Multiple scattering theory for slow neutrons (from thermal to ultracold)

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Abstract

The general theory of neutron scattering is presented, valid for the whole domain of slow neutrons from thermal to ultracold. Particular attention is given to multiple scattering which is the dominant process for ultracold neutrons (UCN). For thermal and cold neutrons, when the multiple scattering in the target can be neglected, the cross section is reduced to the known value. A new expression for inelastic scattering cross section for UCN is proposed. Dynamical processes in the target are taken into account and their influence on inelastic scattering of UCN is analyzed.

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1 Introduction

Thermal and cold neutrons with wave length \(0.03 \text{ nm} \leq \lambda \leq 1 \text{ nm}\) is an important tool for investigation of condensed matter. Due to the absence of charge and considerably weak interaction with electrons and nuclei incident neutron wave goes deep into target almost without distortion and coherently influences on all atoms of the target. The whole specific features of the matter (crystalline and magnetic structure etc.) show themselves in interference of the secondary scattered waves.

Theory of neutron-substance interaction for thermal and cold neutrons is well established (see, e.g., [1, 2, 3]). It is based on the use of Fermi pseudopotential

\[
V(r) = \sum_{\nu} V_{\nu}(r - R_{\nu}) = \sum_{\nu} \frac{2\pi \hbar^2}{m_{\nu}} a_{\nu} \delta(r - R_{\nu}).
\]

Here \(r\) and \(R_{\nu}\) are the position vectors for neutron with mass \(m\) and \(\nu\)-th nucleus with mass \(M_{\nu}\), \(m_{\nu} = mM_{\nu}/(m + M_{\nu})\) is their reduced mass, \(a_{\nu}\) is the amplitude of neutron scattering on free nucleus, connected with the scattering length \(\alpha_{\nu}\) and impact momentum in the center-of-mass system \(k_{\nu}\), in linear on \(k_{\nu}\alpha_{\nu}\) approximation (valid for slow neutrons), by

\[
a_{\nu} = \alpha_{\nu}(1 - i k_{\nu}\alpha_{\nu}).
\]

For thermal and cold neutrons rescattering of secondary waves is unimportant and one may use Born approximation that gives for double differential cross section per one target nucleus

\[
\frac{d^2\sigma}{d\Omega\,d\omega} = \frac{k'}{2\pi N\hbar} \sum_{\nu,\nu'} b'_{\nu} b_{\nu'} \chi(\nu\nu', \kappa, \omega).
\]
Here $\chi(\nu\nu', \kappa, \omega)$ is the Fourier transform

$$
\chi(\nu\nu', \kappa, \omega) = \int_{-\infty}^{+\infty} \chi(\nu\nu', \kappa, t)e^{i\omega t}dt
$$

(4)
of correlation function

$$
\chi(\nu\nu', \kappa, t) = \langle i | e^{-i\kappa R_\nu(t)} e^{i\kappa R_{\nu'}}(0) | i \rangle,
$$

(5)

$\kappa = k - k'$ and $\omega = \epsilon - \epsilon'$ are the neutron momentum and energy transfers. The quantity

$$
b_\nu = \left(\frac{m}{m_\nu}\right)a_\nu
$$

is called scattering amplitude on bound nucleus, and $\hat{R}_\nu(t)$ is time dependent Heisenberg operator of nuclear position.

It is easy to show that rescattering of the secondary waves may be indeed neglected for thermal and cold neutrons. Coherent summation of the secondary waves may be formed only from the volume $\sim \lambda^3$. The sum of all amplitudes from this domain is by the order of magnitude $\sim n\lambda^3(b/\lambda)$, where $n$ is the density of the nuclei ($\sim 10^{22}$ cm$^{-3}$), and $b \sim 10^{-12}$ cm. So far as $nb\lambda^3 \ll 1$, i.e. $\lambda \ll 100$ nm,

(6)

can not be used for UCN.

If the Born approximation is unjustified then one should start from an exact Schrödinger equation for the scattering problem. As the first step one may use a target model with fixed (unmovable) nuclei and consider integral equation

$$
\Psi_k(r) = e^{ikr} - \frac{m}{2\pi\hbar^2} \int e^{ik|r-r'|} V(r') \Psi_k(r')d^3r'.
$$

(7)

With a formal use of the Fermi pseudo-potential $\hat{\chi}$ equation (7) transforms into

$$
\Psi_k(r) = e^{ikr} - \sum_\nu b_\nu e^{ik|r-R_\nu|} \Psi_k(R_\nu).
$$

(8)

The quantity $\Psi_k(R_\nu)$ seems to have the meaning of the neutron wave amplitude on the $\nu$-th nucleus. This wave is composed now from the incident wave and all reflected waves, so its value is not known in advance and consistent equations have to be formulated for these quantities.

It is impossible to get the mentioned equation from (8) just by substitution there for neutron position $r = R_\nu$, due to infinity in diagonal term of the right-hand side. So, it was in fact postulated that a proper equation may be obtained just by throwing away the diagonal term (self-scattering):

$$
\Psi_k(R_\nu) = e^{ikR_\nu} - \sum_\nu b_\nu e^{ik|R_\nu-R_{\nu'}|} \Psi_k(R_{\nu'}).
$$

(9)

The equations (8) and (9) are today the basis for the whole theory of ultracold neutron interaction with matter (see, e.g., [4, 5, 6, 7]). From (9) one can get an effective repulsive (optical) potential on the condensed matter surface, so the neutron wave with the energy below the threshold is exponentially decreasing deep into target.

In general the problem of neutron interaction with matter can be analyzed in the framework of Multiple Scattering Theory (MST) [8, 9, 10, 11]. MST deals with interaction of a projectile with many-body target. In this theory a formal solution of many-body problem takes the form

$$
\Psi^{(+)} = \Psi^0 + \hat{D}^{-1} \sum_\nu \hat{t}_\nu \Psi_\nu,
$$

(10)
with functions $\Psi_\nu$ defined by the set of linear equations

$$\Psi_\nu = \Psi^0 + \hat{D}^{-1} \sum_{\nu' \neq \nu} \hat{t}_{\nu'\nu} \Psi_{\nu'},$$  \hspace{1cm} (11)$$

where operators $\hat{t}_{\nu}$ ($t$-matrixes) are linked with potentials $\hat{V}_\nu$ by

$$\hat{t}_{\nu} = \hat{V}_\nu + \hat{V}_\nu \hat{D}^{-1} \hat{t}_{\nu}.$$  \hspace{1cm} (12)$$

Here $\Psi^0$ is the wave function for noninteracting projectile and target, and $\hat{D}^{-1}$ is the "Green function" (see details in the next section).

There is a widespread opinion in literature that (8) and (9) are just the equations of MST (10) and (11) for fixed nuclei target. In fact, they have similar structure but with some modeled $t_{\nu}$. Consistent derivation of (10) and (11) analogies for fixed nuclei target with realistic potentials was done in [12]. In any way, target model with fixed nuclei can be applied only to elastic scattering. While UCN escape from vessels, that is studied for many years, is due mainly to inelastic scattering. Now quasielastic scattering of UCN with small energy and momentum transfers attracts attention of experimenters as perspective tool for condensed matter studies [13]. Recently observed (see, e.g., [14, 15]) small cooling and heating of UCN in vessels also belong to quasielastic processes.

A step from frozen to moving nuclei target is very dramatic since it requires a transition from one body to many-body function $\Psi(\mathbf{r}, \mathbf{R}_\nu)$. MST does not present any universal solution, since general equations of MST are only a reformulation of the problem in the way where multiple scattering is clearly exhibited (by using iterated (11) in (10)). Practical content of MST is, in fact, a set of approximations applicable for different situations. They were analyzed, e.g., in monograph of Goldberger and Watson [9].

Attempts were made to consider inelastic processes for UCN by using one of approaches developed in MST (see, e.g., [16]). However, approximations used so far for MST cannot be applied for inelastic scattering of UCN. Indeed, the main assumptions, that different approximations of MST were based on, may be formulated as:

(a) energy of projectile is much larger then characteristic energy of target particles ("weak coupling approximation");

(b) mean free path of projectile in target is much larger then its wave length;

(c) mean free path of projectile is much larger then length of effective correlation between target particles.

The first of these assumptions allows to use Born or "impulse" approximation, where each target particle may be considered free when colliding with projectile. The second and the third condition allow to treat multiple scattering as sequential collisions and represent result as sum on number of collisions executed. Due to (b) the energy of projectile between successive collisions is well determined quantity, and due to (c) the target at each collision may be considered being in the ground state.

It is easy to see that all three assumptions are not valid for UCN:

(a) Energy of ultracold neutron is $\sim 10^{-7}$ eV and corresponds to temperature $\sim 10^{-3}$ K which is much smaller then the target temperature even at liquid helium.

(b) The usual definition of mean free path fails for UCN (elastic cross section for mirror like potential is equal to surface area $S$). Thus, one may use for this quantity intrusion length into target, which is of the order of wave length $\sim 10$ nm. It means that neutron energy between collisions is, in fact, uncertain.

(c) The main effect of UCN multiple scattering is appearance of a potential barrier, that is just the product of particle-particle correlation at distances compared with neutron wave length.

The goal of this work is to find solution of MST equations valid for the whole domain of slow neutrons (from thermal to ultracold), starting from realistic neutron – nucleus interaction.
Equations (3) and (8), (9) will follow from this theory as limiting cases. By solution we mean reduction of general equations (10)-(12) to those which allow reasonably simple numerical solution for elastic and inelastic scattering for all practically interesting cases. One numerical solution for inelastic UCN scattering is presented as an example in the last part of the paper.

2 Formulation of the Problem. Plan of Solution

A proper theory for UCN scattering should be based on the following postulates: (i) No Born approximation; (ii) No use of Fermi potential; (iii) Target matter is a dynamical system. So we should start from N+1 body Schrödinger equation

\[
\left( \frac{\hat{p}^2}{2m} + \hat{H}_t + \hat{V} \right) |\Psi_{k,i}\rangle = E_{k,i} |\Psi_{k,i}\rangle, \quad \hat{V} = \sum_{\nu} \hat{V}_{\nu}.
\]

(13)

Here \( \hat{V}_{\nu} \) describes interaction of neutron with \( \nu \)-th nucleus, \( \hat{p} = -i\partial/\partial r \) is the operator of neutron momentum, \( E_{k,i} = \epsilon_k + \epsilon_i \) is the total energy as the sum of neutron energy \( \epsilon_k = k^2/2m \) in the state \( |k\rangle \) and the target initial energy \( \epsilon_i \) in the state \( |i\rangle \) that is the eigenstate of the target Hamiltonian \( \hat{H}_t \). Here and onward we keep \( \hbar = 1 \) till final physical results.

Equation (13) can be written in integral form

\[
|\Psi_{k,i}\rangle = |\Psi_{k,i}^0\rangle + \hat{D}^{-1} \sum_{\nu} \hat{V}_{\nu} |\Psi_{k,i}\rangle,
\]

(14)

where \( |\Psi_{k,i}^0\rangle = |k\rangle |i\rangle \) and \( \hat{D}^{-1} \) is ”Green function” with

\[
\hat{D} = \frac{k^2}{2m} + \epsilon_i - \frac{\hat{p}^2}{2m} - \hat{H}_t + i\eta,
\]

(15)

where positive quantity \( \eta \to 0 \) provides outgoing neutron wave asymptotic.

Note, that the problem can be easily reduced to MST equations (10)-(12). First, equation (14) can be written in the form

\[
|\Psi_{k,i}\rangle - \hat{D}^{-1} \hat{V}_{\nu} |\Psi_{k,i}\rangle = |\Psi_{k,i}^0\rangle + \hat{D}^{-1} \sum_{\nu' \neq \nu} \hat{V}_{\nu'} |\Psi_{k,i}\rangle.
\]

(16)

Then, let define a state vector \( |\Psi_{\nu}\rangle \) and operator \( \hat{i}_{\nu} \) by the relations

\[
|\Psi_{\nu}\rangle = |\Psi_{k,i}\rangle - \hat{D}^{-1} \hat{V}_{\nu} |\Psi_{k,i}\rangle, \quad \hat{i}_{\nu} |\Psi_{\nu}\rangle = \hat{V}_{\nu} |\Psi_{k,i}\rangle.
\]

(17)

(18)

Now one can see that equations (14) and (16) with the help of (17) and (18) turns into (10) and (11), respectively. Finally, we have to show that \( \hat{i}_{\nu} \) obeys (12). For this purpose we use identity

\[
\hat{V}_{\nu} |\Psi_{k,i}\rangle = \hat{V}_{\nu} (|\Psi_{k,i}\rangle - \hat{D}^{-1} \hat{V}_{\nu} |\Psi_{k,i}\rangle) + \hat{V}_{\nu} \hat{D}^{-1} \hat{i}_{\nu} |\Psi_{k,i}\rangle,
\]

(19)

that, with the help of (17), (18), transforms into

\[
\hat{i}_{\nu} |\Psi_{\nu}\rangle = \hat{V}_{\nu} |\Psi_{\nu}\rangle + \hat{V}_{\nu} \hat{D}^{-1} \hat{i}_{\nu} |\Psi_{\nu}\rangle.
\]

(20)

Thus we have demonstrated that MST equations are nothing more than reformulation of the general scattering problem (13) or (14).

It is, of course, impossible to solve the many-body equation (13) or MST equations (10)-(12) and to found the state vectors \( |\Psi_{k,i}\rangle \) or \( |\Psi_{\nu}\rangle \) without any approximations. In our problem there
are two small main parameters: short-range of neutron – target nuclei interaction (as compared with interatomic distance and wave length) and small neutron energy (as compared with depth of interaction potential).

The first condition allows to consider only s-wave part of the wave function of neutron – nucleus center-of-mass motion, when their interaction is evaluated. And the second condition allows in this evaluation to neglect energy of relative neutron – nucleus motion inside the interaction potential area. So, the s-wave function and its derivative, taken at the potential boundary, are independent on neutron energy and are just numerical parameters.

No specific model for neutron – nucleus interaction potential will be needed. Its specific features described above (short range and large depth) allows to use scattering length approximation.

The small parameters allow to simplify our problem. Potential $V_\nu$ is essential only in small vicinity of $R_\nu$. It differs from zero only when the absolute value of deviation $x = r - R_\nu$ does not exceed the potential radius $r_0\nu$. So, using completeness of the neutron states $\sum_r |r\rangle \langle r| = 1$ one has

$$\hat{V}_\nu |\Psi_{k,i}\rangle = \sum_x |R_\nu + x\rangle \langle R_\nu + x| \hat{V}_\nu |\Psi_{k,i}\rangle = \sum_x |R_\nu + x\rangle V_\nu(x) \langle R_\nu + x|\Psi_{k,i}\rangle. \quad (21)$$

Here and onward sums of continue variables mean integrals with the following supposition for position- and momentum–energy variables

$$\sum_R \rightarrow \int dR, \quad \sum_q \rightarrow \int \frac{dq}{(2\pi)^3}, \quad \sum_\omega \rightarrow \int \frac{d\omega}{2\pi}. \quad (22)$$

Using (21) one can transform (14) to

$$|\Psi_{k,i}\rangle = |\Psi_{k,i}^0\rangle + \hat{D}^{-1} \sum_\nu \sum_x |R_\nu + x\rangle V_\nu(x) \langle R_\nu + x|\Psi_{k,i}\rangle. \quad (23)$$

The scalar product of (16) with $\langle R_\nu + x|$ after some rearrangement can be presented as

$$\langle R_\nu + x|\Psi_{k,i}\rangle - \sum_{x'} \langle R_\nu + x'|\hat{D}^{-1}|R_\nu + x'|V_\nu(x') \langle R_\nu + x'|\Psi_{k,i}\rangle = \langle R_\nu + x|\Psi_{k,i}^0\rangle + \sum_{\nu' \neq \nu} \sum_{x'} \langle R_{\nu'} + x|\hat{D}^{-1}|R_{\nu'} + x'\rangle V_{\nu'}(x') \langle R_{\nu'} + x'|\Psi_{k,i}\rangle. \quad (24)$$

Equations (23) and (24), as can be recognized by the structures of their right-hand sides, correspond to MST equations (10) and (11). To make them fully determined it remains to find the only key element, namely $\langle R_\nu + x|\Psi_{k,i}\rangle$, i.e. the exact many-body wave function, but only in the area of short range potential for each nucleus.

So, the many-body problem is reduced to only two-body problem (or, more precisely, three-body, since the nucleus is not free), with the rest of the nuclei as spectators. The solution of the last problem is determined by two parameters: by the values of s-wave amplitude $\chi_\nu(r_0\nu)/r_0\nu$ and its derivative at the boundary of the potential. Since the logarithmic derivative is connected to the scattering length $\alpha_\nu$ (the known physical quantity), the amplitude $\chi_\nu(r_0\nu)$ remains the only free parameter.

Therefore one may hope to express the quantity $\langle R_\nu + x|\Psi_{k,i}\rangle$ by $\chi_\nu(r_0\nu)$ and then to use (24) as a set of linear equations for parameters $\chi_\nu(r_0\nu)$. We will call $\langle R_\nu + x|\Psi_{k,i}\rangle$ for $x = r_0\nu$ as "neutron function at the surface of $\nu$-th nucleus".
Remark. The small quantity $r_0\nu$ will be neglected whenever possible, except in cases where $r_0\nu$ stays near the scattering length (which may be of the same order of magnitude) and in terms with singularity $1/r_0\nu$ till their compensation. Such singularity occurs in both terms in the left-hand side of (24) and requirement of their compensation will give us an additional control of calculations.

3 Neutron function at the surface of $\nu$-th nucleus

Let us transform the basic equation (13) to new variables

$$r, R \rightarrow x = r - R_\nu, R,$$

where $R = \{R_\nu\}$. The Hamiltonian in the new variables takes the form

$$\hat{H} = \hat{H}_n + \hat{H}_t - \frac{\hat{p}_x \hat{P}_\nu}{M_\nu}, \quad \hat{H}_n = \frac{\hat{p}_x^2}{2m_\nu} + V_\nu(x),$$

where $\hat{p}_x = -i\partial/\partial x$, and $\hat{P}_\nu = -i\partial/\partial R_\nu$ is the momentum operator of $\nu$-th nucleus. We assume that the quantity $x$ is small, so that neutron interaction with other nuclei (with $\nu' \neq \nu$) is absent.

We look for the solution of the Schrödinger equation with the Hamiltonian (26) with the energy $E_{k,i} = k^2/2m + \epsilon_i$. In Born approximation in the limit $x \to 0$ solution has the form

$$\Psi_{k,i}(x, R) = \psi(x)e^{ikR_\nu}\Phi_i(R),$$

where $\psi(x)$ is the center-of-mass wave function, and $\Phi_i(R)$ is the initial target state vector. In general case the neutron near the $\nu$-th nucleus may have its energy different from the initial one due to previous collisions. So, it is natural to look for the solution in the form

$$\Psi_{k,i}(x, R) = \varphi(x)e^{igR_\nu}\Phi_j(R),$$

where $\Phi_j(R)$ is the eigenfunction of the target Hamiltonian $H_t$ with the energy $\epsilon_j$ and $g$ is a vector parameter which represents neutron momentum.

If we substitute (28) into Schrödinger equation with the Hamiltonian (24) and take into account that operator $\hat{P}_\nu$ acts on $\Phi_j(R)$ as well as on the exponent, then we obtain the following equation for $\varphi(x)$

$$\left(\hat{H}_n + \frac{g^2}{2M_\nu} + \frac{gG_{j\nu}}{M_\nu}\right)\varphi - \frac{(g + G_{j\nu})\hat{p}_x}{M_\nu}\varphi = (E_{k,i} - \epsilon_j)\varphi,$$

where

$$G_{j\nu} = \left(\frac{\hat{P}_\nu}{\Phi_j}\right)/\Phi_j.$$

Equation (29) after some formal transformation can be displayed as

$$\left(\frac{1}{2m_\nu} \left[\hat{p}_x - \frac{m_\nu}{M_\nu}(g + G_{j\nu})\right]^2 + V_\nu(x)\right)\varphi = E(R)\varphi,$$

where

$$E(R) = E_{k,i} - \epsilon_j - \frac{g^2}{2m} + \frac{1}{2m_\nu}\left[\frac{g}{M_\nu}(g + G_{j\nu})\right]^2.$$
Formally, (31) is an equation only for the function \( \varphi \), and its exact solution, as can be easily proved, may be presented in the form

\[
\varphi(x) = \exp \left( i \frac{m_\nu}{M_\nu} (g + G_{j\nu}) x \right) \Psi(q, x),
\]

where \( \Psi(q, x) \) is the scattering wave-function in the center-of-mass system determined by the equation

\[
\hat{H}_n \Psi(q, x) = \frac{g^2}{2m_\nu} \Psi(q, x),
\]

and the scattering energy is defined from

\[
\frac{q^2}{2m_\nu} = \varepsilon_i - \varepsilon_j + \frac{k^2 - g^2}{2m} + \frac{1}{2m_\nu} \left[ g - \frac{m_\nu}{M_\nu} (g + G_{j\nu}) \right]^2.
\]

So, initial problem of neutron scattering on the bound nucleus seems to be reduced to the problem of scattering on free nucleus. In fact, it cannot be done precisely. Indeed, though (33) is formally an exact solution of the equation (29), its parameter \( q \) – impact momentum – through vector \( G_{j\nu} \) (30) depends on all coordinates of the target \( R \). But such a dependence was not assumed in (28).

However, we are looking for the solution valid for small \( x \). In the limit of small \( x \) only the \( s \)-wave part \( \chi(x)/x \) of the scattering function \( \Psi(q, x) \) is of importance and dependance of \( \chi \) on \( q \) can be neglected. Therefore, expression (33) for small \( x \) is independent on \( R \) and gives the real solution in the form

\[
\Psi_{k,i}(x, R)_{x \to 0} \simeq \frac{\chi(x)}{x} e^{i k R} \Phi_j(R).
\]

So far the target state \( j \) and intermediate neutron momentum \( g \) were not specified. It is evident, that any linear combination of functions (36) is allowed (provided the right-hand side of (35) is non negative), so we finally obtain

\[
\Psi_{k,i}(r = R_{\nu} + x, R)_{x \to 0} \simeq \frac{\chi(x)}{x} e^{i k R_{\nu}} \Phi_j(R).
\]

where

\[
\langle R|\nu \rangle \equiv \Phi_{\nu}(R) = \sum_{g,j} C_{\nu}(g, j) e^{i(g-k)R_{\nu}} \Phi_j(R).
\]

Note, that \( C_{\nu}(g, j) = \delta_{gk} \delta_{ji} \) and \( \Phi_{\nu} \to \Phi_i \) in Born approximation.

Expression (37) defines a local structure of the basic function \( \Psi_{k,i} \) near the point \( r = R_{\nu} \).

It naturally contains a "background target function" \( \Phi_{\nu}(R) = \langle R|\nu \rangle \), separately defined for each nucleus. This function differs from the initial state of the target \( \Phi_i(R) \equiv \langle R|i \rangle \) due to perturbation by the neutron wave. The functions \( \langle R|\nu \rangle \) should be consistently determined in parallel to the amplitudes of the neutron wave \( \chi_{\nu}(r_{0\nu}) \).

Let us now calculate the integral over \( x \) in (31). First, from (37) one finds

\[
\langle R_{\nu} + x|\Psi_{k,i} \rangle \simeq \frac{\chi(x)}{x} e^{i k R_{\nu}} |\nu \rangle.
\]

Second, we note that the state vector \( |R_{\nu} + x \rangle \) due to smooth dependance on \( x \) may be factored out from the integral and taken at \( x = 0 \). Third, from the equation (34) for \( \chi_{\nu} \) inside the potential area it follows

\[
V_{\nu}(x) \chi_{\nu}(x) \simeq \frac{1}{2m_{\nu}} \frac{d^2 \chi_{\nu}(x)}{dx^2}.
\]
Thus, the integration can be performed
\[
\int V_\nu(x) \frac{\chi_\nu(x)}{x} \, dx = -\frac{2\pi}{m_\nu} \frac{\alpha_\nu \chi_\nu(r_{0\nu})}{\alpha_\nu - r_{0\nu}},
\]
where we used the relation between scattering length \(\alpha\) and the logarithmic derivative at the boundary of the potential \(\chi'/\chi\rvert_{x=r_0} = -1/(\alpha - r_0)\). Combining (43) and (41) we get
\[
\sum_x \langle R_\nu + x \rangle V_\nu(x) \langle R_\nu + x \rangle |\Psi_{k,i}\rangle = |R_\nu\rangle \frac{2\pi}{m} e^{ikR_\nu} |\nu\rangle \phi_\nu,
\]
where we have introduced the amplitude
\[
\phi_\nu = -\frac{m}{m_\nu} \frac{\alpha_\nu \chi_\nu(r_{0\nu})}{\alpha_\nu - r_{0\nu}}.
\]

4 Equations for neutron amplitudes

In the previous section integrals over \(x\) in (24) are expressed in terms of the amplitudes \(\phi_\nu\) and state vectors \(|\nu\rangle\). Thus, with the use of (39) the equation (24) takes the form
\[
\frac{\chi_\nu(x)}{x} e^{ikR_\nu} |\nu\rangle - \langle R_\nu + x \rangle \hat{D}^{-1}|R_\nu\rangle \frac{2\pi}{m} e^{ikR_\nu} |\nu\rangle \phi_\nu = e^{ikR_\nu} |i\rangle + \sum_{\nu' \neq \nu} \langle R_\nu | \hat{D}^{-1} | R_{\nu'} \rangle \frac{2\pi}{m} e^{ikR_{\nu'}} |\nu'\rangle \phi_{\nu'}.
\]
The small quantity \(x\) is left only in the terms with singularity \(1/x\) and neglected elsewhere.

Note, that \(x\) in (14) is a free parameter, and for \(x = r_{0\nu}\), when \(\chi_\nu(r_{0\nu})\) and \(\phi_\nu\) are linked by (13), relation (14) may be regarded as a set of linear equations for \(\phi_\nu\), but with operators in target states as coefficients could be hardly used for practical calculations. Our next steps are directed to simplification of (14).

It is useful to transform the terms with \(\hat{D}^{-1}\) as follows
\[
\langle R | \hat{D}^{-1} | R' \rangle = \sum_q e^{iqR} \hat{D}^{-1}_q e^{-iqR'},
\]
where
\[
\hat{D}_q = \langle q | \hat{D} | q \rangle = \frac{k^2 - q^2}{2m} + \varepsilon_i - \hat{H}_t + i\eta.
\]
Then from (44) it is evident that to separate the amplitudes one should multiply both sides by \(e^{-ikR_\nu}\) and take their scalar product with the eigenvector \(|j\rangle\) of \(\hat{H}_t\). Thus, we have
\[
\left[\frac{m_\nu}{m} \left(\frac{1}{\alpha_\nu} - \frac{1}{r_{0\nu}}\right) \langle j | \nu\rangle - \zeta_j(\nu\nu, x) \rvert_{x=r_{0\nu}}\right] \phi_\nu = \delta_{ij} + \sum_{\nu' \neq \nu} \zeta_j(\nu\nu', 0) \phi_{\nu'},
\]
where
\[
\zeta_j(\nu\nu', x) = \frac{2\pi}{m} \sum_q e^{iqx} \langle j | e^{-i(k-q)R_\nu} \hat{D}^{-1}_q e^{i(k-q)R_{\nu'}} |\nu'\rangle.
\]
Expression (18) can be transformed into the other form with the use of the following presentation of the operator \(\hat{D}^{-1}_q\)
\[
\hat{D}^{-1}_q = \frac{1}{i} \int_0^\infty e^{i(x_k - \varepsilon_q + \varepsilon_i - \hat{H}_t + i\eta)t} \, dt.
\]
Then we get the alternative expression for (48)

\[ \zeta_j(\nu \nu', x) = \frac{2\pi}{im} \times \]

\[ \times \sum_q e^{iqx} \int_0^\infty \chi_j(\nu \nu', k - q, t) e^{i(\epsilon_k - \epsilon_q + \epsilon_j + i\eta)t} dt. \]  

(50)

Here the correlation function is introduced

\[ \chi_j(\nu \nu', \kappa, t) = \langle j | e^{-i\kappa \hat{R}_\nu(t)} e^{i\kappa \hat{R}_{\nu'}(0)} | \nu' \rangle, \]  

(51)

which is a generalization of (5).

To make (47) fully determined, we only need to find an explicit expression for diagonal term \( \zeta_j(\nu \nu, x) \) in the limit \( x \to r_0 \nu \). It evidently has a singularity \( 1/r_0 \nu \) which should compensate analogous term on the left-hand side of (47). That can be easily seen from simple scaling analysis. Let introduce new variables and parameters

\[ q' = qx, \quad k' = kx, \quad \epsilon'_i - \epsilon'_j = (\epsilon_i - \epsilon_j) x^2, \quad t' = t/x^2. \]  

(52)

Then small parameter \( x \) remains in (50) only as the common factor \( 1/x \) and inside \( \chi_j \) in the argument of \( \hat{R}_\nu(t) \).

When \( \nu = \nu' \) the operator in matrix element (51) is close to unity with very small deviation \( \sim u\kappa \), where \( u \) is a nuclear shift from equilibrium. Thus, it seems to be a good approximation to integrate over \( t \) in (50) only the exponential factor outside the matrix element. Then the integration over \( q \) gives

\[ \zeta_j(\nu \nu, x) \approx -\frac{e^{ikx}}{x} \langle j | \nu \rangle, \]  

(53)

where

\[ k_j^2 = k^2 + 2m(\epsilon_i - \epsilon_j). \]  

(54)

Note, that \( k_j \) is the absolute value of momentum of inelastically scattered neutron when target remains in the eigenstate \( | j \rangle \).

However, this result is evidently wrong. Since it does not cancel the singularity \( 1/r_0 \) in the left-hand side of (47) due to the additional factor \( m_\nu/m \). So, the matrix element \( \chi_j \) should be more accurately estimated.

The limit \( x \to 0 \) means that only small time interval is of importance in \( \hat{R}_\nu(t) = \hat{R}_\nu(t'x^2) \), and we can use the expansion

\[ \hat{R}_\nu(t) \approx \hat{R}_\nu(0) + \frac{\hat{P}_\nu t}{M_\nu}. \]  

(55)

Each additional power in \( t \) will result in an additional factor \( x^2 \). After substitution of (53) into (51), the matrix element is calculated without any futher approximations. Using the identity \( \exp(\hat{A}) \exp(\hat{B}) = \exp(\hat{A} + \hat{B} + [\hat{A}, \hat{B}]/2) \), which holds when \( \hat{A} \) and \( \hat{B} \) commute with their commutator \( [\hat{A}, \hat{B}] \), we obtain

\[ \chi_j(\nu \nu, k - q, t)_{t \to 0} \rightarrow \]

\[ \langle j | \exp \left( -i \left[ \frac{(k - q)^2}{2M_\nu} + \frac{(k - q)^2}{2M_\nu} \right] t \right) | \nu \rangle. \]  

(56)

Then integration over time and elementary transformation give

\[ \zeta_j(\nu \nu, x)_{x \to 0} = \]

\[ = 4\pi m_\nu m \sum_q \langle j | \frac{e^{iqx}}{k_\nu^2 - q_\nu^2 + 2m_\nu(\epsilon_i - \epsilon_j) + i\eta} | \nu \rangle, \]  

(57)
where
\[ k_\nu = k - \frac{m_\nu}{M_\nu} (\hat{P}_\nu + k), \quad q_\nu = q - \frac{m_\nu}{M_\nu} (\hat{P}_\nu + k). \quad (58) \]
The physical meaning of (58) is evident: \( k_\nu \) and \( q_\nu \) are the momenta in the center-of-mass system. This transition to the center-of-mass system provides additional factor \( m_\nu/m \).

Finally, integrating over \( q \) and taking into account only s-wave part in \( x \) we get
\[ \zeta_j(\nu \nu, x)|_{x \to 0} = -\frac{m_\nu}{m} \left( \frac{1}{x} \langle j|\nu \rangle + i \langle j|\hat{K}_{j\nu}|\nu \rangle \right), \quad (59) \]
where the operator \( \hat{K}_{j\nu} \), defined from
\[ \hat{K}_{j\nu}^2 = \left[ k - \frac{m_\nu}{M_\nu} (\hat{P}_\nu + k) \right]^2 + 2m_\nu (\varepsilon_i - \varepsilon_j), \quad (60) \]
has the meaning of absolute value of the impact momentum in the center-of-mass system for the neutron and \( \nu \)-th target nucleus when the target is in the state \( |j\rangle \). For UCN this quantity is defined mostly by the average absolute value of nuclear momentum.

The limiting value (59) allows to get explicit form of the equation (47) for the amplitudes \( \phi_\nu \). With the help of (59) we verify that for \( x = r_{0\nu} \) singular terms \( 1/r_{0\nu} \) are canceled out and the next terms result in
\[ \frac{1}{\beta_\nu} \langle j|\nu \rangle \phi_\nu + i \frac{m_\nu}{m} \langle j|\hat{K}_{j\nu}|\nu \rangle \phi_\nu = \delta_{ij} + \sum_{\nu' \neq \nu} \zeta_j(\nu \nu') \phi_{\nu'}, \quad (61) \]
where the renormalized scattering length ("on bound nucleus") is introduced
\[ \beta_\nu = \frac{m}{m_\nu} \alpha_\nu. \quad (62) \]
The matrix \( \zeta_j(\nu \nu') \equiv \zeta_j(\nu \nu', 0) \) with the use of (50) can be expressed in terms of Fourier transforms of correlation functions (51)
\[ \zeta_j(\nu \nu') = 4\pi \sum_{q, \omega} \chi_{jj'}(\nu \nu', k - q, \omega). \quad (63) \]
Now we note that any state vector \( |\nu \rangle \) can be presented as series in target eigenfunctions
\[ |\nu \rangle = \sum_j |j\rangle \langle j|\nu \rangle. \quad (64) \]
Therefore the relations (61) are really the linear equations for the amplitudes
\[ \phi^j_\nu = \langle j|\nu \rangle \phi_\nu. \quad (65) \]
Indeed, we get
\[ \frac{1}{\beta_\nu} \phi^j_\nu + i \frac{m_\nu}{m} \sum_{j'} \langle j|\hat{K}_{j\nu}|j' \rangle \phi^j_{\nu'} = \delta_{ij} + \sum_{j', \nu' \neq \nu} \zeta_{jj'}(\nu \nu') \phi^j_{\nu'}. \quad (66) \]
The coefficients of these equations
\[ \zeta_{jj'}(\nu \nu') = \frac{2\pi}{m} \sum_q \langle j|e^{-i(k-q)R_\nu} \hat{D}_q^{-1}e^{i(k-q)R_{\nu'}}|j' \rangle = \]
\[ = 4\pi \sum_{q, \omega} \frac{\chi_{jj'}(\nu \nu', k - q, \omega)}{k_j^2 - q^2 - 2m_\omega + i\eta}. \quad (67) \]
reaction channel. The wave function in the

\[ \chi_{jj'}(\nu\nu', \kappa, \omega) = \int_{-\infty}^{+\infty} \chi_{jj'}(\nu\nu', \kappa, t)e^{i\omega t} dt, \]

(68)

are completely determined by the properties of target matter, i.e., by the matrix elements of the operator of \( \nu \)-th and \( \nu' \)-th nuclei position correlation between the target eigenfunctions.

The equations (66) are obtained from (24) or (11). However, they deal not with N+1 body state vectors \( |\Psi_{k,i}\rangle \) or \( |\Psi_\nu\rangle \) but with numerical parameters \( \phi_\nu^j \). It is easy to see that due to (42) and (23) the total wave function \( |\Psi_{k,i}\rangle \) can be expressed in terms of the same parameters, namely,

\[ |\Psi_{k,i}\rangle = |\Psi_{k,i}^0\rangle + \hat{D}^{-1}\sum_{j,\nu} |R_{\nu}\rangle \frac{2\pi}{m} e^{ikR_{\nu}j} \phi_{\nu}^j. \]

(69)

It means that scattering probability and scattering cross section are also determined by \( \phi_{\nu}^j \). Connection between them is analysed in the next section.

5 Scattering problem and neutron amplitudes

Scattering process with a fixed final state \( \langle j | \) of the target is usually called a transition into \( j \)-th reaction channel. The wave function in the \( j \)-th channel can naturally be defined by

\[ \Psi_{ij}(r) = \langle r, j | \Psi_{k,i} \rangle \]

(70)

From (69) it follows

\[ \Psi_{ij}(r) = \delta_{ij} e^{ikr} + \frac{2\pi}{m} \sum_{j',\nu} \phi_{\nu}^{j'} \langle j | \hat{D}^{-1} |R_{\nu}\rangle e^{ikR_{\nu}j'}. \]

(71)

Then using (45), (46) one has

\[ \Psi_{ij}(r) = \delta_{ij} e^{ikr} - \frac{4\pi}{m} \sum_{j',\nu} \phi_{\nu}^{j'} \langle j | \frac{e^{iq(r-R_{\nu})}}{k_{j'}^2 - q^2 + i\eta} e^{ikR_{\nu}j'}. \]

(72)

where \( k_j \) was introduced by (54). After integration over \( q \) we finally obtain

\[ \Psi_{ij}(r) = \delta_{ij} e^{ikr} - \sum_{j',\nu} \phi_{\nu}^{j'} \langle j | \frac{e^{ik_j |r-R_{\nu}|}}{|r-R_{\nu}|} e^{ikR_{\nu}j'}. \]

(73)

In asymptotic, when \( r \to \infty \), we get from (73) for the scattered wave the usual structure

\[ f_{ij}(k_j, k_j') \frac{e^{ik_j r}}{r}, \]

(74)

where the scattering amplitudes in reaction channels are given by

\[ f_{ij}(k, k') = -\sum_{j',\nu} \phi_{\nu}^{j'} \langle j | e^{i(k-k')^* R_{\nu}} | j' \rangle. \]

(75)

The final momentum \( k' \equiv k_j \) is defined by \( k_j = k_j(r/r) \).

It is instructive to note that one obtains in Born approximation with pseudopotential (1) the following expression for the scattering amplitude:

\[ f_{ij}(k, k') = -\sum_{\nu} b_{\nu} \langle j | e^{i(k-k')^* R_{\nu}} | i \rangle. \]

(76)
It is analogous to (75) but instead of \( \phi_j^i \) it has the scattering amplitude on an bound nucleus, and the matrix element is taken between unperturbed states \( \langle j | i \rangle \).

Remark. A typical target model used for ultracold neutron reflection is semi-infinite substance. The asymptotic procedure used above to extract the scattering amplitude (75) from the wave function, strictly speaking, is incorrect for an infinite target. So, we shall assume our target finite with some plane surface area \( S \), which is large enough to use in parallel planes continuum spectrum, orto-normalized with \( \delta(\mathbf{k}'_\| - \mathbf{k}_\|) \) instead of \( \delta_{\mathbf{k}_\|,\mathbf{k}_\|} \), but allows when necessary to make replacement

\[
\left[ (2\pi)^2 \delta(\mathbf{k}'_\| - \mathbf{k}_\|) \right] \rightarrow S(2\pi)^2 \delta(\mathbf{k}'_\| - \mathbf{k}_\|).
\]

(77)

In the case when transmission is also of importance we need to consider the target of finite width to allow asymptotic in both directions.

The cross section for the reaction \( i \rightarrow j \) can be obtained from the scattering amplitude by

\[
d\sigma_{ij} = \frac{k'}{k} |f_{ij}(\mathbf{k}, \mathbf{k}')|^2 d\Omega',
\]

(78)

but the final state of the target is usually not fixed and inelastic processes are measured by the energy transfer. This process is described by double differential cross section

\[
\frac{d^2\sigma}{d\Omega'd\epsilon'} = \frac{k'}{k} \sum_j 2 \frac{2\pi}{m} f_{ij}(\mathbf{k}, \mathbf{k}')^2 \delta(\epsilon_i - \epsilon_j + \epsilon_k - \epsilon_{k'}). \tag{79}
\]

It is useful to consider the quantity

\[
w(\mathbf{k}, \mathbf{k}') = \sum_j 2 \frac{2\pi}{m} f_{ij}(\mathbf{k}, \mathbf{k}')^2 2\pi \delta(\epsilon_i - \epsilon_j + \epsilon_k - \epsilon_{k'}),
\]

(80)

then \( w(\mathbf{k}, \mathbf{k}') d\mathbf{k}'/(2\pi)^3 \) is the scattering probability per unit time from the fixed state \( |\mathbf{k}\rangle \) to the states \( |\mathbf{k}'\rangle \) into the momentum space element \( d\mathbf{k}' \). The scattering probability (77) divided by the incident neutron flux \( k/m \) gives the cross section to find the final neutron with momentum \( \mathbf{k}' \), and one is free to choose parameters in \( \mathbf{k}' \) to be fixed in the final state and then integrate over the rest of these parameters. The relation between \( w(\mathbf{k}, \mathbf{k}') \) and the cross section is evident from the equality

\[
\frac{m}{k} \int w(\mathbf{k}, \mathbf{k}') \frac{d\mathbf{k}'}{(2\pi)^3} = \int \frac{d^2\sigma}{d\Omega'd\epsilon'} d\Omega'd\epsilon'. \tag{81}
\]

So, the cross section of inelastic scattering with energy loss \( \omega \) is given by

\[
\frac{d\sigma}{d\omega} = \frac{m}{k} \int w(\mathbf{k}, \mathbf{k}') \delta(\epsilon_k - \epsilon_{k'} - \omega) \frac{d\mathbf{k}'}{(2\pi)^3}. \tag{82}
\]

Replacing delta-function in (80) by the integral over \( t \) and using (74) one can sum in (80) over the final states \( j \) as

\[
\sum_j e^{i(\epsilon_j - \epsilon_{j'} t)} \langle j | e^{-i(\mathbf{k} - \mathbf{k}')\hat{R}_\nu} | j' \rangle \langle j' | e^{i(\mathbf{k} - \mathbf{k}')\hat{R}_\nu} | j'' \rangle = \chi_{jj'}(\nu\nu', \mathbf{k} - \mathbf{k}', t), \tag{83}
\]

where \( \chi_{jj'}(\nu\nu', \mathbf{k}, t) \) (as well as its Fourier transform) was introduced by (78). Then (80) takes the form

\[
w(\mathbf{k}, \mathbf{k}') = \left( \frac{2\pi}{m} \right)^2 \sum_{j', \nu', \nu} \phi_{j'}^{\nu'} \phi_j^\nu \chi_{jj'}(\nu\nu', \mathbf{k} - \mathbf{k}', \omega + \epsilon_i - \epsilon_j). \tag{84}
\]
The corresponding equation for double differential cross section is
\[
\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{2\pi k} \sum_{j'\nu'} \phi^{j\nu}_j \phi^{j'\nu'}_{j'} (\nu\nu', k - k', \omega + \varepsilon_i - \varepsilon_j) .
\]
(85)

We have now the scattering amplitude (75) and scattering probability (84) expressed by the neutron amplitudes \(\phi^j_\nu\), which are determined by the equation (66).

6 The case of thermal and cold neutrons

Here we address to the neutrons with momenta in the range
\[
\sqrt{4\pi n} \ll k \ll 1/\alpha ,
\]
(86)
for which the rescattering processes are not important and may be considered as small perturbation.

In the first approximation the last term in (66) may be neglected and we obtain
\[
\phi^j_\nu = \delta_{jj'} \frac{\beta_\nu}{1 + i\langle i|\hat{K}_\nu|i\rangle \alpha_\nu} \simeq \delta_{jj'} \beta_\nu \left(1 - i\langle i|\hat{K}_\nu|i\rangle \alpha_\nu\right) ,
\]
(87)
which is similar to the expression (3) for the amplitude of neutron scattering on the isolated nucleus. The only difference is that instead of impact momentum in (3) (natural parameter for two-body problem), in (87) enters the average value of this parameter over nuclear ensemble in the target. After substitution of (87) into (85) we obtain the known expression (3) for thermal neutron scattering cross section.

7 Renormalized amplitudes for condensed target

Up to now no assumptions were made on the target matter. For a condensed target the results can be presented in more visual form.

Let suppose
\[
R_\nu = \rho_\nu + u_\nu ,
\]
(88)
where for solid state target \(\rho_\nu\) is the equilibrium position of the target nucleus, and \(u_\nu\) is the shift from the equilibrium. For liquids \(\rho_\nu\) and \(u_\nu\) may be understood as an average position and a fluctuation. Note, that index \(\nu\) may be now replaced by \(\rho\). When useful we shall make such replacement without notice.

The matrix \(\chi_{jj'}(\nu\nu', \kappa, t)\) is transformed now into
\[
\chi_{jj'}(\nu\nu', \kappa, t) = e^{-i\kappa(\rho_\nu - \rho_{\nu'})} \langle j|e^{-i\hat{K}_\nu(t)} e^{i\hat{K}_{\nu'}(0)} |j'\rangle .
\]
(89)
For the model with fixed (unmovable) nuclei the matrix element in (89) equals to \(\delta_{jj'}\). In order to separate the effect of nuclei motion let us write
\[
\chi_{jj'}(\nu\nu', \kappa, t) = e^{-i\kappa(\rho_\nu - \rho_{\nu'})} \left(\delta_{jj'} + \tilde{\chi}_{jj'}(\nu\nu', \kappa, t)\right) ,
\]
(90)
where
\[
\tilde{\chi}_{jj'}(\nu\nu', \kappa, t) = \langle j|e^{-i\hat{K}_\nu(t)} e^{i\hat{K}_{\nu'}(0)} - 1 |j'\rangle .
\]
(91)
To simplify the equation (66) let us introduce instead of \(\zeta_{jj'}(\nu\nu')\) (97) a new matrix \(G_{jj'}(\nu\nu')\) from
\[
\zeta_{jj'}(\nu\nu') = -e^{-i\kappa(\rho_\nu - \rho_{\nu'})} G_{jj'}(\nu\nu') .
\]
(92)
Then introducing the new amplitude

\[ \psi_j(\nu) = \frac{1}{\beta_\nu} \phi_j e^{i k \rho_\nu}, \]

(93)

we obtain the equation

\[ \psi_j(\nu) = \delta_{ij} e^{i k \rho_\nu} - \sum_{j' \nu'} G_{jj'}(\nu \nu') \psi_{j'}(\nu') \beta_{\nu'}, \]

(94)

where the diagonal in \( \nu \) and \( \nu' \) term is of the form:

\[ G_{jj}(\nu \nu) = i (m_\nu/m) \langle j | \hat{K}_{j \nu} | j \rangle. \]

Note, that according to (59) this diagonal term equals to \(- \zeta_{jj}(\nu \nu, x)\) in the limit \( x \to 0 \) but without its real part in contrast with the non-diagonal terms. In the long wave length limit the sum in (94) may be replaced by the integral over \( \nu' \). In this case it is not necessary to give special attention to the point \( \nu' = \nu \), since the real part of the term with \( \nu' = \nu \) though singular but integrable and does not contribute into the integral.

For the matrix \( G_{jj'}(\nu \nu') \) we have from (67), (90) and (92)

\[ G_{jj'}(\nu \nu') = \delta_{jj'} G_j(\nu \nu') + \tilde{G}_{jj'}(\nu \nu') \]

(95)

with

\[ G_j(\nu \nu') = -4 \pi \sum_q e^{i q (\nu \nu') / |\rho_\nu - \rho_{\nu'}|}, \]

(96)

\[ \tilde{G}_{jj'}(\nu \nu') = -4 \pi \sum_q \tilde{\chi}_{jj'}(\nu \nu', k - q, \omega) \]

(97)

where Fourier transform of \( \tilde{\chi}_{jj'}(\nu \nu', \kappa, t) \) (91) is introduced.

The scattering amplitudes in reaction channels (75) in the new notations are given by

\[ f_{ij}(k, k') = - \sum_{j' \nu'} e^{-i k \rho_{\nu'}} \langle j | e^{i (k - k') \hat{u}_\nu} | j' \rangle \psi_j(\nu) \beta_{\nu'}. \]

(98)

The scattering probability can be found with (98) and (80) or directly from (84) with (93) and (94).

Remark. In Appendix we obtain an alternative form of (94) and (98), which may be useful for some approximations.

8 Unitarity condition

The flux of neutrons incident on the target should be equal to the total flux in all scattering and reaction channels. As will be proved in this section, this unitarity condition is satisfied by the general theory suggested.

It is convenient to rewrite general equation (94) for neutron amplitudes in the form

\[ \delta_{ij} e^{i k \rho_\nu} = \psi_j(\nu) + \sum_{j' \nu'} G_{jj'}(\nu \nu') \psi_{j'}(\nu') \beta_{\nu'}, \]

(99)

and after complex conjugation

\[ \delta_{ij} e^{-i k \rho_\nu} = \psi_j^*(\nu) + \sum_{j' \nu'} G_{jj'}^*(\nu \nu') \psi_{j'}^*(\nu') \beta_{\nu'}^*. \]

(100)
Multiplying (19) by \( \psi_j^*(\nu)\beta^*_\nu \) and (100) by \( \psi_j(\nu)\beta_\nu \), then summing over \( j, \nu \) and subtracting one equation from the other we get

\[
2i \text{Im} f_{ii}(k, k) = \sum_{j\nu} (-2i \text{Im}\beta_\nu)\psi_j^*(\nu)\psi_j(\nu) + \sum_{j\nu\nu'} \psi_j^*(\nu)\psi_j'(\nu')\beta^*_\nu\beta_\nu' \left( G_{jj'}(\nu\nu') - G^*_{jj'}(\nu'\nu) \right),
\]

where we take into account equation (98) for scattering amplitude.

The kernels \( G \) and \( G^* \), as seen from (67) and (92), differ only in path directions around the poles on complex \( q \) plane, and their difference can be presented in the form

\[
G_{jj'}(\nu\nu') - G^*_{jj'}(\nu'\nu) = -\frac{2\pi}{m} \sum_q e^{i\rho_k'k'} e^{i(k-q)\rho_k} \left( \hat{D}^{-1}_q - (\hat{D}^{-1}_q)^+ \right) e^{i(k-q)\rho_k} \langle j|\psi_j(\nu')|j'\rangle,
\]

where \( k' = k_{jj'}/k_{jj'} \).

Substituting this result in (101) and taking into account (98) we get total cross section \( \sigma_t \) as sum of capture cross section \( \sigma_c \) and total scattering cross section \( \sigma_s \):

\[
\sigma_t = \frac{4\pi}{k} \text{Im} f_{ii}(k, k) = \sigma_c + \sigma_s,
\]

where

\[
\sigma_c = \sum_{j\nu} \left(-\frac{4\pi \text{Im}\beta_\nu}{k}\right)|\psi_j(\nu)|^2,
\]

\[
\sigma_s = \sum_j k_j \int f_{ij}(k, k')^2 d\nu'.
\]

Note that capture cross section is determined by imaginary parts of scattering lengths \( \alpha_\nu \) and \( \beta_\nu = m\alpha_\nu/m_\nu \) (\(-4\pi \text{Im}\alpha/k \) is the capture cross section for free nucleus).

9 Interim summary

Let us sum up our results. To satisfy MST equations one has to find \( N \) state vectors \( \Psi_\nu \) and \( N \) operators \( \hat{t}_\nu \). We have reduced the problem to the set of linear equations (63) for numerical parameters \( \phi^j_\nu \). The price for this reduction is additional index \( j \) which arises due to introduction of unknown state vector \( |\nu\rangle \) for each target nucleus. However, if \( \phi^j_\nu = \langle j|\nu\rangle\phi_\nu \) are found then one can deduce \( \Psi_\nu \) and \( \hat{t}_\nu \).

Indeed, equations (71) and (73) were directly obtained from (14), where the left-hand side has the meaning of \( (R_\nu|\Psi_\nu) \). Following back from (61) to (14) one can deduce for \( \Psi_\nu \)

\[
|\Psi_\nu\rangle = |R_\nu\rangle e^{ikR_\nu} \frac{1}{\beta_\nu} (1 + i\alpha_\nu K_\nu) |\nu\rangle \phi_\nu,
\]
where
\[ \hat{K}_\nu = \sum_j |j\rangle\langle j| \hat{K}_{j\nu}. \] (108)

On the other hand, if to compare (69) with (10), one can obtain combination
\[ \hat{t}_\nu |\Psi_\nu\rangle = \frac{2\pi}{m} |R_\nu\rangle e^{i k \hat{R}_\nu} |\nu\rangle \phi_\nu. \] (109)

From (108) and (109) it follows for \( \hat{t}_\nu \)
\[ \hat{t}_\nu = \frac{2\pi}{m} |R_\nu\rangle e^{i k \hat{R}_\nu} \left( 1 + \frac{i \alpha_\nu \hat{K}_\nu}{\beta_\nu} e^{-i k \hat{R}_\nu} \right)^{-1} \beta_\nu e^{i k \hat{R}_\nu} |\nu\rangle. \] (110)

This expression for \( \hat{t}_\nu \) is rather complicated due to non-commuting in target space operators \( \hat{K}_\nu \) and \( \hat{R}_\nu \).

**Remark.** In (17) \( \Psi_\nu \) seems to be a state vector in \( N+1 \) dimensional space \((r, R)\). However, for short-range \( \hat{t}_\nu \) the total wave function \( \Psi_{k,i} \) is really determined by \( \Psi_\nu \) at \( r = R_\nu \). This part, in fact, is given by (107).

For fixed nuclei \( K_\nu \rightarrow k_\nu \) is the center-of-mass impact momentum and from (110) follows
\[ \langle r|\hat{t}_\nu|r'\rangle \rightarrow \frac{2\pi}{m} \frac{\beta_\nu}{1 + i \alpha_\nu k_\nu} \delta(r - R_\nu) \delta(r - r'), \] (111)

that, with the help of (2) and (62), coincides with Fermi pseudopotential [4]. Just in this approximation (8) and (9) follow from (10) and (11), respectively.

Fortunately, in general case all physical quantities can be obtained directly from the amplitudes \( \phi_j^\nu \) or \( \psi_j(\nu) \) and matrices \( \hat{t}_\nu \) are not needed. Thus we reduce MST equations (10) and (11) to systems (66) for \( \phi_j^\nu \) or (94) for \( \psi_j(\nu) \).

Let us emphasize, that the only approximations used so far are those for the interaction potential. It was assumed a short range and relatively deep, what is equivalent to scattering length approximation for the interaction.

A relation of our equations to the traditional theory for slow neutrons was demonstrated in section 6. For thermal and cold neutrons the structure of equations (66) may be radically simplified due to the physically justifiable neglect of rescattering of the secondary neutron waves in the target.

Our main goal here is UCN. A relation to the traditional theory for the (elastic) scattering of UCN will be in details considered below. Physically evident, that transition to that theory should occur by the neglect of the thermal motion of the target nuclei, which provides the radical simplification of the correlation function (89):
\[ \chi_{jj'}(\nu\nu', \kappa, t) \sim \delta_{jj'} e^{-i\kappa(\rho_\nu - \rho_{\nu'}).} \] (112)

The amplitudes of the thermal motion are indeed small as compared to the UCN wave length and the approximation (112) for \( \chi_{jj'} \) seems to be justified. But if the thermal motion is totally neglected it is no possibility for inelastic scattering. So, for inelastic processes we need to include the thermal motion but may hope for proper simplification since a perturbation procedure is justified.

The rest of the paper is devoted to a perturbational solution of the main equation (94) for \( \psi_j(\nu) \).
10 Expansion over the amplitudes of thermal vibrations

10.1 Zero order (elastic) approximation

In the long wave length limit ($\kappa u \ll 1$) it follows from (91)
\[ \tilde{\chi}_{jj'}(\nu\nu',\kappa,t) \ll 1, \] (113)
which in its turn leads to the inequality
\[ \tilde{G}_{jj'}(\nu\nu') \ll G_j(\nu\nu'). \] (114)

These inequalities open a possibility for the application of a perturbation theory.

Physically (113) and (114) mean that in this limit the basic process of neutron–target interaction is elastic scattering and the probability of inelastic processes is small.

If we neglect $\tilde{\chi}_{jj'}$ then we obtain from (94) an equation for the amplitude $\psi_j^{(0)}(\nu)$ in zero order approximation
\[ \psi_j^{(0)}(\nu) = \delta_{ij} e^{ik\rho_\nu} - \sum_{\nu'} G_j(\nu\nu') \psi_{j'}^{(0)}(\nu') \beta_{\nu'}. \] (115)

As seen from (115), the equations for different $j$ are separated, and since inhomogeneous term contains the factor $\delta_{ij}$, we have
\[ \psi_j^{(0)}(\nu) = \delta_{ij} \psi(\nu), \] (116)

where $\psi(\nu)$ is defined by the equation
\[ \psi(\nu) = e^{ik\rho_\nu} - \sum_{\nu'} G(\nu\nu') \psi(\nu') \beta_{\nu'} \] (117)
with the matrix
\[ G(\nu\nu') \equiv G_i(\nu\nu') = -4\pi \sum_q e^{iq(\rho_\nu-\rho_{\nu'})} = e^{ik|\rho_\nu-\rho_{\nu'}|}. \] (118)

Note, that singular real part of diagonal ($\nu' = \nu$) term in (118) as discussed after (94) should be extracted that results in $G(\nu\nu) = ik$.

The equation (117) is similar to formula (9) customary used for UCN in the target model with fixed (i.e. in fact, infinitely heavy) nuclei and transforms to it by redefinition $\Psi_k(\nu) = \psi(\nu)(1 + ik\beta_{\nu})$ (12). Its solution is basically simplified when the sum over $\nu$ is replaced by the integral over $\rho$. Then after acting on (117) with operator $\Delta + k^2$ it is reduced to Schrödinger equation with the potential
\[ U = 2\pi \frac{m}{n} n\beta, \] (119)
where the density of the target $n$ and scattering length $\beta$ may depend on $\rho$.

Formally, the equation (117) after replacement of the sum by integral $\sum_{\nu} \rightarrow \int n d\rho$, becomes of a linear integral type. Such a replacement, if useful, will be performed below without special notice. On the other hand, to make presentation of general formulae in more compact and transparent form it is useful to consider all $G(\nu\nu')$ as matrices, $\psi(\nu)$ and $e^{ik\rho_\nu}$ as columns, $\psi^*(\nu)$ and $e^{-ik\rho_\nu}$ as rows and omit summation indices $\nu$ and $\nu'$. In this notation (117) looks as
\[ \psi + G \psi \beta = e^{ik\rho}. \] (120)
As seen from (118), the kernel \( G(k, \nu\nu') \) depends on the absolute value \( k \), but a solution \( \psi(k, \nu) \) depends on the vector \( k \), defined by inhomogeneous term on the right-hand side.

The scattering amplitude (28) in zero order approximation is given by

\[
 f_{ij}^{(0)}(k, k') = -\delta_{ij} \psi(k, k'),
\]

where special notation is introduced for \( \beta \)-weighted Fourier-transform of the amplitude \( \psi(k, \nu) \)

\[
 \psi(k, q) = \sum_{\nu} e^{-i q \rho_{\nu}} \psi(k, \nu) \beta_{\nu}.
\]

Scattering probability (80) in zero order approximation is of the form

\[
 w^{(0)}(k, k') = \left(\frac{2\pi}{m}\right)^3 \frac{\delta(\omega)}{m^2} |\psi(k, k')|^2.
\]

Thus from (81) we obtain differential cross section of elastic scattering

\[
 \frac{d\sigma^{(0)}_{el}}{d\Omega} = |\psi(k, k')|^2,
\]

where \( |k'| = |k| \).

### 10.2 Approximations of the first and the second order. Inelastic scattering

Zero order amplitude given by (121) corresponds to elastic scattering. Thus, the probability (80) for inelastic scattering starts from the second order term which is determined by the first order scattering amplitude

\[
 w^{(2)}_{ie}(k, k') = 2\pi \sum_{j} \left| \frac{2\pi}{m} f_{ij}^{(1)}(k, k') \right|^2 \delta(\varepsilon_i - \varepsilon_j + \epsilon_k - \epsilon_{k'}).
\]

Introducing an expansion in \( \kappa u \) for neutron amplitudes

\[
 \psi_j(\nu) = \delta_{ij} \psi(\nu) + \psi_j^{(1)}(\nu) + \ldots,
\]

one obtains from (28)

\[
 f_{ij}^{(1)}(k, k') = -\psi_j^{(1)}(k, k') - \left( k^\sigma - k'^\sigma \right) \sum_{\nu} e^{-ik\rho_{\nu}} (j|\hat{u}_{\nu}^\sigma|j') \psi(\nu) \beta_{\nu},
\]

where the first term is \( \beta \)-weighted Fourier component (122) of the first order amplitudes \( \psi_j^{(1)} \) defined by the equation

\[
 \psi_j^{(1)} + G_j \psi_j^{(1)} \beta = -\tilde{G}_{jj'}^{(1)} \psi_{\beta}.
\]

Matrix \( \tilde{G}_{jj'}^{(1)}(\nu\nu') \) is the first order term which follows from (91) and (97)

\[
 \tilde{G}_{jj'}^{(1)}(\nu\nu') = (\nabla_{\nu} - ik^\sigma) \left( \langle j|\hat{u}_{\nu}^\sigma|j' \rangle G_j^{(1)}(\nu\nu') - G_j(\nu\nu') \langle j|\hat{u}_{\nu}^\sigma|j' \rangle \right),
\]

where \( \nabla_{\nu} = \partial / \partial \rho_{\nu}^\sigma \).
Fourier component $\psi_j^{(1)}(k,k')$ can be found without an explicit solution of equation (128). First, let us introduce the function

$$\tilde{\psi}(k',\nu) = \psi(-k',\nu),$$

(130)
determined by the equation

$$\tilde{\psi} + \beta \tilde{\psi}G = e^{-ik\rho},$$

(131)
where we consider $\tilde{\psi}$ as row, and $\tilde{G} = G_j(\nu\nu')$. Then, multiplying (128) by $\beta \tilde{\psi}$ from the left and using (131), we obtain in the left-hand side just the Fourier component that we are looking for. Therefore we have

$$\psi_j^{(1)}(k,k') = -\beta \tilde{\psi} G_{ji} \psi \beta.$$  

(132)

Right-hand side of this equation can be simplified with the help of (120), (131) and (129). Then, we finally obtain

$$\psi_j^{(1)}(k,k') = \sum_{\nu} \beta_{\nu} \langle j | \tilde{u}_{\nu'} | i \rangle \nabla_{\nu'} (\tilde{\psi}(\nu)\psi(\nu)) - i(k^\sigma - k'^\sigma) \sum_{\nu} e^{-ik\rho_{\nu}} \langle j | \tilde{u}_{\nu'} | i \rangle \psi(\nu) \beta_{\nu}. $$

(133)
Inserting (133) into (127) we get for the first order scattering amplitude

$$f_{ij}^{(1)}(k,k') = -\sum_{\nu} \beta_{\nu} \langle j | \tilde{u}_{\nu} | i \rangle \nabla_{\nu} (\tilde{\psi}(k',\nu)\psi(\nu)).$$

(134)

Remark. An alternative derivation of expressions (121) and (134) is given in Appendix. The probability of inelastic scattering (in the second order) follows from (125) and (134). Summation over $j$ can be explicitly performed according to

$$\sum_{j} e^{i(\epsilon_{j} - \epsilon_{k'} \nu) t} \langle i | \tilde{u}_{\nu'} | j \rangle \langle j | \tilde{u}_{\nu'} | i \rangle = \langle i | \tilde{u}_{\nu'}(t) \tilde{u}_{\nu'}(0) | i \rangle.$$  

(136)

This diagonal matrix element may exhibit a spatial dependence only as a function of $\rho_{\nu} - \rho_{\nu'}$ and therefore allows a Fourier transform

$$\langle i | \tilde{u}_{\nu'}(t) \tilde{u}_{\nu'}(0) | i \rangle = \sum_{q,\omega} e^{i(q \rho_{\nu} - q \rho_{\nu'}) - i\omega t} \Omega^{\sigma\tau}(q,(q,\omega)).$$

(137)

Then, we finally obtain for the probability of inelastic scattering

$$w_{ie}^{(2)}(k,k') =$$

$$= \frac{(2\pi)^3}{m^2} \sum_{q,\omega} \delta(\epsilon_k - \epsilon_{k'} - \omega) B^{\sigma\sigma^*}(q) B^\tau(q) \Omega^{\sigma\tau}(q,(q,\omega)).$$

(138)
where
\[ B(q) = \sum_\nu \beta_\nu e^{-iq\rho_\nu} \nabla_\nu (\bar{\psi}(k',\nu)\psi(k,\nu)). \] (139)

The cross section for neutron to lose energy \( \omega \) can be calculated from (82) and (138)
\[ \frac{d\sigma}{d\omega} = \frac{(2\pi)^2}{mk} \sum_{q,k} \delta(\epsilon_k - \epsilon_{k'} - \omega)B^\sigma*(q)B^\tau(q)\Omega^\sigma\tau(q,\omega). \] (140)

To disclose physical meaning of (140) it is instructive to compare it with corresponding expression which followed from (3). To make the comparison one should transform the correlation function \( \chi(\nu\nu',\kappa,\omega) \) to \( \Omega^\sigma\tau(q,\omega) \) (137). Expanding \( \chi(\nu\nu',\kappa,\omega) \) in \( \kappa \)u by the use of (88) and (89) we get
\[ \chi(\nu\nu',\kappa,\omega) = 2\pi \delta(\omega) e^{-i\kappa(\rho_\nu - \rho_{\nu'})} (1 - \langle (\kappa\hat{u}_\nu)^2 \rangle) + e^{-i\kappa(\rho_\nu - \rho_{\nu'})} \kappa^\sigma\kappa^\tau \int_{-\infty}^{+\infty} \langle i|\hat{u}_\nu^\sigma(t)\hat{u}_{\nu'}^\tau(0)||i \rangle e^{i\omega t} dt. \] (141)

Now it is easy to see that cross section with energy loss (see (81) and (82)), followed from (3) and (141), can be reduced to the form (140) with
\[ \tilde{B}(q) = i(k - k') \sum_\nu b_\nu e^{-iq\rho_\nu} e^{i(k-k')\rho_\nu} \] (142)

instead of \( B(q) \) (139). The difference (apart from factor \( N \)) is that functions \( \psi(k,\nu) \) and \( \bar{\psi}(k',\nu) \) in (139) are replaced by the plane waves \( e^{ik\rho_\nu} \) and \( e^{-ik'\rho_\nu} \), respectively. It is very natural since (3) is obtained in Born approximation.

So, one may say that (140), similar to (3), takes into account interference of two scattered waves (that result in inelasticity), but in addition uses wave functions in both input and output channels modified by rescattering.

The idea to modify (3) for UCN by replacing plane waves with solutions of equation (9) is very natural and was tried in several papers (see, e.g., [17]). But it is evident that if to do it in (142) the result will not coincide with (139).

### 11 Choice of correlation function

Inelastic processes with energy and momentum exchange between neutron and target are essentially determined by the dynamical properties of target matter, i.e. collective excitations that are suitable (for given conservation lows) to provide this exchange. Correlation function that enters into cross section just describes these dynamical properties. The physical meaning of correlation functions – description of space–time evolution of a fluctuation appeared at some moment in some position point.

The field of correlation functions is covered in a number of books and review articles (see, e.g., [3, 18, 19]). So, here we’ll just mention a few details necessary for what follows.

Our function (137) is related to density fluctuations
\[ \frac{1}{2\pi N} \left\langle \int \hat{n}(r' + r, t) \hat{n}(r', 0) dr' \right\rangle = \sum_{q,\omega} e^{iqr-i\omega t} S(q,\omega). \] (143)

Fourier transform \( S(q,\omega) \) (often denoted as ”dynamical structure factor”) can be shown to be connected with (137) by
\[ S(q',\omega) \simeq \frac{n}{2\pi} q^\sigma q^\tau \Omega^\sigma\tau(q,\omega), \] (144)
where the quantities \( q' \) and \( q \) are equal but for crystals may differ by a reciprocal lattice vector.

For simple model of harmonic crystal one can easily obtain (for phonon occupation factors \( n_q \gg 1 \))

\[
\Omega^{\sigma\tau}(q,\omega) \simeq \delta_{\sigma\tau} \frac{2T}{nM^2s^2} \frac{\pi}{|\omega|} \delta \left( q^2 - \frac{\omega^2}{s^2} \right),
\]

(145)

where \( T \) is temperature and \( s \) is velocity of sound.

Sound branch of excitation is effective for large energy and momentum transfer (say, from UCN to thermal), but very ineffective for small transfer (of the order of initial energy and momentum of UCN). The reason is in fact that neutron dispersion low \( \epsilon \sim vk \) is quite different from that of sound \( \omega = sq \) because for UCN \( v/s \sim 10^{-3} \) and one cannot satisfy two requirements \( \Delta \epsilon \sim \omega \) and \( \Delta k \sim q \) simultaneously. For small transfers we need excitations with small \( \omega \) and \( q \).

Limiting value of correlation function for \( \omega, q \to 0 \) is given by ”hydrodynamic value”

\[
\Omega^{\sigma\tau}(q,\omega) \simeq \frac{q^2 q'}{q^2} \frac{2T}{nM^2} \frac{\alpha D}{\omega^2 + D^2 q^4},
\]

(146)

where \( D \) is coefficient of any diffusion-like process, e.g., self- or thermo-diffusion coefficient (in the last case \( \alpha = c_p/c_v - 1 \), in the first case \( \alpha = 1 \)). At normal temperature parameter \( \alpha = c_p/c_v - 1 \) is of the scale of 10\(^{-2} \) for solids and of 10\(^{-1} \) for liquids.

Function (146) for fixed \( q \) has a pick value for \( \omega = 0 \) and width \( \sim Dq^2 \) in contrast to (145), where \( \omega \) and \( q \) are strongly coupled (\( \omega = sq \)). It is useful to introduce instead \( D \) a dimensionless parameter

\[
d = \frac{2mD}{\hbar},
\]

(147)

which appears if one considers dimensionless variables \( \omega/\epsilon_k \) and \( q/k \). One may expect that the optimal conditions for small energy \( \epsilon \sim \hbar \omega \) and momentum \( k \sim q \) transfer would be when this parameter \( d \) is of the scale of unity. In reality at normal temperature \( d \) varies from \( \sim 10^3 \) (metals with high thermoconductivity) to \( \sim 10^{-2} \) (self-diffusion in liquids).

The total correlation function include the phonon part (145) as well as all types of diffusion-like parts (146). All these parts are linearly summed in cross section and their contributions may be calculated separately.

12 Subbarrier inelastic scattering

To consider a specific inelastic scattering problem with general formula (140) one needs, first, to find zero order (elastic) neutron amplitudes for input and output channels \( \psi(k,\nu) \) and \( \tilde{\psi}(k',\nu) \) and, second, to choose a correlation function that is adequately describes collective excitations of target matter in energy–momentum domain of interest.

We consider, as illustrative example, scattering on thick uniform plane target when neutron energies in input and output channels are both below potential barrier. Let \( z \) axis is perpendicular to the surface of the target located at \( z > 0 \). After replacing discreet variable \( \nu \) by uniform \( \rho \), one can reduce integral equations (120) and (131) to Schrödinger equation

\[
(k^2 + \Delta)\psi(r) = u(z)\psi(r),
\]

(148)

where potential \( u(z) = 4\pi\beta n(z) \) is determined by the target density

\[
n(z) = \begin{cases} 
n, & z > 0, \\
0, & z < 0. 
\end{cases}
\]

(149)
Equations for the cross section contain the values of \( \psi(\mathbf{r}) \) and \( \bar{\psi}(\mathbf{r}) \) only inside the target, but solutions for them are determined by the inhomogeneous terms of integral equations (120) and (131), which for solutions of Schrödinger equation (148) have the meaning of waves incident on the target. We expand neutron momentum \( \mathbf{k} \) in input channel into components \( \mathbf{k}_\parallel \) and \( \mathbf{k}_\perp \mathbf{e}_z \) along and normal to the target surface. We use in what follows that \( k_\perp^2 \leq k^2 < u_0 = 4\pi \beta n \).

The solution of (148) for incident neutron in the region \( z > 0 \) is of the form

\[
\psi(\mathbf{r}) = t e^{i \mathbf{k}_\parallel \cdot \mathbf{r} - \alpha z}, \quad t = \frac{2k_\perp}{k_\perp + i\alpha}, \quad \alpha = \sqrt{u_0 - k_\perp^2}. \tag{150}
\]

Neutron momentum in output channel we also expand in sum of longitudinal and transverse components \( \mathbf{k}' = \mathbf{k}'_\parallel + \mathbf{k}'_\perp \mathbf{e}_z \). Thus for the elastic scattering amplitude (121) we get

\[
f^{(0)}(\mathbf{k}, \mathbf{k}') = -\psi(\mathbf{k}, \mathbf{k}') = 2\pi i k_\perp \delta^{(2)}(\mathbf{k}' - \mathbf{k}_\parallel) \frac{k'_\perp + i\alpha}{k_\perp + i\alpha}, \tag{151}
\]

where \( k'_\perp = k_\perp \) for transmission and \( k'_\perp = -k_\perp \) for reflection. Note, that here we take into account diffraction forward scattering (\( \mathbf{k}' = \mathbf{k} \)) which results from finite transverse size of a target (see remark related to equation (77)).

Substituting (151) into (124) and integrating over solid angle around the direction \( \mathbf{k}' = \mathbf{k}_\parallel - k_\perp \mathbf{e}_z \), we obtain zero order cross section of neutron elastic reflection from the semi-infinite target

\[
\sigma_R^{(0)} = S \frac{k_\perp}{k}. \tag{152}
\]

Here \( S \) is area of plain target surface, and \( k_\perp/k = \cos \theta \), where \( \theta \) is the angle of incidence. That is simply the whole target area seen from incident neutron direction. This result is natural for total reflection.

To calculate inelastic scattering to neutron state with momentum \( \mathbf{k}' \) we need the solution \( \bar{\psi}(\mathbf{k}', \mathbf{r}) = \psi(-\mathbf{k}', \mathbf{r}) \). Since subbarrier neutron in output channel is back scattered it is convenient to assume that \( \mathbf{k}' = \mathbf{k}_\parallel - k'_\perp \mathbf{e}_z \), where \( k'_\perp > 0 \). Thus

\[
\bar{\psi}(\mathbf{r}) = t' e^{-i \mathbf{k}_\parallel \cdot \mathbf{r} - \alpha' z}, \quad t' = \frac{2k'_\perp}{k'_\perp + i\alpha'}, \quad \alpha' = \sqrt{u_0 - k'_\perp^2}. \tag{153}
\]

Vector \( \mathbf{B} \) (132) is given by

\[
\mathbf{B}(\mathbf{q}) = n\beta(2\pi)^2 \delta^{(2)}(\mathbf{k}_\parallel - \mathbf{k}'_\parallel - \mathbf{q}_\parallel) T t' \frac{\mathbf{q}_\parallel + i(\alpha + \alpha') \mathbf{e}_z}{q_\perp - i(\alpha + \alpha')} \tag{154}
\]

For simplicity we neglect imaginary parts of amplitude \( \beta \) and potential \( u_0 \) related to radiative capture. Thus, when substituting (154) into (140) we will use

\[
t^* t = \frac{4k_\perp^2}{k_\perp^2 + \alpha^2} = \frac{k_\perp^2}{\pi n \beta}, \tag{155}
\]

and the same for \( t'^* t' \). Taking into account (72), one gets for inelastic cross section the following expression

\[
\frac{d\sigma^{(2)}_\text{ie}}{d\omega} = S \frac{k_\perp}{k} \frac{T}{n M s^2} \frac{k_\perp}{\pi^4 |\omega|^2} \int d\mathbf{k}' \delta(k'^2 + 2m\omega - k^2) \times
\]

\[
\times k'_\perp^2 \int d\mathbf{q} \delta^{(2)}(\mathbf{k}_\parallel - \mathbf{k}'_\parallel - \mathbf{q}_\parallel) \Lambda(k'_\perp, \mathbf{q}). \tag{156}
\]
Here
\[
\Lambda^{\text{ph}}(k'_\perp, q) = \pi \delta \left( q^2 - \frac{\omega^2}{s^2} \right) \frac{q^2}{q^2 + (\omega + \omega')^2} \]
for phonon correlation function (145) and
\[
\Lambda^{\text{hyd}}(k'_\perp, q) = \frac{\alpha \Gamma^2}{q^4 + \Gamma^4} \left( \frac{q^2}{q^2 + (\omega + \omega')^2} - \frac{q^2}{q^2} \right)
\]
for hydrodynamic one (146), where \( \Gamma = \sqrt{|\omega|/D} \).

Dividing the inelastic cross section over the transverse target area \( S k^2 / k \), we get differential probability per one bounce \( dw_{\text{ie}}/d\omega \) for neutron transition to the state with the energy \( \epsilon' = \epsilon - \omega \).

Integration in (156) over \( q'_\parallel \) removes two-dimensional delta-function. Then remaining delta-function allows to perform integration over \( k'_\parallel \). The result is
\[
ds_{\text{ie}} \frac{dw_{\text{ie}}}{d\omega} = \frac{T}{n M s^2} \frac{k_0}{\pi \sqrt{|\omega|}} \int_0^{\frac{k_0^2}{2m\omega}} k'_2 dk'_\perp \times \]
\[
\times \int_0^\pi d\varphi \int d^2 q \Lambda(k'_\perp, q),
\]
where one should keep in mind relations
\[
q^2 = k^2 + k'^2 - 2k k' \cos \varphi, \quad k^2 + k'^2 = k^2 - 2m\omega. \tag{160}
\]

For the phonon model one can easily proceed further using delta-function in \( \Lambda^{\text{ph}} \) and the small value of \( q^2 = q^2 + q'^2 = \omega^2 / s^2 \ll k^2 \). Integration gives
\[
ds_{\text{ie}} \frac{dw_{\text{ph}}}{d\omega} = \frac{2}{\pi} \frac{T}{n M s^2} \frac{k_0 \beta}{U} \frac{v_\perp}{s} \sqrt{\epsilon' - \epsilon_\parallel} \]
\[
\tag{161}
\]
where \( k_0 = \sqrt{2mU/\hbar^2} \) is the momentum at the potential barrier \( U \), \( v_\perp = v \cos \theta \) is the normal component of the incident neutron velocity, and \( \epsilon_\parallel = \epsilon \sin^2 \theta \) is the energy related to the incident neutron motion along the surface plane.

For the hydrodynamic model we can perform in (159) integration over \( q_\parallel \) by closing integration path in complex \( q_\parallel \) plane and suming over pole residues. Then it is useful to write the result in the form similar to (161)
\[
ds_{\text{ie}} \frac{dw_{\text{hyd}}}{d\omega} = \frac{2}{\pi} \frac{T}{n M s^2} \frac{k_0 \beta}{U} f(\epsilon, \theta, \epsilon', d), \tag{162}
\]
where dimensionless function \( f \), depending on \( \epsilon, \theta, \epsilon' \) and parameter \( d = 2mD/\hbar \), is given by
\[
f(\epsilon, \theta, \epsilon', d) = \frac{2}{\pi d} \frac{v_\perp}{v_0} \int_0^{\frac{k_0^2}{2m\omega}} k'_2 dk'_\perp \int_0^\pi d\varphi L(k'_\perp, \varphi). \tag{163}
\]
Here \( v_0 = \hbar k_0 / m \) is the boundary neutron velocity, and
\[
L(k'_\perp, \varphi) = \frac{\sqrt{3}}{\Gamma^3} \left( 1 - 4\lambda^2 \right)^{3/4} \times \]
\[
\times \left( \left( 1 + \frac{1}{\mu} \right) \frac{\mu^2 + \lambda^2}{1 + 2\mu + 2(\mu^2 - \lambda^2)} - \lambda (\lambda + 1) \right), \tag{164}
\]
Figure 1: Function $f(\epsilon, \theta, \epsilon', d)$ from (163) for fixed initial neutron energy $\epsilon = U/2$ and angle of incidence $\theta = \pi/4$ versus final neutron energy $\epsilon'$ and parameter $d$.

$$2\lambda^2 = \frac{q_\parallel^2}{q_\parallel^2 + \sqrt{q_\parallel^4 + \Gamma^4}}, \quad 2\mu^2 = \frac{(\varepsilon + \varepsilon')^2}{q_\parallel^2 + \sqrt{q_\parallel^4 + \Gamma^4}}. \quad (165)$$

To demonstrate the magnitude of the function $f$ (163) and its dependance on the final neutron energy $\epsilon'$ and parameter $d$ we have performed numerical calculation of double integral for typical values of initial neutron energy $\epsilon = U/2$ and angle of incidence $\theta = \pi/4$. The results are shown by solid lines in Fig.1 for $d \ll 1$ and in Fig.2 for $d \geq 0.1$.

It is seen that the spectrum of inelastically scattered neutrons has a peak in the vicinity of the initial neutron energy. In this region parameter $\Gamma = \sqrt{\omega}/D = k_0 \sqrt{|\epsilon' - \epsilon|/(Ud)}$ is small with respect to $\varepsilon + \varepsilon'$ and the main contribution into the integral comes from small $q_\parallel^2(k'_\perp, \varphi)$. Then one may simplify the function $L$ (164) by taking limit $\mu^2 \gg (\lambda^2, 1)$:

$$L \simeq \frac{1}{\sqrt{2}\Gamma^3} \frac{(1 - 4\lambda^2)^{3/4}}{1 + 2\lambda}, \quad (166)$$

which allows to evaluate in (163) all parameter dependence and obtain

$$f(\epsilon, \theta, \epsilon', d) \simeq C \frac{v_0}{v_1} \frac{1}{\sqrt{d}} \sqrt{\frac{\epsilon - \epsilon'}{|\epsilon' - \epsilon|}}. \quad (167)$$

Here $C = 0.47$ is the value of a dimensionless integral.

Approximation (167) is valid for $|\epsilon' - \epsilon| = |\omega| \ll Ud$, and for large parameter $d \gg 1$ (167) may give a good estimate not only for the small $\omega$ peak but for the whole subbarrier area (as seen from Fig.2).

Dependence on $\omega$ is governed mostly by the parameter $d$. For $d \ll 1$ the peak is more pronounced and, when $d$ decreases, becomes more narrow and high but with fixed (independent
Figure 2: Function $f(\epsilon, \theta, \epsilon', d)$ for fixed $\epsilon = U/2$ and $\theta = \pi/4$ versus final neutron energy $\epsilon'$ and parameter $d$. Solid lines – result of exact numerical calculation (163), dash lines – approximation (167).

on $d$ area. Indeed, using approximation (167) one obtains

$$w^{\text{hyd}}_{ie} = \int \frac{dw^{\text{hyd}}_{ie}}{d\omega} d\omega \simeq \frac{4C}{\pi} \frac{\alpha T}{Ms^2} \frac{k_{\perp} \beta}{U} \frac{1}{\sqrt{d}} \int_0^{U/d} \frac{\epsilon_{\perp}}{\omega} d\omega =$$

$$= \frac{8C}{\pi} \frac{\alpha T}{Ms^2} k_{\perp} \beta \sqrt{\frac{\epsilon_{\perp}}{U}}. \quad \text{(168)}$$

Contribution to the peak from phonon model can be neglected since it has smooth behaviour and contains a suppression factor $v/s \sim 10^{-3}$.

For $d > 1$ the small $\omega$ peak becomes less pronounced (see Fig.2) and the probability for neutron to remain under the barrier after inelastic scattering diminishes as $1/\sqrt{d}$ (since in (168) the upper limit of the integral is now $U$).

13 Conclusion

The general theory of neutron scattering is presented, valid for the whole domain of slow neutrons from thermal to ultracold. For thermal and cold neutrons, when the multiple scattering in the target can be neglected, the cross section is reduced to that known for thermal neutrons, which is determined mostly by correlation function for the target matter (section 6).

For UCN the rescattering is the dominant process, but the theory can be simplified by exploiting small parameter $\kappa u$, i.e. the ratio of the amplitude of thermal vibrations (for solid targets) or relaxation lengths (for liquids) to neutron wave length. In zero order approximation in $\kappa u$ (that is equivalent to the scattering on a target with infinitely heavy unmovable nuclei) it
follows the known equation for elastic scattering of UCN \([9]\). Dynamical processes in the target are taken into account in the next orders in \(\kappa u\) and result in inelastic scattering.

A detail analysis of inelastic scattering needs separate publication. Here in section \([12]\) a specific example was considered: scattering with small energy transfer when scattered neutron remains below potential barrier. This quantitative example allows to make some conclusions.

The value of cross section is very sensitive to correlation function used. Phonon model which gives main contribution for UCN excitation into thermal region is quite ineffective for small energy transfer when space-time correlation processes are determined mostly by relaxation (“hydrodynamic”) processes. So, the first condition to obtain reasonable theoretical result for cross section with small energy transfer is the choice of an adequate correlation function.

The second factor that needs a reasonable physical modeling is elastic potential suited for target matter in each specific experiment. Consistence, uniformity, possible existence of surface layers, presence of hydrogen and its distribution – all that may require a change of model potential and therefore the wave functions in input and output channels that enter the cross section.

All effects connected with neutron spin are outside of the scope of this work. For target nuclei with non zero spin the scattering length depends on spin-spin orientation. This would require only replacement in all formulae of scattering length \(\beta\) by weighted average value. (The same prescription is valid for isotope non-uniform target). For large wave length of UCN the averaging is well justified.

Neutron spin interaction with target electrons (“magnetic scattering”) does not present any specific difficulty, but require inclusion of new "spin-spin" correlation function.

Quite different feature have spin-flip processes. Physically interesting is calculation of depolarization probability for stored polarized UCN. This effect (as well as neutron capture \([105]\)) belongs to incoherent processes. They are not considered in this work. It is evident that incoherent processes can be considered by simple perturbation theory with "elastic" functions as zero approximation.

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Appendix: An alternative expression for scattering amplitude

We start with transformation of equation \([14]\). First, using the definition \([14]\) for the matrix \(G_{jj'}(\nu\nu')\) and the expression \([57]\) for the matrix \(\zeta_{jj'}(\nu\nu')\) one obtains for \(G_{jj'}(\nu\nu')\)

\[
G_{jj'}(\nu\nu') = \frac{2\pi}{m} \sum_q e^{iq(\rho_\nu - \rho_{\nu'})} \times \\
\times \langle j | e^{-i(k-q)u_{\nu'}} \tilde{P}_q^{-1} e^{i(k-q)u_{\nu'}} | j' \rangle.
\]  

(A1)

Then it is convenient to introduce the operators

\[
\rightarrow P_{jj'}(\nu) = \langle j | e^{-i(k+\nabla_{\nu})u_{\nu}} | j' \rangle,
\]

\[
\leftarrow P_{jj'}(\nu) = \langle j | e^{i(k-\nabla_{\nu})u_{\nu}} | j' \rangle,
\]  

(A2)

where arrows on operators \(P_{jj'}(\nu)\) denote direction for gradients to act on functions of \(\rho_{\nu}\). Thus, after evident transformation with the help of \([99]\) the matrix \(G_{jj'}(\nu\nu')\) takes the form

\[
G_{jj'}(\nu\nu') = \sum_{j''} \rightarrow P_{jj''} (\nu) \hat{G}_{jj''} (\nu\nu') \leftarrow P_{jj' \nu'} (\nu').
\]  

(A3)
Equation (A4) with the use of (A3) can be written as

$$\psi_j(\nu) + \sum_{j'j''\nu'} \overrightarrow{P}_{j''(\nu)} G_{j''(\nu\nu')} \overrightarrow{P}_{j'j''(\nu')} \psi_{j'}(\nu') \beta_{j'} =$$

$$= \delta_{ij} e^{ik\rho_\nu}. \tag{A4}$$

Note the action of operators $P_{j''(\nu)}$ on exponents with $k$ and $k'$

$$\overrightarrow{P}_{j''(\nu)} e^{ik\rho_\nu} = \delta_{j''j} e^{ik\rho_\nu},$$

$$e^{-ik'\rho_\nu} \overrightarrow{P}_{j''(\nu)} = e^{-ik'\rho_\nu} \langle j| e^{i(k-k')u_\nu} |j'\rangle. \tag{A5}$$

The scattering amplitude (A8), due to (A5), can be represented in the form

$$f_{ij}(k, k') = -\sum_{j'\nu} e^{-ik'\rho_\nu} \overrightarrow{P}_{j''(\nu)} \psi_{j'}(\nu) \beta_{\nu}. \tag{A6}$$

Now let act on all terms of (A4) by the operator $\overrightarrow{P}_{j''(\nu)}^{-1}$ and sum over $j$. The right-hand side, due to (A5), remains unchanged and we obtain a new form of general equation (A4) where the matrix $G_j(\nu\nu')$ is "open" from the left

$$\sum_{j''} \overrightarrow{P}_{j''(\nu)}^{-1} \psi_{j''}(\nu) + \sum_{j''\nu'} G_j(\nu\nu') \overrightarrow{P}_{j''j''(\nu')} \psi_{j''}(\nu') \beta_{j'} =$$

$$= \delta_{ij} e^{ik\rho_\nu}. \tag{A7}$$

We may now multiply (A7) from the left by $\beta_\nu \overrightarrow{\psi}_j^{(0)}(\nu)$, which is a solution of equation (A3), i.e.

$$\sum_\nu \beta_\nu \overrightarrow{\psi}_j^{(0)}(\nu) G_j(\nu\nu') = e^{-ik'\rho_\nu} - \overrightarrow{\psi}_j^{(0)}(\nu'). \tag{A8}$$

Then summing over $\nu$ we get with the help of (A8)

$$\sum_{j'\nu} \beta_\nu \overrightarrow{\psi}_j^{(0)}(\nu) \overrightarrow{P}_{j''(\nu)}^{-1} \psi_{j'}(\nu) +$$

$$+ \sum_{j'\nu} \left(e^{-ik'\rho_\nu} - \overrightarrow{\psi}_j^{(0)}(\nu)\right) \overrightarrow{P}_{j''j''(\nu')} \psi_{j'}(\nu) \beta_{j'} =$$

$$= \delta_{ij} \sum_\nu \beta_\nu \overrightarrow{\psi}_j^{(0)}(\nu) e^{ik\rho_\nu}. \tag{A9}$$

From (A6) and (A9) it follows for the scattering amplitude

$$f_{ij}(k, k') = -\delta_{ij} \sum_\nu \beta_\nu e^{ik\rho_\nu} \overrightarrow{\psi}_j^{(0)}(\nu) -$$

$$- \sum_{j'\nu} \left(\overrightarrow{\psi}_j^{(0)}(\nu) \overrightarrow{P}_{j''(\nu)} \psi_{j'}(\nu) \beta_{j'} -$$

$$- \beta_\nu \overrightarrow{\psi}_j^{(0)}(\nu) \overrightarrow{P}_{j''(\nu)}^{-1} \psi_{j'}(\nu)\right). \tag{A10}$$

where zero order term is explicitly extracted.
As the last step, we perform the action of the operators $P_{jj'}(\nu)$ on $\bar{\psi}_j^{(0)}(\nu)$ and $\psi_j(\nu)$ and arrive at desired relation between scattering amplitude and exact solution $\psi_j(\nu)$ of the general equation \eqref{94}.

\[ f_{ij}(k,k') = -\delta_{ij} \sum_{\nu} \beta_{i\nu} e^{ik\rho_{\nu}} \bar{\psi}_i^{(0)}(\nu) - \sum_{j'} \langle j| e^{iku_{\nu}} (\bar{\psi}_j^{(0)}(\nu_u) \psi_{j'}(\nu) - \bar{\psi}_j^{(0)}(\nu_u) \psi_{j'}(\nu - u_{\nu}) \beta_{\nu}| j' \rangle. \] \tag{A11}

An expansion of (A11) in $u_{\nu}$ gives in zero order (with the use of \eqref{130} and \eqref{122})

\[ f_{ij}^{(0)}(k,k') = -\delta_{ij} \psi(-k',-k), \] \tag{A12}

what, due to time reversal invariance, equals to \eqref{121}. The first order term in (A11) coincides with \eqref{134}.

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\[ f(\varepsilon', d) \]

\[ \varepsilon' / U \]

d=0.001

d=0.01

d=0.1
