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FUNDAMENTAL PRINCIPLES
OF THE PHYSICS OF MAGNETISM
AND THE PROBLEM OF LOCALIZED
AND ITINERANT ELECTRONIC STATES*

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2000

The existence and properties of localized and itinerant magnetism in metals, oxides and alloys and their interplay is an interesting and not yet fully understood problem of quantum theory of magnetism. The most characteristic feature of the recent advancement in basic researches on electronic properties of solids is development of variety of the new class of materials with unusual transport and magnetic properties, such as manganese perovskite oxides , heavy fermion compounds , high T_c superconductors, dilute magnetic semiconductors, magnetic multilayers, etc. An important problem in understanding the physical behaviour of these systems has been the connection between the relevant underlying chemical, crystal and electronic structure and the magnetic and transport properties which continue to be the subject of intensive debates [1]. In last decades a great progress has been made in sample preparation and experimental abilities and sensitivity, low temperature and high field and high pressure techniques and neutron scattering facilities. All of these possibilities make possible more detailed studies of many controversial problems in the field of strong electron correlation , metal-insulator transition, anomalous transport, heavy fermions and magnetism[2-5] , etc. An experimental technique particularly well suited to investigate the magnetic and lattice structure as well as various excitations of magnetic and correlated electron materials is the well-known neutron elastic and inelastic scattering[6-11]. The study of magnetic quasiparticle excitations in transition and rare-earth metals, compounds and alloys has been of considerable interest theoretically and experimentally for a few last decades. The behaviour and the true nature of the electronic and spin states and their quasiparticle dynamics are of central importance to the understanding of the physics of strongly correlated systems[12,13] such as magnetism and Mott-Hubbard metal-insulator transition in metals and oxides, heavy fermion states and their competition with magnetism. In these materials electronic correlation effects are essential and moreover their spectra are complex, i.e. have many branches, etc. This give rise to many

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interesting phenomena but the understanding what is going on is in many cases only partial if exist at all. A principle importance of the studies on strongly correlated electron systems are concerned with a fundamental problem of electronic solid state theory, namely with the tendency of 3(4) d electrons in transition metals and compounds and 4(5) f electrons in rare-earths and compounds and alloys to exhibit both localized and delocalized behaviour. The most celebrated electronic and magnetic features of these substances related intimately to this dual behaviour of relevant electronic states.This confirm the statement that the question about true nature of carriers in copper and manganese oxides is one of the central in the field and is still open. In spite of experimental and theoretical achievements still it remains much to be understood concerning such systems. Clearly a unified picture of competition and interplay of various degrees of freedom and their contribution to the essential physics of magnetic and transport properties is desirable.

In this article we shall discuss briefly these problems in the context of the dual behaviour of the electrons. It is the purpose of this paper to analyse more fully the intriguing dilemma of itinerant and localized behaviour of the carriers in complex oxides and similar substances to understand the nature of electron states which are responsible for many unusual features of these systems and discuss the problem of choice of relevant microscopic models[7,12,13].

Magnetic and correlated electron materials

Strongly correlated d and f electron systems are one of the most important fields in solid state physics[5,12,13]. The central problem of recent efforts is to investigate the interplay and competition of the insulating, metallic, superconducting and heavy fermion behaviour versus the magnetic behaviour, especially in vicinity of a transition to a magnetically ordered state. One more interesting and unsolved problem is related

to the role of orbital degrees of freedom as well as the electron correlation and the lattice effects in manganese oxides. The behaviour and the true nature of the electronic and spin states and their quasiparticle dynamics are of central importance to the understanding of the physics of strongly correlated systems such as magnetism and Mott-Hubbard metal-insulator transition in metals and oxides, heavy fermion states, superconductivity and their competition with magnetism[14]. More recently, considerable attention has been paid to the complex oxides, such as copper oxides after the discovery of high-temperature superconductivity[14-17], certain class of manganese oxides, the manganite perovskites[1, 18,19] and Cr-based chalcogenide spinels[20]. For example, the most characteristic common feature of the magnetic behaviour in the copper oxides is that the undoped parent compounds are insulating antiferromagnets. Upon chemical doping which leads to the metallic and superconducting behaviour the static magnetic order disappear. This is clearly visible in the elastic neutron scattering since the elastic diffraction peaks disappear with doping. Nevertheless, the magnetism of the copper oxides superconductors, which results from the electronic states of the incomplete shells of the copper ions plays an important role[14-17]. There are evidences that the magnetic fluctuations might give rise (along or in combination) to the superconducting pairing. The dual behavior of the electronic states follows from the fact that both antiferromagnetic and superconducting compositions show strong neutron inelastic scattering derived from magnetic fluctuations[17]. Thus, the chemical doping, which induce the metallic behaviour, lead to the changing of the behaviour of relevant electron states from localized to itinerant. Very recently, a direct observation of the appropriate d orbitals become possible in a copper oxide[21], where the high quality charge density maps were obtained by combination of electron and X-ray diffraction. These achievements may help answer questions about bonding in the high-temperature copper oxides superconductors[22] since the charge carriers in active CuO_2 planes are the fundamental degrees of freedom and are primarily responsible for transport and superconductivity.

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From the other side, the plenty of experimental results show that there are a wide class of heavy fermion compounds where the problem of the duality of electron behavior and the magnetic features of heavy-electron system is highly nontrivial. It seems appropriate to point out that there are differences between Ce-based and U-based compounds as regards to the competition with magnetism and to some other aspects. Recently a new development in this field has emerged which is related to alloy systems in which radical changes in physical properties occur with relatively modest changes in chemical composition or structural perfection of the crystall lattice. Due to competing interactions of comparable strength, more complex ground states than usually supposed may be realized. There are many experimental evidences which indicates that various heavy-electron systems at low temperatures are characterized by inhomogeneities of the itinerant electron system, both in real and reciprocal space. Moreover, the strong correlation effects among electrons which lead to the formation of the heavy fermion state take part to some extent in formation of magnetically ordered phase and thus imply that the very delicate competition and interplay of interactions exist in these substances. For most of the heavy fermion superconductors, cooperative magnetism, usually some kind of antiferromagnetic ordering was observed in the "vicinity" of superconductivity. In the case of U-based compounds the two phenomena antiferromagnetism and superconductivity coexist on a microscopic scale, while they seem to compete with each other in the Ce-based systems. For a Kondo lattice system, the formation of a Neel state via the RKKY intersite interaction compete with the formation of a local Kondo singlet . Recent data for many heavy fermion Ce or U based compounds and alloys display a pronounced non-Fermi-liquid behaviour[4,23,24] , which attracted an attention to the problem of duality of electron behaviour again[25]. A number of theoretical scenarios have been proposed and they can be broadly classified into two categories[26] , which deals with the *localized* and *extended* states of f-electrons. Of special interest is the unsolved controversial problem of the reduced magnetic moment in Ce- and U-based alloys and description the heavy fermion state in the presence of the coexisting magnetic

state. In other words, the main interest is in the understanding of the competition of intra-site (Kondo screening) and inter-site (RKKY exchange) interactions. Depending on the relative magnitudes of the Kondo and RKKY scales, materials with different characteristics are found, which are classified as non-magnetic and magnetic concentrated Kondo systems. The latter, "Kondo magnets" are of main interest[25]. They are of conceptual importance because a meaningful theoretical description of the heavy-fermion physics requires a very sophisticated and nontrivial description of many-body correlation effects within the electronic subsystem. The very delicate balance of interactions[25], which result in formation of large effective masses and developing some coherence effects within magnetic degrees of freedom is hardly be expected as tractable with the standard mean-field or perturbation theory methods. Furthermore, there are effects which have very complicated and controversial origination. There are some experimental evidences that peculiar magnetism in quasi-ternary heavy fermion alloys is not that of a localized systems, but have some features of band magnetism. This is very intriguing conjecture which need careful investigation. Thus in addition to the pronounced non-Fermi-liquid effects[4,23,24,26] in thermodynamic and transport properties, the outstanding problems include small magnetic moments and possible transitions from localized moment ordered phase to a kind of "heavy fermion band magnet" [12,25]. This is very intriguing conjecture and confirm the opinion about heavy fermions as "a lasting source of puzzles". These features reflect the very delicate interplay and competition of interactions and changes in chemical composition. This implies that the many-body correlation effects should play a crucial role and behave in an often peculiar and not well understood fashion. It is worthy to underline that in spite of many theoretical efforts, a comprehensive theory and full understanding of the heavy fermion phenomenon is still lacking.

Doped manganites show a complicated interplay of spin, charge, orbital and lattice degrees of freedom [1,5]. It should be emphasized that the colossal magnetoresistance

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effect in these substances have been observed at temperatures close to the insulator-metal transition temperature[5] . Recently there has been considerable interest in identifying the state of the carriers in magnetorestive manganese oxides, where the pronouncing effects of localized-itinerant duality (metal-insulator transitions) were clearly observed . A dramatic increase in the mobility of carriers when they order ferromagnetically is intimately related to the possibility of itinerant (mobile) electrons hops between manganese ions; this mobility of carriers is responsible simultaneously for the electrical conduction and ferromagnetic ("double") exchange[27]. There are some evidences that the origin of the effect of colossal negative magnetoresistance might be attributed to the formation of a kind of magnetic polaron. Magnetic polarons are well known in the magnetic semiconductors[28]. They are charge carriers accompanied by a certain (small, intermediate or large) distortion of the magnetic lattice. The direct demonstration of the existence of polarons in the paramagnetic phase of optimally doped colossal magnetoresistive oxides has been made through detailed combined experiments[29,30] , including neutron scattering.

Exotic and artificial magnetic systems

There are many complex and artificial magnetic systems, which demonstrate unusual and peculiar properties. We will mention a few system only for the demonstration of a wide variety of magnetism. The inter-relation and interaction between spin and orbital degrees of freedom in complex substances determine many unusual features of these systems. Orbital degeneracy plays the important role in the magnetic properties of transition metal compounds. In recent years a lot of attention has been placed on the relation between the magnetic structures and the orbital occupation of the transition metal compounds. The role of orbitals for the magnetic properties of some V oxides have attracted much attention recently. Resonant X-ray scattering has made it possible to determine quite directly the local distortions related to orbital ordering and recent studies of V_2O_3, YVO_3 have revealed

some surprises. Also recent studies of the properties of $LiVO_2$ and YVO_3 display surprising temperature dependent multiple magnetization reversals. For the interpretation of these results it is necessary to take into account the strong coupling between the orbital and spin structure. It was established also very recently that the transition metal oxide compound LiV_2O_4 is the first reported heavy fermion system without f electrons.

There are interesting developments in unusual magnetic properties in hexaborides. Recently Young et al.[31] reported the surprising discovery of ferromagnetism in Ca_{1-x} $La_x B_6$ - a material without d- or f-electrons. The ferromagnetism has special features: it occurs only in the narrow range $0 < x < 0.01$, it has a very small moment ($< 0.1 \mu_B$ /La) , but it has a relative high T_c , about 600 K. One may suppose that the small overlap of valence and conduction bands provides favorable conditions for the formation of a triplet exiton condensate. When doped it is energetically favorable to distribute the carriers asymmetrically between quasiparticle spin directions leading to a ferromagnetic state with a small moment oriented perpendicular to the direction of the triplet condensate . This form of exitonic ferromagnetism may provide an explanation for the unusual properties of ferromagnetism in the hexaborides[32].

Magnetic multilayers form another very interesting artificial magnetic system where there are possibility to change the degree of localization of electronic states not due to the changing of chemical composition but due to changing of the geometry (or topology) of the system. Recent progress in ultra high vacuum preparation and characterization methods resulted in a large variety of novel materials. Among them magnetic multilayers have become one of the mostly investigated system due to the interesting phenomena like oscillating indirect exchange coupling, spin dependent electron transport or large perpendicular anisotropies. An attractive possibility given by the novel technology is to grow the multilayer structures on atomic scale by so-called atomic layer deposition. At the low thickness limit, a multilayer structure, in

which a few atomic layers of different metals are stacked alternately, is expected to be an artificial ordered alloy. Such artificial material, which does not exist in equilibrium bulk phase, was constructed for the first time as the AuFe ordered alloy. The additional investigations of this system proved the existence of the tetragonal phase, which is responsible for the perpendicular anisotropy. The ordering process is influenced by the complicated growth of Fe on Au, as shown by atomic scale investigations. Other similar systems are FeAl (strong ordering mechanism in the bulk) and FeCr (miscible in the wide concentration range) monoatomic superlattices. These investigations of the artificial magnetic systems have a lot of important technological applications. For example, magnetic hard-disk recording density of 20 Gbit/in^2 has been reported recently by using giant magnetoresistive-read sensor in the recording head. In this case the so-called current in plane (CIP) measuring principle was used. However this suffers from several drawbacks and is diminished by shunting and channelling. Measuring with the current perpendicular to the planes (CPP) solves most of the problems, mainly because the electrons cross all magnetic layers. A disadvantage of the CPP mode is that the resistance of the very thin multilayers is too small to be measured by ordinary technologies. The special CPP-MR sensor design was elaborated recently based on the principle of a metal base transistor. In the so-called Spin Valve Transistor (SVT) a CMR multilayer (Co/Cu or NiFe/Co) serves as a base region of an n-Si metal-base structure. There is very interesting field of the investigations, namely the transport through magnetic nanostructures, especially through structures with non-collinear magnetization, like magnetic domain wall and spin-injection devices but this subject deserves of the separate consideration.

Localized and band pictures of magnetism

During the last decades, the physics of magnetic phenomena has been developed into a very extensive branch of modern physical science. To a large degree, the progress in the study of the structural and dynamical properties of magnetic materials is due to the

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achievements of the magnetic neutron-scattering[6-11] . The unique possibilities of the method of thermal neutron scattering make it possible to obtain information about the magnetic and crystal structure, the distribution of magnetic moments, the spectrum of magnetic excitations, critical fluctuations, and so forth. To interpret the data, it is necessary to take into account the electron-electron and electron-nucleus interactions in the system and the Pauli principle, which is the main "player" on the field of magnetism. Thus, magnetism can be understood properly only in the framework of a quantum statistical theory of the condensed matter physics. In the quantum theory of magnetism, the method of model Hamiltonians has proved to be very effective. Without exaggeration, one can say that the great successes in the physics of magnetic phenomena are to a considerably extent due to use of certain very simplified and schematic model representations for the theoretical interpretation. Historically, the first was Heisenberg model of localized spins (and its limiting case, the Ising model). The Heisenberg model is based on the assumption that the wave functions of magnetically active electrons in crystals differ little from the atomic orbitals. The Heisenberg Hamiltonian has the form

$$H_{spin} = \Sigma_{ij} J_{ij} S_i S_j .$$

It is assumed that this model applies basically to substances which are insulator or semiconductors. The size of the coupling constant requires empirically is, however, in many cases very much larger than that calculated for the exchange mechanism originally proposed.

E.Stoner have proposed an alternative, fenomenological band model of magnetism of the transition metals, in which the bands for electrons of different spins are shifted in energy in a way which is favourable to ferromagnetism. The band shift effect is a consequence of strong intra-atomic correlations, as was formulated later by N.Mott, J.van Vleck, P.W.Anderson and J.Hubbard. Since J.Slater first pointed out and

explicitly stated the connection between band states of electrons in crystal and magnetic properties, there has been considerable theoretical interest in setting up microscopic theories of band or itinerant magnetism. The itinerant-electron picture is the alternative conceptual picture for magnetism. The general idea of the energy-band theory of magnetism can be described roughly as follows. The main assumption is that we can set up a potential field in which electron moves, and that the one-electron energy of an electron in this field, as determined by solving Schrodinger equation for the field, represents the energy of the corresponding electron in the real crystal. In an unmagnetized crystal, each energy level will be occupied by two electrons, one of each spin. If it is magnetized, electrons will be removed from the uppermost occupied levels for the unmagnetized crystal, will have their spins reversed, and will be put into the lowest previously empty levels. If we describe the orientation of spin parallel to the magnetization as spin up, the opposite orientation as spin down, we then have levels of both spins occupied up to an energy which is lower than the original Fermi level, and above that we have a set of energy levels occupied only by spin-up electrons, which then constitute the magnetic electrons producing the spin density.

It must be noted that the problem of antiferromagnetism is much more complicated subject and we mention it very briefly. The antiferromagnetism state is characterized by a spatially changing component of magnetization which varies in such a way that the net magnetization of the system is zero. The concept of antiferromagnetism of localized spins[33] which is based on the Heisenberg model and two-sublattice Neel ground state is relatively well founded contrary to the antiferromagnetism of delocalized or itinerant electrons[34]. The simplified band model of an antiferromagnet has been formulated by J.Slater within single-particle Hartree-Fock approximation. In this approach he used the "exchange repulsion" to keep electrons with parallel spins away from each other and to lower the Coulomb interaction energy. Some authors consider Slater model as a prototype of the Hubbard model. However the exchange repulsion was taken proportional to the number of electrons with the same spins only

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and the energy gap between two subbands was proportional to the difference of electrons with up and down spins. In the antiferromagnetic many-body problem there is an additional "symmetry broken" aspect. For an antiferromagnet, contrary to ferromagnet, the one-electron Hartree-Fock potential can violate the translational crystal symmetry. The period of the antiferromagnetic spin structure L is greater than the lattice constant a. To introduce the two-sublattice picture for itinerant model one should assume that L=2a and that the spins of outer electrons on neighbouring atoms are antiparallel to each other. To justify an antiferromagnetic ordering with alternating up and down spin structure we must admit that in effect two different charge distributions will arise concentrated on atoms of sublattices A and B. This picture accounts well for quasi-localized magnetic behavior and is obviously valid only in the simple commensurate two-sublattice case. For the more general case of an incommensurate magnetic structure and spiral states it is necessary to use a more refined description. The antiferromagnetic phase of chromium and its alloys has been satisfactorily explained in terms of the spin density waves (SDW) within a two-band model. It is essential to note that chromium becomes antiferromagnetic in a unique manner. The antiferromagnetism is established in a more subtle way from the spins of the itinerant electrons than the magnetism of collective band electrons in metals like iron and nickel. The essential feature of chromium which makes possible the formation of the SDW is the existence of "nested" portions of Fermi surface. The more fundamental question of whether the Hartree-Fock one-electron approach is really approppriate in describing the quasiparticle excitation spectrum of solids must also be emphasized. Correlation effects, which are entirely neglected in the Hartree-Fock approximation, are well known play an important role in magnetic substances[7,12,13]. The preceding remark should make it clear that in general a theoretically adequate description of the experimentally determined quasiparticle spectrum require more complicated approximations than those provided by the H-F approximation. Antiferromagnetic correlations may play an important role in the possible scenario of normal and superconducting behaviour of heavy fermions and

cuprates . Some of the experimental and theoretical results show that antiferromagnetic spin fluctuations are really involved in the problem. This idea has stirred a great deal of discussion in recent times. An appealing but phenomenological picture of high-temperature superconductors, known as the nearly antiferromagnetic Fermi liquids (NAFL) approach, has been developed to explain many anomalous properties of cuprates. This approach predicts the detailed phase diagram for cuprates and present arguments which suggest that the physical origin of the pseudogap found in quasiparticle spectrum below the critical temperature is the formation of a precursor to a spin-density-wave-state. While the NAFL's scenario is appealing, it has apparently not yet been derived from fully microscopic consideration.

Models of correlated electrons on a lattice

The problem of the adequate description of strongly correlated lattice fermions has been studied intensively during the last decade, especially in the context of heavy fermions and high-Tc superconductivity[12,13]. These investigations call for a better understanding of the nature of solutions (especially magnetic) to the correlated electron models. The microscopic theory of the itinerant ferromagnetism and antiferromagnetism of strongly correlated fermions on a lattice at finite temperatures is one of the important issues of recent efforts in the field. In relation to the duality of localized and itinerant electronic states, G.Wannier showed the importance of the description of the electronic states which reconcile the band and local (cell) concept as a matter of principle. One of the primary aims has been to describe the phenomenon of ferro- and antiferromagnetism . The collective band or itinerant electron model is quite the opposite of the localized spin model but it should be emphasized that these two quite different approaches should be regarded as complimentary rather than competitive since the dilemma between itinerant and localized electrons dominate the physics of many transition and rare-earth metals and compounds[7]. The Hubbard model is in a certain sense an intermediate model (the narrow-band model) and take

into account the specific features of transition metals and their compounds by assuming that the d electrons form a band but are subject to strong Coulomb repulsion at one lattice site. The Hamiltonian of the Hubbard model is:

$$H_{el} = \Sigma_{ij} t_{ij} a^+_{i\sigma} a_{j\sigma} + U/2 \ \Sigma_i n_{i\sigma} n_{i-\sigma}$$

Hubbard model has been widely recognized as a workable model for a study of the correlated itinerant electron systems. For the sake of simplicity we write down the simple single-orbital Hubbard model, however, in general, the multi-orbital Hubbard model should be used. Many magnetic and electronic properties of rare-earth metals and compounds (e.g. magnetic semiconductors) may be interpreted in terms of combined spin-fermion models[35], which include the interacting localized spin and itinerant charge subsystems. This add the richness to physical behaviour and brings in significant and interesting physics, e.g. the bound states and magnetic polarons, heavy fermions and colossal negative magnetoresistance. The Hamiltonian of the spin-fermion model has the form

$$H = H_{spin} + H_{el} + H_{spin-el},$$

where

$$H_{spin-el} = \Sigma_i I \ S_i \ \sigma_i$$

describe the interaction between the localized spin and spin density of itinerant electrons. These three model Hamiltonians (and their simple modifications and combinations) are the most used models in the quantum theory of magnetism.

Quasiparticle excitation spectra

The investigation of the spectrum of magnetic excitations of pure transition metals and their compounds is of great interest for refining our theoretical model representations about the nature of the magnetic states. The most direct and convenient method of experimental study of the spectrum of magnetic excitations is the method of inelastic scattering of thermal neutrons[6-11]. It is known experimentally that the spin wave scattering of slow neutrons in transition metals and compounds can be described on the basis of the Heisenberg model. On the other hand, the mean magnetic moment of the ions in solids differ appreciable from the atomic values and are fractional. The main message of the present paper is that the excitation spectrum of the Hubbard model and some of its modifications is of considerable interest from the point of view of the choice of relevant microscopic model. In other words, if we calculate the neutron scattering cross section, which, in turn, is proportional to the imaginary part of the generalized spin susceptibility

$$d^2\sigma/d\omega\, d\Omega \approx \mathrm{Im}\, \chi(q, \omega)\,,$$

the cross section for the acoustical spin wave scattering will be identical for the Heisenberg and Hubbard model. So, on the level of low-energy, hydrodynamical excitations one cannot distinguish between the models. However, for the Hubbard model the poles of the generalized spin susceptibility will contain, in addition to acoustical spin-wave pole, the continuum of the Stoner excitations, as shown on Fig.1. The spectra of the s-d (or spin-fermion) model and multiorbital (multi-band) Hubbard model are shown for the comparison also. From our point of view[7], the clearest difference between models is manifested in the spectrum of magnetic excitations. The model of correlated itinerant electrons and spin-fermion model have a more complicated spectra than the model of localized spins. These spectra have a great interest from the point of view of the fundamental problem of the nature of magnetism. Since the structure of the generalized spin susceptibility and the form of its poles are determined by the choice of the model Hamiltonian of the system and the
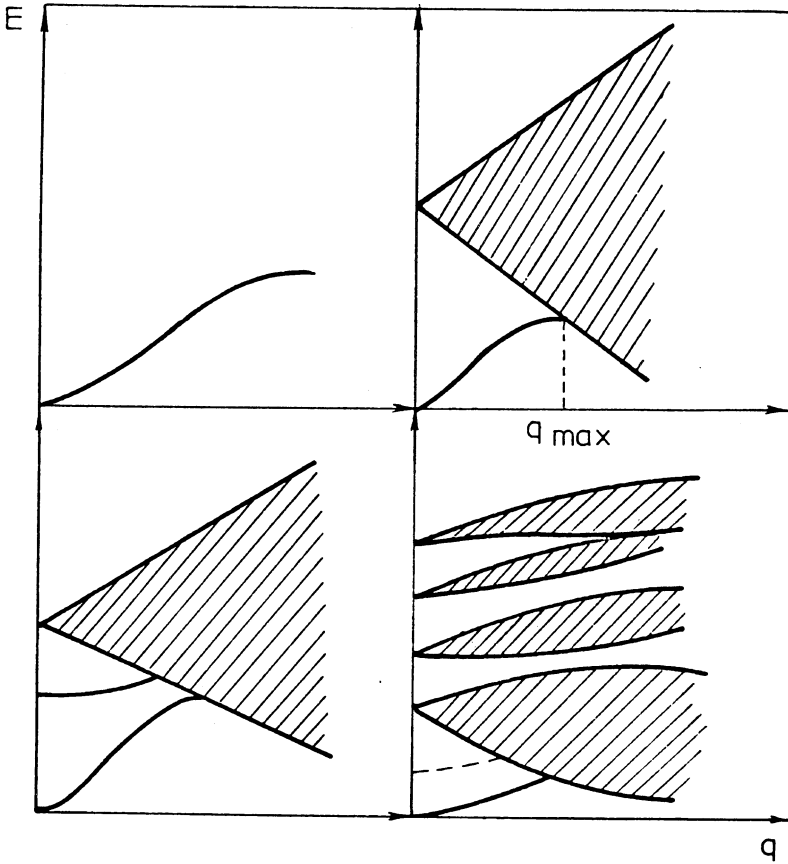
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Fig.1. Schematic form of the excitation spectra of the four microscopic models of magnetism: a) upper-left, the Heisenberg model; b) upper-right, the Hubbard model; c) down-left, the modified Zener (spin-fermion) model; d) down-right, the multiorbital Hubbard model.

approximations made in its calculation, the results of neutron scattering experiments can be used to judge the adequacy of the microscopic models. However, it should be emphasized, that to judge reliably the applicability of a particular model, it is necessary to measure the susceptibility (the cross section) at all points of the reciprocal space and for the wide interval of temperatures, which is not always permitted by the existing experimental techniques. Thus, the further development of experimental facilities will provide a base for further refining of the theoretical models and conceptions about the nature of magnetism.

Conclusions and discussions

The art of "model-making" in physics[36] is one of the main and subtle aspects of the intellectual penetration into the complicated physical situation. In this article, we have shown that many phenomena in transition and rare-earth metal oxides and compounds studied by means of the scattering of slow neutrons and other methods can be reasonably understood from a unified point of view by using the simplified but workable models of correlated electrons on a lattice. The spectrum of magnetic excitations of the Hubbard model reflects the dual behaviour of the magnetically active electrons in transition metals and their compounds. Many magnetic and electronic properties of rare-earth metals and compounds may be interpreted in terms of combined spin-fermion models, which include the interacting spin and charge subsystems. The general properties of rotational invariance of the model Hamiltonians shows that the presence of a spin-wave acoustic pole in the generalized magnetic susceptibility is a direct consequence of the rotational symmetry of the system, as for the isotropic Heisenberg model of localized spins. Thus the acoustical spin-wave branch reflects a certain degree of localization of the relevant electrons; the characteristic quantity D, which determines the spin wave stiffness, can be measured directly in neutron experiments. In contrast, in the simplified Stoner model

of band ferromagnetism, which is based on the assumption of complete collectivization of the magnetic electrons the acoustical spin-waves does not exist. There are only a continuum of single-particle Stoner excitations. The presence of the Stoner continuum for the spectrum of excitations of the Hubbard model is a manifestation of the delocalization of the magnetic electrons. Since the Stoner excitations do not arise in the Heisenberg model, their direct detection and detailed investigation by means of neutron scattering is one of the most intriguing problems of the fundamental physics of magnetic state. Moreover, it is to be expected that measurements in the high-energy ("optical") range will give more interesting results that can be expected on the basis of the single-band Hubbard model, which reflects the basic behaviour of the system but is strongly simplified. The Hubbard model admits natural generalizations that enable one to take into account the many subbands, s-d hybridization, spin-charge and electron-phonon interactions, and so forth. We have demonstrated that even the simpest generalizations of the Hubbard model give a much richer spectrum, and, moreover, precisely in the "optical" range. The acoustical spin-wave pole is preserved if the modified Hamiltonian remains rotationally invariant.

Our understanding of the magnetic phenomena in complex magnetic materials is far from complete. Many new experimental results must be used to judge the extent to which this or that model is applicable. However, at the present time, there are weighty grounds for believing that the duality of itinerant and localized behaviour of electronic states will play a crucial role for our understanding of these complicated materials. The last point is rather remarkable and is the main advantage of the approach we suggest. Clearly, more work is required for both theory and experiment on these perspective materials with unusual combination of the physical properties to clarify ultimately the microscopic origination of their magnetic, superconducting, heavy fermion, colossal negative magnetoresistive and other types of behaviour. Further theoretical and experimental investigations of these systems will deepen our

understanding of the nature of magnetism and more precise model theoretical notions.

In spite that we believe that the models bear the real physics, it is evident, that the model Hamiltonians, which were discussed above are very crude and simplified. According to Sir Rudolf Peierls[36] : "Nevertheless much can be learnt from the model... What is common to all these different types of model is that they serve as aids in thinking more clearly about physical problems, by creating simpler situations, more accessible to our intuition, as steps towards a rational understanding of the actual situation... We can handle them and turn them over, and get a much clearer view of their shape and structure than from real objects, and that is just what the physicist is trying to do with his models".

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Фундаментальные принципы физики магнетизма и проблема
локализованных и делокализованных электронных состояний

E17-2000-32

Дан краткий обзор перспективных направлений в физике магнитных явлений, связанных главным образом с применением метода рассеяния медленных нейтронов. Рассмотрено большое число экспериментальных данных о магнитных и транспортных свойствах сложных соединений и окислов переходных и редкоземельных металлов и их сплавов. Данный класс веществ включает в себя многие материалы с весьма необычными свойствами: высокотемпературные сверхпроводники, купраты; соединения с тяжелыми фермионами; манганиты со структурой перовскита; магнитные d- и f-металлы и др. В отличие от простых металлов, где основные представления о физических свойствах в основном понятны, данная группа веществ характеризуется сильной межэлектронной корреляцией и сложным характером спектра. Корреляционные эффекты определяют многие специфические черты магнитных и транспортных свойств этих веществ. При этом определяющую роль играет то, что электронные состояния проявляют себя как локализованные и делокализованные. Это противоречивое поведение сильно усложняет построение микроскопических корреляционных моделей, адекватно описывающих физическую ситуацию. Наше основное предложение состоит в том, что на основе анализа многих экспериментальных данных по неупругому рассеянию медленных нейтронов, т.е. спектров магнитных квазичастичных возбуждений, можно сформулировать весьма достоверные критерии применимости микроскопических моделей. Данный подход связан с пониманием фундаментальных принципов строения вещества и физики магнитных явлений.

Kuzemsky A.L.

Fundamental Principles of the Physics of Magnetism and the Problem
of Localized and Itinerant Electronic States

E17-2000-32

Some of the remarkably and recently observed features of complex transition metal and rare-earth metal oxides, compounds and alloys concerning mainly of their magnetic behaviour are reviewed in the context of slow neutron scattering. These includes variety of the new class of materials with unusual properties: high Tc superconductors, heavy fermion compounds, perovskite manganites, magnetic d and f transition metals, diluted magnetic semiconductors, etc. Contrary to simple metals where the fundamentals very well known and the electrons can be represented in a way such that they weakly interact with each other, in these materials the electrons interact strongly and moreover their spectra are complex, i.e. have many branches, etc. The behaviour and the true nature of the electronic states are of central importance to the understanding of unusual transport and magnetic properties of this class of materials. We argue that interesting electronic and magnetic properties of these substances are intimately related with dual, itinerant and localized, behaviour of electrons and formulate a criteria what basic picture best describe this dual behaviour. The suggestion is that quasi-particle excitation spectra might provide distinctive signatures and good criteria for the approprite choice of relevant model. The method of inelastic neutron scattering is indispensable and unique tool for study of these spectra.