V. K. Ignatovich

A CATASTROPHE IN QUANTUM MECHANICS

Игнатович В. К.   Е4-2004-45
Катастрофа в квантовой механике

Анализируется стандартная теория рассеяния (СТР) в нерелятивистской квантовой механике (КМ). Вскрываются противоречия СТР. Обсуждается прямой способ вычисления вероятности рассеяния без привлечения конечного объема. Показано, что обоснование СТР в научной литературе неубедительно. Излагается полная теория рассеяния волновых пакетов на фиксированном центре и демонстрируется ее сходство с теорией рассеяния плоских волн. Исследуется рассеяние нейтронов на одноатомном газе и указываются возникающие при этом проблемы. Обнаружена катастрофическая неоднозначность в определении сечения рассеяния. Обсуждается способ преодоления этой неоднозначности.

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A Catastrophe in Quantum Mechanics

The standard scattering theory (SST) in nonrelativistic quantum mechanics (QM) is analyzed. Self-contradictions of SST are deconstructed. A direct way to calculate scattering probability without introduction of a finite volume is discussed. Substantiation of SST in textbooks with the help of wave packets is shown to be incomplete. A complete theory of wave packet scattering on a fixed center is presented, and its similarity to the plane wave scattering is demonstrated. The neutron scattering on a monatomic gas is investigated, and several problems are pointed out. A catastrophic ambiguity of the cross section is revealed, and a way to resolve this ambiguity is discussed.

1. INTRODUCTION

Here we deal with nonrelativistic scattering theory. To be more precise we shall speak about neutron elastic and inelastic scattering, which is met in condensed matter research. We limit ourselves to this case for the sake of simplicity only. Everything we discuss here can be generalized to more complicated processes.

The simplest process is elastic s-wave scattering from a fixed center, which is usually described by the wave function

$$\Psi = \exp\left(i\boldsymbol{kr}\right) - \frac{b}{r}\exp\left(ikr\right), \tag{1}$$

containing an incident plane wave and a scattered spherical wave with a factor b called the scattering amplitude. This amplitude has dimension of length, and it gives cross section $4\pi|b|^2$ with dimension of area.

Such wave function is not appropriate for description of scattering, because it does not satisfy the free Schrödinger equation. According to quantum mechanics we need an asymptotic wave function after scattering, which is a superposition of free states satisfying the free Schrödinger equation. In the next section we show how to do that by nonstationary and stationary methods.

The nonstationary method is well known, and in the 3rd section we briefly discuss how this method is used in some textbooks [1, 2]. These books are considered as providing the proof of validity of the SST. However, their proof is not correct, and we show where. The main point is: the proof starts with an initial wave-packet state, and scattering probability is defined as a transition from the wave packet state to the state of a plane wave. We claim that such transition is impossible, because unitarity is violated. In the mentioned textbooks unitarity is considered as equality of the number of plane wave components before and after scattering. However, this equality means conservation of wave packet normalization. So, to be consistent, we need to find the transition from an initial wave packet state into a final also wave packet state, and in the section 4 we show how to do at least for elastic scattering of a wave packet on a fixed center.

It is of a surprise to find out that the scattering probability of the wave packets does not depend on impact parameter, though this fact can be well explained in

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wave mechanics. However, to get cross section from the scattering probability we need to add to the wave mechanics an additional hypothesis that scattering is absent, when the target is outside of the wave packet.

In section 5 we consider scattering of neutrons from an arbitrary system, taking into account that wave packets scatter like plane waves. The standard approach starting with Fermi golden rule is criticized, and the direct way of calculation of the scattering probability is described. In section 6, this approach is applied to the neutron scattering on a monatomic gas. First we show how to get standard formulas for total and differential cross section. After that we show that the value of the cross section is uncertain, because calculation of it in different ways gives different and even diverging expressions. We conclude that analysis of scattering reveals catastrophic discrepancy inherent in quantum mechanics, and we can only suggest some way to resolve this difficulty.

In the final section we give a summary of the paper, and sum up all our reasonings and contradictions, which were met and resolved here.

2. ASYMPTOTIC WAVE FUNCTION

According to the standard quantum mechanics (SQM), if a system has eigen states ψ_n, its initial state is ψ_i, and the wave function after scattering is Ψ, then to find a result of scattering we need to expand Ψ over eigen states, i.e. to represent it in the form

$$\Psi = \psi_i + \sum_f a_{if}\psi_f, \tag{2}$$

where a_{if} are expansion coefficients, and index i in them points to the initial state before scattering. It immediately follows from (2) that scattering is a transition from the state ψ_i to states ψ_f, and probability of transition from the initial i-state to a definite final $f \neq i$-state is described by dimensionless magnitudes $w_{if} = |a_{if}|^2$. The unitarity condition is

$$|1 + a_{ii}|^2 + \sum_{f \neq i} |a_{if}|^2 = 1. \tag{3}$$

Summation in expression (2) means discrete spectrum, used here for the sake of simplicity, however, it is not essential, and we can (and shall) deal also with continuous spectra of quantum numbers i.

Now we can show that (1) does not correspond to the above principles of calculation of transition probabilities in quantum mechanics.

2.1. What is Wrong in SST . What do we do in SST? Eigen states of a particle are described by plane waves $\psi_i = \exp(i\boldsymbol{k}\boldsymbol{r})$, but the scattered wave function after, say, elastic s-wave scattering, is described by the spherical wave, $\Psi = \psi_i \propto \exp(ikr)/r$, which is not an eigen state, and even is not a solution of the free Schrödinger equation, because

$$[\Delta + k^2]\frac{\exp(ikr)}{r} = -4\pi\delta(\boldsymbol{r}), \tag{4}$$

where the right-hand side contains the Dirac δ-function, which is not identical zero in all the space.

2.2. What Should We Expect According to SQM According to principles of SQM we must represent the scattered wave function as a superposition of plane waves

$$\Psi = \exp(i\boldsymbol{k}\boldsymbol{r}) - \int f(\Omega)d\Omega \, \exp(i\boldsymbol{k}_\Omega \boldsymbol{r}), \tag{5}$$

where Ω is a solid angle of the scattered particle, and $f(\Omega)$ is dimensionless probability amplitude. Then the intensity of scattering into the angle Ω is described by dimensionless probability

$$dw(\Omega) = |f(\Omega)|^2 d\Omega, \tag{6}$$

and the total probability w of scattering is dimensionless integral

$$w = \int dw(\Omega) = \int |f(\Omega)|^2 d\Omega. \tag{7}$$

To satisfy unitarity we must write the incident wave with some amplitude $1 - f(0)$, then the unitarity condition will lead to

$$2\mathrm{Re}f(0) = |f(0)|^2 + w. \tag{8}$$

2.3. How to Meet Our Expectation. To be consistent we need to find asymptotic limit of the wave function (1). It is possible to do that in two ways: to find stationary function after scattering at long distances from the scatterer, or to find nonstationary wave function at long times $t \to +\infty$.

2.3.1. Asymptotic of Stationary Function at Long Distances. The formula (1) can be improved immediately, if we use Fourier expansion for the spherical wave:

$$\frac{\exp(ikr)}{r} = \frac{i}{2\pi}\int \exp(i\boldsymbol{p}_\parallel \boldsymbol{r} + ip_z|z|)\frac{d^2p_\parallel}{p_z}, \tag{9}$$

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where we fix the direction from the scatterer to the observation point as z-axis, and integrate over all components $\boldsymbol{p}_\parallel$ parallel to x, y plane with z-component of the momentum being equal to $p_z = \sqrt{k^2 - p_\parallel^2}$.

The range of integration over $\boldsymbol{p}_\parallel$ (9) is infinite, and, in particular, it includes those $\boldsymbol{p}_\parallel$, for which $p_\parallel^2 > k^2$. At these $\boldsymbol{p}_\parallel$ the component p_z is imaginary, and $\exp(ip_z|z|)$ is an exponentially decaying function. If the distance to the observation point is large enough (later we discuss what does it mean «enough»), we can neglect exponentially decaying terms, and restrict integration to $p_\parallel^2 \leqslant k^2$:

$$\frac{\exp(ikr)}{r} \approx \frac{i}{2\pi} \int\limits_{p_\parallel^2 < k^2} \exp(i\boldsymbol{p}_\parallel \boldsymbol{r} + ip_z|z|) \frac{d^2 p_\parallel}{p_z}. \tag{10}$$

In this integral we can substitute

$$\frac{d^2 p_\parallel}{p_z} = d^3 p \, \delta(p^2/2 - k^2/2) \Theta(p_z z > 0), \tag{11}$$

where $p^2 = p_\parallel^2 + p_z^2$, p_z is a variable, and we introduced the step function $\Theta(x)$, which is unity or zero, when inequality in its argument is satisfied or not, respectively. Substitution of (11) into (10) gives

$$\frac{\exp(ikr)}{r} = \frac{i}{2\pi} \int \exp(i\boldsymbol{p}\boldsymbol{r}) \Theta(p_z z > 0) \, d^3 p \, \delta(p^2/2 - k^2/2) =$$

$$= \frac{ik}{2\pi} \int\limits_{4\pi} \exp(i\boldsymbol{k}_\Omega \boldsymbol{r}) d\Omega, \quad (12)$$

where $\boldsymbol{k}_\Omega$ is the wave vector of the length k pointing into the direction $\boldsymbol{\Omega}$ in the element $d\Omega$ of the solid angle Ω.

Let us now find what values do we neglect excluding exponentially decaying terms from the integrand. For that we calculate the integral

$$\frac{1}{2\pi} \left| \int\limits_{p_\parallel^2 > k^2} \exp(-p_z' z + i\boldsymbol{p}_\parallel \boldsymbol{r}_\parallel) \frac{d^2 p_\parallel}{p_z'} \right| < \frac{1}{2\pi} \int\limits_{p_\parallel^2 > k^2} \exp(-p_z' r) \frac{d^2 p_\parallel}{p_z'} = \frac{1}{r}, \quad (13)$$

where $p_z' = \sqrt{p_\parallel^2 - k^2}$, and we replaced z by the distance r between scatterer and observation point.

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Thus we have found the asymptotical form of the wave function after scattering

$$\Psi(\boldsymbol{k}, \boldsymbol{r}) = \exp{(i\boldsymbol{k}\boldsymbol{r})} - \frac{b}{r}\exp{(ikr)} = \exp{(i\boldsymbol{k}\boldsymbol{r})} - \frac{ibk}{2\pi}\int\limits_{4\pi}\exp{(i\boldsymbol{k}_\Omega\boldsymbol{r})}d\Omega, \quad (14)$$

which is equivalent to (5), with scattering probability amplitude

$$f(\Omega) = \frac{ibk}{2\pi} = i\frac{b}{\lambda}, \quad (15)$$

and scattering probability

$$dw(\Omega) = |f(\Omega)|^2 d\Omega = \left|\frac{b}{\lambda}\right|^2 d\Omega, \quad w = \int\limits_{4\pi} dw(\Omega) = 4\pi\left|\frac{b}{\lambda}\right|^2, \quad (16)$$

where $\lambda = 2\pi/k$ is the neutron wave length. We see that (1) is reduced to (14), when we neglect the terms of the order b/r. Since the decision to neglect or not to neglect this term is at will of the physicist, then the distance r from the center is not asymptotical one, being even of light years size, if he does not neglect it. On the other side, the distances of the order 1 Å are asymptotical ones, if b/r is neglected.

2.3.2. The Nonstationary Derivation of Asymptotic Wave Function at Large Times $t \to \infty$. To find nonstationary asymptotic of the wave function (1) it is sufficient to include in it the time-dependent factor $\exp{(-i\omega_k t)}$, where $\omega_k = k^2/2$, and to use Fourier representation

$$\delta\psi(r, t) = \frac{b}{r}\exp{(ikr - i\omega_k t)} =$$
$$= \frac{b}{(2\pi)^2}\int\frac{d^3p}{\omega_p - \omega_k - i\epsilon}\exp{(i\boldsymbol{p}\boldsymbol{r} - i\omega_k t)}, \qquad \omega_p = p^2/2, \quad (17)$$

for the spherical wave.

We can add and subtract $i\omega_p t$ in the exponent, and represent the field (17) as a superposition of plane waves

$$\delta\psi = \int\widetilde{f}(\boldsymbol{p}, t)\exp{(i\boldsymbol{p}\boldsymbol{r} - i\omega_p t)}d^3p, \quad (18)$$

with amplitudes

$$\widetilde{f}(\boldsymbol{p}, t) = \frac{b}{(2\pi)^2}\frac{\exp{(i[\omega_p - \omega_k]t)}}{\omega_p - \omega_k - i\epsilon}, \quad (19)$$

which depend on time t.

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Now we use the evident relation

$$\frac{\exp\left(i[\omega_p - \omega_k]t\right)}{\omega_p - \omega_k - i\epsilon} = i \int\limits_{-\infty}^{t} \exp\left(i[\omega_p - \omega_k]t'\right)dt', \qquad (20)$$

which in the limit $t \to \infty$ gives the law of energy conservation

$$i \lim_{t\to\infty} \int\limits_{-\infty}^{t} \exp\left(i[\omega_p - \omega_k]t'\right)dt' = 2\pi i\delta(\omega_p - \omega_k) = 4\pi i\delta(p^2 - k^2). \qquad (21)$$

In this limit (18) is

$$\delta\psi = \int \frac{ib}{\pi} \exp\left(i\boldsymbol{pr} - i\omega_p t\right)d^3p\,\delta(p^2 - k^2) = \frac{ibk}{2\pi} \int\limits_{4\pi} d\Omega\,\exp\left(i\boldsymbol{k}_\Omega\boldsymbol{r} - i\omega_k t\right), \quad (22)$$

and we get dimensionless scattering probability amplitude (15) and the total scattering probability $w = 4\pi|b/\lambda|^2$, which coincides with (16).

2.4. Scattering Cross Section. We found dimensionless scattering probability, but almost all the experiments are interpreted in terms of scattering cross sections. To get a cross section we are to introduce a front area A of the incident particle wave function, and suppose that scattering takes place only, if the scattering center crosses this area.

Let us compare experimental and theoretical definitions of the cross section in an experiment schematically shown in Fig. 1. If the detector registers N_s
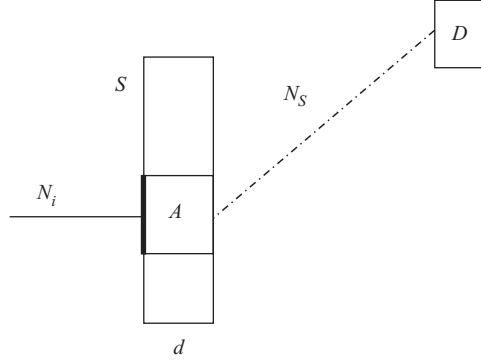

Fig. 1. Definition of cross section for a single atom

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neutrons per unit time, then the total probability W for a single neutron to be scattered in the sample into the given direction is

$$W = \frac{N_s}{N_i} = \frac{N_s}{JS},$$ (23)

where J is the neutron flux density, S is the area of the sample immersed into the neutron flux, and $N_i = JS$ is the total number of neutrons incident on the sample per unit time.

The scattering probability w_1 per unit atom is defined as

$$w_1 = \frac{W}{N_a},$$ (24)

where N_a is the number of atoms on the way of a single neutron. If the neutron wave function has area A, then the number of atoms N_a is equal to $N_0 A d$, where N_0 is atomic density and d is the sample thickness. From (24) we immediately find the scattering cross section of a single neutron per single atom

$$\sigma = A w_1 = \frac{W}{N_0 d} = \frac{N_s}{N_i N_0 d} = \frac{N_s}{J S N_0 d} = \frac{N_s}{J N_0 V},$$ (25)

where V is the sample volume $V = S d$. The second equality in (25) defines experimentally measured quantity for a thin sample with area S wider than the beam area, and the last equality defines the experimentally measured quantity for a small sample with area S smaller than the beam width. To interpret the measured quantity as a cross section we must compare it to $A w_1$. Of course, this A includes also dimension of the single nucleus, so for a point neutron the cross section can be interpreted as cross area of the nucleus. However, in this case we have a paradox: sometimes the cross section σ is several orders of magnitude larger than the nucleus area. We avoid the paradox, if accept that A is considerably larger than nucleus.

It is important to note that the neutron-nucleus scattering process is a consequence of a short range interaction. However, this short range interaction becomes a long range one because of properties of the neutron wave function. This long range property is demonstrated in such effects as total reflection and diffraction in crystals. To calculate probability of these effects it is sufficient to suppose that the wave function is a plane wave. Introduction of the finite front area means that the particle wave function is not a plane wave, but a wave packet.

This wave packet cannot be spreading, because, if it were, the transmission of the sample would decrease, when sample is shifted from source to detector, and no one, in our knowledge, had ever observed such a phenomenon.

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One of the possible candidates for the nonspreading wave packet is the singular de Broglie wave packet (dBWP) [3–5]

$$\psi_{dB}(\boldsymbol{r}, t) = \sqrt{\frac{s}{2\pi}} \exp\left(i\boldsymbol{k}\boldsymbol{r} - i\omega t\right) \frac{\exp\left(-s|\boldsymbol{r} - \boldsymbol{v}t|\right)}{|\boldsymbol{r} - \boldsymbol{v}t|}, \tag{26}$$

where $\omega = [k^2 - s^2]/2$, s determines the packet width, and $\boldsymbol{v}$ is wave packet velocity, which in our units $m = \hbar = 1$ coincides with the wave vector $\boldsymbol{k}$. The front area of (26) can be estimated as $A_{dB} = \pi/s^2$. This area is considerably larger than interatomic distance, because of long range interaction with many atoms, so the dimensions of nuclei can be neglected.

3. THE PROOF OF SST IN TEXTBOOKS AND ITS FLAW

The reader may doubt our definition of the cross section having in mind that in such well-known books as those by Goldberger & Watson [1], and by J. Taylor [2] wave packets are used to proof correctness of SST. We briefly outline here their proof and show its flaw. The main point is the following: the incident wave packet $|\phi\rangle$ is represented as the Fourier expansion $\int d^3 p a(\boldsymbol{p})|\boldsymbol{p}\rangle$, where $|\boldsymbol{p}\rangle$ is a plane wave with wave number $\boldsymbol{p}$, and $a(\boldsymbol{p})$ are Fourier coefficients. After scattering this wave packet is transformed into

$$\int d^3 p a(\boldsymbol{p})|\boldsymbol{p}'\rangle d^3 p' \langle \boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle = \int d^3 p' b(\boldsymbol{p}')|\boldsymbol{p}'\rangle, \tag{27}$$

where $\hat{S}$ is S-matrix, and

$$b(\boldsymbol{p}') = \int^{'} \langle \boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle a(\boldsymbol{p}) d^3 p. \tag{28}$$

The scattering probability is defined as

$$dw(\boldsymbol{p}') = |b(\boldsymbol{p}')|^2 d^3 p', \tag{29}$$

i.e. the scattering probability is defined by Fourier coefficients of the expansion. It is the same as for free wave packet to define scattering probability by $|a(\boldsymbol{p})|^2 d^3 p$. Below we present more details of this proof and arguments against its validity.

3.1. Steps to the Proof

1. In this proof a wave packet $|\phi\rangle$ for initial state of incoming particle long before scattering is introduced. In this state the particle is far from scatterer (target) and therefore its dynamics is described by free Hamiltonian H_0:

$$|\phi(t)\rangle = \exp\left(-iH_0 t\right)|\phi\rangle. \tag{30}$$

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The wave packet is represented by Fourier expansion over plane waves

$$|\phi\rangle \equiv |\phi(\boldsymbol{k})\rangle = \int d^3pa(\boldsymbol{k} - \boldsymbol{p})|\boldsymbol{p}\rangle, \tag{31}$$

where $\boldsymbol{k}$ is momentum of the packet, $|\boldsymbol{p}\rangle$ is eigen function of the momentum operator: $\langle \boldsymbol{r}|\boldsymbol{p}\rangle = \exp{(i\boldsymbol{pr})}$, and $a(\boldsymbol{p})$ are numerical coefficients.

2. A wave function $|\Psi\rangle$ of the particle at the interaction moment $t = 0$ is introduced. At that time dynamics of the particle is described by the full Hamiltonian H containing interaction potential V. The time dependence of this function is determined by expression $|\Psi(t)\rangle = \exp{(-iHt)}|\Psi\rangle$.

3. Two above functions $|\Psi\rangle$ and $|\phi\rangle$ are related to each other by requirement that at $t \to -\infty$ the wave function $\exp{(-iHt)}|\Psi\rangle$ asymptotically transforms into $\exp{(-iH_0t)}|\phi\rangle$, i.e. at $t \to -\infty$ we have

$$\exp{(-iHt)}|\Psi\rangle \to \exp{(-iH_0t)}|\phi\rangle, \tag{32}$$

or

$$|\Psi\rangle = \Omega_+|\phi\rangle, \quad \Omega_+ = \lim_{t \to -\infty} U(0,t), \quad U(0,t) = \mathrm{e}^{iHt}\mathrm{e}^{-iH_0t}. \tag{33}$$

The limiting operator Ω_+ is called Möller operator [2].

4. According to (33) the operator $U(0,t)$ satisfies the differential equation

$$i\frac{\partial}{\partial t}U(0,t) = -\mathrm{e}^{iHt}V\mathrm{e}^{-iH_0t}, \tag{34}$$

because $H - H_0 = V$. It follows from this equation that

$$\Omega_+ = 1 - i\int_{-\infty}^{0} \mathrm{e}^{iHt'}V\,\mathrm{e}^{-iH_0t'}dt', \tag{35}$$

and

$$|\Psi\rangle = \left(1 - i\int_{-\infty}^{0} dt'\,\mathrm{e}^{iHt'}V\,\mathrm{e}^{-iH_0t'}\right)|\phi\rangle =$$

$$= \int d^3pa(\boldsymbol{k} - \boldsymbol{p})\left[1 - i\int_{-\infty}^{0} dt'\,\mathrm{e}^{i(H-E_p)t'}V\right]|\boldsymbol{p}\rangle, \tag{36}$$

where we used the relation $\exp{(-iH_0t)}|\boldsymbol{p}\rangle = \exp{(-iE_pt)}|\boldsymbol{p}\rangle$.

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Integration of (36) over t' leads to

$$\int d^3 p a(\boldsymbol{k} - \boldsymbol{p}) \left[1 - \frac{1}{H - E_p - i\epsilon} V \right] |\boldsymbol{p}\rangle = \int d^3 p a(\boldsymbol{k} - \boldsymbol{p}) |\psi_{\boldsymbol{p}}\rangle, \qquad (37)$$

where the function $|\psi_{\boldsymbol{p}}\rangle$, which replaces plane waves at the time, when interaction is acting, is introduced.

5. This function is

$$|\psi_{\boldsymbol{p}}\rangle = \left[1 - \frac{1}{H - E_p - i\epsilon} V \right] |\boldsymbol{p}\rangle. \qquad (38)$$

It satisfies the full Schrödinger equation with interaction

$$(H - E_p) |\psi_{\boldsymbol{p}}\rangle = 0 \qquad (39)$$

and in agreement with standard representation contains the incident plane and outgoing spherical waves.

6. Using the following identity

$$\frac{1}{A} - \frac{1}{B} = \frac{1}{A}(B - A)\frac{1}{B}, \qquad (40)$$

we find that

$$\frac{1}{H - E_p - i\epsilon} = \frac{1}{H_0 - E_p - i\epsilon} \left(1 - V \frac{1}{H - E_p - i\epsilon} \right). \qquad (41)$$

Therefore $|\psi_{\boldsymbol{p}}\rangle$ is transformed to

$$|\psi_{\boldsymbol{p}}\rangle = \left[1 - \frac{1}{H_0 - E_p - i\epsilon} \mathcal{T} \right] |\boldsymbol{p}\rangle, \qquad (42)$$

where

$$\mathcal{T} = V - V \frac{1}{H - E_p - i\epsilon} V. \qquad (43)$$

7. An asymptotical state $|\chi\rangle$ of the particle after scattering is defined. Its dynamics is again determined by the free Hamiltonian H_0: $|\chi(t)\rangle = \exp(-iH_0 t)|\chi\rangle$. This state is also a wave packet $|\chi\rangle = \int d^3 p |\boldsymbol{p}\rangle a_s(\boldsymbol{k}, \boldsymbol{p})$.

8. A correspondence between $|\psi\rangle$ and $|\chi\rangle$ is established by the requirement that at $t \to +\infty$ the wave function $\exp(-iHt)|\Psi\rangle$ transforms into $\exp(-iH_0 t)|\chi\rangle$:

$$\exp(-iHt)|\Psi\rangle \to \exp(-iH_0 t)|\chi\rangle, \qquad (44)$$

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or

$$|\chi\rangle = \lim_{t\to\infty} e^{iH_0t}\, e^{-iHt} \int d^3p\, a(\boldsymbol{k}-\boldsymbol{p})|\psi_{\boldsymbol{p}}\rangle =$$

$$= \lim_{t\to\infty} e^{iH_0t} \int d^3p\, a(\boldsymbol{k}-\boldsymbol{p})\, e^{-iE_pt}|\psi_{\boldsymbol{p}}\rangle, \quad (45)$$

where in the last equality equation (39) is taken into account.

9. The function $|\psi_{\boldsymbol{p}}\rangle$ is expanded over plane waves. Then (45) becomes

$$|\chi\rangle = \lim_{t\to\infty} \int d^3p\, a(\boldsymbol{k}-\boldsymbol{p}) \int d^3p'\, e^{iE_{p'}t}|\boldsymbol{p}'\rangle\langle\boldsymbol{p}'||\psi_{\boldsymbol{p}}\rangle\, e^{-iE_pt}, \quad (46)$$

with account of $\exp(iH_0t)|\boldsymbol{p}'\rangle = \exp(iE_{p'}t)|\boldsymbol{p}'\rangle$. Substitution of (42) brings

$$|\chi\rangle = \lim_{t\to\infty} \int d^3p'\,|\boldsymbol{p}'\rangle \int d^3p\, a(\boldsymbol{k}-\boldsymbol{p})\times$$

$$\times \left[\delta(\boldsymbol{p}-\boldsymbol{p}') - \frac{e^{i(E_{p'}-E_p)t}}{E_{p'}-E_p-i\epsilon}\langle\boldsymbol{p}'|\mathcal{T}|\boldsymbol{p}\rangle\right]. \quad (47)$$

10. It follows from (20) that

$$|\chi\rangle = \int d^3p'\,|\boldsymbol{p}'\rangle \int d^3p\, a(\boldsymbol{k}-\boldsymbol{p})[\delta(\boldsymbol{p}-\boldsymbol{p}') - 2\pi i\delta(E_{p'}-E_p)T(\boldsymbol{p}',\boldsymbol{p})] =$$

$$= \int d^3p'\,|\boldsymbol{p}'\rangle \int d^3p\,\langle\boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle a(\boldsymbol{k}-\boldsymbol{p}), \quad (48)$$

where $T(\boldsymbol{p}',\boldsymbol{p}) = \langle\boldsymbol{p}'|\mathcal{T}|\boldsymbol{p}\rangle$, and scattering matrix $\hat{S}$ with matrix elements

$$\langle\boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}') - 2\pi i\delta(E_{p'}-E_p)T(\boldsymbol{p}',\boldsymbol{p}) \quad (49)$$

is introduced.

3.2. The flaw of the Proof. Above we presented main steps to the proof, but not the proof itself. The steps are correct and they demonstrate that our approach to get asymptotical state after scattering (compare (20), (21) with (47), (48)) is well justified.

Now we show the next step to the proof, which is not correct. This step introduces probability of scattering. It is suggested that after scattering detectors

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register not a wave packet but a plane wave, so the probability of scattering from the state of the wave packet

$$|\phi\rangle \equiv |\phi(\boldsymbol{k})\rangle = \int d^3 p a(\boldsymbol{k} - \boldsymbol{p})|\boldsymbol{p}\rangle$$

with momentum $\boldsymbol{k}$ into the plane wave $|\boldsymbol{p}'\rangle$ with momentum $\boldsymbol{p}'$ is

$$dw = d^3 p' |\langle \boldsymbol{p}' || \chi \rangle|^2 = d^3 p' \left| \int d^3 p \langle \boldsymbol{p}' | \hat{S} | \boldsymbol{p} \rangle a(\boldsymbol{k} - \boldsymbol{p}) \right|^2. \tag{50}$$

Since the state $|\boldsymbol{p}\rangle$ is nonnormalizable, such a definition violates unitarity: the normalized state transforms into nonnormalizable, so the norm is not conserved.

In all the textbooks pointed above the unitarity is considered as equality of number plane wave components in the initial and final wave packets, but not as equality of norms of the initial and final states. We think it is not correct.

From unitarity of the S-matrix it follows that norm of the wave function is conserved, so if $|\phi\rangle$ is a wave packet normalized to unity, then the final wave function $|\chi\rangle$ after scattering must be also normalized to unity. It would be more consistent, if the final state is represented as a superposition of wave packets

$$|\chi\rangle = \int d^3 k' b(\boldsymbol{k} \to \boldsymbol{k}')|\phi(\boldsymbol{k}')\rangle, \tag{51}$$

and $b(\boldsymbol{k} \to \boldsymbol{k}') = \langle \phi(\boldsymbol{k}') | \hat{S} | \phi(\boldsymbol{k}) \rangle$ defines the amplitude of transition probability from the wave packet state $|\phi(\boldsymbol{k})\rangle$ with momentum $\boldsymbol{k}$ into wave packet state $|\phi(\boldsymbol{k}')\rangle$ with momentum $\boldsymbol{k}'$.

In fact, in the books [1, 2] and others only scattering of plane waves is considered, and the initial wave packet defines only spectrum of plane waves in the incident beam. However, in this case it is more accurate to find probability amplitude of the plane wave scattering

$$df = -2\pi i T(\boldsymbol{p}', \boldsymbol{p})\delta(p^2/2 - p'^2/2)d^3 p' = 2\pi i p T(\boldsymbol{p}', \boldsymbol{p})d\Omega' \tag{52}$$

into solid angle element $d\Omega'$, to make with it the probability of scattering

$$dw = |2\pi p T(\boldsymbol{p}', \boldsymbol{p})|^2 d\Omega',$$

and to average this probability over the spectrum of initial states

$$< dw > = \left(\int |a(\boldsymbol{k} - \boldsymbol{p})|^2 d^3 p |2\pi p T(\boldsymbol{p}', \boldsymbol{p})|^2 \right) d\Omega'. \tag{53}$$

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However, in this case we obtain only dimensionless probability, and it is impossible to find a cross section because plane waves do not have finite dimension of the wave front.

With definition (50) of scattering probability it is possibly to define the scattering cross section but even in this case, to get a cross section from probability you need an additional hypothesis, which was never clearly formulated because it looks evident from the common sense.

3.3. Transformation of Probability into Cross Section. This transformation is slightly different in different books, and it is useful to look at this difference. We present here only two ways presented in books [1, 2].

3.3.1. Transition to Cross Section According to Goldberger & Watson. According to (50) the scattering probability is defined by the Fourier coefficient in expansion (48) over plane waves $|\boldsymbol{p}'\rangle$:

$$dw = d^3p'(2\pi)^2 T(\boldsymbol{p}',\boldsymbol{p}_1)T^*(\boldsymbol{p}',\boldsymbol{p}_2)a(\boldsymbol{k}-\boldsymbol{p}_1)a^*(\boldsymbol{k}-\boldsymbol{p}_2)\times$$
$$\times d^3p_1 d^3p_2 \delta(p_1^2/2 - p_2^2/2)\delta(p'^2/2 - p_1^2/2), \quad (54)$$

it means that the incident wave packet is considered as a coherent unity, and not as incoherent superposition of plane waves in the incident beam.

The momenta $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ in matrix elements $T(\boldsymbol{p}',\boldsymbol{p}_{1,2})$ are replaced by the average momentum $\boldsymbol{k}$ of the initial wave packet. As a result we obtain: $T(\boldsymbol{p}',\boldsymbol{p}_1)T^*(\boldsymbol{p}',\boldsymbol{p}_2) \approx |T(\boldsymbol{p}',\boldsymbol{k})|^2$. The momentum p_1 in $\delta(p'^2/2 - p_1^2/2)$ is also replaced by k, and in result the product $d^3p'\delta(p'^2/2 - p_1^2/2)$ is transformed to $kd\Omega'$, where Ω' is the solid angle in the space of vectors $\boldsymbol{p}'$. The δ-function $\delta(p_1^2/2 - p_2^2/2)$ is represented as

$$\delta(p_1^2/2 - p_2^2/2) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} dt\exp\left(it(p_1^2 - p_2^2)/2\right). \quad (55)$$

The difference $p_1^2 - p_2^2$ in the exponent is replaced by
$$p_1^2 - p_2^2 = (\boldsymbol{p}_1 + \boldsymbol{p}_2)(\boldsymbol{p}_1 - \boldsymbol{p}_2) \approx 2\boldsymbol{k}(\boldsymbol{p}_1 - \boldsymbol{p}_2). \quad (56)$$

After that expression (54) becomes

$$dw = d\Omega' k 2\pi |T(\boldsymbol{p}',\boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dt|\phi(t\boldsymbol{k})|^2, \quad (57)$$

where the representation

$$\phi(\boldsymbol{r}) = \langle\boldsymbol{r}|\phi\rangle = \int d^3p\, a(\boldsymbol{k}-\boldsymbol{p})\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \int d^3p\, a(\boldsymbol{k}-\boldsymbol{p})\exp\left(i\boldsymbol{pr}\right) \quad (58)$$

of the wave packet $|\phi\rangle$ is used.

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If we choose the coordinate system with z-axis along $\boldsymbol{k}$, then (57) becomes identical to

$$dw = d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dz |\phi(0,0,z)|^2. \qquad (59)$$

Since the wave packet ϕ is normalized to unity

$$\int d^3 r |\phi(r)|^2 = 1, \qquad (60)$$

the integral $\int |\phi(0,0,z)|^2 dz$ has dimensionality 1/cm^2, therefore it can be considered as density of the incident particles J. It follows immediately that

$$d\sigma = \frac{dw}{J} = d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2, \qquad (61)$$

and the obtained cross section does not depend on the form of the wave packet. However it is important to note, that the target scatterer is supposed to cross through the wave packet $|\phi\rangle$.

3.3.2. Transition to Cross Section According to J. Taylor. According to (57) the scattering center crosses the wave packet of the scattered particle, and at the moment $t = 0$ it coincides with the packet center [1], as is shown in Fig. 2. Just because of that the expression contains $\phi(\boldsymbol{k}t)$:

$$\phi(\boldsymbol{k}t) = \langle \boldsymbol{r} | \phi \rangle |_{\boldsymbol{r}=\boldsymbol{k}t} = \int d^3 p\, a(\boldsymbol{k}-\boldsymbol{p}) \exp{(i\boldsymbol{p}\boldsymbol{k}t)} \qquad (62)$$

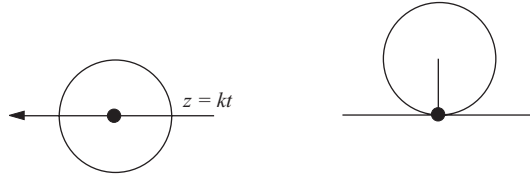instead of $\phi(\boldsymbol{r})$ (58).

Fig. 2. Position of scatterer at $t = 0$ with respect to wave packet of scattered particle. On the left-hand side the packet center coincides with scatterer. Such a position is used in [1]. On the right-hand side the position of the packet center is characterized by the impact parameter $\boldsymbol{\rho}$. Such a parameter is used for derivation of cross section in [2]

J. Taylor in his book [2] introduces an impact parameter $\boldsymbol{\rho} \perp \boldsymbol{k}$ of the wave packet center with respect to scatterer. With the impact parameter expression (62) changes to

$$\phi(\boldsymbol{k}t + \boldsymbol{\rho}) = \int d^3p a(\boldsymbol{k} - \boldsymbol{p}) \exp{(i\boldsymbol{p}\boldsymbol{k}t + i\boldsymbol{p}\boldsymbol{\rho})}, \tag{63}$$

and Eq. (57) and (59), respectively, take the form

$$dw(\boldsymbol{\rho}) = d\Omega' k 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dt |\phi(t\boldsymbol{k} + \boldsymbol{\rho})|^2, \tag{64}$$

$$dw(\boldsymbol{\rho}) = d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dz |\phi(\rho_x, \rho_y, z)|^2. \tag{65}$$

We see that the scattering probability into element $d\Omega'$ depends on $\boldsymbol{\rho}$. The cross section is defined as an integral over impact parameters

$$d\sigma = \int d^2\rho\, dw(\boldsymbol{\rho}) = d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} d^3r |\phi(\boldsymbol{r})|^2 =$$
$$= d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2, \quad (66)$$

where normalization condition (60) is used. The result completely coincides with (61) in agreement with SST. However, we want to note again, that it is implicitly assumed that there are no scattering, if the impact parameter is larger than the wave packet radius, though the final result does not depend on wave packet dimensions.

4. SCATTERING OF WAVE PACKETS

We see that the proof of validity of SST is not perfect because of unacceptable definition of probability of scattering, according to which a wave packet after scattering transforms to plane waves, though according to unitarity it should remain a wave packet. Now we want to show how to calculate scattering of wave packets at least in the simplest case of elastic scattering from a fixed center. We consider a wave packet not as a preparation of a particle in some state, but as an intimate property of the particle, which means that the particle after scattering is the same packet as before scattering. In general all the wave packets can be

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represented as Fourier expansion

$$\psi(\boldsymbol{k}, \boldsymbol{r}, s, t) = G(s|\boldsymbol{r} - \boldsymbol{k}t|) \, \exp{(i\boldsymbol{k}\boldsymbol{r} - i\omega(k)t)} =$$

$$= \int d^3p \, a(\boldsymbol{k}, \boldsymbol{p}) \, \exp{[i\boldsymbol{p}\boldsymbol{r} - i\omega(\boldsymbol{p}, \boldsymbol{k})t]}, \quad (67)$$

where parameter s determines width of the packet, $a(\boldsymbol{k}, \boldsymbol{p})$ and $\omega(\boldsymbol{p}, \boldsymbol{k})$ are functions of invariant variables $\boldsymbol{k}^2$, $\boldsymbol{p}^2$ and $\boldsymbol{k}\boldsymbol{p}$.

4.0.1. Elastic Scattering of Wave Packets on a Center. The primary wave packet describes a free incident particle. Its Fourier expansion contains plane waves $\exp{(i\boldsymbol{p}\boldsymbol{r})}$, which satisfy the free equation

$$[\Delta + p^2] \, \exp{(i\boldsymbol{p}\boldsymbol{r})} = 0. \quad (68)$$

In the presence of a potential $u(\boldsymbol{r})/2$ the plane wave should be replaced by the wave function $\psi_{\boldsymbol{p}}(\boldsymbol{r})$, which is a solution of the equation

$$[\Delta + p^2 - u(\boldsymbol{r})]\psi_p(\boldsymbol{r}) = 0 \quad (69)$$

containing $\exp{(i\boldsymbol{p}\boldsymbol{r})}$ as the incident wave. Substitution into (67) transforms it to

$$\psi(\boldsymbol{k}, \boldsymbol{r}, t) = \int d^3p \, a(\boldsymbol{k}, \boldsymbol{p})\psi_p(\boldsymbol{r}) \, \exp{[-i\omega(\boldsymbol{p}, \boldsymbol{k})t]}. \quad (70)$$

After scattering on a fixed center with impact parameter $\boldsymbol{\rho}$ the incident plane wave transforms to a superposition of plane waves

$$\psi_p(\boldsymbol{r}) = \exp{(i\boldsymbol{p}\boldsymbol{\rho})} \int d\Omega f(\Omega) \, \exp{(i\boldsymbol{p}_\Omega[\boldsymbol{r} - \boldsymbol{\rho}])}, \quad (71)$$

where $f(\Omega)$ is the probability amplitude of a plane wave with wave vector $\boldsymbol{p}$ to be transformed to the plane wave with wave vector $\boldsymbol{p}_\Omega$ pointing into direction $\boldsymbol{\Omega}$ in the element of solid angle $d\Omega$. This amplitude for isotropic scattering is $f(\Omega) = bp/2\pi$. Dependence on p is an irritating moment, however, since the spectrum of wave packets has a sharp peak at $p = k$, we can approximate $f(\Omega)$ by $bk/2\pi$.

The vector $\boldsymbol{p}_\Omega$ in (71) is of length p, but it is turned by angle Ω from $\boldsymbol{p}$. Substitution of (71) into (67) for $\exp{(i\boldsymbol{p}\boldsymbol{r})}$ transforms (67) to the form

$$\psi(\boldsymbol{k}, \boldsymbol{r}, t) = \int d^3p \, a(\boldsymbol{k}, \boldsymbol{p}) \, \exp{(i\boldsymbol{p}\boldsymbol{\rho})}d\Omega f(\Omega) \, \exp{[i\boldsymbol{p}_\Omega[\boldsymbol{r} - \boldsymbol{\rho}] - i\omega(\boldsymbol{p}, \boldsymbol{k})t]}. \quad (72)$$

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Since $a(\boldsymbol{k}, \boldsymbol{p})$, $\boldsymbol{p}\boldsymbol{\rho}$ and $\omega(\boldsymbol{k}, \boldsymbol{p})$ are invariant with respect to rotation, we can replace them with $a(\boldsymbol{k}_\Omega, \boldsymbol{p}_\Omega)$, $\boldsymbol{p}_\Omega\boldsymbol{\rho}_\Omega$ and $\omega(\boldsymbol{k}_\Omega, \boldsymbol{p}_\Omega)$. After that we can transform integration variable $\boldsymbol{p} \rightarrow \boldsymbol{p}_\Omega$, and drop index Ω of $\boldsymbol{p}$. As a result we transform (72) to the form

$$\psi(\boldsymbol{k}, \boldsymbol{r}, t) = \int d^3 p \, a(\boldsymbol{k}_\Omega, \boldsymbol{p}) \, \exp\left(i\boldsymbol{p}\boldsymbol{\rho}_\Omega\right) d\Omega f(\Omega) \times$$

$$\times \exp[i\boldsymbol{p}[\boldsymbol{r} - \boldsymbol{\rho}] - i\omega(\boldsymbol{p}, \boldsymbol{k}_\Omega) t], \quad (73)$$

which can be represented as

$$\psi(\boldsymbol{k}, \boldsymbol{r}, t) = \int d\Omega f(\Omega) \psi_0(\boldsymbol{k}_\Omega, \boldsymbol{r} - \boldsymbol{\rho} + \boldsymbol{\rho}_\Omega, t), \quad (74)$$

where ψ_0 denotes the wave packet of the the same form as that of the incident particle. Now we see that the packet as a whole is scattered with probability $dw = |f(\Omega)|^2 d\Omega = |bk/2\pi| d\Omega$, which, surprisingly, has no dependence on impact parameter $\boldsymbol{\rho}$ as in the case of plane waves. It shows that scattering of wave packets almost the same as that for plane waves. The difference between them is of the order s/k, where s is the wave packet width in the momentum space, as in the case of the de Broglie wave packet (26).

To get cross section from probability we need an additional hypothesis that the scattering takes place only when the particle wave packet overlaps the target position. This hypothesis is outside of the wave mechanics, so we can say that without this hypothesis the wave mechanics is incomplete theory, i.e. it is insufficient to describe scattering of particles.

With the additional hypothesis we can write cross section as $\sigma = Aw$, where A is the cross area of the particle wave packet. In the case of the de Broglie wave packet (26) this area is π/s^2. To show that the de Broglie singular wave packet (26) is the most appropriate one, we consider below three types of wave packets.

4.1. Three Types of the Wave Packets. All the packets are representable in the form (67), and they differ by the Fourier coefficients $a(\boldsymbol{p}, \boldsymbol{k})$ and dispersion $\omega(\boldsymbol{p}, \boldsymbol{k})$. We consider three types of the wave packets and discuss which one is the most appropriate for description of particles.

4.1.1. The Gaussian Wave Packet. The most popular in the literature is the Gaussian wave packet

$$\psi_G(\boldsymbol{r}, \boldsymbol{k}, t, s) = \left(\frac{s}{\sqrt{\pi}(1 + its^2)}\right)^{3/2} e^{i\boldsymbol{k}\boldsymbol{r} - ik^2 t/2} \exp\left(-\frac{s^2[\boldsymbol{r} - \boldsymbol{k}t]^2}{2[1 + its^2]}\right). \quad (75)$$

This packet is normalized to unity, satisfies the free Schrödinger equation, but spreads in time. Because of this spreading its form in space does not coincide with that shown in (67).

Its Fourier components are

$$F_g(\boldsymbol{p},\boldsymbol{k},s) = \left(\frac{1}{2\pi s\sqrt{\pi}}\right)^{3/2} \exp\left(-(\boldsymbol{k}-\boldsymbol{p})^2/2s^2\right), \quad \omega(\boldsymbol{p},\boldsymbol{k}) = p^2/2, \quad (76)$$

where s is the width in momentum space. The spectrum of wave vectors $\boldsymbol{p}$ is spherically symmetrical with respect to the central point $\boldsymbol{p} = \boldsymbol{k}$ and decays away from it according to Gaussian law.

The cross area of this packet can be defined as

$$A_G = \int \pi\rho^2 d^3r |G(\boldsymbol{r},\boldsymbol{k},t,s)|^2 =$$

$$= \int \rho^2 d^2\rho \frac{s^2}{1+t^2s^4} \exp\left(-\frac{s^2\rho^2}{1+t^2s^4}\right) = \pi\frac{1+t^2s^4}{s^2}. \quad (77)$$

4.1.2. Nonsingular de Broglie Wave Packet. It is known that there are no nonspreading normalizable wave packets, which satisfy the free Schrödinger equation. However, nonnormalizable wave packets do exist. As an example we can demonstrate nonsingular de Broglie wave packet [3]

$$\psi_{ns}(\boldsymbol{r},\boldsymbol{k},t,s) = \exp\left(i\boldsymbol{k}\boldsymbol{r} - i\omega t\right) j_0(s|\boldsymbol{r}-\boldsymbol{v}t|), \quad (78)$$

in which $\omega_k = k^2/2 + s^2/2$ and $\boldsymbol{v} = \boldsymbol{k}$ in units $\hbar^2/m = 1$. The packet (78) is a spherical Bessel function $j_0(sr) \exp\left(-is^2t/2\right)$, which center is moving with the speed $\boldsymbol{v}$. This packet satisfy the free Schrödinger equation. Its Fourier components are

$$F(\boldsymbol{p},\boldsymbol{k},s) = F_{ns}(\boldsymbol{p},\boldsymbol{k},s) \propto \delta((\boldsymbol{k}-\boldsymbol{p})^2 - s^2), \quad \omega(\boldsymbol{p},\boldsymbol{k}) = p^2/2, \quad (79)$$

and spectrum of $\boldsymbol{p}$ is a sphere of radius s in momentum space with centrum at the point $\boldsymbol{p} = \boldsymbol{k}$. Since it is not normalizable, its front area is infinite like in the plane wave case.

4.1.3. The singular de Broglie Wave Packet The singular de Broglie wave packet [3]

$$\psi_{dB}(\boldsymbol{r},\boldsymbol{k},t,s) = C \exp\left(i\boldsymbol{k}\boldsymbol{r} - i\omega t\right)\frac{\exp\left(-s|\boldsymbol{r}-\boldsymbol{v}t|\right)}{|\boldsymbol{r}-\boldsymbol{v}t|} \quad (80)$$

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is normalizable one with normalization constant $C = \sqrt{s/2\pi}$ defined by the relation

$$\int d^3 r |\psi(s, \boldsymbol{v}, \boldsymbol{r}, t)|^2 = 1. \tag{81}$$

The parameter s is the width of the packet in momentum space and reciprocal width in coordinate space, $\boldsymbol{v}$ is the packet speed, and $\omega = (v^2 - s^2)/2$. We see that ω is less than kinetic energy by the term $s^2/2$, which can be considered as the bound energy of the packet.

The singular de Broglie wave packet satisfies inhomogeneous Schrödinger equation

$$\left[i\frac{\partial}{\partial t} + \frac{\Delta}{2} \right] \psi_{dB}(\boldsymbol{r}, \boldsymbol{v}, t, s) = -2\pi C e^{i(v^2 + s^2)t/2} \delta(\boldsymbol{r} - \boldsymbol{v}t), \tag{82}$$

which right-hand side is zero everywhere except one point along trajectory in free space.

The Fourier coefficients of the singular de Broglie wave packet are

$$F(\boldsymbol{p}, \boldsymbol{k}, s) = F_{dB}(\boldsymbol{p}, \boldsymbol{k}) = \sqrt{\frac{s}{2\pi}} \frac{4\pi}{(2\pi)^3} \frac{1}{(\boldsymbol{p} - \boldsymbol{k})^2 + s^2} \tag{83}$$

and

$$\omega(\boldsymbol{p}, \boldsymbol{k}) = [2\boldsymbol{k}\boldsymbol{p} - k^2 + s^2]/2 = [p^2 - (\boldsymbol{k} - \boldsymbol{p})^2 - s^2]/2. \tag{84}$$

The spectrum of wave vectors $\boldsymbol{p}$ is spherically symmetrical with respect to the central point $\boldsymbol{p} = \boldsymbol{k}$ and decays away from it according to Lorenzian law with width s.

The Fourier coefficients (83) and frequency (84) become the same as for spherical wave

$$\exp\left(-ik^2 t/2\right) \frac{\exp\left(ikr\right)}{r} = \frac{4\pi}{(2\pi)^3} \int \exp\left(i\boldsymbol{p}\boldsymbol{r}\right) \frac{\exp\left(-ik^2 t/2\right) d^3 p}{p^2 - k^2 - i\epsilon}, \tag{85}$$

after substitution $\boldsymbol{k} \to 0$ and $s \to ik$.

The front area of the singular de Broglie wave packet can be defined as

$$A_{dB} = \frac{s}{2\pi} \int\limits_{0}^{\infty} 2dx\pi d\rho^2 \pi \rho^2 \frac{\exp\left(-2s\sqrt{\rho^2 + x^2}\right)}{\rho^2 + x^2}. \tag{86}$$

After change of variables $y = x/\rho$ we get

$$A_{dB} = 2\pi s \int\limits_{0}^{\infty} dy d\rho \rho^2 \frac{\exp\left(-2s\rho\sqrt{1 + y^2}\right)}{1 + y^2} = \frac{\pi}{2s^2} \int\limits_{0}^{\infty} \frac{dy}{(1 + y^2)^{5/2}} = \frac{\pi}{3s^2}. \tag{87}$$

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4.1.4. Genesis of the singular de Broglie Wave Packet. The singular de Broglie wave packet descends from the spherical wave. Indeed, let us consider the spherical wave with energy $q^2/2$

$$\psi(r,t,q) = \exp\left(-iq^2 t/2\right)\frac{\exp\left(iqr\right)}{r}. \tag{88}$$

This wave satisfies inhomogeneous Schrödinger equation

$$\left[i\frac{\partial}{\partial t} + \frac{\Delta}{2}\right]\psi(r,t,q) = -2\pi\exp\left(-iq^2 t/2\right)\delta(\boldsymbol{r}). \tag{89}$$

The right-hand side describes the center radiating the spherical wave. If we change to the reference system moving with the speed $\boldsymbol{v} = \boldsymbol{k}$ then we must transform the function ψ

$$\psi(r,t,q) \to \Psi(\boldsymbol{r},\boldsymbol{k},t,q) = \exp\left(i\boldsymbol{k}\boldsymbol{r} - ik^2 t/2 - iq^2 t/2\right)\frac{\exp\left(iq|\boldsymbol{r} - \boldsymbol{k}t|\right)}{|\boldsymbol{r} - \boldsymbol{k}t|}. \tag{90}$$

The transformed function is the spherical wave around moving center. It satisfies the equation

$$\left[i\frac{\partial}{\partial t} + \frac{\Delta}{2}\right]\Psi = -2\pi\,\exp\left(i[k^2 - q^2]t/2\right)\delta(\boldsymbol{r} - \boldsymbol{k}t). \tag{91}$$

If the energy of the wave (88) is negative: $q^2 = -s^2$, i.e. the wave (88) describes a bound state around the center, then (90) becomes

$$\Psi(\boldsymbol{r},\boldsymbol{k},t,is) = \exp\left(i\boldsymbol{k}\boldsymbol{r} - ik^2 t/2 + is^2 t/2\right)\frac{\exp\left(-s|\boldsymbol{r} - \boldsymbol{k}t|\right)}{|\boldsymbol{r} - \boldsymbol{k}t|}. \tag{92}$$

With normalization constant C expression (92) becomes identical to (80). Thus the singular de Broglie wave packet is the spherical Hankel function of imaginary argument moving with the speed $\boldsymbol{v}$.

4.1.5. Genesis of the Nonsingular de Broglie Wave Packet. The nonsingular de Broglie wave packet is obtained by transformation to the moving reference frame of the nonsingular spherical wave

$$j_0(qr)\,\exp\left(-iq^2 t/2\right),$$

which satisfies the homogeneous Schrödinger equation. This way we can construct a lot of nonsingular wave packets corresponding to different angular momenta l.

4.1.6. Resume. We considered three types of spherically symmetrical wave packets. However, only one of them is normalizable, and is not spreading. This is the singular de Broglie wave packet, so it looks as the most appropriate one for description of elementary particles. The scattering cross section, $\sigma = Aw$, obtained with it coincides with generally accepted one $\sigma = 4\pi|b|^2$, if the cross area of the packet A_{dB} is proportional to λ^2. It is equivalent to $s \propto k$. In that case the packet width in coordinate space decreases with energy. Such a behavior is in accord with the intuitive expectations that the slow particles have wave properties, whereas the more fast ones are better described by corpuscular mechanics.

5. SCATTERING FROM AN ARBITRARY SYSTEM

Since probability of scattering can be calculated in the same way as for plane waves we want to address the following question: is it possible to calculate this probability in a direct way, without introduction of some finite volume L^3, which plays an auxiliary role, and is excluded at final stage? We shall show that the direct method exists, and in general it gives a result different from that of SST. We apply the direct method to neutron scattering by monatomic gas and find, when our result can be identical to that of SST. At the same time we find that the result is ambiguous, which proves once again that the wave mechanics and with it quantum mechanics are incomplete theories.

5.1. Scattering According to SST. Here we remind to the reader, following the textbooks [6,7], how cross sections are calculated in SST. We find there a list of rules one must to follow to get an expression for the cross section.

5.1.1. Rules for Calculation of Scattering from an Arbitrary System in SST. First we consider general rules for an arbitrary scattering system.

1. The starting point is the «Fermi Golden Rule», according to which one defines **probability of scattering per unit time** (though it does not depend on time)

$$dw(\boldsymbol{k}_i \to \boldsymbol{k}_f, t) = \frac{2\pi}{\hbar} \left| \langle \lambda_f, \boldsymbol{k}_f | V | \lambda_i, \boldsymbol{k}_i \rangle \right|^2 \rho(E_{fk}) \tag{93}$$

of the neutron in an initial state $|\boldsymbol{k}_i>$ from the system in a state $|\lambda_i>$ to final neutron and system states $|\boldsymbol{k}_f>$, $|\lambda_f>$ respectively. Here V is interaction potential, which we can represent in the form

$$V = \frac{\hbar^2}{2m} 4\pi b \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2), \tag{94}$$

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where r_1, r_2 are neutron and atom coordinates, respectively, $\rho(E_{fk})$ is the density of final states of the neutron per unit energy E_{fk}:

$$\rho(E_k) = \left(\frac{L}{2\pi}\right)^3 \frac{d^3k}{dE_k} = \left(\frac{L}{2\pi}\right)^3 \frac{mkd\Omega_k}{\hbar^2},$$

$$d^3k = k^2 dk d\Omega_k, \quad dE_k = \frac{\hbar^2}{m}kdk, \tag{95}$$

$d\Omega_k$ is an element of the solid angle in k-space, L is some (arbitrary large) size of a space cell, and the law of energy conservation is **assumed**.

Note that here we use normal units without $m = \hbar = 1$.

2. The neutron states are represented as

$$|k_{i,f}\rangle = \frac{1}{L^{3/2}} \exp(ik_{i,f}r). \tag{96}$$

3. The expression (93) is multiplied by

$$1 \equiv dE_{fk}\delta(E_{fk} + E_{f\lambda} - E_{ik} - E_{i\lambda}),$$

where $E_{i,fk}$ are initial and final neutron energies $\hbar^2 k_{i,f}^2/2m$, and $E_{i,f\lambda}$ are initial and final energies of the scattering system. After multiplication one obtains the double differential probability of scattering **per unit time**

$$\frac{d^2}{d\Omega_f dE_{fk}}w(k_i \to k_f, t) =$$

$$= \frac{2\pi}{\hbar}|\langle\lambda_f, k_f|V|\lambda_i, k_i\rangle|^2 \left(\frac{L}{2\pi}\right)^3 \frac{mk}{\hbar^2}\delta(E_{fk} + E_{f\lambda} - E_{ik} - E_{i\lambda}), \tag{97}$$

which after substitution of (94) becomes

$$\frac{d^2}{d\Omega_f dE_{fk}}w(k_i \to k_f, t) =$$

$$= \frac{\hbar k_f}{mL^3}|b|^2|\langle\lambda_2|\exp(i\kappa r)|\lambda_1\rangle|^2 \delta(E_{fk} + E_{f\lambda} - E_{ik} - E_{i\lambda}), \tag{98}$$

where $\kappa = k_1 - k_2$ is momentum transferred to the scatterer.

4. This double differential probability is divided by the incident flux

$$\frac{\hbar k_i}{mL^3},$$

and as a result one obtains the double differential scattering cross section

$$\frac{d^2}{d\Omega_f dE_{fk}}\sigma(k_i \to k_f, \lambda_i \to \lambda_f) =$$

$$= \frac{k_f}{k_i}|b|^2|\langle\lambda_f|\exp(i\kappa r)|\lambda_i\rangle|^2 \delta(E_{fk} + E_{f\lambda} - E_{ik} - E_{i\lambda}), \tag{99}$$

or a triple differential neutron cross section

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i,\lambda_i \to \boldsymbol{k}_f,\lambda_f) =$$

$$= \frac{\hbar^2}{m}\frac{1}{k_i}|b|^2 \left|\langle\lambda_f|\exp{(i\boldsymbol{\kappa r})}|\lambda_i\rangle\right|^2 \delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}) \quad (100)$$

for given initial and final states $|\lambda_{i,f}>$ of the scatterer.

5. After that we sum (99) over final states of the scatterer, average over its initial states and find

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_1 \to \boldsymbol{k}_2,\mathcal{P}) = \frac{m}{\hbar^2 k_i}|b|^2 \sum_{\lambda_i,\lambda_f} \mathcal{P}(\lambda_i) \left|\langle\lambda_f|\exp{(i\boldsymbol{\kappa r})}|\lambda_i\rangle\right|^2 \times$$

$$\times\, \delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}), \quad (101)$$

where $\mathcal{P}(\lambda_i)$ is probability for the scatterer to have initial state $|\lambda_i\rangle$.

If $\mathcal{P}(\lambda_i)$ is the Maxwellian distribution $\mathcal{M}(E_\lambda/k_B T)$, where T is temperature, and k_B is the Boltzmann constant, then

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_1 \to \boldsymbol{k}_2,T) = \frac{m}{\hbar^2 k_i}|b|^2 \sum_{\lambda_i,\lambda_f} \mathcal{M}\left(\frac{E_{\lambda_i}}{k_B T}\right) \left|\langle\lambda_f|\exp(i\boldsymbol{\kappa r})|\lambda_i\rangle\right|^2 \times$$

$$\times\, \delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}). \quad (102)$$

5.1.2. Scattering from a Monatomic Gas. Now we look how these general rules are applied to such a simple system like a monatomic gas. In this case the states of the scatterer, $|\lambda\rangle$, are similar to those of neutrons, i.e. they are plane waves $|\lambda\rangle \equiv |\boldsymbol{p}\rangle = L^{-3/2}\exp{(i\boldsymbol{pr})}$.

1. The matrix elements are

$$\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle = 4\pi b\frac{\hbar^2}{2m}\int \frac{d^3r}{L^6}\exp{(i[\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f]\boldsymbol{r})} =$$

$$= \frac{2\pi b\hbar^2}{mL^6}(2\pi)^3\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f).$$

The square of this matrix element, according to step 1, is equal to square of the δ-function, and it is represented as $\delta^2 = [L^3/(2\pi)^3]\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)$. With this representation one obtains (93) in the form

$$dw(i \to f) = \frac{(2\pi)^3\hbar k_f}{m}\frac{|b|^2}{L^6}\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)d\Omega_f. \quad (103)$$

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2. After steps 3 one obtains

$$\frac{d^2}{d\Omega_f dE_{fk}} w(\boldsymbol{k}_i \to \boldsymbol{k}_f, t) =$$

$$= \frac{\hbar k_f (2\pi)^3}{mL^6} |b|^2 \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f) \delta(E_{fk} + E_{fp} - E_{ik} - E_{ip}), \quad (104)$$

where $E_k = \hbar^2 k^2 / 2m$, $E_p = \hbar^2 p^2 / 2M$, and M is the atomic mass.

3. After the step 4 one obtains

$$\frac{d^2}{d\Omega_f dE_{fk}} \sigma(\boldsymbol{k}_i, \boldsymbol{p}_f \to \boldsymbol{k}_f, \boldsymbol{p}_i) =$$

$$= \frac{k_f}{k_i} \frac{(2\pi)^3}{L^3} |b|^2 \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f) \delta(E_{fk} + E_{fp} - E_{ik} - E_{ip}), \quad (105)$$

or the triple differential neutron cross section

$$\frac{d^3}{dk_f^3} \sigma(\boldsymbol{k}_i, \boldsymbol{p}_i \to \boldsymbol{k}_f, \boldsymbol{p}_f) =$$

$$= \frac{(2\pi)^3}{L^3 k_i} |b|^2 \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f) \delta(k_f^2/2 + \mu p_f^2/2 - k_i^2/2 - \mu p_i^2/2), \quad (106)$$

where $\mu = m/M$.

4. Summation over final states in the step 5 is integration over $d^3 p_f$ with weight $L^3 d^3 p_f / (2\pi)^3$, which defines number of final states in the volume L^3.

Averaging over the same Maxwellian distribution as above gives

$$\frac{d^2 \sigma(\boldsymbol{k}_1 \to \boldsymbol{k}_2, T)}{dE_{fk} \Omega_{fk}} = |b|^2 \frac{k_f}{k_i} \int d^3 p_f \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f) \times$$

$$\times \delta(E_{ik} + E_{ip} - E_{fk} - E_{fp}) \mathcal{M}\left(\frac{\hbar^2 p_i^2}{2Mk_BT}\right) d^3 p_i$$

or

$$\frac{d^3}{dk_f^3} \sigma(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = \frac{2}{k_i} |b|^2 \int \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f) d^3 p_f \times$$

$$\times \delta(k_f^2 + \mu p_f^2 - k_i^2 - \mu p_i^2) \mathcal{M}\left(\frac{\hbar^2 p_i^2}{2Mk_BT}\right) d^3 p_i. \quad (107)$$

5. Now it is convenient to redefine temperature $T \to m\hbar^2 k_B T$, or to choose unities $\hbar = m = k_B = 1$, then the Maxwellian distribution is

$$\mathcal{M}\left(\frac{\mu p^2}{2T}\right) = \left(\frac{\mu}{2\pi T}\right)^{3/2} \exp\left(-\mu \frac{p^2}{2T}\right). \tag{108}$$

Substitution of it into (107) and integration over $d^3 p_f$ gives

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) =$$

$$= \frac{1}{k_i}|b|^2 \int \delta(E_R - \omega + \mu\boldsymbol{\kappa}\boldsymbol{p}_i)\left(\frac{\mu}{2\pi T}\right)^{3/2} \exp\left(-\mu\frac{p_i^2}{2T}\right) d^3 p_i, \tag{109}$$

where $E_R = \mu\kappa^2/2$ is recoil energy, and $\omega = (k_i^2 - k_f^2)/2$ is energy transferred to the gas. After integration over $d^3 p_i$ we get the triple differential cross section

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = \frac{1}{\kappa k_i}|b|^2\frac{1}{\sqrt{2\pi\mu T}}\exp\left(-\frac{(\omega - E_R)^2}{4E_R T}\right). \tag{110}$$

6. Integration over $d^3 k_f$ gives total cross section

$$\sigma(k_i, T) = \frac{4\pi}{\sqrt{\pi E_r}}\frac{|b|^2}{(1+\mu)^2}\left(\exp\left(-E_r\right) + \frac{\sqrt{\pi}}{2\sqrt{E_r}}(2E_r + 1)\Phi\left(\sqrt{E_r}\right)\right), \tag{111}$$

where $E_r = k_i^2/2\mu T$ is reduced energy of the incident neutron, and $\Phi(x)$ is the error function

$$\Phi(x) = \frac{2}{\sqrt{\pi}}\int\limits_0^x dz \exp\left(-z^2\right).$$

5.2. Direct Calculation of Scattering. After repeating all the steps of SST calculations, which involve an artificial introduction of a finite volume L^3, one wonders, whether it is impossible to derive the scattering cross section without that? Now we want to show how to make direct calculations without L.

5.2.1. The Direct Calculation of Scattering from an Arbitrary System. Let the scatterer to be described by the Hamiltonian H', which for the sake of simplicity is supposed to have a discrete spectrum E_λ. The neutron scattering is determined from solution of the Schrödinger equation

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\Delta_1 - H' + V(\boldsymbol{r}_1, \boldsymbol{r}_2)\right]\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = 0, \tag{112}$$

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where interaction potential V is shown in (94). Solution of Eq. (112) in perturbation theory is represented in the form

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = \psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2, t) - \delta\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t),$$

where $\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2, t)$ is initial wave function before scattering,

$$\delta\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t) =$$
$$= \int G(\boldsymbol{r}_1, \boldsymbol{r}_2, t; \boldsymbol{r}_1', \boldsymbol{r}_2', t') V(\boldsymbol{r}_1', \boldsymbol{r}_2') \psi_0(\boldsymbol{r}_1', \boldsymbol{r}_2', t') d^3 r_1' d^3 r_2' dt', \quad (113)$$

and G is the Green function of Eq. (112) without interaction

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \Delta_1 - H' \right] G(\boldsymbol{r}_1, \boldsymbol{r}_2, t; \boldsymbol{r}_1', \boldsymbol{r}_2', t') =$$
$$= -\delta(\boldsymbol{r}_1 - \boldsymbol{r}_1') \delta(\boldsymbol{r}_2 - \boldsymbol{r}_2') \delta(t - t'). \quad (114)$$

For the function before scattering we take

$$\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = \Phi_{\lambda_i}(\boldsymbol{r}_2) \, e^{-iE_{\lambda_i} t} \, e^{i\boldsymbol{k}_i \boldsymbol{r}_1 - iE_{ik} t}, \quad (115)$$

where $\Phi_{\lambda_i}(\boldsymbol{r})$ and E_{λ_i} are eigen function and eigen value of the Hamiltonian H', and $\boldsymbol{k}_i$, $E_{ik} = \hbar^2 k_i^2 / 2m$ are wave vector and energy of the incident neutron.

The Green function of the Eq. (112) without interaction is

$$G(\boldsymbol{r}_1 - \boldsymbol{r}_1', \boldsymbol{r}_2 - \boldsymbol{r}_2', t - t') = \frac{1}{(2\pi)^4} \sum_{\lambda_f} \int e^{i\boldsymbol{k}_f \boldsymbol{r}_1 - i\omega t} \Phi_{\lambda_f}(\boldsymbol{r}_2) \times$$
$$\times \frac{d^3 k_f d\omega}{E_{fk} + E_{\lambda_f} - \omega - i\epsilon} e^{-i\boldsymbol{k}_f \boldsymbol{r}_1' + i\omega t'} \Phi_{\lambda_f}^*(\boldsymbol{r}_2'), \quad (116)$$

which is easily checked by substitution of (116) into Eq. (114).

Substitution of (94), (116) and (115) into (113) gives

$$\delta\psi = \frac{1}{(2\pi)^4} \sum_{\lambda_f} \int e^{i\boldsymbol{k}_f \boldsymbol{r}_1 - i\omega t} \Phi_{\lambda_f}(\boldsymbol{r}_2) \frac{d^3 k_f d\omega}{E_{fk} + E_{\lambda_f} - \omega - i\epsilon} e^{-i\boldsymbol{k}_f \boldsymbol{r}_1' + i\omega t'} \times$$

$$\times \Phi_{\lambda_f}^*(\boldsymbol{r}_2') \frac{\hbar^2}{2m} 4\pi b \delta(\boldsymbol{r}_1' - \boldsymbol{r}_2') \Phi_{\lambda_i}(\boldsymbol{r}_2') \exp\left(-iE_{\lambda_i} t'\right) \exp\left(i\boldsymbol{k}_i \boldsymbol{r}_1' - iE_{ik} t'\right) =$$

$$= \frac{1}{(2\pi)^3} \sum_{\lambda_f} \int \frac{d^3 k_f \Phi_{\lambda_f}(\boldsymbol{r}_2) \langle \lambda_f, \boldsymbol{k}_f | V | \lambda_i, \boldsymbol{k}_i \rangle}{E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i} - i\epsilon} e^{i\boldsymbol{k}_f \boldsymbol{r}_1 - i(E_{ik} + E_{\lambda_i}) t}, \quad (117)$$

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where

$$\langle\lambda_f, \boldsymbol{k}_f|V|\lambda_i, \boldsymbol{k}_i\rangle = \frac{\hbar^2}{2m}4\pi b \int d^3 r \Phi^*_{\lambda_f}(\boldsymbol{r}) \exp(i\boldsymbol{\kappa r})\Phi_{\lambda_i}(\boldsymbol{r}) \qquad (118)$$

is a matrix element of the interaction potential, and $\boldsymbol{\kappa} = \boldsymbol{k}_i - \boldsymbol{k}_f$ is the momentum transferred.

At $t \to \infty$ one can use the limit

$$\lim_{t\to\infty} \frac{\exp\left(i(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i})t\right)}{E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i} - i\epsilon} = 2\pi i\delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}), \quad (119)$$

which upon substitution into (117) gives the asymptotical wave function

$$\delta\psi = \frac{i}{(2\pi)^2}\sum_{\lambda_f}\int d^3 k_f\langle\lambda_f, \boldsymbol{k}_f|V|\lambda_i, \boldsymbol{k}_i\rangle\times$$

$$\times\,\delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i})\Phi_{\lambda_f}(\boldsymbol{r}_2)\,\mathrm{e}^{-iE_{\lambda_f}t}\,\mathrm{e}^{i\boldsymbol{k}_f\boldsymbol{r}_1 - iE_{fk}t}. \quad (120)$$

The probability amplitude of transition from the initial state $|\lambda_i, \boldsymbol{k}_i\rangle$ to final state $|\lambda_f, \boldsymbol{k}_f\rangle$ is

$$df(\boldsymbol{k}_i, \lambda_i \to \boldsymbol{k}_f, \lambda_f) = \frac{id^3 k_f}{(2\pi)^2}\langle\lambda_f, \boldsymbol{k}_f|V|\lambda_i, \boldsymbol{k}_i\rangle\delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}) =$$

$$= i\frac{m}{\hbar^2}\frac{k_f d\Omega_f}{(2\pi)^2}\langle\lambda_f, \boldsymbol{k}_f|V|\lambda_i, \boldsymbol{k}_i\rangle, \quad (121)$$

where

$$k_f = \sqrt{k_i^2 + \frac{2m}{\hbar^2}(E_{\lambda_i} - E_{\lambda_f})},$$

and Ω_f characterizes direction of the scattered neutron.

It follows from (121) that the probability of neutron scattering into element of solid angle $d\Omega_f$ and of transition of the system from the state $|\lambda_i\rangle$ into state $|\lambda_f\rangle$ is

$$dw(\boldsymbol{k}_i, \Omega_f, \lambda_i \to \lambda_f) = \frac{1}{(2\pi)^4}\left|\frac{m}{\hbar^2}\right|^2 k_f^2 d\Omega_f\,|\langle\lambda_f, \boldsymbol{k}_f|V|\lambda_i, \boldsymbol{k}_i\rangle|^2. \quad (122)$$

If we replace

$$\frac{m}{\hbar^2}k_f d\Omega_f = d^3 k_f \delta(E_{ik} + E_{\lambda_i} - E_{fk} - E_{\lambda_f}),$$

i.e. make transition reciprocal to (121), we obtain

$$dw(\boldsymbol{k}_i, \Omega_f, \lambda_i \to \lambda_f) =$$
$$\frac{mk_f}{\hbar^2} \frac{d^3 k_f}{(2\pi)^4} \left| \langle \lambda_f, \boldsymbol{k}_f | V | \lambda_i, \boldsymbol{k}_i \rangle \right|^2 \delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}). \quad (123)$$

Substitution of the potential (94) gives

$$dw(\boldsymbol{k}_i, \Omega_f, \lambda_i \to \lambda_f) =$$
$$= |b|^2 \frac{\hbar^2}{m} k_f \frac{d^3 k_f}{(2\pi)^2} \left| \langle \lambda_f | \exp(i\boldsymbol{\kappa}\boldsymbol{r}) | \lambda_i \rangle \right|^2 \delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_f}). \quad (124)$$

To get the cross section we must multiply the probability by the wave front area A. We obtain an agreement with standard formula (106), if we suppose that $A = (2\pi)^2 / k_i k_f$.

5.2.2. Some Remarks. The above considerations for neutron scattering by an arbitrary system are valid only, if both the neutron and the systems are described by the same Schrödinger equation, which has a single derivative on time. If the system obeys a different equation with double derivative on time (this is the case, when we consider scattering on oscillators), we need to use not the Schrödinger but different equation. What to do in this case needs separate considerations.

5.2.3. Direct Calculation of Scattering from a Monatomic Gas. When we consider neutron scattering from monatomic gas, we must treat the neutron and atom of the gas in the same way. Collision of two particles changes the state of both, thus we need to solve the Schrödinger equation for both particles:

$$\left[i\frac{\partial}{\partial t} + \frac{\Delta_1}{2} + \frac{\mu \Delta_2}{2} - \frac{u(\boldsymbol{r}_1 - \boldsymbol{r}_2, t)}{2} \right] \psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = 0, \quad (125)$$

where potential u is given in (94), $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, m, M are coordinates and masses of the neutron and atom, respectively, $\mu = m/M$, and we use unities in which $m = \hbar = 1$.

The Green function of the equation (125) without interaction is

$$G(\boldsymbol{r}_1 - \boldsymbol{r}_1', \boldsymbol{r}_2 - \boldsymbol{r}_2', t - t') =$$
$$= \int \frac{\exp(i\boldsymbol{k}_f(\boldsymbol{r}_1 - \boldsymbol{r}_1') + \boldsymbol{p}_f(\boldsymbol{r}_2 - \boldsymbol{r}_2') - i\omega(t - t'))}{E_{fk} + E_{fp} - \omega - i\epsilon} \frac{d^3 k_f d^3 p_f d\omega}{(2\pi)^7}, \quad (126)$$

where $E_{fk} = k_f^2 / 2$, $E_{fp} = \mu p_f^2 / 2$.

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The scattered part of the wave function is

$$\delta\psi = \frac{2\pi b}{(2\pi)^7} \int \frac{d^3 k_f d^3 p_f d\omega d^3 r'_1 d^3 r'_2 dt'}{E_{fk} + E_{fp} - \omega - i\epsilon} \times$$

$$\times \exp\left(i\boldsymbol{k}_f(\boldsymbol{r}_1 - \boldsymbol{r}'_1) + i\boldsymbol{p}_f(\boldsymbol{r}_2 - \boldsymbol{r}'_2) - i\omega(t - t')\right)\times$$

$$\delta(\boldsymbol{r}'_1 - \boldsymbol{r}'_2) \exp\left(i\boldsymbol{k}_i\boldsymbol{r}'_1 + i\boldsymbol{p}_i\boldsymbol{r}'_2 - i(E_{ik} + E_{ip})t'\right) =$$

$$= \frac{b}{(2\pi)^2} \int \frac{d^3 k_f d^3 p_f \delta(\boldsymbol{k}_f + \boldsymbol{p}_f - \boldsymbol{k}_i - \boldsymbol{p}_i)}{E_{fk} + E_{fp} - E_{ik} - E_{ip} - i\epsilon} \times$$

$$\times \exp\left(i\boldsymbol{k}_f\boldsymbol{r}_1 + i\boldsymbol{p}_f\boldsymbol{r}_2 - i(E_{ik} + E_{ip})t\right), \quad (127)$$

where $\exp\left(i\boldsymbol{k}_i\boldsymbol{r}_1 - iE_{ik}t\right)$, $\exp\left(i\boldsymbol{p}_i\boldsymbol{r}_2 - iE_{ip}t\right)$ describe incident plane waves of the neutron and atom, respectively, with their energies $E_{ik} = k_i^2/2$, and $E_{ip} = \mu p_i^2/2$.

The wave function (127) can be represented as a superposition of plane waves describing final states of the neutron, $\exp\left(i\boldsymbol{k}_f\boldsymbol{r}_1 - iE_{fk}t\right)$, and the atom, $\exp\left(i\boldsymbol{p}_f\boldsymbol{r}_2 - iE_{fp}t\right)$:

$$\delta\psi = \int \widetilde{f}(\boldsymbol{k}_i, \boldsymbol{p}_i \to \boldsymbol{k}_f, \boldsymbol{p}_f, t) d^3 k_f d^3 p_f \times$$

$$\times \exp(i\boldsymbol{k}_f\boldsymbol{r}_1 + i\boldsymbol{p}_f\boldsymbol{r}_2 - iE_{fk}t - iE_{fp}t),$$

where

$$\widetilde{f}(\boldsymbol{k}_i, \boldsymbol{p}_i \to \boldsymbol{k}_f, \boldsymbol{p}_f, t) = \frac{b}{(2\pi)^2} \frac{\delta(\boldsymbol{k}_i + \boldsymbol{p}_f - \boldsymbol{k}_i - \boldsymbol{p}_i)}{E_{fk} + E_{fp} - E_{ik} - E_{ip} - i\epsilon} \times$$

$$\times \exp\left(i(E_{fk} + E_{fp} - E_{ik} - E_{ip})t\right).$$

With the relation (20) we find in the limit $t \to \infty$ that the probability amplitude for the particle to leave in the state $\boldsymbol{k}_f$, and for the atom to leave in the state $\boldsymbol{p}_f$ is:

$$\lim_{t\to\infty} \widetilde{f}(\boldsymbol{k}_i, \boldsymbol{p}_i \to \boldsymbol{k}_f, \boldsymbol{p}_f, t) d^3 k_f d^3 p_f =$$

$$= d^3 k_f d^3 p_f \frac{ib}{2\pi} \delta(\boldsymbol{k}_f + \boldsymbol{p}_f - \boldsymbol{k}_i - \boldsymbol{p}_i)\delta(E_{fk} + E_{fp} - E_{ik} - E_{ip}),$$

and after integration over final momenta $d^3 p_f$ of the atom we obtain probability amplitude of scattering from an atom with momentum $\boldsymbol{p}_i$

$$f(\boldsymbol{k}_i \to \boldsymbol{k}_f, \boldsymbol{p}_i) = d^3 k_f \frac{ib}{\pi} \delta(k_f^2 + \mu(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f)^2 - k_i^2 - \mu p_i^2). \quad (128)$$

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Some remarks. Let's note that we sum the amplitude over final states, not the probability, and it is more correct, because, if we are not interested what is the final state of the atom, we must sum over them, since amplitudes with different atomic states can interfere with each other.

More over, usually cross sections are averaged over initial states, however the amplitude should also be averaged over initial states. The amplitude averaged in this way is the coherent amplitude, and its square gives coherent contribution to coherent probabilities and coherent cross sections.

Averaging the squared amplitude over initial states gives total probability and cross section, which consists of coherent and incoherent parts, and there is an interesting problem how to separate them experimentally.

5.2.4. Scattering in the Center- of Mass-System. Let us represent the argument of the δ-function in the form

$$k_f^2 + \mu(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f)^2 - k_i^2 - \mu p_i^2 =$$

$$(1 + \mu)\left(\boldsymbol{k}_f - \frac{\mu}{1+\mu}\boldsymbol{P}\right)^2 - \frac{q^2}{1+\mu}, \quad (129)$$

where $\boldsymbol{P} = \boldsymbol{k}_i + \boldsymbol{p}_i$ is the total momentum of the center of mass, and $\boldsymbol{q} = \boldsymbol{k}_i - \mu \boldsymbol{p}_i$ is the relative speed of the neutron and atom.

The change of variables

$$\boldsymbol{k}_{cm} = \boldsymbol{k}_f - \mu \boldsymbol{P}/(1 + \mu), \quad (130)$$

and integration over dk_{cm} reduces (128) to

$$df(\boldsymbol{k}_i, \Omega_{cm}, \boldsymbol{p}_i) = \frac{ibq}{2\pi(1+\mu)^2}d\Omega_{cm}. \quad (131)$$

The scattering cross section from an atom with momentum $\boldsymbol{p}_i$ is

$$d\sigma(\boldsymbol{k}_i, \Omega_{cm}, \boldsymbol{p}_i) = A\left|\frac{ibq}{2\pi(1+\mu)^2}\right|^2 d\Omega_{cm}, \quad (132)$$

and the total scattering cross section from an atom with momentum $\boldsymbol{p}_i$ is

$$\sigma(\boldsymbol{k}_i, \boldsymbol{p}_i) = 4\pi A\left|\frac{ibq}{2\pi(1+\mu)^2}\right|^2, \quad (133)$$

where A is the neutron wave front area.

Total cross section for atom at rest. In the case $\boldsymbol{p}_i = 0$, the cross section (132) becomes

$$d\sigma(\boldsymbol{k}_i, \Omega_{cm}, \boldsymbol{p}_i = 0) = A\left|\frac{bk_i}{2\pi(1+\mu)^2}\right|^2 d\Omega_{cm}, \quad (134)$$

because in that case $q = k_i$. Integration over $d\Omega_{cm}$ gives total cross section of scattering from atom at rest

$$\sigma(k_i, \boldsymbol{p}_i = 0) = 4\pi A \left| \frac{bk_i}{2\pi(1+\mu)^2} \right|^2. \tag{135}$$

Total cross section for scattering from monatomic gas. To get cross section for scattering from monatomic gas at temperature T we must average (132) over $\boldsymbol{p}_i$ with Maxwellian distribution (108)

$$d\sigma(\boldsymbol{k}_i, \Omega_{cm}, T) = \int d^3 p_i \mathcal{M}\left(\frac{\mu p_i^2}{2T}\right) A \left| \frac{bq}{2\pi(1+\mu)^2} \right|^2 d\Omega_{cm}. \tag{136}$$

If area A does not depend on neutron energy, then the total cross section is

$$\sigma(k_i, T) = 4\pi A \left| \frac{ib}{2\pi(1+\mu)^2} \right|^2 \int d^3 p_i \left(\frac{\mu}{2\pi T}\right)^{3/2} \exp\left(-\mu \frac{p_i^2}{2T}\right) \times$$

$$\times (k_i^2 + \mu^2 p_i^2) = 4\pi A \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 (2\mu T) \left(\frac{3}{2} + \frac{k_i^2}{2\mu T}\right). \tag{137}$$

It is seen that the cross section grows linearly with increase of the temperature.

However, it is not this cross section which is measured in an experiment. In the experiment the probability of neutron scattering from a gas sample of width d and density N_0 is measured. This probability is proportional to the flight time $t_f = d/k_i$ of the neutron through the sample, and to the number $\nu(\boldsymbol{k}_i, \boldsymbol{p}_i)$ of collisions per unit time, which in its turn is proportional to N_0, σ and to relative velocity $q = |\boldsymbol{k}_i - \mu \boldsymbol{p}_i|$. So, the full probability of a single neutron scattering in the sample is

$$W = N_0 \frac{d}{k_i} \int d^3 p_i q \sigma(\boldsymbol{k}_i, \boldsymbol{p}_i) \mathcal{M}\left(\mu \frac{p_i^2}{2T}\right).$$

After substitution of (133) in the case of constant A we obtain an expression, which grows at high temperatures $\propto T^{3/2}$. Experiment shows that the grows is only $\propto T^{1/2}$. It means that $A = \alpha/q^2$ with constant α. With such A the total scattering probability after change of variables $\boldsymbol{p} = \boldsymbol{p}_i/\sqrt{2T/\mu}$ and $\boldsymbol{k}_r = \boldsymbol{k}_i/\sqrt{2\mu T}$ becomes

$$W = N_0 d \frac{4\pi\alpha}{\pi^{3/2} k_r} \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 \int p^2 dp d\Omega \exp\left(-p^2\right) \sqrt{(\boldsymbol{k}_r - \boldsymbol{p})^2}.$$

Thus, the experimentally measured cross section $\sigma_{\text{exp}} = W?N_0 d$ should be compared with theoretical one

$$\sigma_{\text{eff}} = \frac{4\pi\alpha}{\pi^{3/2}k_r} \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 \int p^2 dp d\Omega \, \exp\left(-p^2\right)\sqrt{(\boldsymbol{k}_r - \boldsymbol{p})^2}. \qquad (138)$$

The integral at the right-hand side is

$$I = \frac{4\pi}{3k_r} \int_0^\infty p dp \{[p(3k_r^2 + p^2)\Theta(p < k_r)+$$

$$+ k_r[3p^2 + k_r^2]\theta(p > k_r)\} \exp(-p^2) =$$

$$= \frac{2\pi}{3k_r} \left(\int_0^{E_r} dp^2 [p(3k_r^2 + p^2) - k_r(3p^2 + k_r^2)]e^{-p^2} + \right.$$

$$\left. + \int_0^\infty dp^2 k_r[3p^2 + k_r^2]e^{-p^2} \right) = \frac{\pi}{k_r}\left(k_r e^{-k_r^2} + \frac{\sqrt{\pi}}{2}[1 + 2k_r^2]\Phi(k_r) \right).$$

So cross section (138) is

$$\sigma_{eff} = 4\pi \frac{\alpha}{\sqrt{\pi}k_r} \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 \left(e^{-k_r^2} + \frac{\sqrt{\pi}}{2k_r}[1 + 2k_r^2]\Phi(k_r) \right),$$

which coincides with the standard expression (111), if $\alpha = [2\pi(1+\mu)]^2$, because $k_r = \sqrt{E_r}$.

We can also show that the differential cross section in this case does also coincide with the standard one (110). For that we replace

$$d\Omega_q \to \frac{(1+\mu)^2}{q} d^3 k_2 \delta(k_f^2/2 + \mu(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f)^2/2 - k_i^2/2 - \mu p_i^2/2), \quad (139)$$

which means transition reciprocal to the one from (128) to (131). After this replacement we represent (134) in the form

$$d\sigma(k_i \to \boldsymbol{k}_f, \boldsymbol{p}_i) = A d^3 k_f \left| \frac{b}{2\pi(1+\mu)} \right|^2 \frac{\delta(E_R - \omega + \mu \boldsymbol{p}_i \boldsymbol{\kappa})}{\sqrt{(\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2}}, \qquad (140)$$

where $E_R = \mu\kappa^2/2$, $\boldsymbol{\kappa} = \boldsymbol{k}_i - \boldsymbol{k}_f$, and $\omega = k_i^2/2 - k_f^2/2$.

In (140) we can integrate over dk_f, then we obtain differential scattering cross section

$$d\sigma(k_i, \Omega_f, \boldsymbol{p}_i) = A d^3 k_f \left| \frac{b}{2\pi(1+\mu)} \right|^2 \times$$

$$\times \frac{(\mu \boldsymbol{Pn} \pm \sqrt{\mu^2(\boldsymbol{Pn})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2})^2}{(1+\mu)\sqrt{(\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2}\sqrt{\mu^2(\boldsymbol{Pn})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2}}, \quad (141)$$

where $\boldsymbol{n}$ is a unit vector, pointing into direction of $\boldsymbol{k}_f$ scattered neutron.

In the case of $A = \alpha/q^2$ the probability of neutron scattering in the sample to the state $\boldsymbol{k}_f$, averaged over Maxwellian distribution is equal to

$$dW_s(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = N_a \frac{d}{k_i} \alpha d^3 k_f \left| \frac{b}{2\pi(1+\mu)} \right|^2 \times$$

$$\times \int d^3 p \left(\frac{1}{2\pi\mu T} \right)^{3/2} e^{-p^2/2\mu T} \delta(E_R - \omega + \boldsymbol{p\kappa}), \quad (142)$$

where $\boldsymbol{p} = \mu \boldsymbol{p}_i$, and we used (140). After integration over $d^3 p$ we obtain the cross section

$$d\sigma_{eff}(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = \frac{\alpha d^3 k_f}{k_i \kappa \sqrt{2\pi\mu T}} \left| \frac{b}{2\pi(1+\mu)} \right|^2 \exp\left(-\frac{(E_R - \omega)^2}{4 E_R T} \right), \quad (143)$$

identical to (110), if $\alpha = [2\pi(1+\mu)]^2$.

5.3. An Alternative Calculation. Catastrophe in Quantum Mechanics
Above we considered probability amplitude (131) calculated in the center-of-mass coordinate system. It means that the argument of δ-function in (128) was represented in the form (129), and after change of variables (130) and integration over dk_{cm} we obtained (131), and the cross section (132). Transition from the cm system to laboratory one was performed with reciprocal transformation (139), which led to (140) and after integration over dk_f — to (141).

Now we proceed differently. We integrate (128) directly over dk_f. Then we obtain probability amplitude of scattering into direction $\boldsymbol{\Omega}_f$ of the wave vector $\boldsymbol{k}_f$ in laboratory coordinate system

$$f(\boldsymbol{k}_i \to \boldsymbol{k}_f, \boldsymbol{p}_i) = d^3 k_f \frac{ib}{\pi} \delta(k_f^2 + \mu(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f)^2 - k_i^2 - \mu p_i^2) =$$

$$df(\boldsymbol{k}_i, \boldsymbol{\Omega}_f, \boldsymbol{p}_i) = \frac{ibd\Omega_f}{2\pi} \frac{k_f^2}{|k_f(1+\mu) - \mu \boldsymbol{nP}|}, \quad (144)$$

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where

$$k_f = \frac{\mu \boldsymbol{P} \boldsymbol{n} \pm \sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2}}{1 + \mu} > 0, \tag{145}$$

$\boldsymbol{P} = \boldsymbol{k}_i + \boldsymbol{p}_i$, and $\boldsymbol{n}$ is the unit vector pointing into direction $\boldsymbol{\Omega}_f$. With the help of amplitude (144) we obtain the scattering cross section

$$d\sigma(\boldsymbol{k}_i, \boldsymbol{\Omega}_f, \boldsymbol{p}_i) = d\Omega_f A \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 \times$$

$$\times \frac{\left(\mu \boldsymbol{P} \boldsymbol{n} \pm \sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2} \right)^4}{|\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2|}. \tag{146}$$

Now we can make transformation

$$d\Omega \frac{\left| \mu \boldsymbol{P} \boldsymbol{n} \pm \sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2} \right|^2}{2(1+\mu)^2 \sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2}} =$$

$$= d^3 k_f \delta(k_f^2 + \mu(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f)^2 - k_i^2 - \mu p_i^2), \tag{147}$$

which is reciprocal to the one, used in (144), then we obtain

$$d\sigma(\boldsymbol{k}_i \rightarrow \boldsymbol{k}_f, \boldsymbol{p}_i) = A d^3 k_f k_f^2 \left| \frac{b}{2\pi} \right|^2 \frac{\delta(E_R - \omega + \mu \boldsymbol{\kappa} \boldsymbol{p}_i)}{\sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2}}. \tag{148}$$

We can replace $\sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2 P^2 + (\boldsymbol{k}_i - \mu \boldsymbol{p}_i)^2}$ in denominator by $|(1 + \mu)k_f - \mu \boldsymbol{P} \boldsymbol{n}|$, multiply it by k_f, replace $\boldsymbol{p}_i \boldsymbol{k}_f$ by $\mu \boldsymbol{p}_i \boldsymbol{k}_i - \mu \boldsymbol{p}_i \boldsymbol{\kappa}$, and substitute according to the argument of the δ-function $\mu \boldsymbol{p}_i \boldsymbol{k}_i = \omega - E_R$. After some rearrangement the Eq. (148) becomes

$$d\sigma(\boldsymbol{k}_i \rightarrow \boldsymbol{k}_f, \boldsymbol{p}_i) = A d^3 k_f k_f^3 \left| \frac{b}{2\pi} \right|^2 \frac{\delta(E_R - \omega + \mu \boldsymbol{\kappa} \boldsymbol{p}_i)}{|s - \mu \omega - \mu \boldsymbol{k}_i \boldsymbol{p}_i|}, \tag{149}$$

where $s = k_i^2/2 + k_f^2/2$. We see that this expression strongly differs from (140). If we substitute $A = \alpha/q^2$, introduce number $\nu(\boldsymbol{k}_i \rightarrow \boldsymbol{k}_f)$ of collisions per unit time, which give scattering from $\boldsymbol{k}_i$ to $\boldsymbol{k}_f$, and flight time $t_f = d/k_i$ through the sample, and average over distribution of $\boldsymbol{p}_i$, then we obtain the effective cross section

$$d\sigma_{\text{eff}}(\boldsymbol{k}_i, \rightarrow \boldsymbol{k}_f, T) =$$

$$= \frac{\alpha}{k_i} d^3 k_f k_f^3 \left| \frac{b}{2\pi} \right|^2 \int \mathcal{P}(\boldsymbol{p}_i) d^3 p_i \frac{\delta(E_R - \omega + \mu \boldsymbol{\kappa} \boldsymbol{p}_i)}{|\boldsymbol{k}_i - \mu \boldsymbol{p}_i||s - \mu \omega - \mu \boldsymbol{k}_i \boldsymbol{p}_i|}. \tag{150}$$

5.3.1. Scattering from the Atom at Rest. As an exercise let us consider the case $\mathcal{P}(\boldsymbol{p}_i) = \delta(\boldsymbol{p}_i)$. In this case expression (150) becomes

$$d\sigma_{eff}(\boldsymbol{k}_i, \rightarrow \boldsymbol{k}_f, p_i = 0) = \frac{\alpha}{k_i^2} d^3 k_f k_f^3 \left| \frac{b}{2\pi} \right|^2 \frac{\delta(E_R - \omega)}{s - \mu\omega}. \qquad (151)$$

To find the total cross section we first integrate over angles and obtain

$$d\sigma_{\text{eff}}(k_i, \rightarrow k_f, p_i = 0) = \frac{2\pi\alpha}{\mu k_i^3} k_f^4 dk_f \left| \frac{b}{2\pi} \right|^2 \frac{\Theta(|\mu s - \omega| < \mu k_i k_f)}{s - \mu\omega}. \qquad (152)$$

After change of variables $k_f = k_i x$ we obtain the integral

$$\sigma_{\text{eff}}(k_i, p_i = 0) = \frac{4\pi\alpha}{\mu(1+\mu)} \left| \frac{b}{2\pi} \right|^2 \int_\gamma^1 \frac{x^4 dx}{x^2 + \gamma} =$$

$$= 4\pi\alpha \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 \left(\frac{8}{3}\mu^2 + \frac{(1-\mu^2)^{3/2}}{\mu} \arctan\left(\frac{\mu}{\sqrt{1-\mu^2}} \right) \right), \qquad (153)$$

where $\gamma = (1 - \mu)/(1 + \mu)$. This expression differs from (135), where for comparison $A = \alpha/k_i^2$ should be substituted. The difference can be described by the factor

$$C(\mu) = \frac{1}{(1+\mu)^2} \left(\frac{8}{3}\mu^2 + \frac{(1-\mu^2)^{3/2}}{\mu} \arctan\left(\frac{\mu}{\sqrt{1-\mu^2}} \right) \right).$$

This difference is the first evidence of the catastrophe, because it shows that there is an ambiguity in definition of the cross section. This ambiguity is the result of definition of probability as a square of probability amplitude.

5.3.2. Scattering from the Maxwellian Gas. Now we take $\mathcal{P}(\boldsymbol{p}_i)$ to be Maxwellian. Substitution of (108) into (150) gives

$$d\sigma_{\text{eff}}(\boldsymbol{k}_i, \rightarrow \boldsymbol{k}_f, T) = \frac{\alpha}{k_i} d^3 k_f k_f^3 \left| \frac{b}{2\pi} \right|^2 \int \left(\frac{\mu}{2\pi T} \right)^{3/2} \times$$

$$\times \exp\left(-\mu \frac{p_i^2}{2T} \right) d^3 p_i \frac{\delta(E_R - \omega + \mu\boldsymbol{\kappa}\boldsymbol{p}_i)}{|\boldsymbol{k}_i - \mu\boldsymbol{p}_i||s - \mu\omega - \mu\boldsymbol{k}_i\boldsymbol{p}_i|}. \qquad (154)$$

In the integral we can change variables $\boldsymbol{p} = \mu\boldsymbol{p}_i$ and integrate over one component of $\boldsymbol{p}_\kappa$ along $\boldsymbol{\kappa}$. Then we obtain the result

$$d\sigma_{\text{eff}}(\boldsymbol{k}_i, \rightarrow \boldsymbol{k}_f, T) =$$

$$= \frac{\alpha d^3 k_f}{\kappa k_i \sqrt{2\pi\mu T}} \left| \frac{b}{2\pi} \right|^2 \exp\left(-\frac{(\omega - E_R)^2}{4E_R T} \right) F(\kappa^2, \omega, s), \qquad (155)$$

which has an additional factor $F(\kappa^2, \omega, s)$ comparing to (110)

$$F(\kappa^2, \omega, s) = k_f^3 \int \frac{d^2 p_\perp}{2\pi\mu T} \exp\left(-\frac{p_\perp^2}{2\mu T}\right) \frac{1}{|\mathbf{k}_i - \mathbf{p}||s - \mu\omega - \mathbf{k}_i\mathbf{p}|}. \quad (156)$$

To calculate this factor we represent $\mathbf{k}_i$ as $\mathbf{k}_\kappa + \mathbf{k}_\perp$, where

$$\mathbf{k}_\kappa = \frac{(\mathbf{k}_i\boldsymbol{\kappa})\boldsymbol{\kappa}}{\kappa^2} = \frac{\omega + \kappa^2/2}{\kappa^2}\boldsymbol{\kappa},$$

and $\mathbf{k}_\perp \mathbf{k}_\kappa = 0$. Then

$$(\mathbf{k}_i - \mathbf{p})^2 = \frac{(\omega + \kappa^2/2 - \omega + E_R)^2}{\kappa^2} + (\mathbf{k}_\perp - \mathbf{p}_\perp)^2 =$$

$$= \frac{1}{4}\kappa^2(1 + \mu)^2 + (\mathbf{k}_\perp - \mathbf{p}_\perp)^2$$

and

$$s - \mu\omega - \mathbf{k}_i\mathbf{p} = s - \mu\omega - \frac{(\omega + \kappa^2/2)(\omega - E_R)}{\kappa^2} - \mathbf{k}_\perp \mathbf{p}_\perp.$$

Substitution into (156) and change of variables $\mathbf{q} = \mathbf{p}_\perp - \mathbf{k}_\perp$ gives

$$F(\kappa^2, \omega, s) = \int \frac{d^2 q}{2\pi\mu T} \exp\left(-\frac{(\mathbf{q} + \mathbf{k}_\perp)^2}{2\mu T}\right) \times$$

$$\times \frac{4k_f^3}{\sqrt{\kappa^2(1 + \mu)^2 + 4q^2}|(\omega + \kappa^2/2)(1 + \mu) + 2\mathbf{k}_\perp \mathbf{q}|}. \quad (157)$$

It is easy to see that this integral diverges at the point $2\mathbf{k}_\perp \mathbf{q} = -(\omega + \kappa^2/2)(1 + \mu)$. This divergence, in principle, can be eliminated with the help of imaginary part, which will be needed to satisfy unitarity condition, however this imaginary part does not solve the main problem — the difference of two probabilities, which is seen in the case of scattering on a free atom at rest, where divergence is absent.
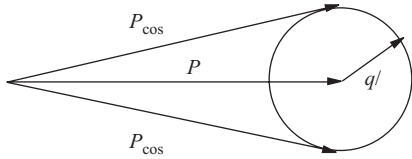

Fig. 3. Geometry of the experiment with scattering of the neutron beam on an atomic beam. $P = |\mathbf{k}_i + \mathbf{p}_i|$ is the total momentum of neutrons and atoms, $q = |\mathbf{k}_i - \mu\mathbf{p}_i|$ is relative velocity of neutrons and atoms, θ is direction of the scattered neutrons with respect to total momentum. In this direction scattering cross section has a maximum

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We see the only way to resolve the paradox, is to quantize angular distribution, i.e. to make the particle scattering only at discrete angles. In that case the number of scattering angles will be the same in center-of-mass system and in the laboratory reference frame. Therefore both way of probability calculations will give the same result. We do not know now how to define the quantum of angle, however, it seems that any size can be of use for resolution of this paradox. The quantum $\Delta\Omega$ must be defined in a reference system, where angular distribution is uniform. Transition to other reference systems changes this quantum and makes it dependent on angle $\Delta\Omega(\Omega)$. It seems that introduction of a finite space sell L serves like this angular quantization, however, we cannot find direct relation between them.

6. CONCLUSION

Simple consideration of scattering processes shows a contradiction hidden in the standard approach. On one side, we use plane waves as eigenstates of a particle, and on the other side describe scattered particles with spherical waves, which are not even solutions of the free Schrödinger equation. Rigorous approach permits to calculate only dimensionless probabilities of scattering. To get cross section we are to introduce some front area of the wave function for the incident particle, and a hypothesis that scattering takes place only when the scatterer is inside this front area. Without this hypothesis the quantum or wave mechanics is incomplete theory. However, even with this hypothesis QM is not a complete theory, because it does not permit to find a unique scattering cross section.

In to-day science all the measured cross sections are compared to theoretical ones calculated with the help of a set of rules, which do not represent a self-consistent theory. In this paper we could only demonstrate this fact with the help of a single example. We cannot now propose an alternative theory, but think that our research will liberate the physical community from the prejudice that QM is a perfect and complete theory, and stimulate the search for more adequate and self-consistent theory of microworld.

It is possible to test experimentally the scattering cross section (146) and (141) by scattering a collimated neutron beam on an atomic beam. According to both formulas the probability of scattering has maximum at some direction with respect to total momentum $\boldsymbol{P} = \boldsymbol{k}_i + \boldsymbol{p}_i$. Vector diagram of the experiment is presented in Fig. 5.3.2. The momentum k_f after scattering is equal to $\mu P \cos\theta/(1 + \mu)$. Measurement at two different P can discriminate between two expressions.

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