E4-2001-42

V.K.Ignatovich

APOCRYPHA OF STANDARD SCATTERING THEORY (SST) AND QUANTUM MECHANICS OF THE DE BROGLIE WAVE PACKET

1 Introduction

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

The simplest process is elastic s-wave scattering on a fixed center, which is 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.

We found that the SST is inconsistent with principles of QM. Thus we need to improve it. However, it is so widely applied and trusted that our claim looks like an Apocrypha to the Holy Bible. We recognize that, but we are faithful to the Holy spirit of knowledge and will serve it even at the menace of Crusiphication.

To prove that (1) is not consistent with SQM, we need to remind the principles of SQM.

1.1 Canons of the SQM

According to QM, if a system has eigen states ψ_n, its initial state is ψ_i, and scattering is described by $\delta\psi$, then to find results of scattering we need to expand $\delta\psi$ over eigen states, i.e. represent the total wave function in the form

$$\psi = \psi_i + \sum_f a_{if}\psi_f. \tag{2}$$

The probability of scattering from the state ψ_i to state ψ_f is described by dimensionless magnitudes $w_{if} = |a_{if}|^2$. In expression (2) for simplicity we used summation as if the particle had a discrete spectrum, however it is not essential, and we can (and shall) deal also with continuous spectra.

Let us show that (1) contradicts these principles.

1.2 The sin of the SST

What do we do in SST? Eigen states of a particle are described by plane waves $\exp(i\boldsymbol{kr})$, and the scattered wave function $\delta\psi$ after, say, elastic s-wave scattering, is described by the spherical wave, $\delta\psi \propto \exp(ikr)/r$, which is not an eigen state, and even it is not a solution of the homogeneous Schrödinger equation, because

$$[\Delta + k^2]\frac{\exp(ikr)}{r} = -4\pi\delta(\boldsymbol{r}), \tag{3}$$

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

According to principles of SQM we must represent the scattered wave function as a superposition of plane waves:

$$\psi = \exp(i\boldsymbol{kr}) - \int f(\Omega)d\Omega \exp(i\boldsymbol{k}_\Omega \boldsymbol{r}), \tag{4}$$

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

$$dw(\Omega) = |f(\Omega)|^2 d\Omega, \tag{5}$$

and total probability of scattering is the dimensionless integral

$$\int dw(\Omega) = \int |f(\Omega)|^2 d\Omega.$$

In the next section we show rigorous derivation of scattering probabilities, find the probability for elastic and inelastic scattering of neutrons on a fixed and moving center. Calculate scattering on an ideal monoatomic gas, and show how to calculate inelastic scattering on other systems.

We shall show that rigorous derivation leads to some problems. The main problem is met when we attempt to calculate transmission of a sample. With dimensionless probabilities we cannot introduce cross section, and for that reason need to introduce area of the sample or an area of the neutron wave front. However, if the neutron wave front has limited area, its wave function cannot be a plane wave, and we arrive to notion of a wave packet. This wave packet must not spread, because otherwise we should observe dependence of transmission on distance of sample from a source, and we did not do yet.

This consideration leads us very naturally to the de Broglie wave packet (dBWP), for which we show, how to calculate reflection and transmission of a one dimensional potential barrier. We justify correctness of such a calculation comparing it to the same for a well known spherical wave, which can be considered as a particular case of the dBWP.

At the end we formulate the problems which should be solved for development of full quantum mechanics for dBWP.

The paper contains Appendix, where detailed calculations are given for neutron scattering on monoatomic gas.

2 Treatment of the SST

Now we shall show how to improve the SST and to obtain the dimensionless probability of elastic scattering. First we shall do it with the help of standard stationary scattering theory. It is not satisfactory, however it is instructive because it gives the same result as the more rigorous nonstationary approach.

2.1 Simplest, but not satisfactory treatment

The formula (1) can be improved immediately, if we use Fourier expansion for the spherical wave:

$$\frac{\exp(ikr)}{r} = \frac{i}{2\pi}\int \exp(i\boldsymbol{p}_{||}\boldsymbol{r} + ip_z|z|)\frac{d^2p_{||}}{p_z}, \tag{6}$$

where $p_z = \sqrt{k^2 - p_{||}^2}$. Every plane wave $\psi_p(\boldsymbol{r})$ under the integral satisfies the homogeneous Schrödinger equation (HSE)

$$[\Delta + k^2]\psi_p(\boldsymbol{r}) = 0$$

everywhere except one point $z = 0$. However, not all $\psi_p(\boldsymbol{r})$ are plane waves. Since integration in (6) extends over all $p_{||}$, there are such $p_{||}^2 > k^2$ under the integral, for which magnitude of the component p_z is imaginary, and the wave $\psi_p(\boldsymbol{r})$ exponentially decays away from $z = 0$. If we neglect exponentially decaying waves and limit integration in (6) only to $p_{||}^2 \le k^2$, then the integral in (6) can be transformed as follows

$$\frac{i}{2\pi}\int_{p_{||}^2<k^2} e^{i\boldsymbol{p}_{||}\boldsymbol{r}+ip_z|z|}\frac{d^2p_{||}}{p_z} = \frac{i}{2\pi}\int e^{i\boldsymbol{p}\boldsymbol{r}}2d^3p\delta(p^2-k^2) = \frac{ik}{2\pi}\int e^{i\boldsymbol{k}_\Omega\boldsymbol{r}}d\Omega, \tag{7}$$

where k_Ω is a vector of length k, pointing into direction of solid angle Ω.

If we substitute (7) into (6) and subsequently into (1), we obtain (4) with

$$f(\Omega) = \frac{ibk}{2\pi} = \frac{ib}{\lambda} \to \int d\Omega|f(\Omega)|^2 = 4\pi\frac{b^2}{\lambda^2}, \tag{8}$$

where $\lambda = 2\pi/k$ is the neutron wave length. We see that, indeed, the total scattering probability is determined by dimensionless magnitude.

Of course, such a simple derivation is not satisfactory because it is not rigorous at many points. We decided to show it only because to our surprise it gives the same result as the more rigorous derivation presented in the next subsection.

2.2 The rigorous derivation of (4) for elastic s-wave scattering

Now we shall show a derivation which will be rigorous and appropriate for all the processes: elastic and inelastic ones. In this approach we shall see that scattering is a nonstationary process.

Suppose we have a single scattering center described by the potential

$$\frac{u(\boldsymbol{r},t)}{2}=2\pi b\delta(\boldsymbol{r}-\boldsymbol{r}_0).$$

In the following we shall use the units, for which $\hbar^2/m=1$, where m is the neutron mass.

For scattering particle we use nonstationary HSE

$$\left[i\frac{\partial}{\partial t}+\frac{\Delta}{2}-\frac{u(\boldsymbol{r},t)}{2}\right]\psi(\boldsymbol{r},t)=0. \qquad (9)$$

Solution of (9) can be represented in the form

$$\psi(\boldsymbol{r},t)=\psi_0(\boldsymbol{r},t)-\delta\psi(\boldsymbol{r},t), \qquad (10)$$

where $\psi_0(\boldsymbol{r},t)$ denotes an incident wave $\psi_0(\boldsymbol{r},t)=\exp(i\boldsymbol{k}_0\boldsymbol{r}-i\omega_0 t)$ with $\omega_0=k_0^2/2$.

Substitution of (10) into (9) gives equation for $\delta\psi(\boldsymbol{r},t)$. Its solution in the first order of perturbation theory is

$$\delta\psi(\boldsymbol{r},t)=\int d^3r'dt'G(\boldsymbol{r}-\boldsymbol{r}',t-t')2\pi b\delta(\boldsymbol{r}'-\boldsymbol{r}_0)\psi_0(\boldsymbol{r}',t'), \qquad (11)$$

where G is the Green function, which can be represented as the Fourier expansion

$$G(\boldsymbol{r}-\boldsymbol{r}',t-t')=\frac{1}{(2\pi)^4}\int\frac{d^3pd\omega}{p^2/2-\omega-i\epsilon}\exp(i\boldsymbol{p}[\boldsymbol{r}-\boldsymbol{r}']-i\omega[t-t']). \quad (12)$$

The Green function is a solution of the equation

$$\left[i\frac{\partial}{\partial t}+\frac{\Delta}{2}\right]G(\boldsymbol{r}-\boldsymbol{r}',t-t')=-\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t'). \qquad (13)$$

Substitution of (12) into (11) gives

$$\delta\psi(\boldsymbol{r},t)=\frac{2\pi b}{(2\pi)^4}\int\frac{d^3pd\omega d^3r'dt'}{p^2/2-\omega-i\epsilon}e^{i\boldsymbol{p}[\boldsymbol{r}-\boldsymbol{r}']-i\omega[t-t']}\delta(\boldsymbol{r}'-\boldsymbol{r}_0)e^{i\boldsymbol{k}_0\boldsymbol{r}'-i\omega_0 t'}=$$

$$= \frac{b}{(2\pi)^2}\int \frac{d^3p\exp(i\boldsymbol{q}\boldsymbol{r}_0)}{\omega_p-\omega_0-i\epsilon}\exp(i\boldsymbol{p}\boldsymbol{r}-i\omega_0 t), \qquad \boldsymbol{q}=\boldsymbol{k}_0-\boldsymbol{p}, \quad \omega_p = p^2/2. \tag{14}$$

We can add and subtract $i\omega_p t$ in the exponent, and represent the field (14) as a superposition of plane waves

$$\delta\psi = \int f(\boldsymbol{p})\exp(i\boldsymbol{p}\boldsymbol{r}-i\omega_p t)d^3p, \tag{15}$$

with amplitudes

$$f(\boldsymbol{p}) = \frac{b}{(2\pi)^2}\frac{\exp(i[\omega_p-\omega_0]t)}{\omega_p-\omega_0-i\epsilon}\exp(i\boldsymbol{q}\boldsymbol{r}_0). \tag{16}$$

Now we use the following relation

$$\frac{\exp(i[\omega_p-\omega_0]t)}{\omega_p-\omega_0-i\epsilon} = i\int\limits_{-\infty}^{t}\exp(i[\omega_p-\omega_0]t')dt', \tag{17}$$

which is the main trick of our apocrypha. This relation is absolutely rigorous and shows that all the scattering processes are nonstationary ones. We can find a definite result of scattering only in the limit $t\to\infty$, where relation (17) gives the law of energy conservation:

$$i\lim_{t\to\infty}\int\limits_{-\infty}^{t}\exp(i[\omega_p-\omega_0]t')dt' = 2\pi i\delta(\omega_p-\omega_0) = 4\pi i\delta(p^2-k^2). \tag{18}$$

Substitution of (18) into (16) and (15) gives

$$\delta\psi = \int\frac{ib}{\pi}e^{i\boldsymbol{q}\boldsymbol{r}_0}e^{i\boldsymbol{p}\boldsymbol{r}-i\omega_p t}d^3p\delta(p^2-k_0^2) = \frac{ibk}{2\pi}\int\limits_{4\pi}e^{i\boldsymbol{q}\boldsymbol{r}_0}d\Omega e^{i\boldsymbol{k}_\Omega\boldsymbol{r}-i\omega_p t}, \tag{19}$$

from which it follows that probability amplitude of scattering is

$$f(\Omega) = \frac{ibk}{2\pi}\exp(i\boldsymbol{q}\boldsymbol{r}_0), \tag{20}$$

and the total probability of scattering $w=4\pi|b/\lambda|^2$ is the same as above in (8).

The result (20) immediately shows that scattering by a set of scatterers is described by dimensionless amplitude

$$f(\Omega) = \sum_j\frac{ib_j}{\lambda}\exp(i\boldsymbol{q}\boldsymbol{r}_j), \tag{21}$$

from which we can define coherent part

$$f_{coh}(\Omega) = < f(\Omega) > = \frac{i}{\lambda}\sum_j b_{j,coh}\exp(i\boldsymbol{q}\boldsymbol{r}_j) = \frac{iF(\boldsymbol{q})}{\lambda}, \tag{22}$$

where $F(\boldsymbol{q})$ is structure factor, and $< g >$ means averaging over isotopes or spin states of the scatterers.

Now we can define coherent and incoherent scattering probabilities

$$dw_{coh}(\Omega) = \left|\frac{F(\boldsymbol{q})}{\lambda}\right|^2, \quad dw_{inc}(\Omega) = < |f(\Omega)|^2 > = \sum_j \left|\frac{b_{j,inc}}{\lambda}\right|^2. \tag{23}$$

2.3 An important "defect" of the dimensionless scattering probability

The above result discloses a very interesting fact: with dimensionless probability we cannot define transmission of a sample as in SST!

Indeed, extinction of a plane wave depends on total number of scatterers met along its way. The total number of scatterers in a sample of thickness d and cross area S is N_0dS, where N_0 is density of the scatterers. Thus transmission exponent, which in SST is

$$T = \exp(-N_0\sigma d), \tag{24}$$

where σ is scattering cross section, now becomes

$$T = \exp(-N_0wSd), \tag{25}$$

where w is probability of scattering. However this expression would mean that the larger is cross area S of the sample, the larger is extinction. It is evident that such a conclusion is not supported by experiments. Thus we should conclude that the area S in (25) is not cross area of the sample, but the front area of the incident particle, and we inevitably arrive at a conclusion that the particle cannot be an infinite plane wave. It should have a restricted front area, which means that the particle wave function is a wave packet.

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

If front area S is proportional to λ^2: $S = \alpha^2\lambda^2$, where α^2 is a dimensionless factor, then transmission T becomes

$$T = \exp(-4\pi\alpha^2|b|^2N_0d), \tag{26}$$

which is the same as in SST, but the amplitude b is renormalized to $b' = \alpha b$.

The best candidate for the nonspreading wave packet is the singular de Broglie wave packet (dBWP) [2, 3, 4]

$$\psi_{dB}(\boldsymbol{r},t) = \sqrt{\frac{s}{2\pi}}\exp(i\boldsymbol{kr} - i\omega t)\frac{\exp(-s|\boldsymbol{r}-\boldsymbol{v}t|}{|\boldsymbol{r}-\boldsymbol{v}t|}, \tag{27}$$

where $\omega = [k^2 - s^2]/2$, s determines the packet width, and $\boldsymbol{v}$ in our units coincide with $\boldsymbol{k}$. The front area of (27) can be estimated as $S_{dB} = \pi/s^2$. If, for example, s is proportional to k: $s = \xi k = 2\pi\xi/\lambda$, then $S_{dB} = \pi\lambda^2/(2\pi\xi)^2$, and the renormalization factor is $\alpha = 1/2\sqrt{\pi}\xi$.

3 Inelastic processes

3.1 Scattering on a free moving atom

Collision of two particles changes the state of both. Thus, to be correct, we need to solve SE not for a single neutron but for both particles:

$$\left[i\frac{\partial}{\partial t} + \frac{\Delta_1}{2} + \frac{\mu\Delta_2}{2} - \frac{u(\boldsymbol{r}_1-\boldsymbol{r}_2,t)}{2}\right]\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,t) = 0, \tag{28}$$

where $u(\boldsymbol{r}_1-\boldsymbol{r}_2) = 4\pi b\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$, $\mu = m/M$, $\boldsymbol{r}_1$ is the neutron coordinate, and $\boldsymbol{r}_2$ is the one of the nucleus.

The Green function of the equation (28) is

$$G(\boldsymbol{r}_1,\boldsymbol{r}_2,t) = \int \frac{\exp(i\boldsymbol{p}_1\boldsymbol{r}_1 + \boldsymbol{p}_2\boldsymbol{r}_2 - i\omega t)}{p_1^2/2 + \mu p_2^2/2 - \omega - i\epsilon}\frac{d^3p_1d^3p_2d\omega}{(2\pi)^7}, \tag{29}$$

from which it follows that

$$\delta\psi = \frac{2\pi b}{(2\pi)^7}\int\frac{d^3p_1d^3p_2d\omega d^3r_1'd^3r_2'dt'}{p_1^2/2 + \mu p_2^2/2 - \omega - i\epsilon}\exp(i\boldsymbol{p}_1[\boldsymbol{r}_1-\boldsymbol{r}_1'] + i\boldsymbol{p}_2[\boldsymbol{r}_2-\boldsymbol{r}_2'] - i\omega[t-t'])$$

$$\times\delta(\boldsymbol{r}_1'-\boldsymbol{r}_2')\exp(i\boldsymbol{k}_1\boldsymbol{r}_1' + i\boldsymbol{k}_2\boldsymbol{r}_2' - i[\omega_{10}+\omega_{20}]t') =$$

$$= \frac{b}{(2\pi)^2}\int\frac{d^3p_1d^3p_2\delta(\boldsymbol{p}_1+\boldsymbol{p}_2-\boldsymbol{k}_1-\boldsymbol{k}_2)}{p_1^2/2 + \mu p_2^2/2 - \omega_{10} - \omega_{20} - i\epsilon}\exp(i\boldsymbol{p}_1\boldsymbol{r}_1 + i\boldsymbol{p}_2\boldsymbol{r}_2 - i[\omega_{10}+\omega_{20}]t), \tag{30}$$

where $\omega_{10} = k_1^2/2$, and $\omega_{20} = \mu k_2^2/2$.

This wave function can be represented as a superposition of plane waves describing final states of the neutron and nucleus

$$\delta\psi = \int f(\boldsymbol{p}_1,\boldsymbol{p}_2,t)d^3p_1d^3p_2\exp(i\boldsymbol{p}_1\boldsymbol{r}_1 + i\boldsymbol{p}_2\boldsymbol{r}_2 - i\omega_1 t - i\omega_2 t),$$

where $\omega_1 = p_1^2/2$, $\omega_2 = \mu p_2^2/2$, and

$$f(\boldsymbol{p}_1, \boldsymbol{p}_2, t) = \frac{b}{(2\pi)^2} \frac{\delta(\boldsymbol{p}_1 + \boldsymbol{p}_2 - \boldsymbol{k}_1 - \boldsymbol{k}_2)}{\omega_1 + \omega_2 - \omega_{10} - \omega_{20} - i\epsilon} \exp(i[\omega_1 + \omega_2 - \omega_{10} - \omega_{20}]t).$$

Using the same trick as in (17) we find the probability amplitude for the particle to leave in the state $\boldsymbol{p}_1$, and for the atom to leave in the state $\boldsymbol{p}_2$ is $dF(\boldsymbol{k}_1 \to \boldsymbol{p}_1, \boldsymbol{k}_2 \to \boldsymbol{p}_2) =$

$$f(\boldsymbol{p}_1, \boldsymbol{p}_2) d^3p_1 d^3p_2 = d^3p_1 d^3p_2 \frac{ib}{2\pi} \delta(\boldsymbol{p}_1 + \boldsymbol{p}_2 - \boldsymbol{k}_1 - \boldsymbol{k}_2) \delta(\omega_1 + \omega_2 - \omega_{10} - \omega_{20}) =$$

$$d^3p_1 \frac{ib}{\pi} \delta(p_1^2 + \mu(\boldsymbol{k}_1 + \boldsymbol{k}_2 - p_1)^2 - k_1^2 - \mu k_2^2) = d^3p_1 \frac{ib}{\pi} \delta(\mu\kappa^2 - k_1^2 + p_1^2 + 2\mu\boldsymbol{\kappa}\boldsymbol{k}_2), \tag{31}$$

where $\boldsymbol{\kappa} = \boldsymbol{k}_1 - \boldsymbol{p}_1$.

Change of variables $\boldsymbol{p}_1 \to \boldsymbol{\kappa}$ transforms (31) to

$$d^3\kappa \frac{ib}{\pi} \delta(\mu\kappa^2 - k_1^2 + (\boldsymbol{k}_1 - \boldsymbol{\kappa})^2 + 2\mu\boldsymbol{\kappa}\boldsymbol{k}_2), \tag{32}$$

and subsequent change

$$\boldsymbol{\kappa} + \frac{\mu\boldsymbol{k}_2 - \boldsymbol{k}_1}{1 + \mu} = \boldsymbol{q}, \tag{33}$$

transforms (32) to

$$dF(\boldsymbol{k}_1 \to \boldsymbol{p}_1, \boldsymbol{k}_2 \to \boldsymbol{p}_2) = \frac{ib}{\pi} d^3q \delta\left(q^2(1 + \mu) - \frac{(\boldsymbol{k}_1 - \mu\boldsymbol{k}_2)^2}{1 + \mu}\right) = \frac{ibq d\Omega_q}{2\pi(1 + \mu)}, \tag{34}$$

where $q = |\boldsymbol{k}_1 - \mu\boldsymbol{k}_2|/(1 + \mu) = |\boldsymbol{\xi}|/(1 + \mu)$, and $\boldsymbol{\xi} = \boldsymbol{k}_1 - \mu\boldsymbol{k}_2$ is the relative velocity.

In laboratory reference frame differential probability of scattering into the element of solid angle $d\Omega_q$ is accompanied with change of absolute magnitude of the neutron momentum $k_1 \to p_1$, and to find probability of total scattering we need to find ratio of fluxes in all the directions to the incident flux. In other words probability of total scattering on a nucleus with the given momentum $\boldsymbol{k}_2$ is

$$w = \frac{b^2 q^2}{4\pi^2(1 + \mu)^2} \int \frac{p_1}{k_1} d\Omega_q = \frac{b^2}{4\pi^2(1 + \mu)^4 k_1} \xi^2 \int p_1 d\Omega_q. \tag{35}$$

3.1.1 Total scattering

To get total scattering we should integrate over Ω_q. According to (33)

$$p_1 = \frac{|\boldsymbol{\xi} + \mu \boldsymbol{P}|}{1+\mu} = \frac{1}{1+\mu}\sqrt{\xi^2 + \mu^2 P^2 + 2\mu\xi P \cos\vartheta_\xi},$$

where $\boldsymbol{P} = \boldsymbol{k}_1 + \boldsymbol{k}_2$, and we substituted $\boldsymbol{q} = \boldsymbol{\xi}/(1+\mu)$, $\Omega_q \equiv \Omega_\xi$.

Substitution of p_1 into (35) gives

$$\int p_1 d\Omega_q = \frac{2\pi}{3\mu(1+\mu)\xi P}[|\xi + \mu P|^3 - |\xi - \mu P|^3] =$$

$$\frac{4\pi}{3P\mu(1+\mu)}[\xi^2 + 3\mu^2 P^2]\Theta(\xi < \mu P) + \frac{4\pi}{3\xi(1+\mu)}[3\xi^2 + \mu^2 P^2]\Theta(\xi > \mu P), \tag{36}$$

where $\Theta(x)$ is a step function equal to 1 or 0, when inequality in its argument is satisfied or not, respectively.

Now, probability of total scattering for given $\boldsymbol{k}_2$ is $w =$

$$\frac{b^2\xi}{3\pi(1+\mu)^5 k_1}\left\{\frac{\xi}{P\mu}[\xi^2 + 3\mu^2 P^2]\Theta(\xi < \mu P) + [3\xi^2 + \mu^2 P^2]\Theta(\xi > \mu P)\right\}, \tag{37}$$

and we need to average it over distribution $M(\mu k_2^2/2T)d^3k_2$ of momentum $\boldsymbol{k}_2$ of initial nucleus. If the nucleus is initially at rest, then distribution is $M = \delta(\boldsymbol{k}_2)$, which gives $k_2 = 0$, $\xi = P = k_1$, $\xi > \mu P$ and

$$< w >= \frac{b^2 k_1^2 (1 + \mu^2/3)}{\pi(1+\mu)^5}. \tag{38}$$

For Maxwellian distribution we have:

$$< w >= C\int M\left(\frac{\mu k_2^2}{2T}\right) k_2^2 dk_2 \int d\cos\vartheta_{k2} \times$$

$$\left\{\frac{\xi^2}{P\mu}[\xi^2 + 3\mu^2 P^2]\Theta(\xi < \mu P) + \xi[3\xi^2 + \mu^2 P^2]\Theta(\xi > \mu P)\right\}. \tag{39}$$

where

$$C = \frac{2b^2}{3(1+\mu)^5 k_1}, \qquad M\left(\frac{\mu k_2^2}{2T}\right) = \left(\frac{\mu}{2\pi T}\right)^{3/2} \exp\left(-\frac{\mu k_2^2}{2T}\right), \tag{40}$$

and at $T = 0$ expression (39) must be reduced to (38).

Calculation of the integral (39) is done analytically in Appendix A. The result (118) is a complicated function of two dimensionless parameters: $\mu = m/M$ and $\tau = T/E_1$, where T is temperature, and E_1 is the incident neutron energy.

The dependence on τ in the range $0.1 \leq \tau \leq 10$ for $\mu = 0.25$, which corresponds to ^{4}He gas, is presented in fig. 1. For comparison here also the dependence of scattering cross section of standard scattering theory [1] is presented:

$$\sigma = 4\pi\frac{b^2}{(1+\mu)^2}\left(\exp(-1/\mu\tau)\sqrt{\frac{\mu\tau}{\pi}} + \left[1+\frac{\mu\tau}{2}\right]\Phi(\sqrt{1/\mu\tau})\right). \qquad (41)$$

Of course, we cannot compare dimensionless probability with dimensional cross section, so we imagine some extinction by a thin sample, and for convenience normalized two curves to the same magnitude at $\tau = 2$.

Asymptotic behavior of (41) and (118) are different. At large τ the expression (41) gives

$$\sigma = 4\pi\frac{b^2}{(1+\mu)^2}2\sqrt{\frac{\mu\tau}{\pi}}, \qquad (42)$$

and for small τ it gives

$$\sigma = 4\pi\frac{b^2}{(1+\mu)^2},$$

whereas the expression (118) have asymptotics (119) and (120) which for large τ grows more steep than (42). It is very interesting to check the result (118), and even, if it will be found to contradict experimental data, it will mean that the whole quantum theory needs some revision.

3.1.2 Partial scattering

We can also find scattering with given energy. For that we represent (35) in the form

$$dw = \frac{b^2}{2\pi^2(1+\mu)^2}\frac{p_1}{k_1}|\boldsymbol{k}_1 - \mu\boldsymbol{k}_2|d^3q\delta\left((1+\mu)q^2 - \frac{(\boldsymbol{k}_1-\mu\boldsymbol{k}_2)^2}{1+\mu}\right) =$$

$$\frac{b^2}{4\pi^2(1+\mu)^2}\frac{p_1}{k_1}|\boldsymbol{k}_1 - \mu\boldsymbol{k}_2|d^3p_1\delta(\mu\kappa^2/2 - \omega + \mu\boldsymbol{k}_2\boldsymbol{\kappa}), \qquad (43)$$

where $\omega = (k_1^2 - p_1^2)/2$, $\boldsymbol{\kappa} = \boldsymbol{k}_1 - \boldsymbol{p}_1$. If we represent d^3p_1 as $p_1 d(p_1^2/2)d\Omega_{p1}$, then we can define

$$\frac{d^2w}{dE_{p1}d\Omega_{p1}} = \frac{b^2}{4\pi^2(1+\mu)^2}\frac{p_1^2}{k_1}|\boldsymbol{k}_1 - \mu\boldsymbol{k}_2|\delta(\mu\kappa^2/2 - \omega + \mu\boldsymbol{k}_2\boldsymbol{\kappa}). \qquad (44)$$

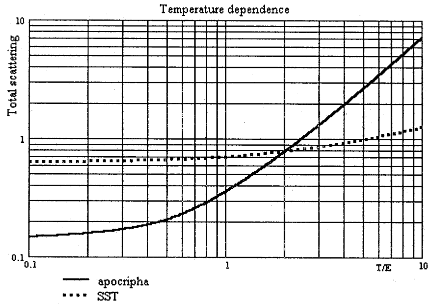

Figure 1: Total scattering probability as an extinction of a beam by a thin sample of ^{4}He gas ($\mu = m/M = 0.25$) in dependence on ratio of temperature T to the incident neutron energy E. The curve for standard scattering theory is plotted according to (41). The curve for apocrypha is plotted according to (118). For comparison the two curves are normalized to the same magnitude at $T/E = 2$

Now we must average this expression over distribution of $\boldsymbol{k}_2$. For Maxwellian one we have

$$< \frac{d^2w}{dE_{p1}d\Omega_{p1}} >= \int M\left(\frac{\mu k_2^2}{2T}\right)\frac{b^2d^3k_2|\boldsymbol{k}_1-\mu\boldsymbol{k}_2|}{4\pi^2(1+\mu)^2}\frac{p_1^2}{k_1}\delta(\mu\kappa^2/2-\omega+\mu\boldsymbol{k}_2\boldsymbol{\kappa}). \tag{45}$$

It is a complicated integral, because it depends on angles between $\boldsymbol{k}_2$ and $\boldsymbol{\kappa}$, and also between $\boldsymbol{k}_2$ and $\boldsymbol{k}_1$. For some particular cases it can be represented analytically, but we shall not do it here.

3.1.3 Dull rules of SST

It is useful to compare our approach with that of the standard textbooks. Let us follow, for instance, the book [1] from the very beginning, where elementary theory of scattering is explained, and no correlation functions introduced yet. We can find a list of rules one must to follow to put down an expression for cross section.

1. According to Fermi golden rule one defines a probability of scattering from state $|\boldsymbol{k}_i>$ to state $|\boldsymbol{k}_f>$ in a unit time

$$w(i\to f) = 2\pi|<\boldsymbol{k}_f|V|\boldsymbol{k}_i>|^2, \quad |\boldsymbol{k}_{i,f}>= \frac{1}{L^{3/2}}\exp(i\boldsymbol{k}_{i,f}\boldsymbol{r}), \tag{46}$$

   where V is interaction potential, $<\boldsymbol{k}_f|V|\boldsymbol{k}_i>$ is matrix element of scattering, L is some dimension of a space cell, and the law of energy conservation is assumed.

2. Then we multiply (46) by

$$\delta(E_f - E_i),$$

3. by number of final states

$$\frac{L^3 d^3 k_f}{(2\pi)^3},$$

4. and divide by the incident flux

$$\frac{k_i}{L^3}.$$

5. After that we sum over final states of scatterer, average over initial state of scatterer and find $d\sigma/d\Omega_f dE_f$.

Let us see how it works for gases.

Atoms are also described by plane waves $L^{-3/2}\exp(i\boldsymbol{p}_{if}\boldsymbol{r})$, and the matrix element is

$$4\pi b \int \frac{d^3r}{L^6} \exp(i[\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f]\boldsymbol{r}) = \frac{4\pi b}{L^6}(2\pi)^3 \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f).$$

The square of this matrix element, according to step 1, gives the square of δ-function, which is transformed as follows: $\delta^2 = [L^3/(2\pi)^3]\delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)$, after which we have

$$w(i \to f) = 2\pi \frac{|4\pi b|^2}{L^9}(2\pi)^3 \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f).$$

After steps 2, 3 and 4 we have

$$d\sigma = 2\pi \frac{|4\pi b|^2}{k_i L^3} \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)\delta(E_{ki} + E_{pi} - E_{kf} - E_{pf}) d^3 k_f,$$

where $E_k = k^2/2$, and $E_p = \mu p^2/2$. The number of final states of scatterer is $L^3 d^3 p_f/(2\pi)^3$, and averaging is done over the same Maxwellian distribution as above. So, after step 5 we have $d^2\sigma/dE_{kf}d\Omega_{kf} =$

$$|b|^2 \frac{k_f}{k_i} \int d^3 p_f \delta(\boldsymbol{k}_i + \boldsymbol{p}_i - \boldsymbol{k}_f - \boldsymbol{p}_f)\delta(E_{ki} + E_{pi} - E_{kf} - E_{pf}) M\left(\frac{\mu p_i^2}{2T}\right) d^3 p_i.$$

The total scattering cross section we obtain immediately:

$$\sigma = 2|b|^2 \frac{1}{k_i} d^3 k_f \delta(k_f^2 + \mu(\boldsymbol{P} - k_f)^2 - k_i^2 - \mu p_i^2) M\left(\frac{\mu p_i^2}{2T}\right) d^3 p_i.$$

It can be easily integrated over d^3k_f as above and we obtain

$$\sigma = \frac{4\pi|b|^2}{(1+\mu)^2}\frac{|\boldsymbol{k}_i - \mu\boldsymbol{p}_i|}{k_i}M\left(\frac{\mu p_i^2}{2T}\right)d^3p_i.$$

After integration over p_i we obtain the above expression (41).

Along this derivation we made several artificial steps. First, it was introduction of the space cell L^3, second, it was a strange rule to replace square of δ-function, third, we did not introduce the outgoing flux, though we divide by incoming flux, and the last, it was a strange rule to introduce the law of energy conservation only at the final stage of cross section calculation. Sometimes it is introduced at the stage of evaluation of matrix elements, but then we obtain a square of this delta function and need to replace it with $2\pi t\delta$, where some time cell t is introduced, and consequent division by it gives a rate of the scattering process.

In short, everything is artificial and has no relation to quantum mechanics. We are dealing with some rules invented by somebody, and have no firm theoretical grounds under them. Even if we have good agreement between these rules and experiment, we need to understand why do these rules work. The good agreement of these rules with experiment tells nothing about validity of standard quantum mechanics.

3.1.4 Inelastic scattering on an arbitrary system

To show that this approach can be used for more complicated processes let us consider neutron interaction with an arbitrary system described by Hamiltonian H', which, for simplicity, is assumed to have a discrete spectrum E_i. The Schrödinger equation for the full system is

$$\left[i\frac{\partial}{\partial t} + \frac{\Delta}{2} - H' + \frac{u(\boldsymbol{r}_1 - \boldsymbol{r}_2, t)}{2}\right]\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = 0, \tag{47}$$

where $u(\boldsymbol{r}_1 - \boldsymbol{r}_2) = 4\pi b\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$, the coordinate $\boldsymbol{r}_1$ is related to neutron, and $\boldsymbol{r}_2$ is related to the scattering system.

A stationary solution without interaction is described by

$$\Psi_{n,k}(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = \Phi_n(\boldsymbol{r}_2)\exp(i\boldsymbol{k}\boldsymbol{r}_1 - i[E_k + E_n]t), \tag{48}$$

where $\Phi_n(\boldsymbol{r})$ and E_n are eigen functions and eigen values of the Hamiltonian H', and $E_k = k^2/2$ is the neutron energy.

The Green function of the equation (47) without interaction is

$$G(\boldsymbol{r}_1 - \boldsymbol{r}_1', \boldsymbol{r}_2, \boldsymbol{r}_2', t) = \sum_n \int \frac{\exp(i\boldsymbol{p}[\boldsymbol{r}_1 - \boldsymbol{r}_1'] - i\omega t)\Phi_n(\boldsymbol{r}_2)\Phi_n^*(\boldsymbol{r}_2')}{E_p + E_n - \omega - i\epsilon}\frac{d^3p\,d\omega}{(2\pi)^4}, \tag{49}$$

and scattering in perturbation theory is described by

$$\delta\psi = \frac{2\pi b}{(2\pi)^4}\sum_n\int\frac{d^3pd\omega d^3r_1'd^3r_2'dt'}{E_p+E_n-\omega-i\epsilon}\exp(i\boldsymbol{p}_1[\boldsymbol{r}_1-\boldsymbol{r}_1']-i\omega[t-t'])\Phi_n(\boldsymbol{r}_2)\Phi^*(\boldsymbol{r}_2')$$

$$\times\delta(\boldsymbol{r}_1'-\boldsymbol{r}_2')\Phi_{n_0}(\boldsymbol{r}_2')\exp(i\boldsymbol{k}\boldsymbol{r}_1'-i[E_k+E_{n_0}]t') =$$

$$= \frac{b}{(2\pi)^2}\sum_n\int\frac{d^3pM_{n,n_0}(\boldsymbol{k}-\boldsymbol{p})}{E_p+E_n-E_k-E_{n_0}-i\epsilon}\exp(i\boldsymbol{p}\boldsymbol{r}_1-i[E_k+E_{n_0}]t), \qquad (50)$$

where

$$M_{n,n_0}(\boldsymbol{q}) = \int d^3r\Phi_{n_0}(\boldsymbol{r})\exp(i\boldsymbol{q}\boldsymbol{r})\Phi_n^*(\boldsymbol{r}) \qquad (51)$$

is a matrix element of the interaction.

It is evident that the scattered function is representable in the form

$$\delta\psi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \sum_n\int f_{n,n_0}(\boldsymbol{p},\boldsymbol{k},t)d^3p\Phi_n(\boldsymbol{r}_2)\exp(i\boldsymbol{p}\boldsymbol{r}_1-iE_pt-iE_nt),$$

and the probability amplitude to find the particle in a state $\boldsymbol{p}$, and the system in the state E_n is

$$dF(\boldsymbol{k}\to\boldsymbol{p},n_0\to n,t) = f_{n,n_0,t}(\boldsymbol{p},\boldsymbol{k})d^3p.$$

Thus

$$dF(\boldsymbol{k}\to\boldsymbol{p},n_0\to n,t) = \frac{bd^3p_1}{(2\pi)^2}M_{n,n_0}(\boldsymbol{k}-\boldsymbol{p})\frac{\exp(i[E_p+E_n-E_k-E_{n_0}]t)}{E_p+E_n-E_k-E_{n_0}-i\epsilon}.$$

This result is representable in the form

$$dF(\boldsymbol{k}\to\boldsymbol{p},n_0\to n,t) = \frac{ibd^3p}{(2\pi)^2}M_{n,n_0}(\boldsymbol{k}-\boldsymbol{p})\int\limits_{-\infty}^{t}\exp(i[E_p+E_n-E_k-E_{n_0}]t'),$$

and in the limit $t\to\infty$, we obtain $dF(\boldsymbol{k}\to\boldsymbol{p},n_0\to n) =$

$$d^3p\frac{ib}{2\pi}M_{n,n_0}(\boldsymbol{k}-\boldsymbol{p})\delta(E_p+E_n-E_k-E_{n_0}) = pd\Omega\frac{ib}{2\pi}M_{n,n_0}(\boldsymbol{k}-\boldsymbol{p}), \qquad (52)$$

where $p=\sqrt{k^2+2(E_{n_0}-E_n)}$, and in the last equality we integrated over dp.

From (52) it follows that the differential probability of scattering is equal to $dW(\boldsymbol{k}\to\boldsymbol{p},n_0\to n)/d\Omega =$

$$\left|\frac{dF(\boldsymbol{k}\to\boldsymbol{p},n_0\to n)}{d\Omega}\right|^2\frac{p(\Omega)}{k} = \left|\frac{b}{\lambda_p}M_{n,n0}(\boldsymbol{k}-\boldsymbol{p})\right|^2\frac{p(\Omega)}{k}, \qquad (53)$$

where we introduced the ratio p/k of particle fluxes after and before scattering.

To get total probability of scattering we must sum (53) over all possible states n, average over n_0, and integrate over $d\Omega$:

$$W(\boldsymbol{k}\to\boldsymbol{p})=\int d\Omega\sum_n\left\langle\left|\frac{dW(\boldsymbol{k}\to\boldsymbol{p},n_0\to n)}{d\Omega}\right|^2\right\rangle_{n0}=$$

$$\int d\Omega\sum_n\left|\frac{b}{\lambda_p}\right|^2\frac{p(\Omega)}{k}<|M_{n,n0}(\boldsymbol{k}-\boldsymbol{p})|^2>_{n0}. \tag{54}$$

where $< f >_n = \sum_n f(n)\rho(n)$, $\rho(n)$ is corresponding distribution density, and $\lambda_p = 2\pi/p$.

3.1.5 Some remarks

Again, we obtain a dimensionless probability, and need to define front area of the incident particle wave function, which leads naturally to dBWP. We also need to point out that the considerations with an arbitrary system above are valid only if both systems are described with the same Schrödinger equation. However this equation has a single derivative on time. If an interesting for us system obeys a different equation with double derivative on time, we need to consider not the Schrödinger but different equation. What to do in this case will be considered in a next paper.

4 Introduction to quantum mechanics of the de Broglie wave packet

Now we see that the dBWP naturally appears in a rigorous theory of scattering, however from the very start we should confess that there are no quantum mechanics of the de Broglie wave packet (dBWP) yet. We have some hints, some ideas, which seem to be interesting, and give a new life to the de Broglie hypothesis advanced almost at the birth days of quantum mechanics (QM). He himself abandoned his hypothesis, because not he not anybody till recent times could tell, what can one do with such a construction. Only recently the dBWP was revived, and it happened because standard quantum mechanics was not able to explain a phenomenon, which is known as ultracold neutrons (UCN) anomaly - two orders of magnitude higher losses of UCN at a single collision with the wall, than is predicted by the standard QM. After its resurrection, however, it became clear, that dBWP deserves its own life independent of UCN anomaly.

The dBWP is described by the function (27)

$$\psi_{dB}(\boldsymbol{r},\boldsymbol{k},s,t)=\sqrt{\frac{s}{2\pi}}\exp(i\boldsymbol{kr}-i\omega t)\frac{\exp(-s|\boldsymbol{r}-\boldsymbol{v}t|)}{|\boldsymbol{r}-\boldsymbol{v}t|}. \tag{55}$$

It contains two parameters: the wave vector $\boldsymbol{k}$ related to velocity $\boldsymbol{v}$: $\boldsymbol{k}=m\boldsymbol{v}/\hbar\equiv\boldsymbol{v}$ $(\hbar/m=1)$, and the parameter s, which determines the width $1/s$ of the packet in coordinate space.

This packet is not a solution of the usual Schrödinger equation (SE). It is a solution of the equation

$$\left[i\frac{i\partial}{\partial t}+\frac{\Delta}{2}\right]\psi(\boldsymbol{r},t)=-4\pi\sqrt{\frac{s}{2\pi}}e^{i\Omega t}\delta(\boldsymbol{r}-\boldsymbol{v}t), \tag{56}$$

where $\Omega=[k^2+s^2]/2$, and the right hand side contains the Dirac δ-function, which is not zero at one point $\boldsymbol{r}=\boldsymbol{v}t$. This fact should not be considered as a reason for immediate rejection of dBWP from the very start, because in everyday life we routinely use the construction, which is also not a solution of the homogeneous SE. I mean the spherical wave, described by the spherical Hankel function.

4.1 Genesis of dBWP

We want to show here that dBWP is a particular case of a spherical wave. Indeed, let us look at a spherical wave

$$\psi(\boldsymbol{r},t)=\frac{\exp(isr)}{r}\exp(-is^2t/2), \tag{57}$$

which satisfies the equation

$$\left[i\frac{\partial}{\partial t}+\frac{\Delta}{2}\right]\psi(\boldsymbol{r},t)=-2\pi\delta(\boldsymbol{r})\exp(-is^2t/2). \tag{58}$$

This spherical wave corresponds to energy $E=s^2/2$ and has a fixed center. Now, let us transform our reference frame to a coordinate system moving with velocity $\boldsymbol{v}\equiv\boldsymbol{k}$. The Schrödinger equation will preserve its form if we not only change $\boldsymbol{r}\to\boldsymbol{r}-\boldsymbol{v}t$, but also multiply function (57) by the phase factor $\exp(i\boldsymbol{kr}-ik^2t/2)$, which transforms (57,58) to

$$\Psi(\boldsymbol{r},\boldsymbol{k},s,t)=\exp(i\boldsymbol{kr}-i\omega t)\frac{\exp(is|\boldsymbol{r}-\boldsymbol{v}t|)}{|\boldsymbol{r}-\boldsymbol{v}t|}, \tag{59}$$

$$\left[i\frac{\partial}{\partial t}+\frac{\Delta}{2}\right]\psi(\boldsymbol{r},t)=-2\pi\delta(\boldsymbol{r})\exp(i[k^2-s^2]t/2), \tag{60}$$

where ω in (59) is $(k^2+s^2)/2$.

Thus we see, that dBWP is immediately obtained from (59), if we suppose that $s^2<0$ and s is purely imaginary. It means that dBWP can be interpreted as a spherical wave bound by a universe negative potential.

The expression (59) shows that, if we accept a possibility to consider singular spherical waves, we should accept also the whole set of possible states like (59), and also their superposition:

$$\psi(\boldsymbol{r},E,t)=\exp(-iEt)\int\delta(E-k^2/2-s^2/2)A(\boldsymbol{k})\Psi(\boldsymbol{r},\boldsymbol{k},s)d^3k.$$

In (57) we considered only s-wave spherical function, but we can also consider other spherical functions, singular and nonsingular ones, with different orbital moments l. However the dBWP is the simplest one, and we want to limit ourselves to it now.

In the papers [3, 4] there was considered transmission of dBWP through a thin layer of matter, which is described by a rectangular potential. Here we want to present some justification for these calculations. For justification we compare our approach in [3] with the well known one for the spherical function. We shall show that our approach applied to the spherical wave gives well known correct result. This demonstration serves as a justification for our approach to the dBWP.

5 Spherical wave

Let us consider transmission through the rectangular barrier of the familiar stationary spherical wave

$$\psi(\boldsymbol{r})=\frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}_0|)}{|\boldsymbol{r}-\boldsymbol{r}_0|}. \tag{61}$$

It is not a solution of the Schrödinger equation

$$[\Delta+k^2]\psi(\boldsymbol{r})=0, \tag{62}$$

but it is the solution of the inhomogeneous one

$$[\Delta+k^2]\psi(\boldsymbol{r})=-4\pi\delta(\boldsymbol{r}-\boldsymbol{r}_0), \tag{63}$$

where the right hand side is the Dirac δ-function, which is not zero at the point $\boldsymbol{r}=\boldsymbol{r}_0$. However it is zero at all other points, and equation (63) at all but one points coincides with (62).

The equation (63) is for free space, but it can be easily generalized to the case of the space with an external potential. In particular, we can imagine a some matter layer of thickness d, described by optical potential of height $u/2$, then (63) becomes

$$[\Delta + k^2 - u\Theta(0 \le z \le d)]\psi(\boldsymbol{r}) = -4\pi\delta(\boldsymbol{r} - \boldsymbol{r}_0), \tag{64}$$

where Θ-function is equal to 1 or 0, when the inequality in its argument is satisfied or not respectively. We can solve (64) precisely for $\boldsymbol{r}_0$ inside and outside the potential. Here we consider it outside i.e. $z_0 < 0$

The equation (64) can be solved in two ways, but in both ways we use Fourier expansion. The Fourier expansion of (61) is

$$\psi(\boldsymbol{r}) = \frac{\exp(ik|\boldsymbol{r} - \boldsymbol{r}_0|)}{|\boldsymbol{r} - \boldsymbol{r}_0|} = \frac{4\pi}{(2\pi)^3}\int \frac{\exp(i\boldsymbol{p}[\boldsymbol{r} - \boldsymbol{r}_0])d^3p}{p^2 - k^2 - i\epsilon}. \tag{65}$$

We can easily check it. Indeed, integration over angles in the last integral gives

$$\psi(\boldsymbol{r}) = \frac{1}{2\pi i|\boldsymbol{r} - \boldsymbol{r}_0|}\int\limits_0^\infty [\exp(ip|\boldsymbol{r}-\boldsymbol{r}_0|) - \exp(-ip|\boldsymbol{r}-\boldsymbol{r}_0|)]\frac{dp^2}{p^2 - k^2 - i\epsilon}, \tag{66}$$

which after transformation of variable $p^2 = x$ can be represented as an integral over contour C_1 around the cut in complex x-plane from 0 to ∞ as is shown in fig. 2. This contour can be closed by the infinite circle and transformed into a little circle around $k^2 + i\epsilon$, as is also shown in fig. 2, and as a result of complex integration around the pole we obtain

$$\frac{1}{2\pi i}\oint\limits_{C_1} \frac{\exp(i\sqrt{x}|\boldsymbol{r} - \boldsymbol{r}_0|)dx}{x - k^2 - i\epsilon} = \frac{1}{2\pi i}\oint\limits_{C_0} \frac{\exp(i\sqrt{x}|\boldsymbol{r} - \boldsymbol{r}_0|)dx}{x - k^2 - i\epsilon} = \exp(ik|\boldsymbol{r} - \boldsymbol{r}_0|),$$

which after substitution into (66) gives the function identical to (61).

The Fourier expansion (65) can be integrated over, say, p_z component of the vector $\boldsymbol{p}$, closing the contour of integration by a semi circle at infinity in the upper or lower half of p_z complex plane. Then (65) is reduced to the form:

$$\frac{\exp(ikr)}{r} = \frac{i}{2\pi}\int \exp(i\boldsymbol{p}_{||}\boldsymbol{r} + ip_z|z|)\frac{d^2p_{||}}{p_z}, \tag{67}$$

where $p_z = \sqrt{k^2 - p_{||}^2}$.

Now we shall see how to find the solution of equation (64) with rectangular potential taking (61) as the incident wave. This solution will give us transmission through the rectangular barrier, and we can obtain this transmission in two ways. They both use Fourier expansions either (65) or (67). However the last case is simpler, and for that reason we start with it. Of course we can also consider the case, when $\boldsymbol{r}_0$ is inside the potential. Here, without accounting for boundaries, the spherical wave for $k^2 < u$ looks like a 'localized' function $\exp(-\sqrt{u-k^2}r)/r$, but this case is not interesting for us now.

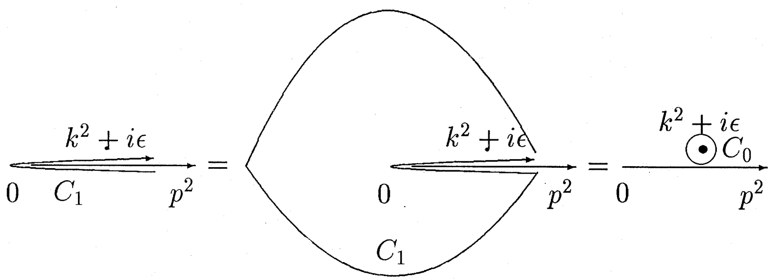

Figure 2: Contour of integration C_1 in (65) can be closed by an infinite circle and transformed into a little circle around the pole at $p^2 = k^2 + i\epsilon$

5.1 Transmission of the rectangular barrier calculated with expansion (6)

In the free space every plane wave component $\psi_p(\boldsymbol{r}) = \exp(i\boldsymbol{pr})$ of the Fourier expansion (67) satisfies equation (63). When we have a potential, the plane waves should be replaced with some functions $\psi_p(\boldsymbol{r})$ satisfying the equation

$$[\Delta + k^2 - u\Theta(0 \le z \le d)]\psi_p(\boldsymbol{r}) = 0. \qquad (68)$$

In our case potential depends only on z, and the function $\psi_p(\boldsymbol{r})$ can be represented as the product $\exp(i\boldsymbol{p}_{||}\boldsymbol{r})\psi_p(z)$, which after substitution into (6) gives

$$\psi(\boldsymbol{r}) = \frac{i}{2\pi}\int \exp(i\boldsymbol{p}_{||}[\boldsymbol{r}-\boldsymbol{r}_0])\psi_p(z)\frac{d^2p_{||}}{p_z}, \qquad (69)$$

where $\psi_p(z)$ is a solution of one dimensional SE equation

$$[\frac{d^2}{dz^2} + k^2 - p_{||}^2 - u\Theta(0 \le z \le d)]\psi_p(z) = 0 \qquad (70)$$

with incident wave $\exp(ip_z[z-z_0])$, and we suppose for now that $z_0 < 0$, i.e. it lies outside of our potential.

Solution of (70) is

$$\psi_p(z) = e^{-ip_z z_0}\{[e^{ip_z z}\Theta(z_0 < z < 0) + \rho(p_z)e^{-ip_z z}\Theta(z < 0)] +$$

$$\tau(p_z)\exp(ip_z[z-d])\Theta(z>d)\}+\exp(-ip_z[z-z_0])\Theta(z<z_0), \quad (71)$$

where ρ and τ are reflection and transmission amplitudes for rectangular potential of height u and width d:

$$\rho(p_z)=\frac{\rho_0(p_z)[1-\exp(2ip'_zd)]}{1-\rho_0^2(p_z)\exp(2ip'_zd)}, \quad \tau(p_z)=\frac{\exp(ip'_zd)[1-\rho_0^2(p_z)]}{1-\rho_0^2(p_z)\exp(2ip'_zd)},$$

$$\rho_0(p_z)=\frac{p_z-p'_z}{p_z+p'_z}, \qquad p'_z=\sqrt{p_z^2-u}=\sqrt{k^2-p_{||}^2-u}, \quad (72)$$

and for simplicity we omitted the part of $\psi_p(z)$ inside the potential $0\le z\le d$.

For $z>d$ after substitution of (71) into (69) we obtain

$$\frac{i}{2\pi}\int\tau(p_z)\exp(i\boldsymbol{p}_{||}[\boldsymbol{r}-\boldsymbol{r}_0]+ip_z[z-d-z_0])\frac{d^2p_{||}}{p_z}. \quad (73)$$

This can be called transmitted part of the wave (61). The total transmission is the normal flux through an infinite plane, which is perpendicular to z-axis at some point $z>d$:

$$J_z=\frac{-i}{2}\int d^2r_{||}\left(\psi^*(\boldsymbol{r})\frac{d}{dz}\psi(\boldsymbol{r})-\psi(\boldsymbol{r})\frac{d}{dz}\psi^*(\boldsymbol{r})\right)=\int|\tau(p_z)|^2\frac{d^2p_{||}}{p_z}\Theta(p_z^2>0). \quad (74)$$

Integration over $p_{||}$ can be reduced to integration over p_z as follows: $d^2p_{||}=d\phi p_zdp_z$, which transforms (74) into

$$J_z=2\pi\int_0^k|\tau(p_z)|^2dp_z. \quad (75)$$

All the factors here have very clear physical meaning. The factor 2π, for instance, means that every infinite plane subtends solid angle 2π.

Transmitted part (75) can be compared with the flux J_0 incident onto the plane at $z=0$:

$$J_0=\int\frac{d^2p_{||}}{p_z}\Theta(p_z^2>0)=2\pi k.$$

Thus transmission probability is

$$W=\int_0^k|\tau(p_z)|^2\frac{dp_z}{k}. \quad (76)$$

If the total energy k^2 is less than u, then transmission is exponentially small, because according to (72)

$$|\tau(p_z)|^2\propto\exp(-2\sqrt{u-p_z^2}d)<\exp(-2\sqrt{u-k^2}d).$$

5.2 Transmission calculated with expansion (65)

We can also use the expansion (65). In this case the exponents $\psi_p(\boldsymbol{r}) = \exp(i\boldsymbol{p}(\boldsymbol{r}-\boldsymbol{r}_0))$ do not satisfy equation (62), but instead they are solution of the equation

$$[\Delta + p^2]\psi_p(\boldsymbol{r}) = 0, \tag{77}$$

and with potential u we should replace them with the solutions of the equation

$$[\Delta + p^2 - u\Theta(0 \le z \le d)]\psi_p(\boldsymbol{r}) = 0. \tag{78}$$

Since our potential depends only on z, we can again represent $\psi_p(\boldsymbol{r})$ as the product

$$\psi_p(\boldsymbol{r}) = \exp(i\boldsymbol{p}_{||}\boldsymbol{r})\psi_p(z), \tag{79}$$

so (65) is represented now as

$$\psi(\boldsymbol{r}) = \frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}_0|)}{|\boldsymbol{r}-\boldsymbol{r}_0|} = \frac{4\pi}{(2\pi)^3}\int \frac{\exp(i\boldsymbol{p}_{||}[\boldsymbol{r}-\boldsymbol{r}_0])d^3p}{p^2-k^2-i\epsilon}\psi_p(z), \tag{80}$$

where $\psi_p(z)$ is a solution of the one dimensional equation

$$[d^2/dz^2 + p_z^2 - u\Theta(0 \le z \le d)]\psi_p(z) = 0, \tag{81}$$

with incident plane wave equal to $\exp(ip_z[z-z_0])$.

Solution of this equation is the same as (71), but p_z is now an independent variable. After substitution of (71) into (80) we obtain transmitted wave at $z > d$ equal to

$$\frac{4\pi}{(2\pi)^3}\int \tau(p_z)\exp(i\boldsymbol{p}_{||}[\boldsymbol{r}-\boldsymbol{r}_0] + ip_z[z-d-z_0])\frac{d^3p}{p^2-k^2-i\epsilon}, \tag{82}$$

where p_z now is not equal to $\sqrt{k^2-p_{||}^2}$.

According to (74) and (82) the flux through the plane at $z > d$ is

$$J_z = \int_{-\infty}^{\infty}\frac{dp_{1z}}{\pi}\int_{-\infty}^{\infty}\frac{dp_{2z}}{\pi}\tau(p_{1z})\tau^*(p_{2z})\frac{p_{1z}+p_{2z}}{2}\times$$

$$\int \frac{d^2p_{||}\exp(i[p_{1z}-p_{2z}][z-d-z_0])}{(p_{||}^2+p_{1z}^2-k^2-i\epsilon)(p_{||}^2+p_{2z}^2-k^2+i\epsilon)}, \tag{83}$$

where $\tau^*(x)$ is complex conjugate of $\tau(x)$. We see that now we should take into account both positive and negative values of p_{1z} and p_{2z}, because we need the total flux. After integration over $d^2p_{||}$ we obtain

$$J_z = \iint_{-\infty}^{\infty} e^{i(p_{1z}-p_{2z})(z-d-z_0)}\frac{dp_{1z}dp_{2z}\tau(p_{1z})\tau^*(p_{2z})}{2\pi[p_{2z}-p_{1z}(1-i\epsilon)]}\ln\left(\frac{p_{2z}^2-k^2+i\epsilon}{p_{1z}^2-k^2-i\epsilon}\right). \tag{84}$$

For further integration we need to identify all singular points of the function under the integral in complex planes of p_{1z} and p_{2z}. The singular points are contained in transmission amplitudes τ, under the logarithm function and there is also a pole at $p_{1z} = p_{2z}$.

5.2.1 Geography of cuts, poles and paths in (84)

Now we shall analyze where lie all the singular points in the integral (84), and where lie the paths of integrations.

Function $\tau(p_z)$ depends on $p_z' = \sqrt{p_z^2 - u}$, which means that there are two branch points at $p_z = \pm\sqrt{u}$ that can be connected with the cut between them as is shown in fig. 3. The path of the integration over p_{1z} should go above this cut because transmission amplitude $\tau(p_{1z})$, which contains $\exp(2ip_{1z}')$ for $p_{1z}^2 > u$ should become exponentially decaying. It means that, when p_{1z} crosses the point $\sqrt{u}$, the magnitude $\sqrt{p_{1z}^2 - u}$ becomes $+i\sqrt{u - p_{1z}^2}$, i.e. integration path should turn π counter clockwise and go above the cut.

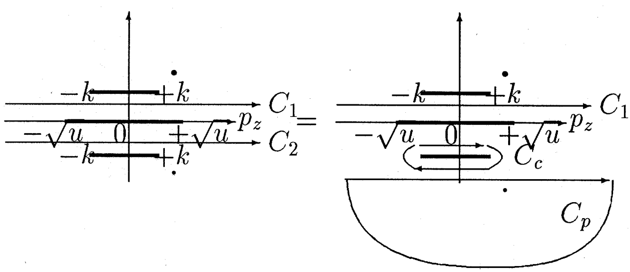

Figure 3: Contour C_1 of integration over p_{1z} lies above the cut $\pm\sqrt{u}$ and below the cut $\pm k$. The contour C_2 of integration over p_{2z} lies below the cut $\pm\sqrt{u}$ and above the cut $\pm k$. After closing C_2 by a semi circle in the low half plane we obtain contribution of the pole and cut $\pm k$.

The logarithm function also gives two branch points $\pm k$ which also can be connected with the cut. It is easy to see, that integration path over p_{1z} should go below this cut, because when going from $p_{1z} > k$ the path crosses the point $p_{1z} = k$, the logarithm argument becomes $-i\epsilon$, which means that the path near the point k makes clockwise turn over $\pi/2$.

The analogous considerations show that integration path over p_{2z} lies below the cut $-\sqrt{u}, +\sqrt{u}$ and above $-k, +k$. We can close this path by a semicircle in lower half of the complex p_{2z} plane because $z - d - z_0 > 0$, and obtain two contributions: contribution of the pole and the cut. The pole contribution is

$$J_z = -i\int_0^\infty dp_{1z}|\tau(p_{1z})|^2 \ln\left(\frac{p_{1z}^2 - k^2 - i\epsilon}{p_{1z}^2 - k^2 - i\epsilon}\right) = 0, \tag{85}$$

because we should substitute $p_{2z}^2 = p_{1z}^2 - 2i\epsilon$ and took into account that the pole gives contribution only for $p_{1z} > 0$. For $p_{1z} < 0$ the pole lies in the upper half plane.

The cut contribution is

$$J_z = i\int_{-\infty}^{\infty} dp_{1z}\int_{-k}^{k} dp_{2z}\tau(p_{1z})\tau^*(p_{2z})\frac{\exp(i[p_{1z} - p_{2z}][z - d - z_0])}{p_{2z} - p_{1z}(1 - i\epsilon)}. \tag{86}$$

In this integral only the pole is remained and the integration path can be closed in the upper half of the complex plane, which gives

$$J_z = 2\pi\int_0^k dp_{2z}|\tau(p_{2z})|^2. \tag{87}$$

It is identical to the result (75), which shows that both ways of calculations give the same result and we are justified to calculate transmission by looking for transmission of every plane wave component of the expansion (65), and apply to it the equation (81).

6 Transmission of the de Broglie wave packet

Now we are ready to start our calculations with dBWP. It is meaningless to suppose that in the equation (27) right hand side has the same value along all the trajectory even inside the potential. If it were so, no reflection at all would happen. So we suppose that equation (27) holds only in free space, and transmission should be calculated quantum mechanically.

The easiest way of calculation is the one, explained in section (5.2). The Fourier expansion of (27) is

$$\psi_{dB}(\boldsymbol{r},t) = \sqrt{\frac{s}{2\pi}}\exp(i\boldsymbol{kr} - i\omega t)\frac{4\pi}{(2\pi)^2}\int d^3p\frac{\exp(i\boldsymbol{p}[\boldsymbol{r} - \boldsymbol{v}t])}{p^2 + s^2}, \tag{88}$$

Or, after change of variables $\boldsymbol{p} - \boldsymbol{k} \to \boldsymbol{p}$, it can be represented as

$$\psi_{dB}(\boldsymbol{r},t) = \sqrt{\frac{s}{2\pi}\frac{4\pi}{(2\pi)^3}}\int d^3p\frac{\exp(i\boldsymbol{pr} + i[k^2 + s^2 - 2\boldsymbol{pv}]t/2)}{(\boldsymbol{p} - \boldsymbol{k})^2 + s^2}. \tag{89}$$

Every plane wave $\exp(i\boldsymbol{pr})$ satisfies the equation (77), and in the potential u it should be replaced with $\psi_p(\boldsymbol{r})$, which satisfies (78), and can be represented as (79), where $\psi_p(z)$ satisfies (81) with incident plane wave equal to $\exp(ip_z z)$. Thus the transmitted function is equal to

$$\psi_{dB}(\boldsymbol{r},t) = \sqrt{\frac{s}{2\pi}}\frac{4\pi}{(2\pi)^3}\int d^3p\tau(p_z)\frac{\exp(i\boldsymbol{pr} + i[k^2 - 2\boldsymbol{pk} + s^2]t/2)}{(\boldsymbol{p}-\boldsymbol{k})^2 + s^2}, \quad (90)$$

and total number of particles having crossed an x,y-plane at some point $z > d$ is

$$N_z = \frac{-i}{2}\int\limits_{-\infty}^{\infty} dt\int d^2r_{\|}\left(\psi^*(\boldsymbol{r})\frac{d}{dz}\psi(\boldsymbol{r}) - \psi(\boldsymbol{r})\frac{d}{dz}\psi^*(\boldsymbol{r})\right) =$$

$$\frac{s}{2\pi}\frac{(4\pi)^2}{(2\pi)^3}\int|\tau(p_z)|^2\frac{p_z}{v_z}\frac{d^3p}{[(\boldsymbol{p}-\boldsymbol{k})^2+s^2]^2}. \quad (91)$$

After integration over $p_{\|}$ it is reduced to

$$N_z = \frac{s}{\pi}\int\limits_{-\infty}^{\infty}|\tau(p_z)|^2\frac{p_z}{k_z}\frac{dp_z}{(\boldsymbol{p}_z - \boldsymbol{k}_z)^2 + s^2}. \quad (92)$$

We are to compare this magnitude with the flux through the plane, say at the point $z = 0$ before the potential. This flux, calculated in the same way will give

$$N_0 = \frac{s}{\pi}\int\limits_{-\infty}^{\infty}\frac{p_z}{k_z}\frac{dp_z}{(\boldsymbol{p}_z-\boldsymbol{k}_z)^2+s^2} = \frac{s}{\pi}\int\limits_{-\infty}^{\infty}\frac{dx}{x^2+s^2} = 1, \quad (93)$$

which could be expected, because from normalization

$$\int|\psi_{dB}(\boldsymbol{r},t)|^2d^3r = 1 \quad (94)$$

we have a single particle in all the space. Thus expression (92) gives transmission probability. We can estimate the integral as

$$W \approx \frac{2s}{\pi}\int\limits_{\sqrt{u}}^{\infty}\frac{dx}{x^2+s^2} = \frac{2}{\pi}\arctan\left(\frac{s}{\sqrt{u}}\right) \approx \frac{2s}{\pi\sqrt{u}}. \quad (95)$$

Thus we can tell that because of the wave vectors spectrum, there is always some non exponential transmission through the rectangular potential, even if neutron velocity is lower than the limiting one: $k^2 < u$.

6.1 Wave function of transmitted particle

We suggest that the wave function of transmitted particle should be the same wave packet (27), and the magnitude (92) gives only probability of transmission. In principle we can represent the transmitted function as a superposition of dBWP. Indeed, let us represent the transmission amplitude as a Fourier expansion:

$$\tau(p_z) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \exp(ip_z\zeta)\tau_F(\zeta)d\zeta. \tag{96}$$

Then the wave function (90) becomes

$$\psi_{dB}(\boldsymbol{r},t) = \sqrt{\frac{s}{2\pi}}\int\limits_{-\infty}^{\infty} d\zeta\frac{\tau_F(\zeta)}{2\pi}e^{i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{\zeta}-\boldsymbol{d})-i\omega t}\frac{\exp(-s|\boldsymbol{r}-\boldsymbol{\zeta}-\boldsymbol{d}-\boldsymbol{v}t|)}{|\boldsymbol{r}-\boldsymbol{\zeta}-\boldsymbol{d}-\boldsymbol{v}t|}, \tag{97}$$

where vectors $\boldsymbol{\zeta}$ and $\boldsymbol{d}$ have components $\boldsymbol{\zeta} = (0,0,\zeta)$, $\boldsymbol{d} = (0,0,d)$. The expression (97) means that with some probability $|\tau_F(\zeta)|^2$ we register the transmitted neutron at time $t = (\zeta + d)/v_z$, because it is delayed by ζ. It is interesting to investigate how to discriminate this time delay from inelastic scattering, which is measured by time of flight technique. We cannot do it for now, and for that reason too, we can tell that there is no QM of the dBWP yet.

6.2 Wave function in the potential

We can easily find the wave function inside the potential, because we know it everywhere. From (89) it follows that

$$\psi_{dB}(\boldsymbol{r},t) = \sqrt{\frac{s}{2\pi}}\frac{4\pi}{(2\pi)^3}\int d^3p\frac{\exp(i\boldsymbol{p}_{\|}\boldsymbol{r} + i[k^2+s^2-2\boldsymbol{p}\boldsymbol{v}]t/2)}{(\boldsymbol{p}-\boldsymbol{k})^2+s^2}\psi_p(z), \tag{98}$$

where $\psi_p(z)$ outside of the potential looks like (71). Inside the potential it is

$$\psi_p(z) = A(p_z)\{exp(ip'_z z) - \exp(ip'_z d)\rho_0(p_z)\exp(-ip'_z[z-d])\}\Theta(0 \le z \le d), \tag{99}$$

where

$$A(p_z) = \frac{\tau_0(p_z)}{1-\rho_0^2(p_z)\exp(2ip_z d)}, \qquad \tau_0(p_z) = \frac{2p_z}{p_z+p'_z}.$$

Somehow this wave function should be represented as a superposition of different dBWPs with different trajectories and velocities. We cannot represent such a superposition now, because we do not know trajectories velocities and widths of dBWP in the potential. If we apply the SE operator

$$\hat{L}=i\frac{i\partial}{\partial t}+\frac{\Delta}{2}-\frac{u}{2}$$

to the function (98), we obtain

$$\hat{L}\psi_{dB}(\boldsymbol{r},t)=-\sqrt{\frac{s}{2\pi}}\delta(\boldsymbol{r}_{\|}-\boldsymbol{v}_{\|}t)\exp(i[k^2+s^2]t/2)\Theta(0\le z\le d)\times$$

$$\int\limits_{-\infty}^{\infty}dp_zA(p_z)\exp(-i\boldsymbol{p}_zv_zt)\{\exp(ip'_zz)-\exp(ip'_zd)\rho_0(p_z)\exp(-ip'_z[z-d])\}. \tag{100}$$

It follows that along the surface trajectory is the same as in the original dBWP (27), but the motion along normal z is not of the δ-function type. It is very complicated, we cannot characterize it, and because of that, we cannot tell that we know QM of the dBWP.

7 Conclusion

Simple consideration of scattering processes shows a contradiction hidden in the standard approach. On one side we use plane waves as eigen states of a particle, and on the other side describe scattered particles with spherical waves, which are not even solutions of the Schrödinger equation. Rigorous approach improves the theory, however it is unable to describe even the simplest experimental process — transmission of particles through a sample. When we try to do that we arrive at necessity to limit wave front of particle plane wave, i.e. we need to use wave packets instead plane waves. The wave packet should not spread and we naturally arrive at the de Broglie wave packet. However we have not yet a mathematical apparat to describe even a simplest scattering of dBWP on a fixed center. We hope that it can be elaborated, because at least we can correctly describe transmission and reflection of dBWP by one dimensional rectangular barriers. Investigation in this direction will help to understand the role of wave function and its relation to trajectories and to motion of the particle itself.

A Calculations of total scattering on monoatomic gas

We need to calculate

$$<w>=C\int M\left(\frac{\mu k_2^2}{2T}\right)k_2^2dk_2\int d\cos\vartheta\times$$

$$\left\{\frac{\xi^2}{P\mu}[\xi^2+3\mu^2P^2]\Theta(\xi<\mu P)+\xi[3\xi^2+\mu^2P^2]\Theta(\xi>\mu P)\right\}. \tag{101}$$

where ϑ is the angle between neutron, $\boldsymbol{k}_1$, and nucleus, $\boldsymbol{k}_2$, moments,

$$C=\frac{2b^2}{3(1+\mu)^5k_1},\qquad M\left(\frac{\mu k_2^2}{2T}\right)=\left(\frac{\mu}{2\pi T}\right)^{3/2}\exp\left(-\frac{\mu k_2^2}{2T}\right), \tag{102}$$

$\xi=|\boldsymbol{k}_1-\mu\boldsymbol{k}_2|$, $P=|\boldsymbol{k}_1+\boldsymbol{k}_2|$, $E=k_1^2+\mu k_2^2$, and inequalities in Θ-functions are equivalent to

$$\xi^2\neq\mu^2P^2=(\boldsymbol{k}_1-\mu\boldsymbol{k}_2)^2\neq\mu^2(\boldsymbol{k}_1+\boldsymbol{k}_2)^2=$$
$$(1-\mu^2)k_1^2\neq 2\mu(1+\mu)\boldsymbol{k}_1\boldsymbol{k}_2=(1-\mu)k_1^2\neq 2\mu\boldsymbol{k}_1\boldsymbol{k}_2.$$

At the beginning we need to integrate over angle.

A.1 $\xi<\mu P$

Since $\xi^2=(1+\mu)E-\mu P^2$, we have $\xi^2<\mu^2P^2\to P^2>E/\mu$, and the integral over angle in the first term of (101) is equivalent to integral over P^2:

$$w_1(k_2)=\int\limits_{P_-}^{P_+}\frac{[(1+\mu)E-\mu P^2]}{k_1k_2\mu}[(1+\mu)E-\mu(1-3\mu)P^2]dP\Theta(P^2>E/\mu)=$$

$$\left[(1+\mu)^2E^2P-\frac{\mu}{3}(1+\mu)(2-3\mu)EP^3+\frac{\mu^2}{5}(1-3\mu)P^5\right]\frac{\Theta(P^2>E/\mu)}{k_1k_2\mu}\Bigg|_{P_-}^{P_+},$$

where $P_+=k_1+k_2$, and P_- is defined below. It is evident that the integral is not zero if at least upper limit satisfies $P_+^2=(k_1+k_2)^2>E/\mu$. It is satisfied only for $k_2>(1-\mu)k_1/2\mu$.

To find the lower limit we notice that $2k_1k_2\cos\vartheta>(1-\mu)k_1^2/\mu$, i.e. for $\mu\le 1$ it is positive, which means that at lower limit $P_-=\sqrt{E/\mu}$. Thus we have

$$w_1(k_2)=\Theta\left(\frac{k_2}{k_1}>\frac{1-\mu}{2\mu}\right)\frac{1}{k_1k_2\mu}\times$$
$$\left[(1+\mu)^2E^2P-\mu\frac{2-\mu-3\mu^2}{3}EP^3+\mu^2\frac{1-3\mu}{5}P^5\right]_{\sqrt{E/\mu}}^{(k_1+k_2)^2}. \tag{103}$$

If we introduce new variable $x=k_2/k_1$, denote $x_1=(1-\mu)/2\mu$, $P=1+x$, and $E=1+\mu x^2$ we represent (103) in the form

$$w_1(k_2)=\Theta(x>x_1)\frac{k_1^3}{\mu x}\left\{(1+\mu)^2E^2\left[P-\sqrt{\frac{E}{\mu}}\right]-\right.$$

$$\mu\frac{2-\mu-3\mu^2}{3}E\left[P^3-\left(\frac{E}{\mu}\right)^{3/2}\right]+\mu^2\frac{1-3\mu}{5}\left[P^5-\left(\frac{E}{\mu}\right)^{5/2}\right]\Bigg\}. \quad (104)$$

A.2 $\xi > \mu P$

Now we consider the second term in (101).

$$w_2(k_2)=\int \xi[3\xi^2+\mu^2P^2]\Theta(\xi^2>\mu^2P^2)d\cos\vartheta. \quad (105)$$

Because $\mu^2P^2=\mu(\mu+1)E-\mu\xi^2$, we can represent $\xi^2>\mu^2P^2$ as $\xi^2>\mu E$, and the integral (105) over angles can be transformed into the one over ξ^2 in the interval $(k_1-\mu k_2)^2\le\xi^2\le(k_1+\mu k_2)^2$:

$$w_2(k_2)=\int\limits_{\xi_-}^{\xi_+}\frac{\xi^2d\xi}{\mu k_1k_2}[(3-\mu)\xi^2+\mu(1+\mu)E]=\frac{1}{\mu k_2k_1}\left[\frac{3-\mu}{5}\xi^5+\mu\frac{1+\mu}{3}E\xi^3\right]_{\xi_-}^{\xi_+}. \quad (106)$$

The upper limit $\xi_+=k_1+\mu k_2$ for $\mu\le1$ is always higher than $\mu P=\mu(k_1+k_2)$. The lower limit is $\xi_-=\max(|k_1-\mu k_2|,\sqrt{\mu E})$. For $0<k_2<(1-\mu)k_1/2\mu$ we have $k_1>\mu k_2$ and $(k_1-\mu k_2)^2>\mu E$. Thus $\xi_-=k_1-\mu k_2$. For $(1-\mu)k_1/2\mu<k_2$ we have $(k_1-\mu k_2)^2<\mu E$, and for ξ_- we must take $\xi_-=\sqrt{\mu E}$.

We again can introduce variable $x=k_2/k_1$, then (106) is representable as $w_2(x)=$

$$\frac{k_1^3}{\mu x}\Bigg\{\frac{3-\mu}{5}[(1+x\mu)^5-(1-x\mu)^5]+\mu\frac{1+\mu}{3}E[(1+\mu x)^3-(1-x\mu)^3]+$$
$$\Theta(x>x_1)\left(\frac{3-\mu}{5}[(1-x\mu)^5-(\mu E)^{5/2}]+\right.$$
$$\left.\mu\frac{1+\mu}{3}E[(1-\mu x)^3-(\mu E)^{3/2}]\right)\Bigg\}. \quad (107)$$

The first term in (107), which is valid for x in the whole range $0\le x<\infty$, can be rearranged as follows

$$w_{21}(x)=2k_1^3\left[3+\mu^2+\frac{1}{3}(21-2\mu+\mu^2)x^2\mu^2+\frac{2}{15}(7+\mu)x^4\mu^4\right]. \quad (108)$$

A.3 Integration over k_2

Integration over k_2 in (101) after change of variables $k_2\to x=k_2/k_1$ is reduced to the form

$$<w>=C\int\limits_0^\infty\frac{x^2dx}{\alpha^3\pi^{3/2}}\exp(-x^2/\alpha^2)[w_1(x)+w_{21}(x)+w_{22}(x)], \quad (109)$$

where $\alpha^2 = 2T/\mu k_1^2 = T/\mu E_1$, $E_1 = k_1^2/2$.

For w_{21} (108) integration can be easily done, and we obtain

$$< w_{21} >= \frac{b^2 k_1^2}{3\pi(1+\mu)^5}\left[3+\mu^2+\frac{1}{2}(21-2\mu+\mu^2)\alpha^2\mu^2+\frac{1}{2}(7+\mu)\alpha^4\mu^4\right], \tag{110}$$

or after substitution of $\alpha^2 = 2T/k_1^2\mu$, it is

$$< w_{21} >= \frac{b^2 k_1^2}{3\pi(1+\mu)^5}\left[3+\mu^2+\frac{T\mu}{2E_1}(21-2\mu+\mu^2)+\frac{T^2\mu^2}{2E_1^2}(7+\mu)\right]. \tag{111}$$

In particular, for $\mu = 1$ we have

$$< w_{21} >= \frac{b^2 k_1^2}{24\pi}\left[1+\frac{5}{2}\frac{T}{E_1}+\frac{T^2}{E_1^2}\right], \tag{112}$$

for $\mu = 0$ we obtain the result of elastic scattering on a fixed center:

$$< w_{21} >= \frac{b^2 k_1^2}{\pi},$$

and at $T = 0$ we obtain the scattering probability

$$< w_{21} >= \frac{b^2 k_1^2}{\pi(1+\mu)^5}(1+\mu^2/3)$$

on a free nucleus at rest.

The terms $< w_1 + w_{22} >$ after summation of (104) with the second term in (107) is: $w_1(x) + w_{22}(x) =$

$$\Theta(x>x_1)\frac{k_1^3}{\mu x}\left\{(1+\mu)^2E^2\left[P-\sqrt{\frac{E}{\mu}}\right]-\mu\frac{2-\mu-3\mu^2}{3}E\left[P^3-\left(\frac{E}{\mu}\right)^{3/2}\right]+\right.$$
$$\mu^2\frac{1-3\mu}{5}\left[P^5-\left(\frac{E}{\mu}\right)^{5/2}\right]+$$
$$\left.\frac{3-\mu}{5}[(1-x\mu)^5-(\mu E)^{5/2}]+\mu\frac{1+\mu}{3}E[(1-\mu x)^3-(\mu E)^{3/2}]\right\}. \tag{113}$$

This expression contains a polynomial of 5-th order in power of x, and the term proportional to $E^{5/2}$:

$$w_1(x) + w_{22}(x) = \Theta(x>x_1)\frac{k_1^3}{\mu x}\left\{\sum_{k=0}^{5}a_k(\mu)x^k - A(\mu)\left(\frac{E}{\mu}\right)^{5/2}\right\}, \tag{114}$$

where $a_0 = (4+\mu)(3+2\mu+3\mu^2)/15$,

$$a_1 = (1-\mu)^3, \quad a_2 = \frac{2\mu^2}{3}(19-2\mu+3\mu^2), \quad a_3 = \frac{\mu}{3}(1-\mu)(4+17\mu-10\mu^2+\mu^3),$$

$$a_4 = 8\mu^4, \quad a_5 = \frac{2\mu^2}{15}(4+13\mu+15\mu^2-7\mu^3-\mu^4), \quad A(\mu) = \frac{2\mu^2}{15}(4+\mu)(1+\mu)^3. \tag{115}$$

After substitution of (114) into (109) and calculation of the integral by parts we obtain

$$< w_1+w_{22} >= -C_1\sqrt{\frac{\tau}{\mu\pi}}[q_1(\mu)+q_2(\mu)\tau]\exp\left(-\frac{(1-\mu)^2}{4\mu\tau}\right)+I(\tau,\mu), \tag{116}$$

where $C_1 = b^2k_1^2/3(1+\mu)^5\pi$,

$$\tau = \frac{T}{E_1}, \quad q1(\mu) = -\frac{1}{2\mu}\left[\sum_{k=2}^{5} ka_k(\mu)x_1^{k-2} - 5A(\mu)\left(\frac{1+\mu}{2\mu}\right)^3\right] = (1-\mu)^2,$$

$$q2(\mu) = \frac{-1}{4\mu^2}\left[8a_4(\mu)+15a_5(\mu)x_1 - 15A(\mu)\frac{1+\mu}{2\mu}\right] = \frac{4+13\mu-10\mu^2+\mu^3}{2}.$$

The first term in (116) for small $\mu\tau \to 0$ decreases exponentially, and for $\mu\tau \to \infty$ grows in absolute magnitude as

$$-C_1\sqrt{\frac{\tau}{\mu\pi}}[q_1(\mu)+q_2(\mu)\tau].$$

The second term in (116) is

$$I(\tau,\mu) = \frac{C_1}{\sqrt{\mu\tau}}\frac{1}{\sqrt{\pi}}\int_{x_1}^{\infty}\exp\left(-\frac{\mu x^2}{\tau}\right)dx\times$$

$$[q_3(\mu)+\tau q_4(\mu)+\tau^2 q_5(\mu)-\tau^2 q_6(\mu)\sqrt{\mu/(1+\mu x^2)}], \tag{117}$$

$$q_3(\mu) \equiv a_1(\mu) = (1-\mu)^3, \quad q_4(\mu) = \frac{3}{2\mu}a_3(\mu) = \frac{1}{2}(1-\mu)(4+17\mu-10\mu^2+\mu^3),$$

$$q_5 = \frac{15}{4\mu^2}a_5(\mu) = \frac{1}{2}(4+13\mu+15\mu^2-7\mu^3-\mu^4),$$

$$q_6(\mu) = \frac{15}{4\mu^2}A(\mu) = \frac{1}{2}(4+\mu)(1+\mu)^3.$$

The integral (117) is equal to

$$I(\tau,\mu) = \frac{C_1}{2\mu}\left\{[q_3(\mu)+\tau q_4(\mu)+\tau^2 q_5(\mu)]\Psi\left(\frac{1-\mu}{2\sqrt{\mu\tau}}\right) - \right.$$

$$q_6(\mu)\tau^2 \exp\left(\frac{1}{\tau}\right)\Psi\left(\frac{1+\mu}{2\sqrt{\mu\tau}}\right)\Bigg\}.$$

Here we introduced the function $\Psi(z) = 1 - \Phi(z)$, where

$$\Psi(z) = \frac{2}{\sqrt{\pi}}\int_z^\infty e^{-x^2}dx \equiv 1 - \Phi(z), \quad \text{where} \quad \Phi(z) = \frac{2}{\sqrt{\pi}}\int_0^z \exp(-x^2)dx$$

is the error function. The total result is

$$< w >= \frac{b^2k_1^2}{3\pi(1+\mu)^5}\Bigg\{\left[3+\mu^2+\frac{\tau\mu}{2}(21-2\mu+\mu^2)+\frac{\tau^2\mu^2}{2}(7+\mu)\right] -$$

$$\sqrt{\frac{\tau}{\mu\pi}}\left[(1-\mu)^2+\frac{\tau}{2}(4+13\mu-10\mu^2+\mu^3)\right]\exp\left(-\frac{(1-\mu)^2}{4\mu\tau}\right)+$$

$$\frac{1}{2\mu}\Bigg[[(1-\mu)^3+\frac{\tau}{2}(1-\mu)(4+17\mu-10\mu^2+\mu^3)+$$

$$\frac{\tau^2}{2}(4+13\mu+15\mu^2-7\mu^3-\mu^4)]\Psi\left(\frac{1-\mu}{2\sqrt{\mu\tau}}\right)-$$

$$\frac{\tau^2}{2}(4+\mu)(1+\mu)^3\exp\left(\frac{1}{\tau}\right)\Psi\left(\frac{1+\mu}{2\sqrt{\mu\tau}}\right)\Bigg]\Bigg\}. \qquad (118)$$

This function has asymptotics ($k^2 = 2mE/\hbar^2$):

$$< w(\mu,E,T) >= \frac{b^2k^2}{3\pi(1+\mu)^5}\left[3+\mu^2+\frac{T\mu}{2E}(21-2\mu+\mu^2)\right], \text{ for } \mu\frac{T}{E}\to 0, \qquad (119)$$

$$\text{and} \quad < w(\mu,E,T) >= \frac{b^2k^2}{3\pi(1+\mu)^5}\left(\frac{T}{E}\right)^{3/2}\frac{16}{\sqrt{\mu}} \text{ for } \mu\frac{T}{E}\to\infty. \qquad (120)$$

References

[1] W.Marshall and S.W.Lovesey, *Theory of Thermal Neutron Scattering.* Clarendon Press, Oxford, 1971.

[2] L. de Broglie, *Non-Linear Wave Mechanics: A Causal Interpretation.* Elsevier, Amsterdam, 1960.

[3] V.K. Ignatovich, M. Utsuro, *Phys. Lett.* **A225**, pp. 195-202, 1997.

[4] M. Utsuro, V. Ignatovich, P. Geltenbort et al, *Proceedings of VII International Seminar on Interaction of Neutrons with Nuclei: Neutron Spectroscopy, Nuclear Structure, Related Topics, Dubna, May 25-28, 1999,* **E3-98-212**, pp. 110-125, JINR, Dubna, 1999.

Received by Publishing Department
on March 15, 2001.

Игнатович В.К. E4-2001-42
Апокриф стандартной теории рассеяния
и квантовая механика волнового пакета де Бройля

Показано, что стандартная теория рассеяния не соответствует принципам канонической квантовой механики. Излагается более последовательная теория и приводятся некоторые ее результаты. Рассмотрено отражение и пропускание волнового пакета де Бройля тонкими слоями вещества.

Работа выполнена в Лаборатории нейтронной физики им. И.М.Франка ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна, 2001

Ignatovich V.K. E4-2001-42
Apocrypha of Standard Scattering Theory (SST)
and Quantum Mechanics of the de Broglie Wave Packet

It is shown that the Standard Scattering Theory (SST) does not correspond to the principles of Standard Quantum Mechanics (SQM). The more consistent theory is formulated. Some new results are obtained. Reflection and transmission of the de Broglie wave packet by thin layers of matter is considered.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna, 2001

Макет Т.Е.Попеко

Подписано в печать 29.03.2001
Формат 60 × 90/16. Офсетная печать. Уч.-изд. листов 3,33
Тираж 360. Заказ 52569. Цена 4 р.

Издательский отдел Объединенного института ядерных исследований
Дубна Московской области