l_k(\mathbf{x}, \hat{\rho}) - \frac{1}{3}\delta_{ik}) \tag{10}$$

can be defined indirectly a unit anisotropy vector (director) in terms of order parameter for uniaxial liquid crystal. Let's introduce spatial anisotropy vector operator in accordance with approach [5]

$$\delta l_k(\mathbf{x}, \hat{\rho}) \equiv \mathrm{Sp}\delta\rho \hat{l}_k(\mathbf{x}, \hat{\rho}). \tag{11}$$

We have to find explicit form of operator $\hat{l}_k(\mathbf{x}, \hat{\rho})$ in terms of order parameter operator $\hat{Q}_{ik}(\mathbf{x})$. This will allow us to obtain dynamical equations for set of parameters of abridge description and to establish connection between proposed microscopic approach and Hamilton approach. Varying of (10) and taking into account indentity $l_i(\mathbf{x}, \hat{\rho})\hat{l}_i(\mathbf{x}, \hat{\rho})$, one can obtain

$$\hat{l}_j(\mathbf{x}, \hat{\rho}) = \frac{\hat{Q}_{uv}(\mathbf{x}) l_v(\mathbf{x}, \hat{\rho})}{Q(\mathbf{x})} \delta^{\perp}_{uj}(\mathbf{l}(\mathbf{x}, \hat{\rho})). \tag{12}$$

In accordance with (10),(12) we obtain the following expression:

$$i\mathrm{Sp}\hat{\rho}[\, \hat{\pi}_i(\mathbf{x}), \hat{l}_\lambda(\mathbf{x}, \hat{\rho})\,] = -l_i(\mathbf{x}', \hat{\rho})\delta^{\perp}_{u\lambda}(\mathbf{l}(\mathbf{x}, \hat{\rho})\nabla'_u \delta(\mathbf{x}-\mathbf{x}') - \delta(\mathbf{x}-\mathbf{x}')\nabla_i l_\lambda(\mathbf{x}, \hat{\rho}). \tag{13}$$

At the investigation of condensed matter with spontaneously broken symmetry within microscopic approach, an important role is paid of local transformations

with the generator of broken symmetry. For liquid crystals it's necessary to consider local spatial deformations, defined by the following unitary operator

$$U_f = \exp(-i) \int d^3x\, f_i(\mathbf{x}) \hat{\pi}_i(\mathbf{x}), \tag{14}$$

where $f_i(\mathbf{x})$ is some arbitrary function of spatial coordinates, that determines a unitary transformation of deformations U_f. The field operators are transformed thereby as

$$U_f^+ \hat{\psi}(\mathbf{x}) U_f = \left| \frac{\partial x'}{\partial x} \right|^{1/2} \hat{\psi}(\mathbf{x}), \quad U_f^+ \hat{\psi}^+(\mathbf{x}) U_f = \left| \frac{\partial x'}{\partial x} \right|^{1/2} \hat{\psi}^+(\mathbf{x}), \tag{15}$$

where $x'_i = x_i - u_i(\mathbf{x})$,$|\frac{\partial x'}{\partial x}| = \det \frac{\partial x'_i}{\partial x_j} = \det b_{ij} = J(\mathbf{x})$, where $u_i(\mathbf{x})$ — vector of displacement, being a transformation parameter functional $f_i(\mathbf{x})$ and point x_i:$u_i(\mathbf{x}) = u_i(f_i(\mathbf{x}')\mathbf{x})$, whereby $u_i(0, \mathbf{x}) = 0$. At transformations arbitrary deformations (15) $\hat{\rho}_f = U_f \hat{\rho} U_f^+$ director $l_i(\mathbf{x}, \hat{\rho})$ changes as follows:

$$l_i(\mathbf{x}, U_f^+ \hat{\rho} U_f) = l_i(\mathbf{x}'(f_i(\mathbf{x}')\mathbf{x}), \hat{\rho}).$$

In case of infinitesimal transformations $\delta\hat{\rho}_f = i \int d^3x' \delta f_j(\mathbf{x}') [\, \hat{\pi}_j(\mathbf{x}', \hat{\rho}\,]$, taking into account (13), (15), one can obtain:

$$\delta l_i(\mathbf{x}) = \delta f_j(\mathbf{x}) \nabla_j l_i(\mathbf{x}) + l_j(\mathbf{x}) \delta^{\perp}_{ik}(\mathbf{l}(\mathbf{x})) \nabla_k \delta f_j(\mathbf{x}). \tag{16}$$

Let's consider local-equilibrium states of liquid crystals. Statistical operator for such states according to (1), (6) has the form:

$$\hat{w}_\nu(Y, \mathbf{l}) \equiv \exp\{\Omega_\nu(Y, \mathbf{l}) - \int d^3x\, Y_a(\mathbf{x}) \hat{\zeta}_a(\mathbf{x}) - \nu \int d^3x\, \underline{l}_i \underline{l}_k U_f^+ \hat{Q}_{ik}(\mathbf{x}) U_f\}. \tag{17}$$

Here thermodynamic forces $Y_a(\mathbf{x})$ and director $l_k(\mathbf{x}') \equiv \underline{l}_j b_{kj}(\mathbf{x}')/|\underline{l}_\lambda b_{p\lambda}(\mathbf{x}')|$, ($\underline{l}_j$- const) are arbitrary functions of the coordinates. Varying the thermodynamic potential

$$\Omega = \Omega(Y(\mathbf{x}'), \mathbf{l}(\mathbf{x}')) = \int d^3x\, \omega(\mathbf{x}, Y(\mathbf{x}'), \mathbf{l}(\mathbf{x}')) \tag{18}$$

(18) with respect to the thermodynamics forces and to director, we obtain the form of the second law of thermodynamics for the local equilibrium state:

$$\delta\omega = \frac{\partial \omega}{\partial Y_a} \delta Y_a + \left(\frac{\partial \omega}{\partial l_i} - \nabla_k \frac{\partial \omega}{\partial \nabla_k l_i} \right) \delta l_i, \tag{19}$$

where ω is a density of thermodynamic potential. Now, let us find the expression for flux densities of additive integral of motion in local-equilibrium state. We find flux density of energy from relations [6]:

$$\underline{Y}_a (Y_k \underline{\zeta}_a + Y_0 \underline{\zeta}_{ak}) = 0, \tag{20}$$

which is adequate also in the given case. According to (7)–(9), (15), (16) flux densities of additive integral of motion have the form

$$\zeta_{ak} = -\frac{\partial}{\partial Y_a}\frac{\omega Y_k}{Y_0} + \left[\frac{\partial\omega}{\partial\nabla_k l_j}\nabla_i l_j + \frac{\partial\omega}{\partial l_k}l_i - l_i\nabla_j\frac{\partial\omega}{\partial\nabla_k l_j}\right]\frac{\partial}{\partial Y_a}\frac{Y_i}{Y_0}. \qquad (21)$$

Let us establish connection between given microscopic approach and Hamilton approach. For this reason we define Poisson bracket by equality

$$\{\, a(\mathbf{x}), b(\mathbf{x}')\,\} \equiv -i\mathrm{Sp}\,\hat\rho[\,\hat a(\mathbf{x},\hat\rho)\hat b(\mathbf{x}',\hat\rho)\,].$$

Here in the right-hand side of this relation $\hat a(\mathbf{x},\hat\rho)\hat b(\mathbf{x}',\hat\rho)$ are a variation of physical values operators. Since these are explicit form of additive integrals of motion and order parameter in terms of field operators, we obtain Poisson brackets

$$\{\, n(\mathbf{x}), n(\mathbf{x}')\,\} = 0,\ \ \{\, \pi_i(\mathbf{x}), n(\mathbf{x}')\,\} = n(\mathbf{x})\nabla'_i\delta(\mathbf{x}-\mathbf{x}'),$$

$$\{\, \pi_i(\mathbf{x}), \pi_k(\mathbf{x}')\,\} = -\pi_i(\mathbf{x})\nabla_k\delta(\mathbf{x}-\mathbf{x}') + \pi_k(\mathbf{x})\nabla'_i\delta(\mathbf{x}-\mathbf{x}'),$$

$$\{\, \pi_i(\mathbf{x}), l_\lambda(\mathbf{x}')\,\} = \delta(\mathbf{x}-\mathbf{x}')\nabla_i l_\lambda(\mathbf{x}) + l_i(\mathbf{x}')\delta^\perp_{\lambda u}(\mathbf{l}\mathbf{x}')\nabla'_u\delta(\mathbf{x}-\mathbf{x}') +$$

$$e^{-W(\mathbf{x}')}\tfrac{1}{2}\delta^\perp_{\lambda\nu}(\mathbf{l}\mathbf{x}')l_u(\mathbf{x}')\nabla_i[\nabla_u(\delta(\mathbf{x}-\mathbf{x}')\nabla_\nu h(\mathbf{x})) + \nabla_\nu(\delta(\mathbf{x}-\mathbf{x}')\nabla_u h(\mathbf{x}))],$$

$$\{\, n(\mathbf{x}), l_\lambda(\mathbf{x}')\,\} = 2\pi_\nu(\mathbf{x}')e^{-W(\mathbf{x}')}\nabla'_u\delta(\mathbf{x}-\mathbf{x}')[l_\nu(\mathbf{x}')\delta^\perp_{\lambda u}(\mathbf{l}\mathbf{x}') + l_u(\mathbf{x}')\delta^\perp_{\lambda\nu}(\mathbf{l}\mathbf{x}')],$$

$$\{\, n(\mathbf{x}), W(\mathbf{x}')\,\} = 4\pi_j(\mathbf{x}')e^{-W(\mathbf{x}')}\nabla'_j\delta(\mathbf{x}-\mathbf{x}'),$$

$$\{\, \pi_i(\mathbf{x}), W(\mathbf{x}')\,\} = 2l_i(\mathbf{x}')l_j(\mathbf{x}')\nabla_j\delta(\mathbf{x}-\mathbf{x}') + \nabla'_i\delta(\mathbf{x}-\mathbf{x}') +$$

$$\nabla_i W(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}') + e^{-W(\mathbf{x}')}\nabla_i\nabla_j[\delta(\mathbf{x}-\mathbf{x}')\nabla_j n(\mathbf{x})],$$

where $W(\mathbf{x}) \equiv \ln Q(\mathbf{x})$. It is obvious from represented formulas, that for harmonization of Poisson brackets algebra it's necessary to supplement the total set of hydrodynamic parameters by an additional value $W(\mathbf{x})$, being physically the smectic variable parameter. When $W \gg 1$, Poisson brackets can be simplified, eventually becoming [2,3].

$$\{\, n(\mathbf{x}), W(\mathbf{x}')\,\} = 0, \{\, n(\mathbf{x}), l_i(\mathbf{x}')\,\} = 0, \{\, \pi_i(\mathbf{x}), W(\mathbf{x}')\,\} = \nabla_i W(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}'),$$

$$\{\, \pi_i(\mathbf{x}), l_\lambda(\mathbf{x}')\,\} = \nabla_i l_\lambda(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}') + l_i(\mathbf{x}')\delta^\perp_{\lambda u}(\mathbf{l}\mathbf{x}')\nabla'_u\delta(\mathbf{x}-\mathbf{x}'). \qquad (22)$$

Hypothesis of abridged description in latter case for nematic liquid crystals is expressed like

$$\hat\rho(t) \xrightarrow[t\gg\tau]{} \hat\rho(\zeta(x,t),\mathbf{l}(x,t)), \qquad (23)$$

where τ is relaxation time, and smectic properties are not considered here. Equations of motion for parameters of abridge description using equations (11), (13), (22), (23) have the form

$$\dot\zeta_a(\mathbf{x}) = -\nabla_k\mathrm{Sp}\hat\rho(\zeta,\mathbf{l})\hat\zeta_{ak}(\mathbf{x}), \dot l_i(\mathbf{x}) = i\mathrm{Sp}\hat\rho(\zeta,\mathbf{l})[\,\hat H, \hat l_i(\mathbf{x})\,]. \qquad (24)$$

In the leading approximation with respect to the gradients of thermodynamic forces and to director, we obtain hydrodynamic equation of nematics

$$\dot{\zeta}_a(\mathbf{x}) = -\nabla_k \zeta_{ak}(\mathbf{x}), \quad \dot{l}_i(\mathbf{x}) = -(Y_k(\mathbf{x})/Y_0(\mathbf{x}))\nabla_k l_i(\mathbf{x}) - l_k(\mathbf{x})\delta^{\perp}_{ik}(\mathbf{lx})\nabla_j(Y_k(\mathbf{x})/Y_0(\mathbf{x})). \tag{25}$$

Following from equations (25) and definition of entropy density $\sigma = -\omega + Y_a\zeta_a$, there appears an adiabaticity of motion of considering condensed matter $\dot{\sigma} = \nabla_i(\sigma Y_i/Y_0)$.

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ЯДЕРНАЯ ФИЗИКА

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ASYMPTOTIC LAWS IN RELATIVISTIC NUCLEAR PHYSICS AND THEIR EXPERIMENTAL VERIFICATION

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1. INTRODUCTION

Relativistic nuclear physics was born in Dubna and Berkeley in the early 1970s. In Dubna at the Synchrophasotron, deuterons and then more heavy nuclei up to the sulfur nuclei with an energy of 4.5 GeV/nucleon were first accelerated. At Berkeley beams of different relativistic nuclei, but with less energy were also obtained. An active research of nuclear interactions in GeV nuclear beams was then started.

At the Joint Institute for Nuclear Research a specialized superconductive accelerator of relativistic nuclei — Nuclotron, able to accelerate practically all the nuclei at an energy of 6 GeV/nucleon [1] was built (Fig. 1).

Fig. 1. The Synchrophasotron and the Nuclotron of the Laboratory of High Energies of the Joint Institute for Nuclear Research

In connection with N.N.Bogoliubov's anniversary we would like to remember how he understood the main problem of relativistic nuclear physics. In his talk at a general 1985 meeting of the USSR Academy of Sciences [2] he paid attention to the fact that over the past years the ideas of the theory of color quarks had started to penetrate more deeply in nuclear physics and the major problem is to explain the nature and the basic regularities of nuclear forces

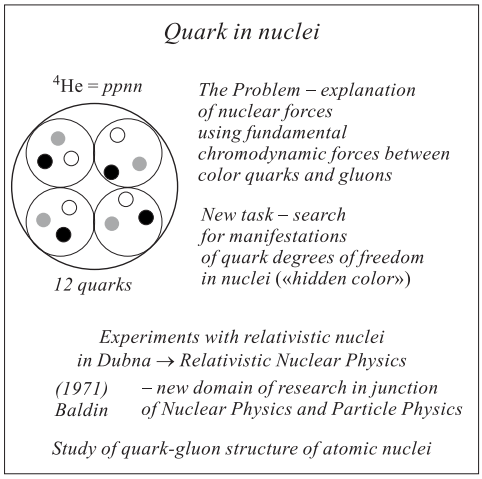

Fig. 2. A fragment from the talk of N.N.Bogoliubov [2]

proceeding from fundamental chromodynamic interactions of quarks and gluons. Figure 2 gives a fragment from Bogoliubov's talk. As is seen from this fragment, he considers that the main problem of relativistic nuclear physics is the search for manifestations of quark degrees of freedom in nuclei.

Being the Director of JINR, N.N.Bogoliubov gave constant support to the work on the Nuclotron. It is known that he was the author of the theory of superconductivity and he was interested in the quantum system with length of a quarter of kilometer. Figure 3 presents a photo on which Academicians N.N.Bogoliubov and A.M.Baldin are discussing the magnetic system of the Nuclotron.

Fig. 3. Academicians N.N.Bogoliubov (right) and A.M.Baldin are discussing the magnetic system of the Nuclotron

2. CUMULATIVE EFFECT

First experiments with the deuteron beam of the Synchrophasotron carried out by the group of V.S.Stavinsky have resulted in the discovery of a nuclear cumulative effect [3] predicted earlier by A.M.Baldin [4].

The idea of this effect consists in the following: collisions of relativistic nuclei result in the production of particles in the region of energies, forbidden for one nucleon interactions. Otherwise, because the secondary particles have the momentum and energy, observed in experiment, it's necessary to suppose that several nucleons take part in the interaction, i.e., it's impossible to consider that the nucleons in the nucleus are quasi-free. Figure 4 gives a schematic view of the cumulative effect.

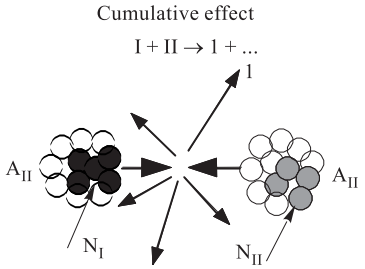

Fig. 4. A schematic view of the cumulative effect. Two nuclei with atomic numbers A_I and A_{II} interact between them and produce an inclusive particle 1. For the description of the kinematic parameters of inclusive particle 1 it is necessary to suppose that N_I nucleons from nucleus I participate with N_{II} from nucleus II

Later on the cumulative effect was investigated in detail in Dubna and in other scientific centres.

This research has resulted in the discovery of the quark-parton structure function of the nucleus analogous to the quark-parton structure function of the hadron. It was established that the experimental data for all nuclei from helium to uranium can be described by the following approximate equation for the cross sections

$$\sigma(A_I A_{II} \to h_1 + \dots) = k A_I^n A_{II}^{m(N_I)} \exp\left(-N_I/\langle N_I\rangle\right) \tag{1}$$

at $0.5 \le N_I \le 3.3$ (cumulative region at $N_I > 1$),

$$\begin{array}{ll} m(N_I) = 2/3 + N_I/3 & (0.5 \le N_I \le 1) \\ m(N_I) \approx 1 & (N_I > 1). \end{array}$$

$N_I \approx 0.14$ characterises the sizes of a multi-quark system, from which cumulative particles are emitted. In this way, the nuclear quark-parton structure function can be taken as:

$$G(N_I) \sim \exp\left(-N_I/\langle N_I\rangle\right). \tag{2}$$

In a more general case the cumulative effect can be realized in both nuclei A_I and A_{II} (double cumulative effect, Fig. 4), but with smaller probability.

3. DESCRIPTION OF INTERACTIONS OF RELATIVISTIC NUCLEI IN FOUR-VELOCITY SPACE

A relativistic invariant description of multiple particle processes in relative 4-velocity space was suggested by A.M.Baldin [6]. This approach turned out to be very fruitful and made it possible to obtain a number of new properties of relativistic nuclear interactions. The process of the interaction of two nuclei can be written as follows:

$$I + II \to 1 + 2 + \dots \tag{3}$$

where I and II are the interacting nuclei, and $1, 2, 3, \dots$ are the secondary particles. Following this approach relativistic invariant quantities:

$$b_{ik} = -(u_i - u_k)^2 \tag{4}$$

were introduced, where $u_i = p_i/m_i$, $u_k = p_k/m_k$ are 4-velocity particles i and k; $p_{i,k}$ and $m_{i,k}$ are their 4-momenta and masses. The distributions of the secondary particles as functions of b_{ik} have universal properties, which points to a common interaction mechanism on the quark-gluon level.

An important principle introduced in 4-velocity space by A.M.Baldin, is the correlation depletion principle (CDP) analogous to the Bogoliubov's CDP. CDP has been suggested by Bogoliubov in statistical physics as a universal property of the probability distributions for particle location in an ordinary space-time. The principle is based on an intuitive idea that the correlation between largely spaced parts of a macroscopic system practically vanishes and the distribution is factorized. From the mathematical point of view the principle means that probability distributions are desintegrated in independent factors (Fig. 5).

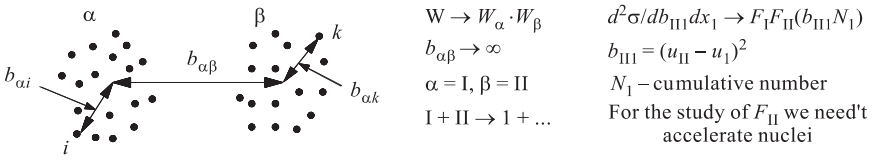

Fig. 5. Schematic view of the correlation depletion principle in four-velocity space. Correlation between largely spaced parts α and β of the particle system vanishes when the distance $b_{\alpha\beta}$ in four-velocity space between the centres of systems α and β tends to infinity. The probability distribution which characterizes the system is factorized $W \to W_\alpha \cdot W_\beta$ at $b_{\alpha\beta} \to \infty$

This principle makes it possible to study in detail cumulative processes as target nucleus fragmentation processes using intense proton beams as projectiles. In this case acceleration of relativistic nuclei is found to be unnecessary.

The second important property of relativistic nuclear interactions, which was used in four-velocities space, is the automodelity.

The introduction of a self-similarity parameter Π [7]:

$$\Pi = \min\,[\frac{1}{2}\sqrt{(u_I N_I + u_{II} N_{II})^2}] \tag{5}$$

leads to the description of the invariant production cross section for an inclusive particle in the form [8]:

$$E(d^3\sigma/d^3p) = C_1 \cdot A_I^{1/3+N_I/3} \cdot A^{1/3+N_{II}/3} \cdot \exp\,(-\Pi/C_2), \tag{6}$$

where $C_1 = 1.9 \cdot 10^4$ mb·GeV$^{-2} \cdot$ c^3·st^{-1}, $C_2 = 0.125 \pm 0.002$.

This equation describes a very large amount of experimental data in a wide region of change of the cross sections (by 10 orders of magnitude) and of the energy for different particles and interacting nuclei.

4. ASYMPTOTICS IN RELATIVISTIC NUCLEAR PHYSICS

Using the self-similarity parameter Π (5) an analytical expression was obtained for the inclusive invariant cross section of production of particles, nuclear fragments and antinuclei in relativistic nuclear collisions in the central rapidity region [9,10].

The quantities N_I and N_{II} become measurable if we take into account the law of conservation of four-momentum in the form

$$(N_I m_0 u_I + N_{II} m_0 u_{II} - m_1 u_1)^2 = (N_I m_0 + N_{II} m_0 + \Delta)^2, \tag{7}$$

neglecting the relative motion of the remaining not detected particles. Here m_0 is the nucleon mass, Δ is the mass of the particles providing conservation of the baryon number, strangeness and other quantum numbers. For antinuclei and K^- mesons (the case of antimatter formation) $\Delta = -m_1$. For particles produced without accompanying antiparticles (π mesons, jets and others) $\Delta = 0$.

Using condition (7) it is possible to find value (5) in the central rapidity region (here $N_I = N_{II} = N$):

$$\Pi = \frac{1}{2}\sqrt{2N^2 + 2N^2(u_I u_{II})} = \frac{N}{\sqrt{2}}\sqrt{1 + (u_I u_{II})} = N \cosh Y, \tag{8}$$

where Y is the rapidity of colliding nuclei in the c.m. system.

In the region of the rapidity of the inclusive particle $y = 0$ we have obtained

$$N = [1 + \sqrt{(\Phi_\delta/\Phi^2) + 1}] \cdot [\frac{m_T}{m_0} \cosh Y + \frac{\Delta}{m_0}] \cdot [1/(2 \sinh^2 Y)], \tag{9}$$

where

$$\Phi = \frac{1}{m_0} \cdot [m_T \cosh Y + \Delta] \cdot (1/2 \sinh^2 Y),$$

$$\Phi_\delta = (\Delta^2 - m_1^2)/(4m_0^2 \sinh^2 Y), \tag{10}$$

m_1 — the inclusive particle mass, $m_T = \sqrt{m_1^2 + p_T^2}$ — the transverse mass.

Now we consider the asymptotic behaviour of the self-similarity parameter with increasing interaction energy:

$$s/(2m_I m_{II}) \approx (u_I u_{II}) = \cosh 2Y \to \infty.$$

In the collider energy region the self-similarity parameter Π assumes the finite value

$$\Pi_\infty = \frac{m_T}{2m_0}\Big[1 + \sqrt{1 + (\Delta^2 - m_1^2)/m_T^2}\Big]. \tag{11}$$

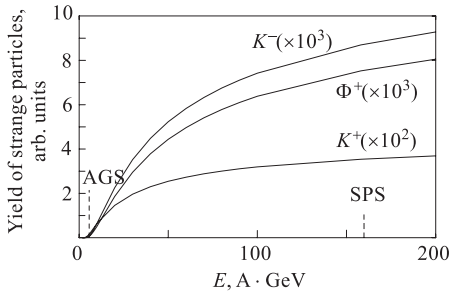

Fig. 6. Yield of strange particles in the central rapidity region (for $y = 0$) as a function of the collision energy

As is seen from Eq. (9), the effective number of the nucleons is involved in the reaction $N \to 0$ at $\cosh Y \to \infty$. In this connection, we may say with certainty that the hopes for obtaining dence and hot matter (in any case, for detecting it by fast inclusive particles) in ultrarelativistic nuclear collisions are not feasible.

The analytical representation for Π enables us to draw the following new conclusions:

1. There exists the limiting value of Π described by Eq.(11).

2. For $\Phi_\delta = 0$ the expression for Π is factorized and proportionality of it to the inclusive particle mass m_1 makes it possible to test in detail the self-similarity laws. From Eq.(9) it follows that the cross section (6) exponentially quickly decreases with increasing m_1. In particular, this implies that the probability of observing even light antinuclei and fragments in the region $y = 0$ is insignificantly small.

3. The yield of strange particles in the central rapidity region increases with increasing collision energy (Fig. 6).

4. The effective number of nucleons involved in the reaction decreases with increasing $\cosh Y$ (9).

5. A strong factorizable dependence of Π on m_T we have discovered explains the observed m_T scaling.

The results of our calculations for AGS and SPS energy are presented in the Table. Experimental results from Refs. 11–13 are also presented there.

Table

Ratios of the yields	$\bar{p}/p$	$\bar{d}/d$	K^-/K^+
Calculation (160 A · GeV) (the present paper) ($p_T = 0$)	0.16	0.027	0.25
NA52 (160 A · GeV)	≈ 0.1	≈ 0.01	$\approx 0{,}2$
NA44 (160 A · GeV)	≈ 0.08	-	≈ 0.4
Calculation (11 A · GeV) (the present paper) ($p_T = 0$)	0.00039	-	0.11
E866 (11 A · GeV)	≈ 0.0003	-	≈ 0.2

The results of our calculations are in satisfactory agreement with experiment.

Our predictions of the ratios of the production cross section for antiparticles to that for particles are presented in Fig. 7. The calculations were carried out for a fixed target and energy of incident nuclei in laboratory system.

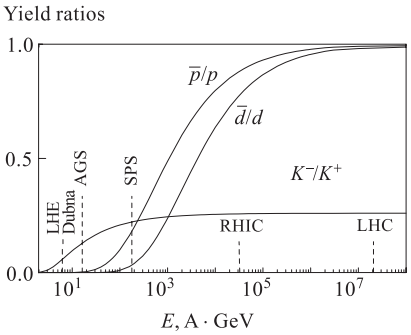

Fig. 7. Predictions of production cross section ratios for antiparticles to particles versus laboratory collision energy

5. CONCLUSIONS

For inclusive production cross sections for particles, nuclear fragments and antinuclei in relativistic nuclear collisions in the central rapidity region ($y = 0$)

- the analytical expression is obtained;
- the results of calculations are in agreement with available experimental data;
- the asymptotic behaviour as a function of increasing interaction energy is discovered;
- the predictions for RHIC and LHC energy are presented.

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«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
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УДК 539.14

DESCRIPTION OF TRANSITIONAL NUCLEI IN THE FRAMEWORK OF «QUADRUPOLE PLUS PAIRING» COLLECTIVE MODEL

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The «quadrupole plus pairing» collective model is constructed and adopted to describe the quadrupole collective states in even-even transitional nuclei. An approximation scheme of solving the model is given. Exemplary results of microscopic calculations within the framework of the model are shown.

Since more than 30 years the General Bohr Hamiltonian (GBH) remains the main tool for description of collective states in even-even transitional nuclei (e.g., [1–5]). This is because of two important features of such a model. The former is that the collective Hamiltonian is a rotational scalar and its eigenfunctions are of a definite angular momentum. The latter is that a rotation-vibration coupling, so important for transitional nuclei, is taken into account. To be sure, algebraic collective models of the type of Interacting Boson Model (IBM) possess similar features (cf. [7]). However, such models act usually as purely phenomenological approaches whereas there exist efficient methods of microscopic constructing the GBH. Two standard microscopic approaches are: (i) the cranking model (see [6] for formulae and references quoted therein) which, however, gives a classical Hamiltonian and, therefore, requires a requantization procedure, (ii) the Gaussian Overlap Approximation (GOA) of the Generator Coordinate Method (GCM) [8]. But it should be admitted that the GBH treats collective excitations as an adiabatic phenomenon and does not take into account a coupling with other degrees of freedom, in particular, with two-quasiparticle excitations.

It is known for a long time that the GBH, when constructed microscopically, gives results which are not compatible with experimental data [3]. The calculated excitation energies of collective levels are not in a proper scale. This seems as if the inertial parameters are two to three times too small. These inertial parameters

are sensitive functions of the pairing energy gaps and can easily be made bigger by an artificial weakening of pairing forces [3]. This observation has brought us to the conclusion that a coupling between the quadrupole and the pairing degrees of freedom should be taken into account [9,10]. It can be done by the construction of a collective Hamiltonian for both, the quadrupole and the pairing vibrations.

Below we present the «quadrupole plus pairing» collective model and discuss a way of its approximate solving. Next, we show some exemplary results of calculations and compare them with experimental data. At the end we draw some conclusions.

Apart from the five usual collective variables, namely, $\beta,\ \gamma$, the Bohr deformation parameters describing the nuclear shape or the quadrupole moment in the intrinsic frame, and $\phi,\ \theta,\ \psi$, the Euler angles describing the orientation of the intrinsic frame, we introduce a further four dynamical variables to the collective model, namely, $\Delta^{\rm p},\ \Delta^{\rm n}$, the proton and neutron energy gaps describing the proton and neutron pairing correlations, and $\Phi^{\rm p},\ \Phi^{\rm n}$, the proton and neutron gauge angles describing rotations in the proton and neutron gauge spaces or transfer of the proton and neutron pairs (cf. [11–13]). We assume the «quadrupole plus pairing» collective Hamiltonian (QPCH) of the following structure:

$$\begin{aligned}\hat{\mathcal{H}}_{\rm quad-pair} &= \hat{\mathcal{T}}_{\rm vib}(\beta,\gamma;\Delta^{\rm n},\Delta^{\rm p}) + V_{\rm def}(\beta,\gamma,\Delta^{\rm n},\Delta^{\rm p}) \\ &+\hat{\mathcal{H}}_{\rm rot}(\phi,\theta,\psi;\beta,\gamma,\Delta^{\rm n},\Delta^{\rm p}) \\ &+ \sum_{\rm t=p,n}\Big[\hat{\mathcal{T}}^{\rm (t)}_{\rm pair}(\Delta^{\rm t},\Phi^{\rm t};\beta,\gamma) + V^{\rm (t)}_{\rm pair}(\beta,\gamma,\Delta^{\rm t}) \\ &+ \hat{\mathcal{T}}^{\rm (t)}_{\rm quad-pair}(\beta,\gamma,\Delta^{\rm t})\Big]. \end{aligned} \tag{1}$$

The operators which enter into the Hamiltonian of Eq. (1) are differential operators of the second order in the arguments given in front of semicolon; $\hat{\mathcal{T}}^{\rm (t)}_{\rm quad-pair}$ is a differential operator in all of its arguments. We do not write down here exact forms of all terms of the Hamiltonian which are more or less obvious. We only mention that it is determined by the following functions of β, γ, $\Delta^{\rm p}$ and $\Delta^{\rm n}$

- $V_{\rm def},\ V^{\rm (p)}_{\rm pair},\ V^{\rm (n)}_{\rm pair}$, the deformation and pairing potentials,
- $B_{\beta\beta},\ B_{\beta\gamma},\ B_{\gamma\gamma}$, the quadrupole vibrational inertial functions (mass parameters),
- $\mathcal{J}_1,\ \mathcal{J}_2,\ \mathcal{J}_3$, the quadrupole moments of inertia,
- $B_{\Delta^{\rm t}\Delta^{\rm t}}$ for t = p, n, the pairing vibrational inertial functions,
- $B_{\beta\Delta^{\rm t}},\ B_{\gamma\Delta^{\rm t}}$ for t = p, n, the quadrupole–pairing mixed vibrational inertial functions,

– $\mathcal{J}_{\Phi^t}$ for t = p, n, the pairing moments of inertia,

– $\lambda^{(t)}$ for t = p, n, the chemical potentials.

To calculate electromagnetic characteristics of nuclei, like reduced probabilities of γ-transitions, electric and magnetic multipole moments, collective multipole operators, which are determined again by some functions of β, γ, Δ^p and Δ^n, should be constructed. All these functions determining the collective Hamiltonian and multipole operators can be calculated from a microscopic theory. This problem is discussed elsewhere [6].

Solving the collective model formulated above may consist in the numerical diagonalizing the set of operators: $\hat{\mathcal{H}}_{\mathrm{quad-pair}}$, the collective Hamiltonian, $\hat{I}^2$, $\hat{I}_z$, the total angular momentum and its projection onto a lab axis z, $\hat{N}_t = -i\partial/\partial\Phi_t$ for t = p, n, the particle number excess operators. We do not solve this eigenvalue problem exactly as yet. Instead, we have adopted an approximation scheme, which proceeds in the following steps:

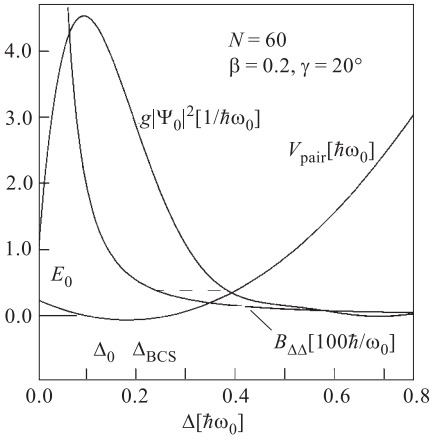

Fig. 1. Zero-point pairing vibration of neutrons in ^{104}Ru at deformation $\beta = 0.2$, $\gamma = 20^\circ$. The equilibrium value of the energy gap is $\Delta_{\mathrm{BCS}} \approx 0.14\hbar\omega_0$ whereas the most probable value is $\Delta_0 \approx 0.09\hbar\omega_0$. The oscillator frequency is $\hbar\omega_0 \approx 41/A^{1/3}$ MeV

1. Neglect the quadrupole-pairing coupling in the kinetic energy, i.e., put $\hat{\mathcal{T}}^{(t)}_{\mathrm{quad-pair}}(\beta, \gamma, \Delta^t) = 0$ for t = p, n in Eq. (1).

2. Find the zero-point pairing vibration of neutrons and protons for given β and γ solving the eigenvalue problem

$$\hat{\mathcal{H}}^{(t)}_{\mathrm{pair}}(\Delta^t; \beta, \gamma)\Psi_0(\Delta^t; \beta, \gamma) = E^{(t)}_0(\beta, \gamma)\Psi_0(\Delta^t; \beta, \gamma), \qquad (2)$$

$$\hat{N}_t(\Phi^t)\Psi_0(\Delta^t; \beta, \gamma) = 0, \qquad (3)$$

where

$$\hat{\mathcal{H}}^{(t)}_{\mathrm{pair}}(\Delta^t; \beta, \gamma) = \hat{\mathcal{T}}^{(t)}_{\mathrm{pair}}(\Delta^t; \beta, \gamma) + V^{(t)}_{\mathrm{pair}}(\Delta^t, \beta, \gamma) \qquad (4)$$

and the collective pairing kinetic energy (excluding the pair transfer effect) reads [12, 13]

$$\hat{\mathcal{T}}^{(\mathrm{t})}_{\mathrm{pair}} = -\frac{\hbar^2}{2\sqrt{g(\Delta^{\mathrm{t}})}}\frac{\partial}{\partial\Delta^{\mathrm{t}}}\frac{\sqrt{g(\Delta^{\mathrm{t}})}}{B_{\Delta^{\mathrm{t}}\Delta^{\mathrm{t}}}(\Delta^{\mathrm{t}})}\frac{\partial}{\partial\Delta^{\mathrm{t}}}; \tag{5}$$

here $g(\Delta^{\mathrm{t}},\beta,\gamma)$ is a normalization weight.

3. Find the most probable neutron or proton energy gap $\Delta^{\mathrm{t}}_0(\beta,\gamma)$, i.e., the value of Δ^{t}_0 for which $g|\Psi_0|^2$ takes its maximum (see Fig. 1).

4. Solve the eigenvalue problem for the following general Bohr Hamiltonian

$$\begin{aligned}\hat{\mathcal{H}}_{\mathrm{coll}} &= \hat{\mathcal{T}}_{\mathrm{vib}}(\beta,\gamma;\Delta^{\mathrm{n}}_0(\beta,\gamma),\Delta^{\mathrm{p}}_0(\beta,\gamma)) + V_{\mathrm{coll}}(\beta,\gamma,\Delta^{\mathrm{n}}_0(\beta,\gamma),\Delta^{\mathrm{p}}_0(\beta,\gamma))\\ &+ \hat{\mathcal{H}}_{\mathrm{rot}}(\phi,\theta,\psi;\beta,\gamma,\Delta^{\mathrm{n}}_0(\beta,\gamma),\Delta^{\mathrm{p}}_0(\beta,\gamma)),\end{aligned} \tag{6}$$

where the quadrupole collective potential is

$$V_{\mathrm{coll}} = V_{\mathrm{def}} + E^{(\mathrm{n})}_0 + E^{(\mathrm{p})}_0 \tag{7}$$

and the quadrupole kinetic energy reads

$$\begin{aligned}\hat{\mathcal{T}}_{\mathrm{vib}} = -\frac{\hbar^2}{2\sqrt{wr}}\Bigg\{\frac{1}{\beta^4}\Bigg[\partial_\beta\Bigg(\beta^4\sqrt{\frac{r}{w}}B_{\gamma\gamma}\partial_\beta\Bigg) - \partial_\beta\Bigg(\beta^3\sqrt{\frac{r}{w}}B_{\beta\gamma}\partial_\gamma\Bigg)\Bigg]\\ +\frac{1}{\beta\sin3\gamma}\Bigg[\frac{1}{\beta}\partial_\gamma\Bigg(\sqrt{\frac{r}{w}}\sin3\gamma B_{\beta\beta}\Bigg)\partial_\gamma - \partial_\gamma\Bigg(\sqrt{\frac{r}{w}}\sin3\gamma B_{\beta\gamma}\partial_\beta\Bigg)\Bigg]\Bigg\},\end{aligned} \tag{8}$$

$$\hat{\mathcal{H}}_{\mathrm{rot}} = \frac{1}{2}\sum_{k=1}^{3}\hat{I}^2_k/\mathcal{J}_k; \tag{9}$$

here $\hat{I}_1$, $\hat{I}_2$, $\hat{I}_3$ are the operators of intrinsic angular momenta (differential operators in the Euler angles). The GBH of Eq. (6) is Hermitian with the volume element

$$\mathrm{d}\tau = \beta^4\sqrt{wr}|\sin3\gamma|\mathrm{d}\beta\mathrm{d}\gamma\sin\theta\mathrm{d}\theta\mathrm{d}\phi\mathrm{d}\psi, \tag{10}$$

where $w = B_{\beta\beta}B_{\gamma\gamma} - B^2_{\beta\gamma}$ and $r = \mathcal{J}_1\mathcal{J}_2\mathcal{J}_3/(4\beta^6\sin^2 3\gamma)$.

The physical meaning of the above approximation consists in taking into account an effect of the zero-point pairing vibration on the quadrupole collective excitations.

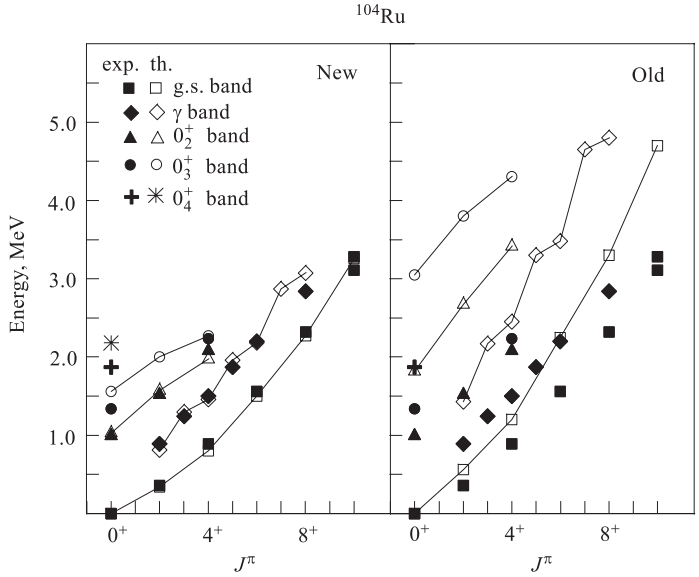

Fig. 2. Experimental (black figures) and theoretical (open figures connected by straight lines) energy levels in ^{104}Ru versus angular momentum J^π. The theoretical levels are calculated with («new») and without («old») the effect of zero-point pairing vibration taken into account

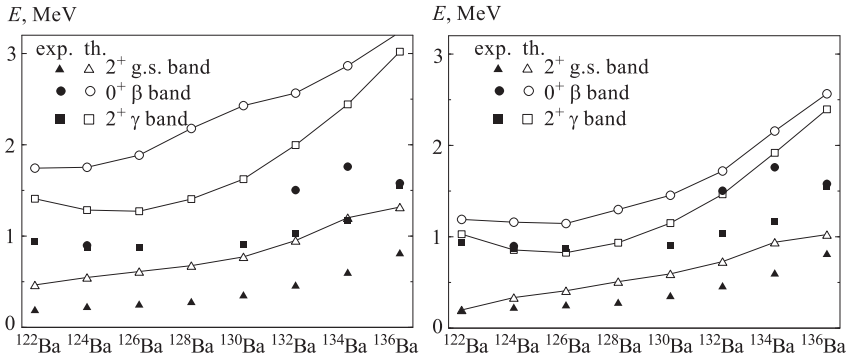

Fig. 3. Experimental (black figures) and theoretical (open figures connected by straight lines) values of the lowest excited 2^+ levels and band-heads of the β- and the γ-band in the Ba isotopes. The theoretical levels are calculated without (left part) and with (right part) the effect of zero-point pairing vibration taken into account

Results of calculations show that the zero-point-pairing-vibration effect is really essential for the quadrupole excitations and improves considerably an agree-

ment with experimental data. It is easily seen in Fig. 2, where the collective energy levels in ^{104}Ru calculated without («old») and with («new») this effect taken into account, are compared with experimental levels [14]. The «new» calculation reproduces the data almost perfectly. The ground-state rotational bands in isotopes of Erbium, $^{152-166}$Er are reproduced equally well and the γ-bands only a little bit worse (Fig. 4). From Fig. 3 we see that the effect of pairing vibration improves the results also for isotopes of Barium. However, it does not make the job in this case. The qudrupole-pairing coupling in the kinetic energy and also a coupling with the octupole degrees of freedom may probably play a role in the quadrupole excitations of the neutron-deficient nuclei of $50 < Z, N < 82$.

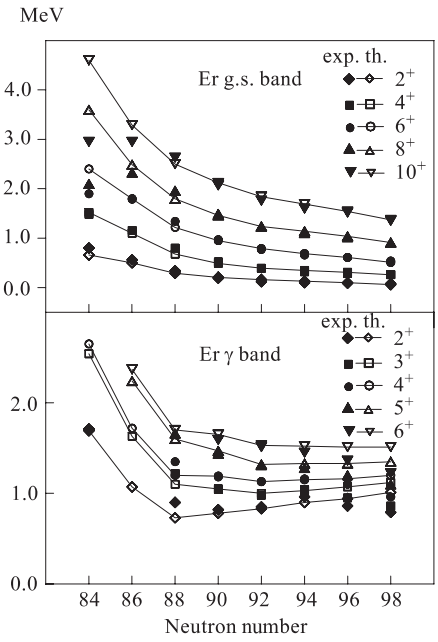

Fig. 4. Experimental (black figures) and theoretical (open figures connected by straight lines) rotational bands in the Er isotopes. The upper part shows the ground-state band, the lower — γ-band

In conclusion, the «quadrupole plus pairing» collective model can successfully be applied to the description of collective states in even-even transitional nuclei. An essential role of the zero-point pairing vibration in the behaviour of quadrupole excitations is observed. When the pairing vibration is taken into account, microscopic calculations with no free parameters yield results which are in good agreement with experimental data. However, it is still an open question whether the description of low-lying collective states by the «quadrupole plus pairing» model takes all main and/or proper effects into account.

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