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CONTRADICTIONS IN SCATTERING THEORY

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Abstract

The standard scattering theory (SST) in non relativistic quantum mechanics (QM) is analyzed. Self-contradictions of SST are demonstrated. 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 packets 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

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

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

Such a 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 3-rd 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 a transition is impossible, because unitarity is violated. In mentioned textbooks unitarity is considered as equality of 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 that 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 wave mechanics. However, to get cross section from 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 eigenstates 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 eigenstates, 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? Eigenstates of a particle are described by plane waves $\psi_i = \exp(i\boldsymbol{kr})$, but the scattered wave function after, say, elastic s-wave scattering, is described by the spherical wave, $\Psi \propto \exp(ikr)/r$, 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:

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

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:

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

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 $\boldsymbol{p}_\parallel$ in (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 $p_\parallel^2 \leq k^2$:

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

In this integral we can substitute

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

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

$$\begin{aligned} \frac{\exp(ikr)}{r} &= \frac{i}{2\pi} \int \exp(i\boldsymbol{p}\boldsymbol{r})\Theta(p_z z > 0)\, d^3p\delta(p^2/2 - k^2/2) = \\ &= \frac{ik}{2\pi} \int\limits_{4\pi} \exp(i\boldsymbol{k}_\Omega \boldsymbol{r}) d\Omega, \end{aligned} \tag{12}$$

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

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

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

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

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

which is equivalent to (5) with scattering probability amplitude

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

and scattering probability

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

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

$$\begin{aligned}\delta\psi(r,t) &= \tfrac{b}{r}\exp(ikr - i\omega_k t) = \\ &= \tfrac{b}{(2\pi)^2}\int \tfrac{d^3p}{\omega_p - \omega_k - i\epsilon}\exp(i\boldsymbol{pr} - i\omega_k t),\end{aligned} \tag{17}$$

where $\omega_p = p^2/2$ 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

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

with amplitudes

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

which depend on time t.

Now we use the evident relation

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

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

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

In this limit (18) is

$$\begin{aligned}\delta\psi &= \int \tfrac{ib}{\pi}\exp(i\boldsymbol{pr} - i\omega_p t)d^3p\,\delta(p^2 - k^2) = \\ &= \tfrac{ibk}{2\pi}\int\limits_{4\pi} d\Omega\exp(i\boldsymbol{k}_\Omega\boldsymbol{r} - i\omega_k t),\end{aligned} \tag{22}$$

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 spoke above about dimensionless scattering probability, while almost all the experiments (exceptions are reflectometry and diffractometry) are interpreted in terms of scattering cross sections. Here we compare different definitions of scattering cross section and show that to get a cross section from probability we have to introduce a parameter A with dimension of area, characterizing the size of the neutron wave function.

2.4.1 Definition of the scattering cross section in an experiment

For definition of the scattering cross section we can look at an experiment schematically shown in fig. 1. If the detector registers N_s scattered neutrons per unit time, then the total probability W for a single neutron to be scattered in the sample into the given direction is

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

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.

Experimentalists divide this value by dimensional parameter $N_0 d$, where N_0 is atomic number density in the sample, and d is the sample

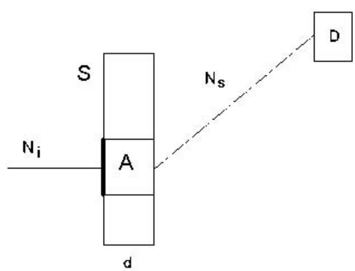

Figure 1: Definition of cross section for a single atom

width, and as a result obtain the cross section (we assume the sample to be thin for not to take into account self-shielding)

$$\sigma = \frac{N_s}{N_i N_0 d} = \frac{N_s}{JSN_0 d} = \frac{N_s}{JV}, \tag{24}$$

where $V = Sd$ is the volume of the sample illuminated by the incident neutron flux. The expression (24) is commonly accepted, but gives no insight about interaction of a single neutron with a single atom.

It looks more reasonable from total probability W (23) of scattering of a single neutron in the whole sample to find the scattering probability w_1 of a single neutron on a single atom:

$$w_1 = \frac{W}{N_a}, \tag{25}$$

where N_a is the number of atoms met by a single neutron on its way during the flight through the sample. To find the number of atoms on the neutron's way we have 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. So, let the neutron wave function to have area A, then $N_a = N_0 Ad$. From (25) we immediately find the scattering cross section of a single neutron per single atom:

$$\sigma = Aw_1 = \frac{W}{N_0 d} = \frac{N_s}{N_i N_0 d} = \frac{N_s}{JSN_0 d} = \frac{N_s}{JN_0 V}, \tag{26}$$

which coincides with (24). The left hand side is the cross section we must calculate, the right hand side is the experimentally defined cross section. To compare theory with experiment we must be able to calculate w_1 and A.

2.4.2 Phenomenological definition of the scattering cross section

According to all the textbooks the scattering cross section is defined as a ratio of the count rate N_s of scattered particles to the flux density, J, of the incident particles:

$$\sigma = \frac{N_s}{J}. \tag{27}$$

If, for instance, we have a small sample, the above ratio gives the cross section of the whole sample, and if we divide this ratio by the total number of atoms in the sample, $N_a = N_0 V$, illuminated by the incident flux, we obtain the result (24), which defines the cross section per one atom. We call it a phenomenological definition, because it says nothing about interaction of a single neutron with a single atom.

2.4.3 Theoretical definition of the scattering cross section

Theoretically, if you want to find a number of scattered particles for a single target atom and a given incident flux J, you must first find, how a single particle is scattered, and how this scattering depends on impact parameter. After that we should integrate over all particles in the incident flux, and average over all possible positions of the scatterer. This procedure gives the number N_s of scattered particles for the given J. The ratio N_s/J is an average cross section Aw_1, and it can be compared with the phenomenological one.

The parameter A includes also the size of a single nucleus. If we suppose that the widely used plane wave describes point neutrons propagating like rays of the wave, then A is equal to the size σ_N of the nucleus, and the total cross section can never be larger than σ_N, because the total probability w_1 can never be larger than unity. This contradicts to the well known facts, that some capture cross sections can be many orders of magnitude larger than σ_N. To avoid this contradiction, we have to assume that A is considerably larger than σ_N.

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, though this wave packet should be sufficiently wide.

The 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.

One of possible candidates for the nonspreading wave packet is the singular de Broglie wave packet (dBWP) [3, 4, 5]

$$\psi_{dB}(\boldsymbol{r},t)=\sqrt{\frac{s}{2\pi}}\exp(i\boldsymbol{k}\boldsymbol{r}-i\omega t)\frac{\exp(-s|\boldsymbol{r}-\boldsymbol{v}t|}{|\boldsymbol{r}-\boldsymbol{v}t|}, \tag{28}$$

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 (28) 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 $\int d^3pa(\boldsymbol{p})|\boldsymbol{p}\rangle$, 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

$$\int d^3pa(\boldsymbol{p})|\boldsymbol{p}'\rangle d^3p'\langle\boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle=\int d^3p'b(\boldsymbol{p}')|\boldsymbol{p}'\rangle, \tag{29}$$

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

$$b(\boldsymbol{p}')=\int' \langle\boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle a(\boldsymbol{p})d^3p. \tag{30}$$

The scattering probability is defined as

$$dw(\boldsymbol{p}')=|b(\boldsymbol{p}')|^2d^3p', \tag{31}$$

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 $|a(\boldsymbol{p})|^2d^3p$. 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:

$$|\phi(t)\rangle = \exp(-iH_0t)|\phi\rangle. \tag{32}$$

   The wave packet is represented by Fourier expansion over plane waves

$$|\phi\rangle \equiv |\phi(\boldsymbol{k})\rangle = \int d^3pa(\boldsymbol{k}-\boldsymbol{p})|\boldsymbol{p}\rangle, \tag{33}$$

   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

$$\exp(-iHt)|\Psi\rangle \to \exp(-iH_0t)|\phi\rangle, \tag{34}$$

   or

$$|\Psi\rangle = \Omega_+|\phi\rangle, \quad \Omega_+ = \lim_{t\to-\infty} U(0,t), \quad U(0,t) = e^{iHt}e^{-iH_0t}. \tag{35}$$

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

4. According to (35) the operator $U(0,t)$ satisfies the differential equation

$$i\frac{\partial}{\partial t}U(0,t) = -e^{iHt}Ve^{-iH_0t}, \tag{36}$$

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

$$\Omega_+ = 1 - i \int\limits_{-\infty}^{0} e^{iHt'} V e^{-iH_0 t'} dt', \tag{37}$$

and

$$\begin{aligned} |\Psi\rangle &= \left(1 - i \int\limits_{-\infty}^{0} dt' e^{iHt'} V e^{-iH_0 t'}\right) |\phi\rangle = \\ &= \int d^3p a(\boldsymbol{k} - \boldsymbol{p}) \left[1 - i \int\limits_{-\infty}^{0} dt' e^{i(H - E_p)t'} V\right] |\boldsymbol{p}\rangle, \end{aligned} \tag{38}$$

where we used the relation $\exp(-iH_0 t)|\boldsymbol{p}\rangle = \exp(-iE_p t)|\boldsymbol{p}\rangle$.

Integration of (38) over t' leads to

$$\begin{aligned} &\int d^3p a(\boldsymbol{k} - \boldsymbol{p}) \left[1 - \tfrac{1}{H - E_p - i\epsilon} V\right] |\boldsymbol{p}\rangle = \\ &\qquad = \int d^3p a(\boldsymbol{k} - \boldsymbol{p}) |\psi_{\boldsymbol{p}}\rangle, \end{aligned} \tag{39}$$

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

5. This function is

$$|\psi_{\boldsymbol{p}}\rangle = \left[1 - \frac{1}{H - E_p - i\epsilon} V\right] |\boldsymbol{p}\rangle. \tag{40}$$

It satisfies the full Schrödinger equation with interaction

$$(H - E_p)|\psi_{\boldsymbol{p}}\rangle = 0 \tag{41}$$

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

6. Using the following identity

$$\frac{1}{A} - \frac{1}{B} = \frac{1}{A}(B - A)\frac{1}{B}, \tag{42}$$

we find that

$$\frac{1}{H-E_p-i\epsilon}=\frac{1}{H_0-E_p-i\epsilon}\left(1-V\frac{1}{H-E_p-i\epsilon}\right). \qquad (43)$$

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

$$|\psi_{\boldsymbol{p}}\rangle=\left[1-\frac{1}{H_0-E_p-i\epsilon}\mathcal{T}\right]|\boldsymbol{p}\rangle, \qquad (44)$$

where

$$\mathcal{T}=V-V\frac{1}{H-E_p-i\epsilon}V. \qquad (45)$$

7. An asymptotical state $|\chi\rangle$ of the particle after scattering is defined. Its dynamics is again determined by the free hamiltonian H_0: $|\chi(t)\rangle=\exp(-iH_0t)|\chi\rangle$. This state is also a wave packet $|\chi\rangle=\int d^3p|\boldsymbol{p}\rangle a_s(\boldsymbol{k},\boldsymbol{p})$.

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 $\exp(-iH_0t)|\chi\rangle$:

$$\exp(-iHt)|\Psi\rangle\to\exp(-iH_0t)|\chi\rangle, \qquad (46)$$

or

$$\begin{aligned}|\chi\rangle &= \lim_{t\to\infty}e^{iH_0t}e^{-iHt}\int d^3pa(\boldsymbol{k}-\boldsymbol{p})|\psi_{\boldsymbol{p}}\rangle= \\ &= \lim_{t\to\infty}e^{iH_0t}\int d^3pa(\boldsymbol{k}-\boldsymbol{p})e^{-iE_pt}|\psi_{\boldsymbol{p}}\rangle,\end{aligned} \qquad (47)$$

where in the last equality equation (41) is taken into account.

9. The function $|\psi_{\boldsymbol{p}}\rangle$ is expanded over plane waves. Then (47) becomes

$$|\chi\rangle=\lim_{t\to\infty}\int d^3pa(\boldsymbol{k}-\boldsymbol{p})\int d^3p'e^{iE_{p'}t}|\boldsymbol{p}'\rangle\langle\boldsymbol{p}'||\psi_{\boldsymbol{p}}\rangle e^{-iE_pt}, \qquad (48)$$

with account of $\exp(iH_0t)|\boldsymbol{p}'\rangle = \exp(iE_{p'}t)|\boldsymbol{p}'\rangle$. Substitution of (44) brings

$$\begin{aligned}|\chi\rangle = \lim_{t\to\infty}\int d^3p'|\boldsymbol{p}'\rangle\int d^3pa(\boldsymbol{k}-\boldsymbol{p})\times \\ \times\left[\delta(\boldsymbol{p}-\boldsymbol{p}') - \frac{e^{i(E_{p'}-E_p)t}}{E_{p'}-E_p-i\epsilon}\langle\boldsymbol{p}'|\mathcal{T}|\boldsymbol{p}\rangle\right].\end{aligned} \tag{49}$$

10. It follows from (20) that

$$\begin{aligned}|\chi\rangle &= \int d^3p'|\boldsymbol{p}'\rangle\int d^3pa(\boldsymbol{k}-\boldsymbol{p})[\delta(\boldsymbol{p}-\boldsymbol{p}')- \\ &- 2\pi i\delta(E_{p'}-E_p)T(\boldsymbol{p}',\boldsymbol{p})] = \\ &= \int d^3p'|\boldsymbol{p}'\rangle\int d^3p\langle\boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle a(\boldsymbol{k}-\boldsymbol{p}),\end{aligned} \tag{50}$$

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

$$\langle\boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}') - 2\pi i\delta(E_{p'}-E_p)T(\boldsymbol{p}',\boldsymbol{p}) \tag{51}$$

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 (49,50)) 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 register not a wave packet but a plane wave, so the probability of scattering from the state of the wave packet

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

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

$$dw = d^3p'|\langle\boldsymbol{p}'||\chi\rangle|^2 = d^3p'\left|\int d^3p\langle\boldsymbol{p}'|\hat{S}|\boldsymbol{p}\rangle a(\boldsymbol{k}-\boldsymbol{p})\right|^2. \tag{52}$$

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

$$|\chi\rangle = \int d^3k' b(\boldsymbol{k} \to \boldsymbol{k}')|\phi(\boldsymbol{k}')\rangle, \tag{53}$$

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

$$df = -2\pi i T(\boldsymbol{p}', \boldsymbol{p})\delta(p^2/2 - p'^2/2)d^3p' = 2\pi i p T(\boldsymbol{p}', \boldsymbol{p})d\Omega' \tag{54}$$

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

$$< dw >= \left(\int |a(\boldsymbol{k} - \boldsymbol{p})|^2 d^3p |2\pi p T(\boldsymbol{p}', \boldsymbol{p})|^2\right) d\Omega'. \tag{55}$$

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 size of the wave front.

With definition (52) 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 (52) the scattering probability is defined by the Fourier coefficient in expansion (50) over plane waves $|\boldsymbol{p}'\rangle$:

$$\begin{aligned} dw &= d^3p'(2\pi)^2T(\boldsymbol{p}',\boldsymbol{p}_1)T^*(\boldsymbol{p}',\boldsymbol{p}_2)a(\boldsymbol{k}-\boldsymbol{p}_1)\times \\ &\times\ a^*(\boldsymbol{k}-\boldsymbol{p}_2)d^3p_1d^3p_2\delta(p_1^2/2-p_2^2/2)\times \\ &\times\ \delta(p'^2/2-p_1^2/2), \end{aligned} \tag{56}$$

it means that the incident wave packet is considered as a coherent unity, but 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

$$\delta(p_1^2/2-p_2^2/2)=\frac{1}{2\pi}\int\limits_{-\infty}^{\infty}dt\exp(it(p_1^2-p_2^2)/2). \tag{57}$$

The difference $p_1^2-p_2^2$ in the exponent is replaced by

$$p_1^2-p_2^2=(\boldsymbol{p}_1+\boldsymbol{p}_2)(\boldsymbol{p}_1-\boldsymbol{p}_2)\approx 2\boldsymbol{k}(\boldsymbol{p}_1-\boldsymbol{p}_2). \tag{58}$$

After that expression (56) becomes

$$dw = d\Omega' k 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dt |\phi(t\boldsymbol{k})|^2, \tag{59}$$

where the representation

$$\phi(\boldsymbol{r}) = \langle \boldsymbol{r}|\phi\rangle = \int d^3p a(\boldsymbol{k}-\boldsymbol{p})\langle \boldsymbol{r}|\boldsymbol{p}\rangle = \int d^3p a(\boldsymbol{k}-\boldsymbol{p}) \exp(i\boldsymbol{p}\boldsymbol{r}) \tag{60}$$

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

If we choose the coordinate system with z-axis along $\boldsymbol{k}$, then (59) becomes identical to

$$dw = d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dz |\phi(0,0,z)|^2. \tag{61}$$

Since the wave packet ϕ is normalized to unity

$$\int d^3r |\phi(r)|^2 = 1, \tag{62}$$

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

$$d\sigma = \frac{dw}{J} = d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2, \tag{63}$$

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 (59) the scattering center crosses the wave packet of the scattered particle, and at the moment $t = 0$ it coincides with

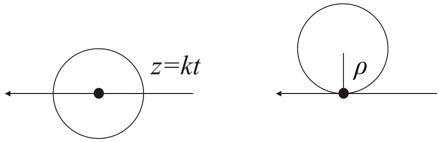

Figure 2: Position of scatterer at $t = 0$ with respect to wave packet of scattered particle. On the left hand side the packet center coincides with scatterer. Such a position is used in [1]. On the right hand side the position of the packet center is characterized by the impact parameter $\boldsymbol{\rho}$.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

the packet center [1], as is shown in fig. 2. Just because of that the expression contains $\phi(\boldsymbol{k}t)$:

$$\phi(\boldsymbol{k}t) = \langle \boldsymbol{r}|\phi\rangle|_{\boldsymbol{r}=\boldsymbol{k}t} = \int d^3pa(\boldsymbol{k}-\boldsymbol{p})\exp(i\boldsymbol{p}\boldsymbol{k}t). \tag{64}$$

instead of $\phi(\boldsymbol{r})$ (60).

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 (64) changes to

$$\phi(\boldsymbol{k}t+\boldsymbol{\rho}) = \int d^3pa(\boldsymbol{k}-\boldsymbol{p})\exp(i\boldsymbol{p}\boldsymbol{k}t + i\boldsymbol{p}\boldsymbol{\rho}), \tag{65}$$

and Eq-s (59) and (61) respectively take the form

$$dw(\boldsymbol{\rho}) = d\Omega' k 2\pi |T(\boldsymbol{p}',\boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dt|\phi(t\boldsymbol{k}+\boldsymbol{\rho})|^2, \tag{66}$$

$$dw(\boldsymbol{\rho}) = d\Omega' 2\pi |T(\boldsymbol{p}',\boldsymbol{k})|^2 \int\limits_{-\infty}^{\infty} dz|\phi(\rho_x,\rho_y,z)|^2. \tag{67}$$

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:

$$\begin{aligned} d\sigma &= \int d^2\rho dw(\boldsymbol{\rho}) = \\ &= d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2 \int_{-\infty}^{\infty} d^3 r |\phi(\boldsymbol{r})|^2 = \\ &= d\Omega' 2\pi |T(\boldsymbol{p}', \boldsymbol{k})|^2, \end{aligned} \tag{68}$$

where normalization condition (62) is used. The result completely coincides with (63) 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 sizes.

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 represented as Fourier expansion

$$\begin{aligned} \psi(\boldsymbol{k}, \boldsymbol{r}, s, t) &= G(s|\boldsymbol{r} - \boldsymbol{k}t|) \exp(i\boldsymbol{k}\boldsymbol{r} - i\omega(k)t) = \\ &= \int d^3p\, a(\boldsymbol{k}, \boldsymbol{p}) \exp[i\boldsymbol{p}\boldsymbol{r} - i\omega(\boldsymbol{p}, \boldsymbol{k})t], \end{aligned} \tag{69}$$

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 $\boldsymbol{k}\boldsymbol{p}$.

4.0.3 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

$$[\Delta + p^2] \exp(i\boldsymbol{p}\boldsymbol{r}) = 0. \tag{70}$$

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

$$[\Delta + p^2 - u(\boldsymbol{r})]\psi_p(\boldsymbol{r}) = 0 \tag{71}$$

containing $\exp(i\boldsymbol{pr})$ as the incident wave. Substitution into (69) transforms it to

$$\psi(\boldsymbol{k},\boldsymbol{r},t) = \int d^3p\, a(\boldsymbol{k},\boldsymbol{p})\psi_p(\boldsymbol{r})\exp[-i\omega(\boldsymbol{p},\boldsymbol{k})t]. \tag{72}$$

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

$$\psi_p(\boldsymbol{r}) = \exp(i\boldsymbol{p\rho})\int d\Omega f(\Omega)\exp(i\boldsymbol{p}_\Omega[\boldsymbol{r}-\boldsymbol{\rho}]), \tag{73}$$

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 (73) is of length p, but it is turned by angle Ω from $\boldsymbol{p}$. Substitution of (73) into (69) for $\exp(i\boldsymbol{pr})$ transforms (69) to the form

$$\begin{aligned}\psi(\boldsymbol{k},\boldsymbol{r},t) &= \int d^3p\, a(\boldsymbol{k},\boldsymbol{p})\exp(i\boldsymbol{p\rho})d\Omega f(\Omega)\times \\ &\times \exp[i\boldsymbol{p}_\Omega[\boldsymbol{r}-\boldsymbol{\rho}] - i\omega(\boldsymbol{p},\boldsymbol{k})t].\end{aligned} \tag{74}$$

Since $a(\boldsymbol{k},\boldsymbol{p})$, $\boldsymbol{p\rho}$ 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 $\boldsymbol{p}\to\boldsymbol{p}_\Omega$, and drop index Ω of $\boldsymbol{p}$. As a result we transform (74) to the form

$$\begin{aligned}\psi(\boldsymbol{k},\boldsymbol{r},t) &= \int d^3p\, a(\boldsymbol{k}_\Omega,\boldsymbol{p})\exp(i\boldsymbol{p\rho}_\Omega)d\Omega f(\Omega)\times \\ &\times \exp[i\boldsymbol{p}[\boldsymbol{r}-\boldsymbol{\rho}] - i\omega(\boldsymbol{p},\boldsymbol{k}_\Omega)t],\end{aligned} \tag{75}$$

which can be represented as

$$\psi(\boldsymbol{k},\boldsymbol{r},t)=\int d\Omega f(\Omega)\psi_0(\boldsymbol{k}_\Omega,\boldsymbol{r}-\boldsymbol{\rho}+\boldsymbol{\rho}_\Omega,t), \tag{76}$$

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 $dw=|f(\Omega)|^2d\Omega=|bk/2\pi|d\Omega$, 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 (28).

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 (28) this area is π/s^2. To show that the de Broglie singular wave packet (28) 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 (69), 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

$$\begin{aligned}\psi_G(\boldsymbol{r},\boldsymbol{k},t,s) &= \left(\frac{s}{\sqrt{\pi}(1+its^2)}\right)^{3/2} e^{i\boldsymbol{k}\boldsymbol{r}-ik^2t/2}\times\\ &\times \exp\left(-\frac{s^2[\boldsymbol{r}-\boldsymbol{k}t]^2}{2[1+its^2]}\right).\end{aligned} \tag{77}$$

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 (69).

Its Fourier components are

$$F_g(\boldsymbol{p},\boldsymbol{k},s)=\left(\frac{1}{2\pi s\sqrt{\pi}}\right)^{3/2}\exp(-(\boldsymbol{k}-\boldsymbol{p})^2/2s^2),\ \ \omega(\boldsymbol{p},\boldsymbol{k})=p^2/2, \tag{78}$$

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

$$\begin{aligned} A_G &= \int \pi\rho^2 d^3r|G(\boldsymbol{r},\boldsymbol{k},t,s)|^2 = \\ &= \int \rho^2 d^2\rho \tfrac{s^2}{1+t^2s^4}\exp\left(-\tfrac{s^2\rho^2}{1+t^2s^4}\right)=\pi\tfrac{1+t^2s^4}{s^2}. \end{aligned} \tag{79}$$

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]

$$\psi_{ns}(\boldsymbol{r},\boldsymbol{k},t,s)=\exp(i\boldsymbol{kr}-i\omega t)j_0(s|\boldsymbol{r}-\boldsymbol{v}t|). \tag{80}$$

in which $\omega_k=k^2/2+s^2/2$ and $\boldsymbol{v}=\boldsymbol{k}$ in units $\hbar^2/m=1$. The packet (80) is a spherical Bessel function $j_0(sr)\exp(-is^2t/2)$, which center is moving with the speed $\boldsymbol{v}$. This packet satisfy the free Schrödinger equation. Its Fourier components are

$$F(\boldsymbol{p},\boldsymbol{k},s)=F_{ns}(\boldsymbol{p},\boldsymbol{k},s)\propto\delta((\boldsymbol{k}-\boldsymbol{p})^2-s^2),\quad \omega(\boldsymbol{p},\boldsymbol{k})=p^2/2, \tag{81}$$

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]

$$\psi_{dB}(\boldsymbol{r},\boldsymbol{k},t,s) = C\exp(i\boldsymbol{kr}-i\omega t)\frac{\exp(-s|\boldsymbol{r}-\boldsymbol{v}t|)}{|\boldsymbol{r}-\boldsymbol{v}t|}, \tag{82}$$

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

$$\int d^3r|\psi(s,\boldsymbol{v},\boldsymbol{r},t)|^2 = 1. \tag{83}$$

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

$$\left[i\frac{\partial}{\partial t}+\frac{\Delta}{2}\right]\psi_{dB}(\boldsymbol{r},\boldsymbol{v},t,s) = -2\pi C e^{i(v^2+s^2)t/2}\delta(\boldsymbol{r}-\boldsymbol{v}t), \tag{84}$$

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

$$F(\boldsymbol{p},\boldsymbol{k},s) = F_{dB}(\boldsymbol{p},\boldsymbol{k}) = \sqrt{\frac{s}{2\pi}}\frac{4\pi}{(2\pi)^3}\frac{1}{(\boldsymbol{p}-\boldsymbol{k})^2+s^2}. \tag{85}$$

and

$$\omega(\boldsymbol{p},\boldsymbol{k}) = [2\boldsymbol{kp}-k^2-s^2]/2 = [p^2-(\boldsymbol{k}-\boldsymbol{p})^2-s^2]/2. \tag{86}$$

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 (85) and frequency (86) become the same as for spherical wave

$$\exp(-ik^2t/2)\frac{\exp(ikr)}{r} = \frac{4\pi}{(2\pi)^3}\int\exp(i\boldsymbol{pr})\frac{\exp(-ik^2t/2)\,d^3p}{p^2-k^2-i\epsilon}, \tag{87}$$

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

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

$$A_{dB} = \frac{s}{2\pi}\int_0^\infty 2dx\pi d\rho^2 \pi\rho^2 \frac{\exp(-2s\sqrt{\rho^2+x^2})}{\rho^2+x^2}. \tag{88}$$

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

$$\begin{aligned} A_{dB} &= 2\pi s \int_0^\infty dy d\rho \rho^2 \frac{\exp(-2s\rho\sqrt{1+y^2})}{1+y^2} = \\ &= \frac{\pi}{2s^2}\int_0^\infty \frac{dy}{(1+y^2)^{5/2}} = \frac{\pi}{3s^2}. \end{aligned} \tag{89}$$

4.1.4 Genesis of the singular de Broglie wave packet

The singular de Broglie wave packet descends from the spherical wave. Indeed, let's consider the spherical wave with energy $q^2/2$:

$$\psi(r,t,q) = \exp(-iq^2t/2)\frac{\exp(iqr)}{r}. \tag{90}$$

This wave satisfies inhomogeneous Schrödinger equation

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

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:

$$\begin{aligned} \psi(r,t,q) \to \Psi(\boldsymbol{r},\boldsymbol{k},t,q) &= \exp(i\boldsymbol{kr} - ik^2t/2 - iq^2t/2)\times \\ &\times \frac{\exp(iq|\boldsymbol{r}-\boldsymbol{k}t|)}{|\boldsymbol{r}-\boldsymbol{k}t|}. \end{aligned} \tag{92}$$

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

$$\left[i\frac{\partial}{\partial t} + \frac{\Delta}{2}\right]\Psi = -2\pi\exp(i[k^2-q^2]t/2)\delta(\boldsymbol{r}-\boldsymbol{k}t). \tag{93}$$

If the energy of the wave (90) is negative: $q^2 = -s^2$, i.e. the wave (90) describes a bound state around the center, then (92) becomes

$$\Psi(\boldsymbol{r}, \boldsymbol{k}, t, is) = \exp(i\boldsymbol{kr} - ik^2t/2 + is^2t/2)\frac{\exp(-s|\boldsymbol{r} - \boldsymbol{k}t|)}{|\boldsymbol{r} - \boldsymbol{k}t|}. \quad (94)$$

With normalization constant C expression (94) becomes identical to (82). 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

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

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

4.2 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 the 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)

$$dw(\boldsymbol{k}_i \to \boldsymbol{k}_f, t) = \frac{2\pi}{\hbar} \left|\langle \lambda_f, \boldsymbol{k}_f | V | \lambda_i, \boldsymbol{k}_i \rangle\right|^2 \rho(E_{fk}) \qquad (95)$$

   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

$$V = \frac{\hbar^2}{2m} 4\pi b \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2), \qquad (96)$$

   where $\boldsymbol{r}_1$, $\boldsymbol{r}_2$ are neutron and atom coordinates respectively, $\rho(E_{fk})$ is the density of final states of the neutron per unit energy E_{fk}:

$$\begin{aligned}
\rho(E_k) &= \left(\frac{L}{2\pi}\right)^3 \frac{d^3k}{dE_k} = \left(\frac{L}{2\pi}\right)^3 \frac{mkd\Omega_k}{\hbar^2}, \\
d^3k &= k^2 dk d\Omega_k, \qquad (97)\\
dE_k &= \frac{\hbar^2}{m} kdk,
\end{aligned}$$

$d\Omega_k$ is an element of the solid angle in $\boldsymbol{k}$-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

$$|\boldsymbol{k}_{i,f}> = \frac{1}{L^{3/2}} \exp(i\boldsymbol{k}_{i,f}\boldsymbol{r}). \qquad (98)$$

3. The expression (95) 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**

$$\begin{aligned}
\frac{d^2}{d\Omega_f dE_{fk}} w(\boldsymbol{k}_i \to \boldsymbol{k}_f, t) &= \frac{2\pi}{\hbar} \left|\langle \lambda_f, \boldsymbol{k}_f | V | \lambda_i, \boldsymbol{k}_i \rangle\right|^2 \times \\
&\times \left(\frac{L}{2\pi}\right)^3 \frac{mk}{\hbar^2} \delta(E_{fk} + E_{f\lambda} - E_{ik} - E_{i\lambda}), \qquad (99)
\end{aligned}$$

which after substitution of (96) becomes

$$\begin{aligned}
&\frac{d^2}{d\Omega_f dE_{fk}} w(\boldsymbol{k}_i \to \boldsymbol{k}_f, t) = \\
&= \frac{\hbar k_f}{mL^3} |b|^2 \left|\langle \lambda_f | \exp(i\boldsymbol{\kappa}\boldsymbol{r}) | \lambda_i \rangle\right|^2 \times \qquad (100)\\
&\times \delta(E_{fk} + E_{f\lambda} - E_{ik} - E_{i\lambda}),
\end{aligned}$$

where $\boldsymbol{\kappa} = \boldsymbol{k}_i - \boldsymbol{k}_f$ 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
$$\frac{d^2}{d\Omega_f dE_{fk}}\sigma(\boldsymbol{k}_i \to \boldsymbol{k}_f, \lambda_i \to \lambda_f) =$$
$$= |\langle\lambda_f|\exp(i\boldsymbol{\kappa}\boldsymbol{r})|\lambda_i\rangle|^2 \frac{k_f}{k_i}|b|^2 \times$$
$$\times\delta(E_{fk} + E_{f\lambda} - E_{ik} - E_{i\lambda}), \tag{101}$$
or a triple differential neutron cross section
$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i, \lambda_i \to \boldsymbol{k}_f, \lambda_f) =$$
$$= \frac{\hbar^2}{m}\frac{1}{k_i}|b|^2\,|\langle\lambda_f|\exp(i\boldsymbol{\kappa}\boldsymbol{r})|\lambda_i\rangle|^2 \times$$
$$\times\delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}) \tag{102}$$
for given initial and final states $|\lambda_{i,f} >$ of the scatterer.

5. After that we sum (102) over final states of the scatterer, average over its initial states and find
$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_1 \to \boldsymbol{k}_2, \mathcal{P}) =$$
$$= \frac{m}{\hbar^2 k_i}|b|^2 \sum_{\lambda_i,\lambda_f} \mathcal{P}(\lambda_i)\,|\langle\lambda_f|\exp(i\boldsymbol{\kappa}\boldsymbol{r})|\lambda_i\rangle|^2 \times$$
$$\times\delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}), \tag{103}$$
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 $\mathcal{M}(E_\lambda/k_BT)$, where T is temperature, and k_B is the Boltsman constant, then

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_1 \to \boldsymbol{k}_2, T) =$$

$$= \frac{m}{\hbar^2 k_i}|b|^2 \sum_{\lambda_i,\lambda_f} \mathcal{M}\left(\frac{E_{\lambda_i}}{k_BT}\right) |\langle\lambda_f| \exp(i\boldsymbol{\kappa r})|\lambda_i\rangle|^2 \times$$

$$\times\delta(E_{fk} + E_{\lambda_f} - E_{ik} - E_{\lambda_i}). \qquad (104)$$

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

$$\langle\lambda_f, \boldsymbol{k}_f|V|\lambda_i, \boldsymbol{k}_i\rangle = 4\pi b\frac{\hbar^2}{2m}\int\frac{d^3r}{L^6} \times$$

$$\times \exp(i[\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f]\boldsymbol{r}) =$$

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

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 (95) in the form

$$dw(i \to f) = \frac{(2\pi)^3\hbar k_f}{m}\frac{|b|^2}{L^6}\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)d\Omega_f. \qquad (105)$$

2. After steps 3 one obtains

$$\frac{d^2}{d\Omega_f dE_{fk}}w(\boldsymbol{k}_i \to \boldsymbol{k}_f, t) = \frac{\hbar k_f(2\pi)^3}{mL^6}|b|^2 \times$$

$$\times\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)\delta(E_{fk} + E_{fp} - E_{ik} - E_{ip}), \qquad (106)$$

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

$$\frac{d^2}{d\Omega_f dE_{fk}}\sigma(\boldsymbol{k}_i, \boldsymbol{p}_f \to \boldsymbol{k}_f, \boldsymbol{p}_i) = \frac{k_f}{k_i}\frac{(2\pi)^3}{L^3}|b|^2 \times \\ \times\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)\delta(E_{fk} + E_{fp} - E_{ik} - E_{ip}), \quad (107)$$

or the triple differential neutron cross section

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i, \boldsymbol{p}_i \to \boldsymbol{k}_f, \boldsymbol{p}_f) = \frac{(2\pi)^3}{L^3 k_i}|b|^2\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f) \times \\ \times\delta(k_f^2/2 + \mu p_f^2/2 - k_i^2/2 - \mu p_i^2/2), \quad (108)$$

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

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = \frac{2}{k_i}|b|^2\int \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f) d^3 p_f \times \\ \times\delta(k_f^2 + \mu p_f^2 - k_i^2 - \mu p_i^2)\mathcal{M}\left(\frac{\hbar^2 p_i^2}{2Mk_BT}\right) d^3 p_i. \quad (109)$$

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

$$\mathcal{M}\left(\frac{\mu p^2}{2T}\right) = \left(\frac{\mu}{2\pi T}\right)^{3/2}\exp\left(-\mu\frac{p^2}{2T}\right). \quad (110)$$

Substitution of it into (109) and integration over d^3p_f gives

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = \frac{1}{k_i}|b|^2 \int \delta(E_R - \omega + \mu\boldsymbol{\kappa}\boldsymbol{p}_i) \times$$

$$\times \left(\frac{\mu}{2\pi T}\right)^{3/2} \exp\left(-\mu\frac{p_i^2}{2T}\right) d^3p_i, \quad (111)$$

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^3p_i we get the triple differential cross section

$$\frac{d^3}{dk_f^3}\sigma(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = \frac{1}{\kappa k_i}|b|^2 \frac{1}{\sqrt{2\pi\mu T}} \exp\left(-\frac{(\omega - E_R)^2}{4E_R T}\right). \quad (112)$$

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

$$\sigma(k_i, T) = \frac{4\pi}{\sqrt{\pi E_r}} \frac{|b|^2}{(1+\mu)^2} \times$$

$$\times \left(\exp(-E_r) + \frac{\sqrt{\pi}}{2\sqrt{E_r}}(2E_r + 1)\Phi\left(\sqrt{E_r}\right)\right), \quad (113)$$

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

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

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

$$\left[i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\Delta_1-H'+V(\boldsymbol{r}_1,\boldsymbol{r}_2)\right]\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,t)=0, \qquad (114)$$

where interaction potential V is shown in (96). Solution of Eq. (114) 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,

$$\begin{aligned}\delta\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,t) &= \int G(\boldsymbol{r}_1,\boldsymbol{r}_2,t;\boldsymbol{r}_1',\boldsymbol{r}_2',t')V(\boldsymbol{r}_1',\boldsymbol{r}_2')\times \\ &\times \quad \psi_0(\boldsymbol{r}_1',\boldsymbol{r}_2',t')d^3r_1'd^3r_2'dt', \qquad (115)\end{aligned}$$

and G is the Green function of Eq. (114) without interaction

$$\begin{aligned}\left[i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\Delta_1-H'\right]G(\boldsymbol{r}_1,\boldsymbol{r}_2,t;\boldsymbol{r}_1',\boldsymbol{r}_2',t') &= \\ = -\delta(\boldsymbol{r}_1-\boldsymbol{r}_1')\delta(\boldsymbol{r}_2-\boldsymbol{r}_2')\delta(t-t'). \qquad (116)\end{aligned}$$

For the function before scattering we take

$$\psi_0(\boldsymbol{r}_1,\boldsymbol{r}_2,t)=\Phi_{\lambda_i}(\boldsymbol{r}_2)e^{-iE_{\lambda_i}t}e^{i\boldsymbol{k}_i\boldsymbol{r}_1-iE_{ik}t}, \qquad (117)$$

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

The Green function of the Eq. (114) without interaction is

$$\begin{aligned}G(\boldsymbol{r}_1-\boldsymbol{r}_1',\boldsymbol{r}_2-\boldsymbol{r}_2',t-t') &= \frac{1}{(2\pi)^4}\sum_{\lambda_f}\int e^{i\boldsymbol{k}_f\boldsymbol{r}_1-i\omega t}\Phi_{\lambda_f}(\boldsymbol{r}_2)\times \\ &\times\frac{d^3k_f d\omega}{E_{fk}+E_{\lambda_f}-\omega-i\epsilon}e^{-i\boldsymbol{k}_f\boldsymbol{r}_1'+i\omega t'}\Phi^*_{\lambda_f}(\boldsymbol{r}_2'), \qquad (118)\end{aligned}$$

which is easily checked by substitution of (118) into Eq. (116).

Substitution of (96), (118) and (117) into (115) gives

$$\delta\psi = \frac{1}{(2\pi)^4}\sum_{\lambda_f}\int e^{i\boldsymbol{k}_f\boldsymbol{r}_1 - i\omega t}\Phi_{\lambda_f}(\boldsymbol{r}_2)\frac{d^3k_f d\omega}{E_{fk}+E_{\lambda_f}-\omega-i\epsilon}\times$$
$$\times e^{-i\boldsymbol{k}_f\boldsymbol{r}'_1+i\omega t'}\Phi^*_{\lambda_f}(\boldsymbol{r}'_2)\frac{\hbar^2}{2m}4\pi b\delta(\boldsymbol{r}'_1-\boldsymbol{r}'_2)\Phi_{\lambda_i}(\boldsymbol{r}'_2)\times$$
$$\times\exp(-iE_{\lambda_i}t')\exp(i\boldsymbol{k}_i\boldsymbol{r}'_1-iE_{ik}t') =$$
$$= \frac{1}{(2\pi)^3}\sum_{\lambda_f}\int\frac{d^3k_f\Phi_{\lambda_f}(\boldsymbol{r}_2)\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle}{E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_i}-i\epsilon}\times$$
$$\times e^{i\boldsymbol{k}_f\boldsymbol{r}_1-i(E_{ik}+E_{\lambda_i})t}, \quad (119)$$

where

$$\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle = \frac{\hbar^2}{2m}4\pi b\int d^3r\Phi^*_{\lambda_f}(\boldsymbol{r})\exp(i\boldsymbol{\kappa}\boldsymbol{r})\Phi_{\lambda_i}(\boldsymbol{r}) \quad (120)$$

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

$$\lim_{t\to\infty}\frac{\exp(i(E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_i})t)}{E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_i}-i\epsilon} =$$
$$= 2\pi i\delta(E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_i}), \quad (121)$$

which upon substitution into (119) gives the asymptotical wave function

$$\delta\psi = \frac{i}{(2\pi)^2}\sum_{\lambda_f}\int d^3k_f\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle\times$$
$$\times\delta(E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_i})\times$$
$$\times\Phi_{\lambda_f}(\boldsymbol{r}_2)e^{-iE_{\lambda_f}t}e^{i\boldsymbol{k}_f\boldsymbol{r}_1-iE_{fk}t}. \quad (122)$$

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

$$df(\boldsymbol{k}_i,\lambda_i\to\boldsymbol{k}_f,\lambda_f) = \frac{id^3k_f}{(2\pi)^2}\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle\times$$

$$\times\delta(E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_i})=$$
$$=i\frac{m}{\hbar^2}\frac{k_f d\Omega_f}{(2\pi)^2}\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle, \tag{123}$$

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 (123) 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

$$dw(\boldsymbol{k}_i,\Omega_f,\lambda_i\to\lambda_f)=\frac{1}{(2\pi)^4}\left|\frac{m}{\hbar^2}\right|^2 k_f^2 d\Omega_f\left|\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle\right|^2. \tag{124}$$

If we replace

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

i.e. make transition reciprocal to (123), we obtain

$$dw(\boldsymbol{k}_i,\Omega_f,\lambda_i\to\lambda_f)=$$
$$=\frac{mk_f}{\hbar^2}\frac{d^3k_f}{(2\pi)^4}\left|\langle\lambda_f,\boldsymbol{k}_f|V|\lambda_i,\boldsymbol{k}_i\rangle\right|^2\times$$
$$\times\delta(E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_i}). \tag{125}$$

Substitution of the potential (96) gives

$$dw(\boldsymbol{k}_i,\Omega_f,\lambda_i\to\lambda_f)=$$
$$=|b|^2\frac{\hbar^2}{m}k_f\frac{d^3k_f}{(2\pi)^2}\left|\langle\lambda_f|\exp(i\boldsymbol{\kappa}\boldsymbol{r})|\lambda_i\rangle\right|^2\times$$
$$\times\delta(E_{fk}+E_{\lambda_f}-E_{ik}-E_{\lambda_f}). \tag{126}$$

To get the cross section we must multiply the probability by the wave front area A. We obtain an agreement with standard formula (108), if we suppose that $A=(2\pi)^2/k_ik_f$.

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 a 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:

$$\left[i\frac{\partial}{\partial t}+\frac{\Delta_1}{2}+\frac{\mu\Delta_2}{2}-\frac{u(\boldsymbol{r}_1-\boldsymbol{r}_2,t)}{2}\right]\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,t)=0, \tag{127}$$

where potential u is given in (96), $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, 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 (127) without interaction is

$$G(\boldsymbol{r}_1-\boldsymbol{r}_1',\boldsymbol{r}_2-\boldsymbol{r}_2',t-t')=$$
$$=\int\frac{\exp(i\boldsymbol{k}_f(\boldsymbol{r}_1-\boldsymbol{r}_1')+\boldsymbol{p}_f(\boldsymbol{r}_2-\boldsymbol{r}_2')-i\omega(t-t'))}{E_{fk}+E_{fp}-\omega-i\epsilon}\times$$
$$\times\frac{d^3k_fd^3p_fd\omega}{(2\pi)^7}, \tag{128}$$

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

The scattered part of the wave function is

$$\delta\psi=\frac{2\pi b}{(2\pi)^7}\int\frac{d^3k_fd^3p_fd\omega d^3r_1'd^3r_2'dt'}{E_{fk}+E_{fp}-\omega-i\epsilon}\exp(i\boldsymbol{k}_f(\boldsymbol{r}_1-\boldsymbol{r}_1')+$$
$$i\boldsymbol{p}_f(\boldsymbol{r}_2-\boldsymbol{r}_2')-i\omega(t-t'))\times$$
$$\times\delta(\boldsymbol{r}_1'-\boldsymbol{r}_2')\exp(i\boldsymbol{k}_i\boldsymbol{r}_1'+i\boldsymbol{p}_i\boldsymbol{r}_2'-i(E_{ik}+E_{ip})t')=$$

$$= \frac{b}{(2\pi)^2} \int \frac{d^3k_f d^3p_f \delta(\boldsymbol{k}_f + \boldsymbol{p}_f - \boldsymbol{k}_i - \boldsymbol{p}_i)}{E_{fk} + E_{fp} - E_{ik} - E_{ip} - i\epsilon} \times$$
$$\times \exp(i\boldsymbol{k}_f\boldsymbol{r}_1 + i\boldsymbol{p}_f\boldsymbol{r}_2 - i(E_{ik} + E_{ip})t), \quad (129)$$

where $\exp(i\boldsymbol{k}_i\boldsymbol{r}_1 - iE_{ik}t)$, $\exp(i\boldsymbol{p}_i\boldsymbol{r}_2 - iE_{ip}t)$ 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 (129) can be represented as a superposition of plane waves describing final states of the neutron, $\exp(i\boldsymbol{k}_f\boldsymbol{r}_1 - iE_{fk}t)$, and the atom, $\exp(i\boldsymbol{p}_f\boldsymbol{r}_2 - iE_{fp}t)$:

$$\delta\psi = \int \widetilde{f}(\boldsymbol{k}_i, \boldsymbol{p}_i \to \boldsymbol{k}_f, \boldsymbol{p}_f, t) d^3k_f d^3p_f \times$$
$$\times \exp(i\boldsymbol{k}_f\boldsymbol{r}_1 + i\boldsymbol{p}_f\boldsymbol{r}_2 - iE_{fk}t - iE_{fp}t),$$

where

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

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:

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

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

$$f(\boldsymbol{k}_i \to \boldsymbol{k}_f, \boldsymbol{p}_i) = d^3k_f \frac{ib}{\pi} \delta(k_f^2 + \mu(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f)^2 - k_i^2 - \mu p_i^2). \quad (130)$$

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.

Moreover, usually cross sections are averaged over initial states, but 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

$$k_f^2+\mu(\boldsymbol{k}_i+\boldsymbol{p}_i-\boldsymbol{k}_f)^2-k_i^2-\mu p_i^2=(1+\mu)\left(\boldsymbol{k}_f-\frac{\mu}{1+\mu}\boldsymbol{P}\right)^2-\frac{\boldsymbol{q}^2}{1+\mu}. \tag{131}$$

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

$$\boldsymbol{k}_{cm}=\boldsymbol{k}_f-\mu\boldsymbol{P}/(1+\mu), \tag{132}$$

and integration over dk_{cm} reduces (130) to

$$df(\boldsymbol{k}_i,\Omega_{cm},\boldsymbol{p}_i)=\frac{ibq}{2\pi(1+\mu)^2}d\Omega_{cm}. \tag{133}$$

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

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

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

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

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 (134) becomes

$$d\sigma(\boldsymbol{k}_i, \Omega_{cm}, \boldsymbol{p}_i = 0) = A \left| \frac{bk_i}{2\pi(1+\mu)^2} \right|^2 d\Omega_{cm} \qquad (136)$$

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

$$\sigma(k_i, \boldsymbol{p}_i = 0) = 4\pi A \left| \frac{bk_i}{2\pi(1+\mu)^2} \right|^2. \qquad (137)$$

Total cross section for scattering from monatomic gas To get cross section for scattering from monatomic gas at temperature T we must average (134) over $\boldsymbol{p}_i$ with Maxwellian distribution (110):

$$d\sigma(\boldsymbol{k}_i, \Omega_{cm}, T) = \int d^3p_i \mathcal{M}\left(\frac{\mu p_i^2}{2T}\right) A \left| \frac{bq}{2\pi(1+\mu)^2} \right|^2 d\Omega_{cm}. \qquad (138)$$

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

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

$$\times \exp\left(-\mu \frac{p_i^2}{2T}\right) (k_i^2 + \mu^2 p_i^2) = \qquad (139)$$

$$= 4\pi A \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 (2\mu T) \left(\frac{3}{2} + \frac{k_i^2}{2\mu T}\right). \qquad (140)$$

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 (135) 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

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

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

$$\sigma_{eff} = \frac{4\pi\alpha}{\pi^{3/2} k_r} \left| \frac{b}{2\pi(1+\mu)^2} \right|^2 \int p^2 dp d\Omega \exp(-p^2) \sqrt{(\boldsymbol{k}_r - \boldsymbol{p})^2}. \tag{141}$$

The integral at the right hand side is

$$I = \frac{4\pi}{3k_r} \int_0^\infty p dp \{[p(3k_r^2 + p^2)\Theta(p < k_r) + k_r[3p^2 + k_r^2] \times$$
$$\times \theta(p > k_r)\} \exp(-p^2) = \frac{2\pi}{3k_r} \times$$
$$\left(\int_0^{E_r} dp^2 [p(3k_r^2 + p^2) - k_r(3p^2 + k_r^2)] e^{-p^2} + \int_0^\infty dp^2 k_r [3p^2 + k_r^2] e^{-p^2} \right)$$
$$= \frac{\pi}{k_r} \left(k_r e^{-k_r^2} + \frac{\sqrt{\pi}}{2} [1 + 2k_r^2] \Phi(k_r) \right).$$

So cross section (141) 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 (113), 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 (112). For that we replace

$$d\Omega_q \to \frac{(1+\mu)^2}{q} d^3k_2\delta(k_f^2/2 + \mu(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f)^2/2 - k_i^2/2 - \mu p_i^2/2), \tag{142}$$

which means transition reciprocal to the one from (130) to (133). After this replacement we represent (136) in the form

$$d\sigma(k_i \to \boldsymbol{k}_f, \boldsymbol{p}_i) = Ad^3k_f \left|\frac{b}{2\pi(1+\mu)}\right|^2 \frac{\delta(E_R - \omega + \mu\boldsymbol{p}_i\boldsymbol{\kappa})}{\sqrt{(\boldsymbol{k}_i - \mu\boldsymbol{p}_i)^2}}, \tag{143}$$

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

$$d\sigma(k_i, \Omega_f, \boldsymbol{p}_i) = Ad^3k_f \left|\frac{b}{2\pi(1+\mu)}\right|^2 \times$$
$$\times \frac{(\mu\boldsymbol{P}\boldsymbol{n} \pm \sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2P^2 + (\boldsymbol{k}_i - \mu\boldsymbol{p}_i)^2})^2}{(1+\mu)\sqrt{(\boldsymbol{k}_i - \mu\boldsymbol{p}_i)^2}\sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2P^2 + (\boldsymbol{k}_i - \mu\boldsymbol{p}_i)^2}}, \tag{144}$$

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

$$dW_s(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = N_a\frac{d}{k_i}\alpha d^3k_f \left|\frac{b}{2\pi(1+\mu)}\right|^2 \times$$
$$\times \int d^3p \left(\frac{1}{2\pi\mu T}\right)^{3/2} e^{-p^2/2\mu T}\delta(E_R - \omega + \boldsymbol{p}\boldsymbol{\kappa}), \tag{145}$$

where $\boldsymbol{p} = \mu\boldsymbol{p}_i$, and we used (143). After integration over d^3p we obtain the cross section

$$d\sigma_{eff}(\boldsymbol{k}_i \to \boldsymbol{k}_f, T) = \frac{\alpha d^3k_f}{k_i\kappa\sqrt{2\pi\mu T}} \times$$

$$\times \left|\frac{b}{2\pi(1+\mu)}\right|^2 \exp\left(-\frac{(E_R-\omega)^2}{4E_RT}\right), \qquad (146)$$

identical to (112), if $\alpha = [2\pi(1+\mu)]^2$.

5.3 An alternative calculation. Catastrophe in quantum mechanics

Above we considered probability amplitude (133) calculated in center of mass coordinate system. It means that the argument of δ-function in (130) was represented in the form (131), and after change of variables (132) and integration over dk_{cm} we obtained (133), and the cross section (134). Transition from the cm system to laboratory one was performed with reciprocal transformation (142), which led to (143) and after integration over dk_f — to (144).

Now we proceed differently. We integrate (130) 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:

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

$$df(\boldsymbol{k}_i, \boldsymbol{\Omega}_f, \boldsymbol{p}_i) = \frac{ibd\Omega_f}{2\pi}\frac{k_f^2}{|k_f(1+\mu) - \mu\boldsymbol{n}\boldsymbol{P}|}, \qquad (147)$$

where

$$k_f = \frac{\mu\boldsymbol{P}\boldsymbol{n} \pm \sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2P^2 + (\boldsymbol{k}_i - \mu\boldsymbol{p}_i)^2}}{1+\mu} > 0, \qquad (148)$$

$\boldsymbol{P} = \boldsymbol{k}_i + \boldsymbol{p}_i$, and $\boldsymbol{n}$ is the unit vector pointing into direction $\boldsymbol{\Omega}_f$. With the help of amplitude (147) we obtain the scattering cross section

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

$$\times\frac{\left(\mu\boldsymbol{P}\boldsymbol{n} \pm \sqrt{\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2P^2 + (\boldsymbol{k}_i - \mu\boldsymbol{p}_i)^2}\right)^4}{|\mu^2(\boldsymbol{P}\boldsymbol{n})^2 - \mu^2P^2 + (\boldsymbol{k}_i - \mu\boldsymbol{p}_i)^2|}. \qquad (149)$$

Now we can make transformation

$$d\Omega\frac{\left|\mu\boldsymbol{Pn}\pm\sqrt{\mu^2(\boldsymbol{Pn})^2-\mu^2P^2+(\boldsymbol{k}_i-\mu\boldsymbol{p}_i)^2}\right|^2}{2(1+\mu)^2\sqrt{\mu^2(\boldsymbol{Pn})^2-\mu^2P^2+(\boldsymbol{k}_i-\mu\boldsymbol{p}_i)^2}}= \\ =d^3k_f\delta(k_f^2+\mu(\boldsymbol{k}_i+\boldsymbol{p}_i-\boldsymbol{k}_f)^2-k_i^2-\mu p_i^2), \qquad (150)$$

which is reciprocal to the one, used in (147), then we obtain

$$d\sigma(\boldsymbol{k}_i\to\boldsymbol{k}_f,\boldsymbol{p}_i)=Ad^3k_fk_f^2\left|\frac{b}{2\pi}\right|^2\times \\ \times\frac{\delta(E_R-\omega+\mu\boldsymbol{\kappa}\boldsymbol{p}_i)}{\sqrt{\mu^2(\boldsymbol{Pn})^2-\mu^2P^2+(\boldsymbol{k}_i-\mu\boldsymbol{p}_i)^2}}. \qquad (151)$$

We can replace $\sqrt{\mu^2(\boldsymbol{Pn})^2-\mu^2P^2+(\boldsymbol{k}_i-\mu\boldsymbol{p}_i)^2}$ in denominator by $|(1+\mu)k_f-\mu\boldsymbol{Pn}|$, multiply it by k_f, replace $\boldsymbol{p}_i\boldsymbol{k}_f$ by $\boldsymbol{p}_i\boldsymbol{k}_i-\boldsymbol{p}_i\boldsymbol{\kappa}$, 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. (151) becomes

$$d\sigma(\boldsymbol{k}_i\to\boldsymbol{k}_f,\boldsymbol{p}_i)=Ad^3k_fk_f^3\left|\frac{b}{2\pi}\right|^2\frac{\delta(E_R-\omega+\mu\boldsymbol{\kappa}\boldsymbol{p}_i)}{|s-\mu\omega-\mu\boldsymbol{k}_i\boldsymbol{p}_i|}, \qquad (152)$$

where $s=k_i^2/2+k_f^2/2$. We see, that this expression strongly differs from (143). If we substitute $A=\alpha/q^2$, introduce number $\nu(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ 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

$$d\sigma_{eff}(\boldsymbol{k}_i,\to\boldsymbol{k}_f,T)=\frac{\alpha}{k_i}d^3k_fk_f^3\left|\frac{b}{2\pi}\right|^2\int\mathcal{P}(\boldsymbol{p}_i)d^3p_i\times \\ \times\frac{\delta(E_R-\omega+\mu\boldsymbol{\kappa}\boldsymbol{p}_i)}{|\boldsymbol{k}_i-\mu\boldsymbol{p}_i||s-\mu\omega-\mu\boldsymbol{k}_i\boldsymbol{p}_i|}. \qquad (153)$$

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 (153) becomes

$$d\sigma_{eff}(\boldsymbol{k}_i,\to\boldsymbol{k}_f,p_i=0)=\frac{\alpha}{k_i^2}d^3k_fk_f^3\left|\frac{b}{2\pi}\right|^2\frac{\delta(E_R-\omega)}{s-\mu\omega}. \qquad (154)$$

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

$$d\sigma_{eff}(k_i,\to k_f,p_i=0) = \frac{2\pi\alpha}{\mu k_i^3}k_f^4dk_f\left|\frac{b}{2\pi}\right|^2\times \times\frac{\Theta(|\mu s-\omega|<\mu k_ik_f)}{s-\mu\omega}. \quad (155)$$

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

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

$$= 4\pi\alpha\left|\frac{b}{2\pi(1+\mu)^2}\right|^2\left(\frac{8}{3}\mu^2+\frac{(1-\mu^2)^{3/2}}{\mu}\arctan\left(\frac{\mu}{\sqrt{1-\mu^2}}\right)\right), \quad (156)$$

where $\gamma = (1-\mu)/(1+\mu)$. This expression differs from (137), 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 (110) into (153) gives

$$d\sigma_{eff}(\boldsymbol{k}_i,\to\boldsymbol{k}_f,T) = \frac{\alpha}{k_i}d^3k_fk_f^3\left|\frac{b}{2\pi}\right|^2\int\left(\frac{\mu}{2\pi T}\right)^{3/2}\times \times exp\left(-\mu\frac{p_i^2}{2T}\right)d^3p_i\frac{\delta(E_R-\omega+\mu\boldsymbol{\kappa}\boldsymbol{p}_i)}{|\boldsymbol{k}_i-\mu\boldsymbol{p}_i||s-\mu\omega-\mu\boldsymbol{k}_i\boldsymbol{p}_i|}. \quad (157)$$

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

$$d\sigma_{eff}(\boldsymbol{k}_i, \to \boldsymbol{k}_f, T) = \frac{\alpha d^3k_f}{\kappa k_i\sqrt{2\pi\mu T}}\left|\frac{b}{2\pi}\right|^2 \times \\ \times \exp\left(-\frac{(\omega - E_R)^2}{4E_R T}\right) F(\kappa^2, \omega, s), \quad (158)$$

which has an additional factor $F(\kappa^2, \omega, s)$ comparing to (112):

$$F(\kappa^2, \omega, s) = k_f^3 \int \frac{d^2p_\perp}{2\pi\mu T}\exp\left(-\frac{p_\perp^2}{2\mu T}\right)\frac{1}{|\boldsymbol{k}_i - \boldsymbol{p}||s - \mu\omega - \boldsymbol{k}_i\boldsymbol{p}|}. \quad (159)$$

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

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

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

$$\begin{aligned}(\boldsymbol{k}_i - \boldsymbol{p})^2 &= \tfrac{(\omega+\kappa^2/2-\omega+E_R)^2}{\kappa^2} + (\boldsymbol{k}_\perp - \boldsymbol{p}_\perp)^2 = \\ &= \tfrac{1}{4}\kappa^2(1+\mu)^2 + (\boldsymbol{k}_\perp - \boldsymbol{p}_\perp)^2,\end{aligned} \quad (160)$$

and

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

Substitution into (159) and change of variables $\boldsymbol{q} = \boldsymbol{p}_\perp - \boldsymbol{k}_\perp$ gives

$$F(\kappa^2, \omega, s) = \int \frac{d^2q}{2\pi\mu T}\exp\left(-\frac{(\boldsymbol{q} + \boldsymbol{k}_\perp)^2}{2\mu T}\right) \times \\ \times \frac{4k_f^3}{\sqrt{\kappa^2(1+\mu)^2 + 4q^2}|(\omega + \kappa^2/2)(1+\mu) + 2\boldsymbol{k}_\perp\boldsymbol{q}|}. \quad (161)$$

It is easy to see that this integral diverges at the point $2\boldsymbol{k}_\perp\boldsymbol{q} = -(\omega + \kappa^2/2)(1+\mu)$. 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.

5.3.3 A way to solve the contradiction

Our contradiction arises because of the continuous spectrum of angular distribution

$$\psi_s = \int_{2\pi} f(\Omega) d\Omega \exp(i\boldsymbol{k}_\Omega \boldsymbol{r}). \tag{162}$$

No contradiction would appear, if the angular distribution were discrete. It suggests an idea to replace the integral in (162) with the integral sum

$$\psi_s = \sum_{j=1}^{N} f(\Omega_j)\delta\Omega_j \exp(i\boldsymbol{k}_{\Omega_j}\boldsymbol{r}) = \sum_{j=1}^{N} F_j \exp(i\boldsymbol{k}_{\Omega_j}\boldsymbol{r}), \tag{163}$$

where discrete amplitudes $F_j = f(\Omega_j)\delta\Omega_j$ are introduced. In such a representation the probability of scattering into the angle Ω_j is $|F_j|^2$, and probability of scattering into the angular interval covering $2n$ elements $j_1 - n \le j \le j_1 + n$ around some direction Ω_{j1}, is

$$dw_n(\Omega_{j1}) = \sum_{j=j_1-n}^{j_1+n} |F_j|^2 \approx W_{j1}\Delta\Omega,$$

where we denoted

$$\Delta\Omega = \sum_{j=j_1-n}^{j_1+n} \delta\Omega_j \approx 2n\delta\Omega_{j1}, \qquad W_{j1} = |f(\Omega_{j1})|^2 \delta\Omega_{j1},$$

and supposed that W_j are almost constant in the interval $j_1 - n \le j \le j_1 + n$.

Transformation of the integral to the sum can be made with arbitrary choice of Ω_j and $\delta\Omega_j$. So we can make a step in style of quantization, i.e. we can require all the amplitude elements $F_j = f(\Omega_j)\delta\Omega_j$ to be equal, which means that we introduce a quantum of the area $\int_{\delta\Omega} f(\Omega)d\Omega$. In the center of mass reference frame, where $f(\Omega)$ is constant, such a requirement means an introduction of quantum of the angular interval or uncertainty $\delta\Omega$. Below we discuss what value this quantum can be of.

When we transform from one reference frame to the other, we see a deformation of both $f(\Omega)$ and $\delta\Omega$, however the amplitude elements $F(\Omega) = f(\Omega)\delta\Omega$ and the number of such elements in the whole integral $\int_{4\pi} f(\Omega)d\Omega$ remain the same. Therefore, if we take some amount of amplitude elements in the center of mass reference frame, square every element, and after that transform to the laboratory reference frame, then we obtain the same amount of the squared elements in the laboratory frame, and they will be confined in some angular interval. If we transform from center of mass to laboratory frame without squaring the amplitude elements, and square them only after the transformation, we obtain the same number of squared elements in the same angular interval as before. Which means that our result is completely invariant under Galilean transformation. Therefore we have the full right to use center of mass reference frame without a danger to get an ambiguous result after changing of the reference frame.

5.3.4 A value of the scattering amplitude quantum

According to (133) we have

$$f(\Omega_{cm}) = \frac{ibq}{2\pi(1+\mu)^2}. \tag{164}$$

Therefore the scattering amplitude element is

$$F(\Omega_{cm}) = \frac{ibq}{2\pi(1+\mu)^2}\delta\Omega. \tag{165}$$

Probability of scattering into some interval of solid angle $\Delta\Omega = n\delta\Omega$ is

$$\Delta w = n|F(\Omega_{cm})|^2 = \left(\left|\frac{bq}{2\pi(1+\mu)^2}\right|^2 \delta\Omega\right)\Delta\Omega, \tag{166}$$

the differential scattering cross section becomes

$$\frac{d\sigma}{d\Omega} = \frac{\Delta w}{\Delta\Omega}A = \left|\frac{bq}{2\pi(1+\mu)^2}\right|^2 A\delta\Omega, \tag{167}$$

and we immediately obtain that to get $d\sigma/d\Omega = |b|^2/(1+\mu)^2$, we must put

$$\left|\frac{q}{2\pi(1+\mu)}\right|^2 A\delta\Omega = 1. \tag{168}$$

It means that the angular quantum $\delta\Omega$ correlates with the wave packet cross area A! This correlation is very important because it even solves one another contradiction.

5.3.5 The contradiction related to ultracold neutrons anomaly

Ultracold neutrons (UCN) are the neutrons, which can be stored in closed bottles. Their energy is less than the optical potential of the bottle walls, and they are totally reflected from the walls at any incidence angle, because their reflection coefficient is equal to unity:

$$|R|^2 = \left|\frac{k_\perp - i\sqrt{u_0 - k_\perp^2}}{k_\perp + i\sqrt{u_0 - k_\perp^2}}\right|^2 = 1. \tag{169}$$

However (169) is valid only for real potentials $u_0 = 4\pi N_0 b$, i.e. real scattering amplitudes b. The amplitude $b = b' - ib''$ is a complex number, which always contains a negative imaginary part $b'' = k\sigma_l/4\pi$, where σ_l is loss cross section, which includes absorption, σ_a, and inelastic scattering, σ_{inel}, cross sections. Therefore the reflection coefficient $|R|^2$ is always less than unity by amount

$$\mu = 1 - |R|^2 = 2\frac{b''}{b'}\frac{k_\perp}{\sqrt{u_0 - k_\perp^2}}, \tag{170}$$

which is called loss coefficient, where b' is real part of the scattering amplitude.

Measurement of the storage time of the UCN in closed vessels had shown that the loss coefficient can be two orders of magnitude larger than the theoretically predicted one. This discrepancy was labelled "UCN anomaly", and all the attempts to explain it were unsuccessful. At last a hypothesis was proposed that the neutron is described by a wave packet [4], which in the Fourier decomposition contains waves with such wave vectors $\boldsymbol{p}$, that $p^2 > u_0$. These waves can overcome the potential barrier of the vessel walls. The fraction of such waves in the wave packet spectrum determines the probability of UCN penetration through the walls. To explain the anomaly it was necessary to suppose that the wave packet is sufficiently large, i.e. its area A in the case of UCN is of the order of 1 mm^2. The dimensions of faster neutrons can decrease with energy according to the formula $A = \alpha\lambda^2$, however the parameter α, which is of the order of $\approx 10^9$, should be constant.

Above we used expression (26) for the cross section: $\sigma = Aw$, where probability of scattering w is approximately $|b|^2/\lambda^2$. To get agreement with the cross section $\sigma = 4\pi|b|^2$, we must accept that $A \approx \lambda^2$, i.e. $\alpha \approx 1$. It contradicts to $\alpha \approx 10^9$. Of course, we can suppose that it is the product $|b|^2\alpha$, which we call $|b|^2$. So $|b|^2 = |\tilde{b}|^2\alpha$. However, then in the case of large α we have small $\tilde{b} \ll b$, and since $\tilde{b}$ determines the height of the optical potential, this potential becomes many order of magnitude lower than experimentally observed one. Thus we have a contradiction between dimensions of the neutron wave packet and the height of the optical potential.

However now, when we found that the scattering probability contains the angular quantum $\delta\Omega$, and this quantum can be very small, the above contradiction becomes resolved. Now the cross section contains the product of the large parameter A and the small parameter $\delta\Omega$, and they can compensate each other.

6 Conclusion

Simple consideration of a scattering process 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, which resolves this contradiction, creates another one. With this approach we can calculate only dimensionless probabilities of scattering, while for interpretation of experiments we need cross sections with dimensions of area. To resolve this second contradiction and to get cross sections instead of dimensionless probabilities, we are to introduce some front area of the wave function for the incident particle. Thus we arrive at wave packets, and must describe scattering process with wave packets instead of plane waves. However, while doing that we arrive at the third contradiction: the wave packets scatter alike plane waves, and scattering does not depend on whether the scatterer crosses the wave packet or not. This contradiction is a result of linearity of the quantum mechanics. To resolve the third contradiction we must introduce a nonlinearity to assure that scattering takes place only when the scatterer is inside the front area of the wave packet. However, even with this hypothesis in mind, we have the fourth contradiction: the probability of scattering is an ambiguous value, which depends on a way of calculation. To resolve this fourth contradiction we are to quantize the process of scattering. This quantization leads to substitution of angular integrals with discrete integral sums. It is amazing that resolution of the fourth contradiction simultaneously resolves the fifth contradiction, which relates dimensions of neutron wave packets with the height of the optical potential of materials. The last result proves that a valuable truth is contained in our investigations.

Acknowledgement

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6.1 History of submissions and rejections

It is very difficult to publish something critical with respect to existing paradigm. So, may be it will be of interest for history of science to report my attempts.

6.1.1 Rejection from Phys.Lett.A

On July 15, after more than 4 months I received at last the final rejection from Phys.Lett.A:

Dear Dr Ignatovich,

On 09-Mar-2004 you submitted a new paper number to Physics Letters A entitled:

'Dramatic problems of Scattering Theory'

We regret to inform you that your paper has not been accepted for publication. Comments from the editor are:

I apologize for the delay in writing to you about your paper.

Despite my considerable efforts I have been unable to elicit any referee reports on your article and at this stage I do not think I am going to receive any reviews. In the circumstances and to save you losing further time I believe it would be in your interests if you submitted your article to another journal.

Thank you for submitting your work to our journal and I wish you luck in publishing it elsewhere.

Yours sincerely,

J.P. Vigier Editor Physics Letters A

6.1.2 Submission and rejection from Phys.Rev.A

Since no referee report was sent to me during 2.5 months from Phys. Lett.A, I decided to send a more short and concise version to another journal. On May 23 of 2004 I submitted to Phys.Rev. A, because "The journal contains articles on quantum mechanics..." (citation from http://librarians.aps.org/jnldesc.pdf). In my covering letter, I did not propose any referee, but asked not to reject the paper at the level of an associated editor. After 2 weeks I received the rejection

Reply 09.06.2004 Dear Dr. Ignatovich,

We regret to inform you that, in view of the subject matter, your manuscript is not considered suitable for publication in Physical Review. A paper of this nature belongs in a journal on mathematical physics or on foundation concepts. It has pedagogical interest but does not meet the current criterion for Physical Review of research that substantially advances the field.

Yours sincerely,

Lee A. Collins Associate Editor Physical Review A

6.1.3 Submission and rejection from Russian Nuclear Physics (YaF)

On 10 June the same short version was submitted to YaF. On 23 August I received the referee report:

In his paper V.Ignatovich claims that the standard scattering theory contradicts to principles of the nonrelativistic quantum mechanics. This claim is based on a misunderstanding. The motion of the center of mass does not influence the scattering dynamics, so the problem is reduced to scattering of a single particle on a given potential. This process is studied in full details and widely discussed in literature. See, for example, the books [1] and [2] cited by the author. Transition to the laboratory frame is also well known. See, for example, volumes I and II of the Theoretical physics course by Landau and Lifshits for nonrelativistic and relativistic cases respectively. Consistency of the nonrelativistic scattering theory is easily checked in the first order of the perturbation theory (Fermi "Golden" rule). This has been also proven mathematically rigorously. See, for example, the book by K.Hepp and A.Epshtein, "Analytical properties of scattering amplitudes in local quantum field theory" and references therein.

Taking into account all said above, I consider that the paper "Catastrophe..." by V.Ignatovich should not to be published in YaF.

My reply Dear editors.

I received the referee report, but I regret that it is not a report on my paper. The referee listed well known thesises but said nothing about the contradiction formulated on the very first page of my paper. He did not want or could not read it. So, his judgement and verdict "Not to publish" is absolutely unfounded. I don't know even what to reply to him. Yours sincerely, V.Ignatovich.

Decision of the editorial board on October 01 of 2004 Dear author, your paper together with referee report was considered at the editorial board Council. We regret to communicate to you, that the editorial board had to decide to reject your paper in solidarity with the referee opinion.

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