Eur. Phys. J. B **15**, 59–75 (2000)

THE EUROPEAN PHYSICAL JOURNAL B
EDP Sciences

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

A.L. Barabanov[a] and S.T. Belyaev

Kurchatov Institute, 123182 Moscow, Russia

Received 21 July 1999

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.

PACS. 28.20.-v Neutron physics – 61.12.Bt Theories of diffraction and scattering

1 Introduction

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

Such a simple picture is justified when rescattering of secondary neutron waves in the target can be neglected. To estimate rescattering let us compare the amplitude of the secondary waves at some nucleus with that of incoming neutron wave (taken as unity). Secondary waves from the surrounding volume $\sim \lambda^3$ add coherently and result in total amplitude $\sim n\lambda^3(b/\lambda)$, where $n \sim 10^{22}\ \text{cm}^{-3}$ is the density of nuclei and $b \sim 10^{-12}$ cm is the neutron-nucleus scattering length. As long as

$$nb\lambda^2 \ll 1, \quad i.e. \quad \lambda \ll 100\ \text{nm}, \tag{1}$$

the rescattering can be neglected. For ultracold neutrons (UCN), when $\lambda \ge 10$ nm, the rescattering of neutron wave in media is very essential, and for the neutron wave vector k which satisfies $k^2 < 4\pi nb$, the rescattering becomes the dominant process and results in the total reflection from the surface of the target (of course, for positive b). Thus, the cases of thermal and ultracold neutron scattering differ from one another, and there are two separate theories for their description.

[a] e-mail: barab@pretty.mbslab.kiae.ru

For thermal neutron disregard of the rescattering allows to use Born approximation and to model neutron-nucleus interaction by Fermi pseudopotential

$$V(\mathbf{r}) = \sum_\nu V_\nu(\mathbf{r}-\mathbf{R}_\nu) = \sum_\nu \frac{2\pi\hbar^2}{m_\nu} a_\nu \delta(\mathbf{r}-\mathbf{R}_\nu). \tag{2}$$

Here $\mathbf{r}$ and $\mathbf{R}_\nu$ are the position vectors for a neutron with mass m and the νth nucleus with mass M_ν, respectively, $m_\nu = mM_\nu/(m+M_\nu)$ is their reduced mass, a_ν is the amplitude of neutron scattering on free nucleus, connected with the scattering length α_ν and impact momentum in the center-of-mass system k_ν, in linear on $k_\nu\alpha_\nu$ approximation (valid for slow neutrons), by

$$a_\nu = \alpha_\nu(1 - \mathrm{i}k_\nu\alpha_\nu). \tag{3}$$

For thermal neutrons double differential cross-section per one target nucleus is given by (see, *e.g.*, [1–3])

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{k'}{2\pi Nk}\sum_{\nu\nu'} b_\nu^* b_{\nu'}\chi(\nu\nu',\boldsymbol{\kappa},\omega). \tag{4}$$

Here $\chi(\nu\nu',\boldsymbol{\kappa},\omega)$ is the Fourier transform

$$\chi(\nu\nu',\boldsymbol{\kappa},\omega) = \int_{-\infty}^{+\infty} \chi(\nu\nu',\boldsymbol{\kappa},t)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t \tag{5}$$

of correlation function

$$\chi(\nu\nu',\boldsymbol{\kappa},t) = \langle i|\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{R}}_\nu(t)}\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{R}}_{\nu'}(0)}|i\rangle, \tag{6}$$

$\boldsymbol{\kappa} = \mathbf{k} - \mathbf{k}'$ and $\omega = \epsilon - \epsilon'$ are the neutron momentum and energy transfers. The quantity $b_\nu = (m/m_\nu)a_\nu$ is called the scattering amplitude on bound nucleus, and $\hat{\mathbf{R}}_\nu(t)$ is the time dependent Heisenberg operator of nuclear position.

The rescattering, *i.e.* multiple scattering of neutron wave in the target, which is a dominant process for UCN, does not allow to use Born approximation, and 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

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{r}} - \frac{m}{2\pi\hbar^2}\int \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}')\mathrm{d}^3r'. \quad (7)$$

With a formal use of the Fermi pseudo-potential (2) equation (7) transforms into

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{r}} - \sum_\nu b_\nu \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{R}_\nu|}}{|\mathbf{r}-\mathbf{R}_\nu|}\Psi_{\mathbf{k}}(\mathbf{R}_\nu). \quad (8)$$

The quantity $\Psi_{\mathbf{k}}(\mathbf{R}_\nu)$ seems to have the meaning of the neutron wave amplitude on the νth nucleus. This wave combines the incident wave and all reflected waves. Thus, the amplitudes $\Psi_{\mathbf{k}}(\mathbf{R}_\nu)$ are not known in advance, and consistent equations have to be formulated for these quantities. It is impossible to get the mentioned equations from (8) just by substitution for neutron position $\mathbf{r} = \mathbf{R}_\nu$ due to infinity in the 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):

$$\Psi_{\mathbf{k}}(\mathbf{R}_\nu) = \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu} - \sum_{\nu'\neq\nu} b_{\nu'} \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{R}_\nu-\mathbf{R}_{\nu'}|}}{|\mathbf{R}_\nu-\mathbf{R}_{\nu'}|}\Psi_{\mathbf{k}}(\mathbf{R}_{\nu'}). \quad (9)$$

The equations (8, 9) are today the basis for the whole theory of ultracold neutron interaction with matter (see, *e.g.*, [4–7]). 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 frames of fixed-nuclei model used for (8, 9) there are no inelastic processes, and traditional approach to their estimate is, first, to calculate distortion of incoming neutron wave by the target optical potential, and then consider its interaction with some dynamical excitations (phonons, surface waves etc.). Such an approach may be somehow justified for large energy transfer (say, from UCN to thermal domain). As for small energy changes, all estimates gave negligibly small values for probability, then strong theoretical justification seemed to be unimportant.

In recent years inelastic scattering of UCN attracts attention of experimenters and quantitative measurements of small energy changes (small "heating" and "cooling" of UCN – see, *e.g.*, [8,9]) become more and more precise. Behavior of UCN in traps may be influenced by many factors and each experiment needs its own close inspection. But in any case one needs a well based theory of inelastic scattering with proper account of dynamical processes in the trap substance. This appeal from experiments is the first motivation for this article.

The second motivation is purely theoretical. With different ways of looking at neutron scattering in two energy domains a general theory, valid for the whole energy range, seems to be very desirable.

Such a theory should allow expansion in rescattering on the thermal energy side, turn into (4) when the rescattering is completely neglected and provide corrections in the next terms. On the UCN side the theory should allow expansion in dynamical (thermal) motion in the target matter and give results for the fixed nuclei model at the first step, and for inelastic scattering at the next step.

General problem of neutron interaction with matter can be analyzed in the framework of multiple scattering theory (MST) [10–13]. MST deals with interaction of a projectile with many-body target. In this theory a formal solution of many-body problem takes the form

$$\Psi^{(+)} = \Psi^0 + \hat{D}^{-1}\sum_\nu \hat{t}_\nu \Psi_\nu, \quad (10)$$

with functions Ψ_ν defined by the set of linear equations

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

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

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

Here Ψ^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 wide spread opinion in the literature that (8, 9) are just the equations of MST (10, 11) for fixed nuclei target. In fact, they have similar structure but with some modeled t_ν. Consistent derivation of (10, 11) analogies for fixed nuclei target with realistic potentials was done in [14]. In any way, the target model with fixed nuclei can be applied only to elastic scattering. While UCN escape from vessels, which have been studied for many years, is due mainly to inelastic scattering. Now scattering of UCN with small energy and momentum transfers attracts the attention of experimenters as a promising tool for condensed matter studies [15].

A step from frozen to moving nuclei 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)). The practical content of MST is, in fact, a set of approximations applicable for different situations. They were analyzed, *e.g.*, in the monograph of Goldberger and Watson [11].

Attempts were made to consider inelastic processes for UCN by using one of approaches developed in MST (see, *e.g.*, [16]). However, the 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 higher than the characteristic energy of target particles ("weak coupling approximation");
(b) mean free path of projectile in the target is much longer than its wave-length;
(c) mean free path of projectile is much longer than the 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 as free one when colliding with the projectile. The second and the third condition allow to treat multiple scattering as sequential collisions and represent the result as a sum on number of collisions executed. Due to (b) the energy of projectile between successive collisions is a well-determined quantity, and due to (c) the target in each collision may be considered as 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 than the target temperature even for liquid helium.
(b) The usual definition of mean free path fails for UCN (elastic cross-section for mirror like potential is equal to the surface area S). Thus, one may use for this quantity a length of intrusion into the target, which is of the order of wave-length ~ 10 nm. It means that the 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 the solution of MST equations valid for the whole domain of slow neutrons (from thermal to ultracold), starting from realistic neutron-nucleus interaction. Equations (4, 8, 9) will follow from this theory as limiting cases. By the solution we mean the 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 final part of the paper. A more detailed analysis of inelastic scattering in connection with specific experiments needs a separate publication.

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

$$\left(\frac{\hat{\mathbf{p}}^2}{2m} + \hat{H}_{\rm t} + \hat{V}\right)|\Psi_{\mathbf{k},i}\rangle = E_{\mathbf{k},i}|\Psi_{\mathbf{k},i}\rangle, \quad \hat{V} = \sum_\nu \hat{V}_\nu. \tag{13}$$

Here $\hat{V}_\nu$ describes interaction of neutron with νth nucleus, $\hat{\mathbf{p}} = -{\rm i}\partial/\partial\mathbf{r}$ is the operator of neutron momentum, $E_{\mathbf{k},i} = \epsilon_\mathbf{k} + \varepsilon_i$ is the total energy as the sum of neutron energy $\epsilon_\mathbf{k} = k^2/2m$ in the state $|\mathbf{k}\rangle$ and the target initial energy ε_i in the state $|i\rangle$ that is the eigenstate of the target Hamiltonian $\hat{H}_{\rm t}$. Here and below we keep $\hbar = 1$ till final physical results.

Equation (13) can be written in integral form

$$|\Psi_{\mathbf{k},i}\rangle = |\Psi^0_{\mathbf{k},i}\rangle + \hat{D}^{-1}\sum_\nu \hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle, \tag{14}$$

where $|\Psi^0_{\mathbf{k},i}\rangle = |\mathbf{k}\rangle|i\rangle$ and $\hat{D}^{-1}$ is "Green function" with

$$\hat{D} = \frac{k^2}{2m} + \varepsilon_i - \frac{\hat{\mathbf{p}}^2}{2m} - \hat{H}_{\rm t} + {\rm i}\eta, \tag{15}$$

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

$$|\Psi_{\mathbf{k},i}\rangle - \hat{D}^{-1}\hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle = |\Psi^0_{\mathbf{k},i}\rangle + \hat{D}^{-1}\sum_{\nu'\neq\nu}\hat{V}_{\nu'}|\Psi_{\mathbf{k},i}\rangle. \tag{16}$$

Then, let us define a state vector $|\Psi_\nu\rangle$ and operator $\hat{t}_\nu$ by the relations

$$|\Psi_\nu\rangle = |\Psi_{\mathbf{k},i}\rangle - \hat{D}^{-1}\hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle, \tag{17}$$

$$\hat{t}_\nu|\Psi_\nu\rangle = \hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle. \tag{18}$$

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

$$\hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle = \hat{V}_\nu(|\Psi_{\mathbf{k},i}\rangle - \hat{D}^{-1}\hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle) + \hat{V}_\nu\hat{D}^{-1}\hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle, \tag{19}$$

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

$$\hat{t}_\nu|\Psi_\nu\rangle = \hat{V}_\nu|\Psi_\nu\rangle + \hat{V}_\nu\hat{D}^{-1}\hat{t}_\nu|\Psi_\nu\rangle. \tag{20}$$

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 $|\Psi_{\mathbf{k},i}\rangle$ or $|\Psi_\nu\rangle$ without any approximations. In our problem there are two main small 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 the energy of relative neutron-nucleus motion inside the interaction potential area. Thus, the s-wave function and its derivative, taken at the potential boundary, are independent of 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_ν is essential only in a small vicinity of $\mathbf{R}_\nu$. It differs from zero only when the absolute value of deviation $\mathbf{x} = \mathbf{r} - \mathbf{R}_\nu$ does not exceed the potential radius $r_{0\nu}$. Thus, using completeness of the neutron states $\sum_{\mathbf{r}} |\mathbf{r}\rangle\langle\mathbf{r}| = 1$ one has

$$\hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle = \sum_{\mathbf{x}} |\mathbf{R}_\nu + \mathbf{x}\rangle\langle\mathbf{R}_\nu + \mathbf{x}|\hat{V}_\nu|\Psi_{\mathbf{k},i}\rangle = \sum_{\mathbf{x}} |\mathbf{R}_\nu + \mathbf{x}\rangle V_\nu(\mathbf{x})\langle\mathbf{R}_\nu + \mathbf{x}|\Psi_{\mathbf{k},i}\rangle. \tag{21}$$

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

$$\sum_{\mathbf{R}} \longrightarrow \int \mathrm{d}\mathbf{R}, \quad \sum_{\mathbf{q}} \longrightarrow \int \frac{\mathrm{d}\mathbf{q}}{(2\pi)^3}, \quad \sum_{\omega} \longrightarrow \int \frac{\mathrm{d}\omega}{2\pi}\cdot \tag{22}$$

Using (21) one can transform (14) to

$$|\Psi_{\mathbf{k},i}\rangle = |\Psi^0_{\mathbf{k},i}\rangle + \hat{D}^{-1}\sum_{\nu}\sum_{\mathbf{x}} |\mathbf{R}_\nu + \mathbf{x}\rangle V_\nu(\mathbf{x})\langle\mathbf{R}_\nu + \mathbf{x}|\Psi_{\mathbf{k},i}\rangle. \tag{23}$$

After some rearrangement the scalar product of (16) with $\langle\mathbf{R}_\nu + \mathbf{x}|$ can be presented as

$$\begin{aligned}\langle\mathbf{R}_\nu + \mathbf{x}|\Psi_{\mathbf{k},i}\rangle &- \sum_{\mathbf{x}'}\langle\mathbf{R}_\nu + \mathbf{x}|\hat{D}^{-1}|\mathbf{R}_\nu + \mathbf{x}'\rangle V_\nu(\mathbf{x}')\langle\mathbf{R}_\nu + \mathbf{x}'|\Psi_{\mathbf{k},i}\rangle \\ &= \langle\mathbf{R}_\nu + \mathbf{x}|\Psi^0_{\mathbf{k},i}\rangle \\ &+ \sum_{\nu'\neq\nu}\sum_{\mathbf{x}'}\langle\mathbf{R}_\nu + \mathbf{x}|\hat{D}^{-1}|\mathbf{R}_{\nu'} + \mathbf{x}'\rangle V_{\nu'}(\mathbf{x}')\langle\mathbf{R}_{\nu'} + \mathbf{x}'|\Psi_{\mathbf{k},i}\rangle.\end{aligned} \tag{24}$$

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

Therefore, 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 latter 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 α_ν (the known physical quantity), the amplitude $\chi_\nu(r_{0\nu})$ remains the only free parameter.

Thus, one may hope to express the quantity $\langle\mathbf{R}_\nu + \mathbf{x}|\Psi_{\mathbf{k},i}\rangle$ 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 $\langle\mathbf{R}_\nu + \mathbf{x}|\Psi_{\mathbf{k},i}\rangle$ for $x = r_{0\nu}$ as "neutron function at the surface of νth 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 νth nucleus

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

$$\mathbf{r},\, \mathbf{R} \quad \longrightarrow \quad \mathbf{x} = \mathbf{r} - \mathbf{R}_\nu,\, \mathbf{R}, \tag{25}$$

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

$$\hat{H} = \hat{H}_\mathrm{n} + \hat{H}_\mathrm{t} - \frac{\hat{\mathbf{p}}_x\hat{\mathbf{P}}_\nu}{M_\nu}, \quad \hat{H}_\mathrm{n} = \frac{\hat{\mathbf{p}}_x^2}{2m_\nu} + V_\nu(x), \tag{26}$$

where $\hat{\mathbf{p}}_x = -\mathrm{i}\partial/\partial\mathbf{x}$, and $\hat{\mathbf{P}}_\nu = -\mathrm{i}\partial/\partial\mathbf{R}_\nu$ is the momentum operator of νth nucleus. We assume that the quantity $\mathbf{x}$ is small, therefore 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 $E_{\mathbf{k},i} = \mathbf{k}^2/2m + \varepsilon_i$. In Born approximation in the limit $x \to 0$ the solution has the form

$$\Psi_{\mathbf{k},i}(\mathbf{x}, \mathbf{R}) = \psi(\mathbf{x})\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}\Phi_i(\mathbf{R}), \tag{27}$$

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

$$\Psi_{\mathbf{k},i}(\mathbf{x}, \mathbf{R}) = \varphi(\mathbf{x})\mathrm{e}^{\mathrm{i}\mathbf{g}\mathbf{R}_\nu}\Phi_j(\mathbf{R}), \tag{28}$$

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

If we substitute (28) into Schrödinger equation with the Hamiltonian (26) and take into account that operator $\hat{\mathbf{P}}_\nu$ acts on $\Phi_j(\mathbf{R})$ as well as on the exponent, then we obtain the following equation for $\varphi(\mathbf{x})$

$$\left(\hat{H}_\mathrm{n} + \frac{\mathbf{g}^2}{2M_\nu} + \frac{\mathbf{g}\mathbf{G}_{j\nu}}{M_\nu}\right)\varphi - \frac{(\mathbf{g} + \mathbf{G}_{j\nu})\hat{\mathbf{p}}_x}{M_\nu}\varphi = (E_{\mathbf{k},i} - \varepsilon_j)\varphi, \tag{29}$$

where

$$\mathbf{G}_{j\nu} = \left(\hat{\mathbf{P}}_\nu \Phi_j\right)/\Phi_j. \qquad (30)$$

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

$$\left(\frac{1}{2m_\nu}\left[\hat{\mathbf{p}}_x - \frac{m_\nu}{M_\nu}(\mathbf{g}+\mathbf{G}_{j\nu})\right]^2 + V_\nu(x)\right)\varphi = E(\mathbf{R})\varphi, \qquad (31)$$

where

$$E(\mathbf{R}) = E_{\mathbf{k},i} - \varepsilon_j - \frac{g^2}{2m} + \frac{1}{2m_\nu}\left[\mathbf{g} - \frac{m_\nu}{M_\nu}(\mathbf{g}+\mathbf{G}_{j\nu})\right]^2. \qquad (32)$$

Formally, (31) is an equation only for the function φ, and its exact solution, as can be easily proved, may be presented in the form

$$\varphi(\mathbf{x}) = \exp\left(\mathrm{i}\frac{m_\nu}{M_\nu}(\mathbf{g}+\mathbf{G}_{j\nu})\mathbf{x}\right)\Psi(\mathbf{q},\mathbf{x}), \qquad (33)$$

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

$$\hat{H}_{\mathrm{n}}\Psi(\mathbf{q},\mathbf{x}) = \frac{q^2}{2m_\nu}\Psi(\mathbf{q},\mathbf{x}), \qquad (34)$$

and the scattering energy is defined from

$$\frac{q^2}{2m_\nu} = \varepsilon_i - \varepsilon_j + \frac{k^2-g^2}{2m} + \frac{1}{2m_\nu}\left[\mathbf{g} - \frac{m_\nu}{M_\nu}(\mathbf{g}+\mathbf{G}_{j\nu})\right]^2. \qquad (35)$$

Thus, the 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 $\mathbf{q}$ – impact momentum – through vector $\mathbf{G}_{j\nu}$ (30) depends on all coordinates of the target $\mathbf{R}$. 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 $\chi_\nu(x)/x$ of the scattering function $\Psi(\mathbf{q},\mathbf{x})$ is of importance and the dependence of χ_ν on q can be neglected. Therefore, expression (33) for small x is independent of $\mathbf{R}$ and gives the real solution in the form

$$\Psi_{\mathbf{k},i}(\mathbf{x},\mathbf{R})_{|x\to 0} \simeq \frac{\chi_\nu(x)}{x}\mathrm{e}^{\mathrm{i}\mathbf{g}\mathbf{R}_\nu}\Phi_j(\mathbf{R}). \qquad (36)$$

So far the target state j and intermediate neutron momentum $\mathbf{g}$ have not been 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

$$\Psi_{\mathbf{k},i}(\mathbf{r}=\mathbf{R}_\nu+\mathbf{x},\mathbf{R})_{|x\to 0} \simeq \frac{\chi_\nu(x)}{x}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}\langle\mathbf{R}|\nu\rangle, \qquad (37)$$

where

$$\langle\mathbf{R}|\nu\rangle \equiv \Phi_\nu(\mathbf{R}) = \sum_{\mathbf{g},j} C_\nu(\mathbf{g},j)\mathrm{e}^{\mathrm{i}(\mathbf{g}-\mathbf{k})\mathbf{R}_\nu}\Phi_j(\mathbf{R}). \qquad (38)$$

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

Expression (37) defines a local structure of the basic function $\Psi_{\mathbf{k},i}$ near the point $\mathbf{r} = \mathbf{R}_\nu$. It naturally contains a "background target function" $\Phi_\nu(\mathbf{R}) = \langle\mathbf{R}|\nu\rangle$, separately defined for each nucleus. This function differs from the initial state of the target $\Phi_i(\mathbf{R}) \equiv \langle\mathbf{R}|i\rangle$ due to perturbation by the neutron wave. The functions $\langle\mathbf{R}|\nu\rangle$ 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 $\mathbf{x}$ in (21). First, from (37) one finds

$$\langle\mathbf{R}_\nu+\mathbf{x}|\Psi_{\mathbf{k},i}\rangle \simeq \frac{\chi_\nu(x)}{x}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}|\nu\rangle. \qquad (39)$$

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

$$V_\nu(x)\chi_\nu(x) \simeq \frac{1}{2m_\nu}\frac{\mathrm{d}^2\chi_\nu(x)}{\mathrm{d}x^2}. \qquad (40)$$

Thus, the integration can be performed

$$\int V_\nu(x)\frac{\chi_\nu(x)}{x}\mathrm{d}\mathbf{x} = -\frac{2\pi}{m_\nu}\frac{\alpha_\nu\chi_\nu(r_{0\nu})}{\alpha_\nu - r_{0\nu}}, \qquad (41)$$

where we used the relation between scattering length α and the logarithmic derivative at the boundary of the potential $[\chi'/\chi]_{r=r_0} = -1/(\alpha - r_0)$. Combining (39, 41) we get

$$\sum_{\mathbf{x}} |\mathbf{R}_\nu+\mathbf{x}\rangle V_\nu(\mathbf{x})\langle\mathbf{R}_\nu+\mathbf{x}|\Psi_{\mathbf{k},i}\rangle = |\mathbf{R}_\nu\rangle\frac{2\pi}{m}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}|\nu\rangle\phi_\nu, \qquad (42)$$

where we have introduced the amplitude

$$\phi_\nu = -\frac{m}{m_\nu}\frac{\alpha_\nu\chi_\nu(r_{0\nu})}{\alpha_\nu - r_{0\nu}}. \qquad (43)$$

4 Equations for neutron amplitudes

In the previous section the integrals over $\mathbf{x}$ in (24) are expressed in terms of the amplitudes ϕ_ν and state vectors $|\nu\rangle$. Thus, with the use of (39) the equation (24) takes the form

$$\frac{\chi_\nu(x)}{x}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}|\nu\rangle - \langle\mathbf{R}_\nu+\mathbf{x}|\hat{D}^{-1}|\mathbf{R}_\nu\rangle\frac{2\pi}{m}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}|\nu\rangle\phi_\nu$$
$$= \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}|i\rangle + \sum_{\nu'\neq\nu}\langle\mathbf{R}_\nu|\hat{D}^{-1}|\mathbf{R}_{\nu'}\rangle\frac{2\pi}{m}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_{\nu'}}|\nu'\rangle\phi_{\nu'}. \qquad (44)$$

The small quantity x is left only in the terms with singularity $1/x$ and neglected elsewhere.

Note, that x in (44) is a free parameter, and for $x = r_{0\nu}$, when $\chi_\nu(r_{0\nu})$ and ϕ_ν are linked by (43), relation (44) may be regarded as a set of linear equations for ϕ_ν, but with operators in target states as coefficients could be hardly used for practical calculations. Our next steps are directed to simplification of (44).

It is useful to transform the terms with $\hat{D}^{-1}$ as follows

$$\langle \mathbf{R}|\hat{D}^{-1}|\mathbf{R}'\rangle = \sum_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{R}} \hat{D}_q^{-1} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}'}, \qquad (45)$$

where

$$\hat{D}_q = \langle \mathbf{q}|\hat{D}|\mathbf{q}\rangle = \frac{k^2 - q^2}{2m} + \varepsilon_i - \hat{H}_\mathrm{t} + \mathrm{i}\eta. \qquad (46)$$

Then from (44) it is evident that to separate the amplitudes one should multiply both sides by $\mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{R}_\nu}$ and take their scalar product with the eigenvector $\langle j|$ of $\hat{H}_\mathrm{t}$. Thus, we have

$$\left[\frac{m_\nu}{m}\left(\frac{1}{\alpha_\nu} - \frac{1}{r_{0\nu}}\right)\langle j|\nu\rangle - \zeta_j(\nu\nu, \mathbf{x})_{|x\to r_{0\nu}}\right]\phi_\nu = \delta_{ij} + \sum_{\nu'\neq\nu} \zeta_j(\nu\nu', 0)\,\phi_{\nu'}, \qquad (47)$$

where

$$\zeta_j(\nu\nu', \mathbf{x}) = \frac{2\pi}{m}\sum_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}} \langle j|\mathrm{e}^{-\mathrm{i}(\mathbf{k}-\mathbf{q})\hat{\mathbf{R}}_\nu} \hat{D}_q^{-1} \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{q})\hat{\mathbf{R}}_{\nu'}}|\nu'\rangle. \qquad (48)$$

Expression (48) can be transformed into the other form with the use of the following presentation of the operator $\hat{D}_q^{-1}$

$$\hat{D}_q^{-1} = \frac{1}{\mathrm{i}}\int_0^\infty \mathrm{e}^{\mathrm{i}(\epsilon_\mathbf{k} - \epsilon_\mathbf{q} + \varepsilon_i - \hat{H}_\mathrm{t} + \mathrm{i}\eta)t}\mathrm{d}t. \qquad (49)$$

Then we get the alternative expression for (48)

$$\zeta_j(\nu\nu', \mathbf{x}) = \frac{2\pi}{\mathrm{i}m} \times \sum_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}} \int_0^\infty \chi_j(\nu\nu', \mathbf{k}-\mathbf{q}, t)\,\mathrm{e}^{\mathrm{i}(\epsilon_\mathbf{k} - \epsilon_\mathbf{q} + \varepsilon_i - \varepsilon_j + \mathrm{i}\eta)t}\mathrm{d}t. \qquad (50)$$

Here the correlation function is introduced

$$\chi_j(\nu\nu', \boldsymbol{\kappa}, t) = \langle j|\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{R}}_\nu(t)} \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{R}}_{\nu'}(0)}|\nu'\rangle, \qquad (51)$$

which is a generalization of (6).

To make (47) fully determined, we only need to find an explicit expression for diagonal term $\zeta_j(\nu\nu, \mathbf{x})$ 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). This can be easily seen from simple scaling analysis. Let us introduce new variables and parameters

$$\mathbf{q}' = \mathbf{q}x, \quad \mathbf{k}' = \mathbf{k}x, \quad \varepsilon_i' - \varepsilon_j' = (\varepsilon_i - \varepsilon_j)x^2, \quad t' = t/x^2. \qquad (52)$$

Then small parameter x remains in (50) only as the common factor $1/x$ and inside χ_j in the argument of $\mathbf{R}_\nu(t'x^2)$.

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 $\mathbf{q}$ gives

$$\zeta_j(\nu\nu, \mathbf{x}) \simeq -\frac{\mathrm{e}^{\mathrm{i}k_j x}}{x}\langle j|\nu\rangle, \qquad (53)$$

where

$$k_j^2 = k^2 + 2m(\varepsilon_i - \varepsilon_j). \qquad (54)$$

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

However, this result is evidently wrong. Since it does not cancel the singularity $1/r_{0\nu}$ in the left-hand side of (47) due to the additional factor m_ν/m. Thus, the matrix element χ_j should be more accurately estimated.

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

$$\hat{\mathbf{R}}_\nu(t) \simeq \hat{\mathbf{R}}_\nu(0) + \frac{\hat{\mathbf{P}}_\nu t}{M_\nu}\cdot \qquad (55)$$

Each additional power in t will result in an additional factor x^2. After substitution of (55) into (51), the matrix element is calculated without any approximations. Using the identity $\exp(\hat{A})\exp(\hat{B}) = \exp(\hat{A} + \hat{B} + [\hat{A}, \hat{B}]/2)$, we obtain

$$\chi_j(\nu\nu, \mathbf{k}-\mathbf{q}, t)_{|t\to 0} \longrightarrow \langle j|\exp\left(-\mathrm{i}\left[\frac{(\mathbf{k}-\mathbf{q})\hat{\mathbf{P}}_\nu}{M_\nu} + \frac{(\mathbf{k}-\mathbf{q})^2}{2M_\nu}\right]t\right)|\nu\rangle. \qquad (56)$$

Then integration over time and elementary transformation give

$$\zeta_j(\nu\nu, \mathbf{x})_{|x\to 0} = 4\pi\frac{m_\nu}{m}\sum_{\mathbf{q}}\langle j|\frac{\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}}}{k_\nu^2 - q_\nu^2 + 2m_\nu(\varepsilon_i - \varepsilon_j) + \mathrm{i}\eta}|\nu\rangle, \qquad (57)$$

where

$$\mathbf{k}_\nu = \mathbf{k} - \frac{m_\nu}{M_\nu}(\hat{\mathbf{P}}_\nu + \mathbf{k}), \quad \mathbf{q}_\nu = \mathbf{q} - \frac{m_\nu}{M_\nu}(\hat{\mathbf{P}}_\nu + \mathbf{k}). \qquad (58)$$

The physical meaning of (58) is evident: $\mathbf{k}_\nu$ and $\mathbf{q}_\nu$ are the momenta in the center-of-mass system. This transition to the center-of-mass system provides additional factor m_ν/m.

Finally, integrating over $\mathbf{q}$ and taking into account only s-wave part in $\mathbf{x}$ we get

$$\zeta_j(\nu\nu, \mathbf{x})_{|x\to 0} = -\frac{m_\nu}{m}\left(\frac{1}{x}\langle j|\nu\rangle + \mathrm{i}\langle j|\hat{K}_{j\nu}|\nu\rangle\right), \tag{59}$$

where the operator $\hat{K}_{j\nu}$, defined from

$$\hat{K}_{j\nu}^2 = \left[\mathbf{k} - \frac{m_\nu}{M_\nu}(\hat{\mathbf{P}}_\nu + \mathbf{k})\right]^2 + 2m_\nu(\varepsilon_i - \varepsilon_j), \tag{60}$$

has the meaning of absolute value of the impact momentum in the center-of-mass system for the neutron and νth 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 the explicit form of equation (47) for the amplitudes ϕ_ν. 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

$$\frac{1}{\beta_\nu}\langle j|\nu\rangle\phi_\nu + \mathrm{i}\frac{m_\nu}{m}\langle j|\hat{K}_{j\nu}|\nu\rangle\phi_\nu = \delta_{ij} + \sum_{\nu'\neq\nu}\zeta_j(\nu\nu')\phi_{\nu'}, \tag{61}$$

where the renormalized scattering length ("on bound nucleus") is introduced

$$\beta_\nu = \frac{m}{m_\nu}\alpha_\nu. \tag{62}$$

With the use of (50) the matrix $\zeta_j(\nu\nu') \equiv \zeta_j(\nu\nu', 0)$ can be expressed in terms of Fourier transforms of correlation functions (51)

$$\zeta_j(\nu\nu') = 4\pi\sum_{\mathbf{q},\omega}\frac{\chi_j(\nu\nu', \mathbf{k}-\mathbf{q}, \omega)}{k_j^2 - q^2 - 2m\omega + \mathrm{i}\eta}\cdot \tag{63}$$

Now we note that any state vector $|\nu\rangle$ can be presented as a series in target eigenfunctions

$$|\nu\rangle = \sum_j |j\rangle\langle j|\nu\rangle. \tag{64}$$

Therefore the relations (61) are really the linear equations for the amplitudes

$$\phi_\nu^j = \langle j|\nu\rangle\phi_\nu. \tag{65}$$

Indeed, we get

$$\frac{1}{\beta_\nu}\phi_\nu^j + \mathrm{i}\frac{m_\nu}{m}\sum_{j'}\langle j|\hat{K}_{j\nu}|j'\rangle\phi_\nu^{j'} = \delta_{ij} + \sum_{j',\nu'\neq\nu}\zeta_{jj'}(\nu\nu')\phi_{\nu'}^{j'}. \tag{66}$$

The coefficients of these equations

$$\begin{aligned}\zeta_{jj'}(\nu\nu') &= \frac{2\pi}{m}\sum_{\mathbf{q}}\langle j|\mathrm{e}^{-\mathrm{i}(\mathbf{k}-\mathbf{q})\hat{\mathbf{R}}_\nu}\hat{D}_q^{-1}\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{q})\hat{\mathbf{R}}_{\nu'}}|j'\rangle \\ &= 4\pi\sum_{\mathbf{q},\omega}\frac{\chi_{jj'}(\nu\nu', \mathbf{k}-\mathbf{q}, \omega)}{k_j^2 - q^2 - 2m\omega + \mathrm{i}\eta}\end{aligned} \tag{67}$$

with

$$\chi_{jj'}(\nu\nu', \boldsymbol{\kappa}, \omega) = \int_{-\infty}^{+\infty}\chi_{jj'}(\nu\nu', \boldsymbol{\kappa}, t)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t,$$

$$\chi_{jj'}(\nu\nu', \boldsymbol{\kappa}, t) = \langle j|\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{R}}_\nu(t)}\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{R}}_{\nu'}(0)}|j'\rangle, \tag{68}$$

are completely determined by the properties of target matter, *i.e.* by the matrix elements of the operator of νth and ν'th nuclei position correlation between the target eigenfunctions.

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

$$|\Psi_{\mathbf{k},i}\rangle = |\Psi_{\mathbf{k},i}^0\rangle + \hat{D}^{-1}\sum_{j,\nu}|\mathbf{R}_\nu\rangle\frac{2\pi}{m}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}|j\rangle\phi_\nu^j. \tag{69}$$

It means that scattering probability and scattering cross-section are also determined by ϕ_ν^j. The relation between them is analyzed 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 the jth reaction channel. The wave function in the jth channel can naturally be defined by

$$\Psi_{ij}(\mathbf{r}) = \langle\mathbf{r}, j|\Psi_{\mathbf{k},i}\rangle. \tag{70}$$

From (69) it follows

$$\Psi_{ij}(\mathbf{r}) = \delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{r}} + \frac{2\pi}{m}\langle j|\sum_{j',\nu}\phi_\nu^{j'}\langle\mathbf{r}|\hat{D}^{-1}|\mathbf{R}_\nu\rangle\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}_\nu}|j'\rangle. \tag{71}$$

Then using (45, 46) we have

$$\Psi_{ij}(\mathbf{r}) = \delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{r}} + 4\pi\sum_{j',\nu}\phi_\nu^{j'}\langle j|\sum_{\mathbf{q}}\frac{\mathrm{e}^{\mathrm{i}\mathbf{q}(\mathbf{r}-\hat{\mathbf{R}}_\nu)}}{k_j^2 - q^2 + \mathrm{i}\eta}\mathrm{e}^{\mathrm{i}\mathbf{k}\hat{\mathbf{R}}_\nu}|j'\rangle, \tag{72}$$

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

$$\Psi_{ij}(\mathbf{r}) = \delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{r}} - \sum_{j',\nu}\phi_\nu^{j'}\langle j|\frac{\mathrm{e}^{\mathrm{i}k_j|\mathbf{r}-\hat{\mathbf{R}}_\nu|}}{|\mathbf{r}-\hat{\mathbf{R}}_\nu|}\mathrm{e}^{\mathrm{i}\mathbf{k}\hat{\mathbf{R}}_\nu}|j'\rangle. \tag{73}$$

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

$$f_{ij}(\mathbf{k}, \mathbf{k}_j)\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}, \tag{74}$$

where the scattering amplitudes in reaction channels are given by

$$f_{ij}(\mathbf{k},\mathbf{k}') = -\sum_{j',\nu}\phi_\nu^{j'}\langle j|\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\hat{\mathbf{R}}_\nu}|j'\rangle. \qquad (75)$$

The final momentum $\mathbf{k}' \equiv \mathbf{k}_j$ is defined by $\mathbf{k}_j = k_j(\mathbf{r}/r)$.

It is instructive to note that in Born approximation with pseudopotential (2) the following expression for the scattering amplitude can be obtained:

$$f_{ij}(\mathbf{k},\mathbf{k}') = -\sum_\nu b_\nu\langle j|\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\hat{\mathbf{R}}_\nu}|i\rangle. \qquad (76)$$

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

Remark. A typical target model used for ultracold neutron reflection is a 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. Therefore, we shall assume our target to be finite with some plane surface area S, which is large enough to use in parallel planes the continuum spectrum, orto-normalized with $\delta(\mathbf{k}'_\parallel - \mathbf{k}_\parallel)$ instead of $\delta_{\mathbf{k}'_\parallel\mathbf{k}_\parallel}$, but allows us, when necessary, to make the replacement

$$\left[(2\pi)^2\delta(\mathbf{k}'_\parallel - \mathbf{k}_\parallel)\right]^2 \longrightarrow S(2\pi)^2\delta(\mathbf{k}'_\parallel - \mathbf{k}_\parallel). \qquad (77)$$

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 $i \to j$ can be obtained from the scattering amplitude by

$$\mathrm{d}\sigma_{ij} = \frac{k'}{k}|f_{ij}(\mathbf{k},\mathbf{k}')|^2\mathrm{d}\Omega', \qquad (78)$$

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

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega'\mathrm{d}\epsilon'} = \frac{k'}{k}\sum_j|f_{ij}(\mathbf{k},\mathbf{k}')|^2\delta(\varepsilon_i - \varepsilon_j + \epsilon_\mathbf{k} - \epsilon_{\mathbf{k}'}). \qquad (79)$$

It is useful to consider the quantity

$$w(\mathbf{k},\mathbf{k}') = \sum_j\left|\frac{2\pi}{m}f_{ij}(\mathbf{k},\mathbf{k}')\right|^2 2\pi\delta(\varepsilon_i - \varepsilon_j + \epsilon_\mathbf{k} - \epsilon_{\mathbf{k}'}), \qquad (80)$$

then $w(\mathbf{k},\mathbf{k}')\mathrm{d}\mathbf{k}'/(2\pi)^3$ 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 $\mathrm{d}\mathbf{k}'$. The scattering probability (80) 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

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

So, the cross-section of inelastic scattering with energy loss ω is given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = \frac{m}{k}\int w(\mathbf{k},\mathbf{k}')\delta(\epsilon_\mathbf{k} - \epsilon_{\mathbf{k}'} - \omega)\frac{\mathrm{d}\mathbf{k}'}{(2\pi)^3}\cdot \qquad (82)$$

Replacing delta-function in (80) by the integral over t and using (75) one can sum in (80) over the final states j as

$$\sum_{j''}\mathrm{e}^{\mathrm{i}(\varepsilon_j - \varepsilon_{j''})t}\langle j|\mathrm{e}^{-\mathrm{i}(\mathbf{k}-\mathbf{k}')\hat{\mathbf{R}}_\nu}|j''\rangle\langle j''|\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\hat{\mathbf{R}}_{\nu'}}|j'\rangle = \chi_{jj'}(\nu\nu',\mathbf{k}-\mathbf{k}',t), \qquad (83)$$

where $\chi_{jj'}(\nu\nu',\boldsymbol{\kappa},t)$ (as well as its Fourier transform) was introduced by (68). Then (80) takes the form

$$w(\mathbf{k},\mathbf{k}') = \left(\frac{2\pi}{m}\right)^2 \times\sum_{jj'\nu\nu'}\phi_\nu^{j*}\phi_{\nu'}^{j'}\chi_{jj'}(\nu\nu',\mathbf{k}-\mathbf{k}',\omega+\varepsilon_i-\varepsilon_j). \qquad (84)$$

The corresponding equation for the double differential cross-section is

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{k'}{2\pi k}\sum_{jj'\nu\nu'}\phi_\nu^{j*}\phi_{\nu'}^{j'}\chi_{jj'}(\nu\nu',\mathbf{k}-\mathbf{k}',\omega+\varepsilon_i-\varepsilon_j). \qquad (85)$$

We have now the scattering amplitude (75) and scattering probability (84) expressed by the neutron amplitudes ϕ_ν^j, 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

$$\sqrt{4\pi n\alpha} \ll k \ll 1/\alpha, \qquad (86)$$

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

$$\phi_\nu^j = \delta_{ij}\frac{\beta_\nu}{1+\mathrm{i}\langle i|\hat{K}_{i\nu}|i\rangle\alpha_\nu} \simeq \delta_{ij}\beta_\nu\left(1 - \mathrm{i}\langle i|\hat{K}_{i\nu}|i\rangle\alpha_\nu\right), \qquad (87)$$

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), (87) contains the average value of this parameter over nuclear ensemble in the target. After substitution of (87) into (85) we obtain the known expression (4) 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 us suppose

$$\mathbf{R}_\nu = \boldsymbol{\rho}_\nu + \mathbf{u}_\nu, \tag{88}$$

where for solid state target $\boldsymbol{\rho}_\nu$ is the equilibrium position of the target nucleus, and $\mathbf{u}_\nu$ is the shift from the equilibrium. For liquids $\boldsymbol{\rho}_\nu$ and $\mathbf{u}_\nu$ may be understood as an average position and a fluctuation, respectively. Note, that index ν may be now replaced by $\boldsymbol{\rho}$. When useful we shall make such replacement without notice.

The matrix $\chi_{jj'}(\nu\nu',\boldsymbol{\kappa},t)$ is transformed now into

$$\chi_{jj'}(\nu\nu',\boldsymbol{\kappa},t) = \mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}\langle j|\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{u}}_\nu(t)}\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{u}}_{\nu'}(0)}|j'\rangle. \tag{89}$$

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

$$\chi_{jj'}(\nu\nu',\boldsymbol{\kappa},t) = \mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}\left(\delta_{jj'} + \tilde{\chi}_{jj'}(\nu\nu',\boldsymbol{\kappa},t)\right), \tag{90}$$

where

$$\tilde{\chi}_{jj'}(\nu\nu',\boldsymbol{\kappa},t) = \langle j|\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{u}}_\nu(t)}\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\hat{\mathbf{u}}_{\nu'}(0)} - 1|j'\rangle. \tag{91}$$

To simplify the equation (66) let us replace $\zeta_{jj'}(\nu\nu')$ (67) by a new matrix $G_{jj'}(\nu\nu')$ from

$$\zeta_{jj'}(\nu\nu') = -\mathrm{e}^{-\mathrm{i}\mathbf{k}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}G_{jj'}(\nu\nu'). \tag{92}$$

Then introducing the new amplitude

$$\psi_j(\nu) = \frac{1}{\beta_\nu}\phi^j_\nu \mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}, \tag{93}$$

we obtain the equation

$$\psi_j(\nu) = \delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu} - \sum_{j'\nu'} G_{jj'}(\nu\nu')\psi_{j'}(\nu')\beta_{\nu'}, \tag{94}$$

where the diagonal in ν and ν' term is of the form: $G_{jj'}(\nu\nu) = \mathrm{i}(m_\nu/m)\langle j|\hat{K}_{j\nu}|j'\rangle$. Note, that according to (59) this diagonal term is equal to $-\zeta_{jj'}(\nu\nu,\mathbf{x})$ 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 ν'. 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 does not contribute to the integral.

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

$$G_{jj'}(\nu\nu') = \delta_{jj'}G_j(\nu\nu') + \tilde{G}_{jj'}(\nu\nu') \tag{95}$$

with

$$G_j(\nu\nu') = -4\pi\sum_{\mathbf{q}}\frac{\mathrm{e}^{\mathrm{i}\mathbf{q}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}}{k_j^2 - q^2 + \mathrm{i}\eta} = \frac{\mathrm{e}^{\mathrm{i}k_j|\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'}|}}{|\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'}|}, \tag{96}$$

$$\tilde{G}_{jj'}(\nu\nu') = -4\pi\sum_{\mathbf{q},\omega}\mathrm{e}^{\mathrm{i}\mathbf{q}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}\frac{\tilde{\chi}_{jj'}(\nu\nu',\mathbf{k}-\mathbf{q},\omega)}{k_j^2 - q^2 - 2m\omega + \mathrm{i}\eta}, \tag{97}$$

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

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

$$f_{ij}(\mathbf{k},\mathbf{k}') = -\sum_{j',\nu}\mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu}\langle j|\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\hat{\mathbf{u}}_\nu}|j'\rangle\psi_{j'}(\nu)\beta_\nu. \tag{98}$$

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

Remark. In Appendix we obtain an alternative form of (94, 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 the general equation (94) for neutron amplitudes in the form

$$\delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu} = \psi_j(\nu) + \sum_{j'\nu'}G_{jj'}(\nu\nu')\psi_{j'}(\nu')\beta_{\nu'}, \tag{99}$$

and after complex conjugation as

$$\delta_{ij}\mathrm{e}^{-\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu} = \psi^*_j(\nu) + \sum_{j'\nu'}G^*_{jj'}(\nu\nu')\psi^*_{j'}(\nu')\beta^*_{\nu'}. \tag{100}$$

Multiplying (99) by $\psi^*_j(\nu)\beta^*_\nu$ and (100) by $\psi_j(\nu)\beta_\nu$, then summing over j, ν and subtracting one equation from the other we get

$$\begin{aligned}2\mathrm{i}\,\mathrm{Im}f_{ii}(\mathbf{k},\mathbf{k}) = &\sum_{j\nu}(-2\mathrm{i}\,\mathrm{Im}\beta_\nu)\psi^*_j(\nu)\psi_j(\nu)\\ &+\sum_{jj'\nu\nu'}\psi^*_j(\nu)\psi_{j'}(\nu')\beta^*_\nu\beta_{\nu'}\left(G_{jj'}(\nu\nu') - G^*_{j'j}(\nu'\nu)\right),\end{aligned} \tag{101}$$

where equation (98) for scattering amplitude is taken into account.

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

$$\begin{aligned}G_{jj'}(\nu\nu') - G^*_{j'j}(\nu'\nu) = &-\frac{2\pi}{m}\sum_{\mathbf{q}}\mathrm{e}^{\mathrm{i}\mathbf{q}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}\\ &\times\langle j|\mathrm{e}^{-\mathrm{i}(\mathbf{k}-\mathbf{q})\hat{\mathbf{u}}_\nu}\left(\hat{D}_q^{-1} - (\hat{D}_q^{-1})^+\right)\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{q})\hat{\mathbf{u}}_{\nu'}}|j'\rangle.\end{aligned} \tag{102}$$

Operator $\hat{D}_q^{-1}$ has the form $(a+\mathrm{i}\eta)^{-1}$ and due to the equality $(a+\mathrm{i}\eta)^{-1} = -\mathrm{i}\pi\delta(a) + \mathrm{P}(1/a)$ only the delta-function part remains in combination $\hat{D}_q^{-1} - (\hat{D}_q^{-1})^+$. Thus (102) is reduced to

$$G_{jj'}(\nu\nu') - G^*_{j'j}(\nu'\nu) = \frac{\mathrm{i}}{2\pi}\int \mathrm{d}\mathbf{n}'' \sum_{j''} k_{j''} \mathrm{e}^{\mathrm{i}\mathbf{k}_{j''}(\boldsymbol{\rho}_\nu - \boldsymbol{\rho}_{\nu'})} \times \langle j|\mathrm{e}^{-\mathrm{i}(\mathbf{k}-\mathbf{k}_{j''})\hat{\mathbf{u}}_\nu}|j''\rangle\langle j''|\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}_{j''})\hat{\mathbf{u}}_{\nu'}}|j'\rangle, \quad (103)$$

where $\mathbf{n}'' = \mathbf{k}_{j''}/k_{j''}$.

Putting this result in (101) and taking into account (98) we get total cross-section σ_t as a sum of capture cross-section σ_c and total scattering cross-section σ_s:

$$\sigma_\mathrm{t} = \frac{4\pi}{k}\mathrm{Im} f_{ii}(\mathbf{k},\mathbf{k}) = \sigma_\mathrm{c} + \sigma_\mathrm{s}, \quad (104)$$

where

$$\sigma_\mathrm{c} = \sum_{j\nu}\left(-\frac{4\pi\mathrm{Im}\beta_\nu}{k}\right)|\psi_j(\nu)|^2, \quad (105)$$

$$\sigma_\mathrm{s} = \sum_j \frac{k_j}{k}\int |f_{ij}(\mathbf{k},\mathbf{k}')|^2 \mathrm{d}\mathbf{n}'. \quad (106)$$

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

9 Interim summary

Let us sum up our results. To satisfy MST equations we have to find N state vectors Ψ_ν and N operators $\hat{t}_\nu$. The problem is reduced to the set of linear equations (66) for numerical parameters ϕ^j_ν. 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 Ψ_ν and $\hat{t}_\nu$.

Indeed, equations (61, 66) were directly obtained from (44), where the left-hand side has the meaning of $\langle\mathbf{R}_\nu|\Psi_\nu\rangle$. Following back from (61) to (44) one can deduce for Ψ_ν

$$|\Psi_\nu\rangle = |\mathbf{R}_\nu\rangle \mathrm{e}^{\mathrm{i}\mathbf{k}\hat{\mathbf{R}}_\nu}\frac{1}{\beta_\nu}\left(1+\mathrm{i}\alpha_\nu\hat{K}_\nu\right)|\nu\rangle\phi_\nu, \quad (107)$$

where

$$\hat{K}_\nu = \sum_j |j\rangle\langle j|\hat{K}_{j\nu}. \quad (108)$$

On the other hand, if to compare (69) with (10), one can obtain combination

$$\hat{t}_\nu|\Psi_\nu\rangle = \frac{2\pi}{m}|\mathbf{R}_\nu\rangle\mathrm{e}^{\mathrm{i}\mathbf{k}\hat{\mathbf{R}}_\nu}|\nu\rangle\phi_\nu. \quad (109)$$

From (108) and (109) it follows for $\hat{t}_\nu$

$$\hat{t}_\nu = \frac{2\pi}{m}|\mathbf{R}_\nu\rangle\mathrm{e}^{\mathrm{i}\mathbf{k}\hat{\mathbf{R}}_\nu}\left(1+\mathrm{i}\alpha_\nu\hat{K}_\nu\right)^{-1}\beta_\nu\mathrm{e}^{-\mathrm{i}\mathbf{k}\hat{\mathbf{R}}_\nu}\langle\mathbf{R}_\nu|. \quad (110)$$

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

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

For fixed nuclei $\hat{K}_\nu \to k_\nu$ is the center-of-mass impact momentum and from (110) it follows

$$\langle\mathbf{r}|\hat{t}_\nu|\mathbf{r}'\rangle \longrightarrow \frac{2\pi}{m}\frac{\beta_\nu}{1+\mathrm{i}\alpha_\nu k_\nu}\delta(\mathbf{r}-\mathbf{R}_\nu)\delta(\mathbf{r}-\mathbf{r}'), \quad (111)$$

that, with the help of (3, 62), coincides with Fermi pseudopotential (2). Just in this approximation (8, 9) follow from (10, 11), respectively.

Fortunately, in the general case all physical quantities can be obtained directly from the amplitudes ϕ^j_ν or $\psi_j(\nu)$ and matrices $\hat{t}_\nu$ are not needed. Thus we reduce MST equations (10, 11) to systems (66) for ϕ^j_ν 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 to be a short range and relatively deep, which is equivalent to scattering length approximation for the interaction.

The relation of our equations to the traditional theory for thermal 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. The relation to the traditional theory for (elastic) scattering of UCN will be considered in details below. It is physically evident, that transition to that theory should occur due to the neglect of the thermal motion of the target nuclei, which provides the radical simplification of the correlation function (89):

$$\chi_{jj'}(\nu\nu',\boldsymbol{\kappa},t) \simeq \delta_{jj'}\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}(\boldsymbol{\rho}_\nu - \boldsymbol{\rho}_{\nu'})}. \quad (112)$$

The amplitudes of the thermal motion are very small indeed as compared to the UCN wave-length and the approximation (112) for $\chi_{jj'}$ seams to be justified. But if the thermal motion is totally neglected there is no possibility for inelastic scattering. Thus, for inelastic processes we need to include the thermal motion but may expect proper simplification since 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 ($\boldsymbol{\kappa}\mathbf{u} \ll 1$) it follows from (91)

$$\tilde{\chi}_{jj'}(\nu\nu',\boldsymbol{\kappa},t) \ll 1, \quad (113)$$

which, in its turn, leads to the inequality

$$\tilde{G}_{jj'}(\nu\nu') \ll G_j(\nu\nu'). \tag{114}$$

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

Physically (113, 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

$$\psi_j^{(0)}(\nu) = \delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu} - \sum_{\nu'} G_j(\nu\nu')\psi_j^{(0)}(\nu')\beta_{\nu'}. \tag{115}$$

As seen from (115), the equations for different j are separated, and since inhomogeneous term contains the factor δ_{ij}, we have

$$\psi_j^{(0)}(\nu) = \delta_{ij}\psi(\nu), \tag{116}$$

where $\psi(\nu)$ is defined by the equation

$$\psi(\nu) = \mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu} - \sum_{\nu'} G(\nu\nu')\psi(\nu')\beta_{\nu'} \tag{117}$$

with the matrix

$$G(\nu\nu') \equiv G_i(\nu\nu') = -4\pi \sum_{\mathbf{q}} \frac{\mathrm{e}^{\mathrm{i}\mathbf{q}(\boldsymbol{\rho}_\nu - \boldsymbol{\rho}_{\nu'})}}{k^2 - q^2 + \mathrm{i}\eta} = \frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{\rho}_\nu - \boldsymbol{\rho}_{\nu'}|}}{|\boldsymbol{\rho}_\nu - \boldsymbol{\rho}_{\nu'}|} \cdot \tag{118}$$

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

The equation (117) is similar to formula (9) usually used for UCN in the target model with fixed (*i.e.* in fact, infinitely heavy) nuclei and transforms to it by redefinition $\Psi_{\mathbf{k}}(\nu) = \psi(\nu)(1 + \mathrm{i}k\beta_\nu)$ [14]. Its solution is basically simplified when the sum over ν is replaced by the integral over $\boldsymbol{\rho}$. Then after acting on (117) with operator $\Delta + k^2$ it is reduced to Schrödinger equation with the potential

$$U = \frac{2\pi}{m} n\beta, \tag{119}$$

where the density of the target n and scattering length β may depend on $\boldsymbol{\rho}$.

Formally, equation (117) after replacement of the sum by integral $\sum_\nu \to \int n\mathrm{d}\boldsymbol{\rho}$ 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 $\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}$ – as columns, $\psi^*(\nu)$ and $\mathrm{e}^{-\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}$ – as rows and omit summation indices ν and ν'. In this notation (117) looks as

$$\psi + G\psi\beta = \mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}}. \tag{120}$$

As seen from (118), the kernel $G(k, \nu\nu')$ depends on the absolute value k, but the solution $\psi(\mathbf{k}, \nu)$ depends on the vector $\mathbf{k}$, defined by inhomogeneous term on the right-hand side.

The scattering amplitude (98) in zero order approximation is given by

$$f_{ij}^{(0)}(\mathbf{k}, \mathbf{k}') = -\delta_{ij}\psi(\mathbf{k}, \mathbf{k}'), \tag{121}$$

where special notation is introduced for β-weighted Fourier-transform of the amplitude $\psi(\mathbf{k}, \nu)$

$$\psi(\mathbf{k}, \mathbf{q}) = \sum_\nu \mathrm{e}^{-\mathrm{i}\mathbf{q}\boldsymbol{\rho}_\nu}\psi(\mathbf{k}, \nu)\beta_\nu. \tag{122}$$

Scattering probability (80) in zero order approximation has the form

$$w^{(0)}(\mathbf{k}, \mathbf{k}') = \frac{(2\pi)^3}{m^2}\delta(\omega)\left|\psi(\mathbf{k}, \mathbf{k}')\right|^2. \tag{123}$$

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

$$\frac{\mathrm{d}\sigma_{\mathrm{el}}^{(0)}}{\mathrm{d}\Omega} = \left|\psi(\mathbf{k}, \mathbf{k}')\right|^2, \tag{124}$$

where $|\mathbf{k}'| = |\mathbf{k}|$.

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

$$w_{ie}^{(2)}(\mathbf{k}, \mathbf{k}') = 2\pi \sum_j \left|\frac{2\pi}{m} f_{ij}^{(1)}(\mathbf{k}, \mathbf{k}')\right|^2 \delta(\varepsilon_i - \varepsilon_j + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}). \tag{125}$$

Introducing an expansion in $\boldsymbol{\kappa}\mathbf{u}$ for neutron amplitudes

$$\psi_j(\nu) = \delta_{ij}\psi(\nu) + \psi_j^{(1)}(\nu) + \ldots, \tag{126}$$

we obtain from (98)

$$f_{ij}^{(1)}(\mathbf{k}, \mathbf{k}') = -\psi_j^{(1)}(\mathbf{k}, \mathbf{k}') - \mathrm{i}(k^\sigma - k'^\sigma)\sum_\nu \mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu}\langle j|\hat{u}_\nu^\sigma|i\rangle\psi(\nu)\beta_\nu, \tag{127}$$

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

$$\psi_j^{(1)} + G_j\psi_j^{(1)}\beta = -\tilde{G}_{ji}^{(1)}\psi\beta. \tag{128}$$

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

$$\tilde{G}^{(1)}_{jj'}(\nu\nu') = (\nabla^\sigma_\nu - \mathrm{i}k^\sigma)\left(\langle j|\hat{u}^\sigma_\nu|j'\rangle G_{j'}(\nu\nu') - G_j(\nu\nu')\langle j|\hat{u}^\sigma_{\nu'}|j'\rangle\right), \tag{129}$$

where $\nabla^\sigma_\nu = \partial/\partial\rho^\sigma_\nu$.

Fourier component $\psi^{(1)}_j(\mathbf{k},\mathbf{k}')$ can be found without an explicit solution of equation (128). First, let us introduce the function

$$\bar{\psi}(\mathbf{k}',\nu) = \psi(-\mathbf{k}',\nu), \tag{130}$$

determined by the equation

$$\bar{\psi} + \beta\bar{\psi}\bar{G} = \mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}}, \tag{131}$$

where we consider $\bar{\psi}$ as row, and $\bar{G}(\nu\nu') \equiv G_j(\nu\nu')$. Then, multiplying (128) by $\beta\bar{\psi}$ 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

$$\psi^{(1)}_j(\mathbf{k},\mathbf{k}') = -\beta\bar{\psi}\tilde{G}^{(1)}_{ji}\psi\beta. \tag{132}$$

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

$$\psi^{(1)}_j(\mathbf{k},\mathbf{k}') = \sum_\nu \beta_\nu\langle j|\hat{u}^\sigma_\nu|i\rangle\nabla^\sigma_\nu\left(\bar{\psi}(\nu)\psi(\nu)\right) - \mathrm{i}(k^\sigma - k'^\sigma)\sum_\nu \mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu}\langle j|\hat{u}^\sigma_\nu|i\rangle\psi(\nu)\beta_\nu. \tag{133}$$

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

$$f^{(1)}_{ij}(\mathbf{k},\mathbf{k}') = -\sum_\nu \beta_\nu\langle j|\hat{\mathbf{u}}_\nu|i\rangle\boldsymbol{\nabla}_\nu\left(\bar{\psi}(\mathbf{k}',\nu)\psi(\mathbf{k},\nu)\right). \tag{134}$$

Remark. An alternative derivation of expressions (121, 134) is given in Appendix.

The probability of inelastic scattering (in the second order) follows from (125, 134)

$$w^{(2)}_{\mathrm{ie}}(\mathbf{k},\mathbf{k}') = \left(\frac{2\pi}{m}\right)^2 \sum_{j\nu\nu'}\beta^*_\nu\beta_{\nu'} \times \nabla^\sigma_\nu\left(\bar{\psi}(\mathbf{k}',\nu)\psi(\mathbf{k},\nu)\right)^*\nabla^\tau_{\nu'}\left(\bar{\psi}(\mathbf{k}',\nu')\psi(\mathbf{k},\nu')\right) \times \int_{-\infty}^{+\infty}\mathrm{e}^{\mathrm{i}(\varepsilon_i-\varepsilon_j+\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'})t}\langle i|\hat{u}^\sigma_\nu|j\rangle\langle j|\hat{u}^\tau_{\nu'}|i\rangle\mathrm{d}t. \tag{135}$$

Summation over j can be explicitly performed according to

$$\sum_j \mathrm{e}^{\mathrm{i}(\varepsilon_i-\varepsilon_j)t}\langle i|\hat{u}^\sigma_\nu|j\rangle\langle j|\hat{u}^\tau_{\nu'}|i\rangle = \langle i|\hat{u}^\sigma_\nu(t)\hat{u}^\tau_{\nu'}(0)|i\rangle. \tag{136}$$

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

$$\langle i|\hat{u}^\sigma_\nu(t)\hat{u}^\tau_{\nu'}(0)|i\rangle = \sum_{\mathbf{q},\omega}\mathrm{e}^{\mathrm{i}\mathbf{q}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})-\mathrm{i}\omega t}\,\Omega^{\sigma\tau}(\mathbf{q},\omega). \tag{137}$$

Then, we finally obtain for the probability of inelastic scattering

$$w^{(2)}_{\mathrm{ie}}(\mathbf{k},\mathbf{k}') = \frac{(2\pi)^3}{m^2} \times \sum_{\mathbf{q},\omega}\delta(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}-\omega)B^{\sigma*}(\mathbf{q})B^\tau(\mathbf{q})\Omega^{\sigma\tau}(\mathbf{q},\omega), \tag{138}$$

where

$$\mathbf{B}(\mathbf{q}) = \sum_\nu \beta_\nu\mathrm{e}^{-\mathrm{i}\mathbf{q}\boldsymbol{\rho}_\nu}\boldsymbol{\nabla}_\nu\left(\bar{\psi}(\mathbf{k}',\nu)\psi(\mathbf{k},\nu)\right). \tag{139}$$

The cross-section for neutron to lose energy ω can be calculated from (82, 138)

$$\frac{\mathrm{d}\sigma^{(2)}_{ie}}{\mathrm{d}\omega} = \frac{(2\pi)^2}{mk}\sum_{\mathbf{q},\mathbf{k}'}\delta(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}-\omega)B^{\sigma*}(\mathbf{q})B^\tau(\mathbf{q})\Omega^{\sigma\tau}(\mathbf{q},\omega). \tag{140}$$

To disclose physical meaning of (140) it is instructive to compare it with corresponding expression which can be obtained from (4). To make the comparison one should transform the correlation function $\chi(\nu\nu',\boldsymbol{\kappa},\omega)$ to $\Omega^{\sigma\tau}(\mathbf{q},\omega)$ (137). Expanding $\chi(\nu\nu',\boldsymbol{\kappa},\omega)$ in $\boldsymbol{\kappa}\mathbf{u}$ by the use of (88, 89) we get

$$\chi(\nu\nu',\boldsymbol{\kappa},\omega) = 2\pi\delta(\omega)\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}\left(1-\langle(\boldsymbol{\kappa}\hat{\mathbf{u}}_\nu)^2\rangle\right) + \mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}(\boldsymbol{\rho}_\nu-\boldsymbol{\rho}_{\nu'})}\kappa^\sigma\kappa^\tau\int_{-\infty}^{+\infty}\langle i|\hat{u}^\sigma_\nu(t)\hat{u}^\tau_{\nu'}(0)|i\rangle\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t. \tag{141}$$

Now it is easy to see that the cross-section with energy loss (see (81, 82)), obtained from (4, 141), can be reduced to the form (140) with

$$\tilde{\mathbf{B}}(\mathbf{q}) = \mathrm{i}(\mathbf{k}-\mathbf{k}')\sum_\nu b_\nu\mathrm{e}^{-\mathrm{i}\mathbf{q}\boldsymbol{\rho}_\nu}\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\boldsymbol{\rho}_\nu} \tag{142}$$

instead of $\mathbf{B}(\mathbf{q})$ (139). The difference (apart from factor N) is that functions $\psi(\mathbf{k},\nu)$ and $\bar{\psi}(\mathbf{k}',\nu)$ in (139) are replaced by the plane waves $\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}$ and $\mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu}$, respectively. It is very natural since (4) is obtained in Born approximation.

So, it can be said that (140), similar to (4), takes into account the 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 (4) for UCN by replacing the plane waves with the 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 the cross-section just describes these dynamical properties. The physical meaning of correlation function is that it describes 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]). Here we shall just mention a few details necessary for what follows.

Our function (137) is related to density fluctuations

$$\frac{1}{2\pi N}\langle\int \hat{n}(\mathbf{r}'+\mathbf{r},t)\hat{n}(\mathbf{r}',0)\mathrm{d}\mathbf{r}'\rangle = \sum_{\mathbf{q},\omega}\mathrm{e}^{\mathrm{i}\mathbf{qr}-\mathrm{i}\omega t}S(\mathbf{q},\omega). \quad (143)$$

Fourier transform $S(\mathbf{q},\omega)$ (often denoted as "dynamical structure factor") can be shown to be connected with (137) by

$$S(\mathbf{q}',\omega) \simeq \frac{n}{2\pi}q^\sigma q^\tau \Omega^{\sigma\tau}(\mathbf{q},\omega), \quad (144)$$

where the quantities $\mathbf{q}'$ and $\mathbf{q}$ 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 $n_\mathbf{q} \gg 1$)

$$\Omega^{\sigma\tau}(\mathbf{q},\omega) \simeq \delta_{\sigma\tau}\frac{2T}{nMs^2}\frac{\pi}{|\omega|}\delta\left(q^2-\frac{\omega^2}{s^2}\right), \quad (145)$$

where T is the temperature and s is the 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 ω and $\mathbf{q}$.

The limiting value of correlation function for $\omega, q \to 0$ is given by the "hydrodynamic value"

$$\Omega^{\sigma\tau}(\mathbf{q},\omega) \simeq \frac{q^\sigma q^\tau}{q^2}\frac{2T}{nMs^2}\frac{\alpha D}{\omega^2+D^2q^4}, \quad (146)$$

where D is the coefficient of any diffusion-like process, *e.g.*, the self- or thermo-diffusion coefficient (in the latter case $\alpha = c_P/c_V - 1$, in the former 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 ω and q are strongly coupled ($\omega = sq$). Instead of D it is useful to introduce a dimensionless parameter

$$d = \frac{2mD}{\hbar}, \quad (147)$$

which appears when dimensionless variables $\omega/\epsilon_\mathbf{k}$ and q/k are considered. 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 order 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 includes 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 can 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 $\psi(\mathbf{k},\nu)$ and $\bar{\psi}(\mathbf{k}',\nu)$ and, second, to choose a correlation function that adequately describes collective excitations of target matter in energy-momentum domain of interest.

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

$$(k^2+\Delta)\psi(\mathbf{r}) = u(z)\psi(\mathbf{r}), \quad (148)$$

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

$$n(z) = \begin{cases} n, & z>0,\\ 0, & z<0. \end{cases} \quad (149)$$

The 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, 131). For the solutions of Schrödinger equation (148) they have the meaning of waves incident on the target. We split the neutron momentum $\mathbf{k}$ in input channel into components $\mathbf{k}_\parallel$ and $k_\perp\mathbf{e}_z$ along and normal to the target surface. We assume in what follows that $k_\perp^2 \le k^2 < u_0 = 4\pi\beta n$.

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

$$\psi(\mathbf{r}) = t\mathrm{e}^{\mathrm{i}\mathbf{k}_\parallel\mathbf{r}_\parallel-æz}, \quad t = \frac{2k_\perp}{k_\perp+\mathrm{i}æ}, \quad æ = \sqrt{u_0-k_\perp^2}. \quad (150)$$

The neutron momentum in output channel is also split into longitudinal and transverse components

$\mathbf{k}' = \mathbf{k}'_{\|} + k'_{\perp}\mathbf{e}_z$. Thus for the elastic scattering amplitude (121) we get

$$f^{(0)}(\mathbf{k},\mathbf{k}') = -\psi(\mathbf{k},\mathbf{k}') = 2\pi \mathrm{i} k_{\perp}\delta^{(2)}(\mathbf{k}'_{\|} - \mathbf{k}_{\|})\frac{k'_{\perp} + \mathrm{i}æ}{k_{\perp} + \mathrm{i}æ}, \tag{151}$$

where $k'_{\perp} = k_{\perp}$ for transmission and $k'_{\perp} = -k_{\perp}$ for reflection. Note, that (151) contains diffraction forward scattering ($\mathbf{k}' = \mathbf{k}$) which originates from finite transverse size of the target (see the remark related to Eq. (77)).

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

$$\sigma_{\mathrm{R}}^{(0)} = S\frac{k_{\perp}}{k}\cdot \tag{152}$$

Here S is the area of plane target surface, and $k_{\perp}/k = \cos\theta$, where θ 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 the subbarrier neutron in the output channel is back scattered it is convenient to assume that $\mathbf{k}' = \mathbf{k}'_{\|} - k'_{\perp}\mathbf{e}_z$, where $k'_{\perp} > 0$. Thus

$$\bar{\psi}(\mathbf{r}) = t'\mathrm{e}^{-\mathrm{i}\mathbf{k}_{\|}\mathbf{r}_{\|} - æ'z}, \quad t' = \frac{2k'_{\perp}}{k'_{\perp} + \mathrm{i}æ'}, \quad æ' = \sqrt{u_0 - k'^2_{\perp}}. \tag{153}$$

Vector $\mathbf{B}$ (139) is given by

$$\mathbf{B}(\mathbf{q}) = n\beta(2\pi)^2\delta^{(2)}(\mathbf{k}_{\|} - \mathbf{k}'_{\|} - \mathbf{q}_{\|})tt'\frac{\mathbf{q}_{\|} + \mathrm{i}(æ + æ')\mathbf{e}_z}{q_{\perp} - \mathrm{i}(æ + æ')}\cdot \tag{154}$$

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

$$t^*t = \frac{4k_{\perp}^2}{k_{\perp}^2 + æ^2} = \frac{k_{\perp}^2}{\pi n\beta}, \tag{155}$$

and the same for t'^*t'. Taking into account (77), we have for inelastic cross-section the following expression

$$\frac{\mathrm{d}\sigma_{ie}^{(2)}}{\mathrm{d}\omega} = S\frac{k_{\perp}}{k}\frac{T}{nMs^2}\frac{k_{\perp}}{\pi^4|\omega|}\int \mathrm{d}\mathbf{k}'\delta(k'^2 + 2m\omega - k^2) \times k'^2_{\perp}\int \mathrm{d}\mathbf{q}\delta^{(2)}(\mathbf{k}_{\|} - \mathbf{k}'_{\|} - \mathbf{q}_{\|})\Lambda(k'_{\perp},\mathbf{q}). \tag{156}$$

Here

$$\Lambda^{\mathrm{ph}}(k'_{\perp},\mathbf{q}) = \pi\delta\left(q^2 - \frac{\omega^2}{s^2}\right)\frac{q_{\|}^2 + (æ + æ')^2}{q_{\perp}^2 + (æ + æ')^2} \tag{157}$$

for phonon correlation function (145) and

$$\Lambda^{\mathrm{hyd}}(k'_{\perp},\mathbf{q}) = \frac{\alpha\Gamma^2}{q^4 + \Gamma^4}\left(\frac{q_{\|}^2 + (æ + æ')^2}{q_{\perp}^2 + (æ + æ')^2} - \frac{q_{\|}^2}{q^2}\right) \tag{158}$$

for hydrodynamic one (146), where $\Gamma = \sqrt{|\omega|/D}$. Dividing the inelastic cross-section over the transverse target area $Sk_{\perp}/k$, we get the differential probability per one bounce $\mathrm{d}w_{ie}/\mathrm{d}\omega$ for neutron transition to the state with the energy $\epsilon' = \epsilon - \omega$.

Integration in (156) over $\mathbf{q}_{\|}$ removes two-dimensional delta-function. Then the remaining delta-function allows to perform integration over $k'_{\|}$. The result is

$$\frac{\mathrm{d}w_{ie}}{\mathrm{d}\omega} = \frac{T}{nMs^2}\frac{k_{\perp}}{\pi^4|\omega|}\int_0^{\sqrt{k^2-2m\omega}} k'^2_{\perp}\mathrm{d}k'_{\perp} \times \int_0^{\pi}\mathrm{d}\varphi\int_{-\infty}^{+\infty}\mathrm{d}q_{\perp}\Lambda(k'_{\perp},\mathbf{q}), \tag{159}$$

where one should keep in mind relations

$$q_{\|}^2 = k_{\|}^2 + k'^2_{\|} - 2k_{\|}k'_{\|}\cos\varphi, \quad k'^2_{\|} + k'^2_{\perp} = k^2 - 2m\omega. \tag{160}$$

For the phonon model one can easily proceed further using the delta-function in Λ^{ph} and the small value of $q^2 = q_{\|}^2 + q_{\perp}^2 = \omega^2/s^2 \ll k^2$. The integration gives

$$\frac{\mathrm{d}w_{ie}^{\mathrm{ph}}}{\mathrm{d}\omega} = \frac{2}{\pi}\frac{T}{Ms^2}\frac{k_0\beta}{U}\frac{v_{\perp}}{s}\sqrt{\frac{\epsilon' - \epsilon_{\|}}{U}}, \tag{161}$$

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 $\epsilon_{\|} = \epsilon\sin^2\theta$ is the energy related to the incident neutron motion along the surface plane.

For the hydrodynamic model we can perform in (159) integration over $q_{\perp}$ by closing the integration path in complex $q_{\perp}$ plane and summing over the pole residues. Then it is useful to write the result in the form similar to (161)

$$\frac{\mathrm{d}w_{ie}^{\mathrm{hyd}}}{\mathrm{d}\omega} = \frac{2}{\pi}\frac{\alpha T}{Ms^2}\frac{k_0\beta}{U}f(\epsilon,\theta,\epsilon',d), \tag{162}$$

where dimensionless function f, depending on ϵ, θ, ϵ' and parameter $d = 2mD/\hbar$, is given by

$$f(\epsilon,\theta,\epsilon',d) = \frac{2}{\pi d}\frac{v_{\perp}}{v_0}\int_0^{\sqrt{k^2-2m\omega}} k'^2_{\perp}\mathrm{d}k'_{\perp}\int_0^{\pi}\mathrm{d}\varphi L(k'_{\perp},\varphi). \tag{163}$$

Here $v_0 = \hbar k_0/m$ is the boundary neutron velocity, and

$$L(k'_{\perp},\varphi) = \frac{\sqrt{2}}{\Gamma^3}\frac{(1-4\lambda^2)^{3/4}}{1-2\lambda^2} \times \left(\left(1+\frac{1}{\mu}\right)\frac{\mu^2+\lambda^2}{1+2\mu+2(\mu^2-\lambda^2)} - \frac{\lambda(\lambda+1)}{1+2\lambda}\right), \tag{164}$$

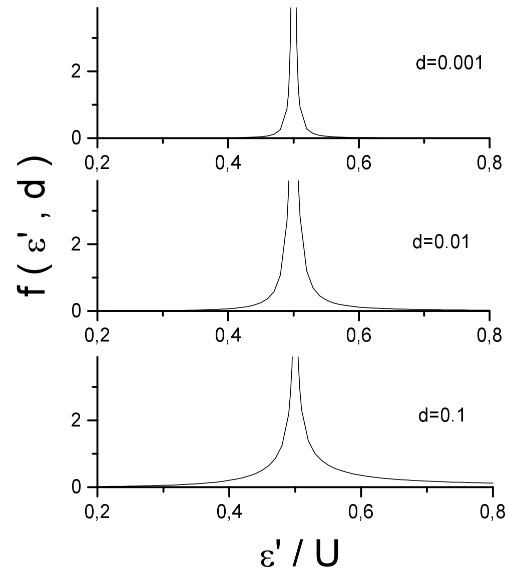

Fig. 1. Function $f(\epsilon,\theta,\epsilon',d)$ from (163) for fixed initial neutron energy $\epsilon = U/2$ and angle of incidence $\theta = \pi/4$ *versus* final neutron energy ϵ' and parameter d.

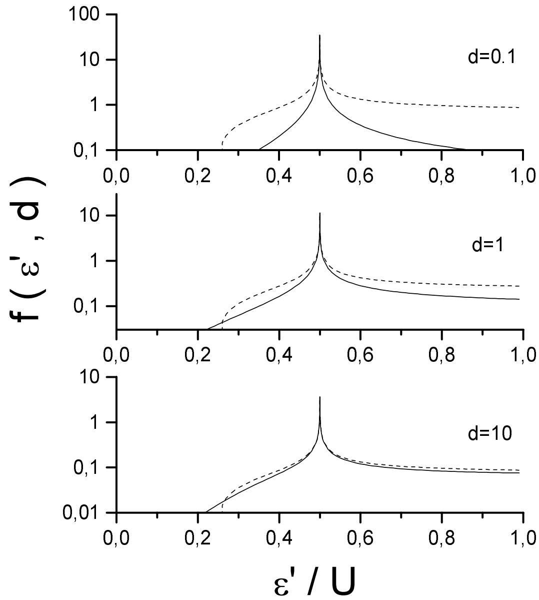

Fig. 2. Function $f(\epsilon,\theta,\epsilon',d)$ for fixed $\epsilon = U/2$ and $\theta = \pi/4$ *versus* final neutron energy ϵ' and parameter d. Solid lines – the result of exact numerical calculation (163), dash lines – approximation (167).

$$2\lambda^2 = \frac{q_\|^2}{q_\|^2 + \sqrt{q_\|^4 + \mathit{\Gamma}^4}}, \quad 2\mu^2 = \frac{(æ + æ')^2}{q_\|^2 + \sqrt{q_\|^4 + \mathit{\Gamma}^4}} \cdot \quad (165)$$

To demonstrate the magnitude of the function f (163) and its dependence on the final neutron energy ϵ' 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 Figure 1 for $d \ll 1$ and in Figure 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. The left side of the broadened line corresponds to the neutron energy loss. Its observation in experiment can be interpreted as "cooling" of UCN. Surely, this process is accompanied by "heating" presented by the right side of the broadened line.

Near the initial energy parameter $\mathit{\Gamma} = \sqrt{|\omega|/D} = k_0\sqrt{|\epsilon' - \epsilon|/(Ud)}$ is small with respect to $æ + æ'$ and the main contribution into the integral comes from small $q_\|^2(k'_\perp, \varphi)$. Then one may simplify the function L (164) by taking limit $\mu^2 \gg (\lambda^2, 1)$:

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

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

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

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 ω peak but for the whole subbarrier area (as seen from Fig. 2).

The dependence on ω 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 on d) area. Indeed, using approximation (167) we obtain

$$w_{ie}^{\rm hyd} = \int \frac{{\rm d}w_{ie}^{\rm hyd}}{{\rm d}\omega}{\rm d}\omega \simeq \frac{4C}{\pi}\frac{\alpha T}{Ms^2}\frac{k_\perp\beta}{U}\frac{1}{\sqrt{d}}\int_0^{Ud}\sqrt{\frac{\epsilon_\perp}{\omega}}{\rm d}\omega$$
$$= \frac{8C}{\pi}\frac{\alpha T}{Ms^2}k_\perp\beta\sqrt{\frac{\epsilon_\perp}{U}} \cdot \quad (168)$$

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

For $d > 1$ the small ω 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 (Sect. 6).

For UCN the rescattering is the dominant process, but the theory can be simplified by exploiting small parameter $\boldsymbol{\kappa}\mathbf{u}$, *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 $\boldsymbol{\kappa}\mathbf{u}$ (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 $\boldsymbol{\kappa}\mathbf{u}$ and result in inelastic scattering.

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

The value of cross-section is very sensitive to correlation function used. The phonon model which gives the 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. Thus, the first condition to obtain reasonable theoretical result for the 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 these may require a change in the model potential and, therefore, the wave functions in the input and output channels that enter the cross-section.

All effects connected with neutron spin are outside 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 β 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 the inclusion of a new "spin-spin" correlation function.

Spin-flip processes need special attention. Physically interesting problem is the 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.

We are grateful to V.I. Morozov for valuable discussions. The work was supported by RFBR grant 96-15-96548.

Appendix: An alternative expression for scattering amplitude

We start with transformation of equation (94). First, using the definition (92) for the matrix $G_{jj'}(\nu\nu')$ and the expression (67) for the matrix $\zeta_{jj'}(\nu\nu')$, one obtains for $G_{jj'}(\nu\nu')$

$$G_{jj'}(\nu\nu') = -\frac{2\pi}{m}\sum_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}(\boldsymbol{\rho}_\nu - \boldsymbol{\rho}_{\nu'})} \times \langle j|\mathrm{e}^{-\mathrm{i}(\mathbf{k}-\mathbf{q})\mathbf{u}_\nu}\hat{D}_q^{-1}\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{q})\mathbf{u}_{\nu'}}|j'\rangle. \quad \text{(A.1)}$$

Then it is convenient to introduce the operators

$$\overrightarrow{P}_{jj'}(\nu) = \langle j|\mathrm{e}^{-\mathrm{i}(\mathbf{k}+\mathrm{i}\nabla_\nu)\mathbf{u}_\nu}|j'\rangle,$$
$$\overleftarrow{P}_{jj'}(\nu) = \langle j|\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathrm{i}\nabla_\nu)\mathbf{u}_\nu}|j'\rangle, \quad \text{(A.2)}$$

where arrows on operators $P_{jj'}(\nu)$ denote the direction for gradients to act on functions of $\boldsymbol{\rho}_\nu$. Thus, after evident transformation with the help of (96) the matrix $G_{jj'}(\nu\nu')$ takes the form

$$G_{jj'}(\nu\nu') = \sum_{j''}\overrightarrow{P}_{jj''}(\nu)G_{j''}(\nu\nu')\overleftarrow{P}_{j''j'}(\nu'). \quad \text{(A.3)}$$

Equation (94) with the use of (A.3) can be written as

$$\psi_j(\nu) + \sum_{j'j''\nu'}\overrightarrow{P}_{jj''}(\nu)G_{j''}(\nu\nu')\overleftarrow{P}_{j''j'}(\nu')\psi_{j'}(\nu')\beta_{\nu'} = \delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}. \quad \text{(A.4)}$$

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

$$\overrightarrow{P}_{jj'}(\nu)\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu} = \delta_{jj'}\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu},$$
$$\mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu}\overleftarrow{P}_{jj'}(\nu) = \mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu}\langle j|\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\mathbf{u}_\nu}|j'\rangle. \quad \text{(A.5)}$$

The scattering amplitude (98), due to (A.5), can be represented in the form

$$f_{ij}(\mathbf{k},\mathbf{k}') = -\sum_{j'\nu}\mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu}\overleftarrow{P}_{jj'}(\nu)\psi_{j'}(\nu)\beta_\nu. \quad \text{(A.6)}$$

Now let us act on all terms of (A.4) by the operator $\overrightarrow{P}^{-1}_{j'j}(\nu)$ and sum over j. The right-hand side, due to (A.5), remains unchanged and we obtain a new form of general equation (94) where the matrix $G_j(\nu\nu')$ is "open" from the left

$$\sum_{j'}\overrightarrow{P}^{-1}_{jj'}(\nu)\psi_{j'}(\nu) + \sum_{j'\nu'}G_j(\nu\nu')\overleftarrow{P}_{jj'}(\nu')\psi_{j'}(\nu')\beta_{\nu'} = \delta_{ij}\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}. \quad \text{(A.7)}$$

We can now multiply (A.7) from the left by $\beta_\nu\bar{\psi}_j^{(0)}(\nu)$, which is a solution of equation (131), *i.e.*

$$\sum_\nu \beta_\nu\bar{\psi}_j^{(0)}(\nu)G_j(\nu\nu') = \mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_{\nu'}} - \bar{\psi}_j^{(0)}(\nu'). \quad \text{(A.8)}$$

Then summing over ν we get with the help of (A.8)

$$\sum_{j'\nu}\beta_\nu\bar{\psi}_j^{(0)}(\nu)\overrightarrow{P}_{jj'}^{-1}(\nu)\psi_{j'}(\nu) + \sum_{j'\nu}\left(\mathrm{e}^{-\mathrm{i}\mathbf{k}'\boldsymbol{\rho}_\nu} - \bar{\psi}_j^{(0)}(\nu)\right)\overleftarrow{P}_{jj'}(\nu)\psi_{j'}(\nu)\beta_\nu = \delta_{ij}\sum_\nu\beta_\nu\bar{\psi}_j^{(0)}(\nu)\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}. \quad (A.9)$$

From (A.6) and (A.9) it follows for the scattering amplitude

$$f_{ij}(\mathbf{k},\mathbf{k}') = -\delta_{ij}\sum_\nu\beta_\nu\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}\bar{\psi}_i^{(0)}(\nu) - \sum_{j'\nu}\Big(\bar{\psi}_j^{(0)}(\nu)\overleftarrow{P}_{jj'}(\nu)\psi_{j'}(\nu)\beta_\nu - \beta_\nu\bar{\psi}_j^{(0)}(\nu)\overrightarrow{P}_{jj'}^{-1}(\nu)\psi_{j'}(\nu)\Big), \quad (A.10)$$

where the 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 the desired relation between scattering amplitude and exact solution $\psi_j(\nu)$ of the general equation (94)

$$f_{ij}(\mathbf{k},\mathbf{k}') = -\delta_{ij}\sum_\nu\beta_\nu\mathrm{e}^{\mathrm{i}\mathbf{k}\boldsymbol{\rho}_\nu}\bar{\psi}_i^{(0)}(\nu) - \sum_{j'\nu}\langle j|\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{u}_\nu}\Big(\bar{\psi}_j^{(0)}(\boldsymbol{\rho}_\nu+\mathbf{u}_\nu)\psi_{j'}(\boldsymbol{\rho}_\nu) - \bar{\psi}_j^{(0)}(\boldsymbol{\rho}_\nu)\psi_{j'}(\boldsymbol{\rho}_\nu-\mathbf{u}_\nu)\Big)\beta_\nu|j'\rangle. \quad (A.11)$$

An expansion of (A.11) in $\mathbf{u}_\nu$ gives in zero order (with the use of (130) and (122))

$$f_{ij}^{(0)}(\mathbf{k},\mathbf{k}') = -\delta_{ij}\psi(-\mathbf{k}',-\mathbf{k}), \quad (A.12)$$

which, due to time reversal invariance, equals to (121). The first order term in (A.11) coincides with (134).

References

1. V.F. Turchin, *Slow Neutrons* (Jerusalem: Israel Programm for Scientific Translations, 1965).
2. I.I. Gurevich, L.V. Tarasov, *Low Energy Neutron Physics* (Amsterdam, North Holland, 1968).
3. S.W. Lovesey, *Theory of Neutron Scattering from Condensed Matter* (Oxford, Clarendon Press, 1984), Vols. 1 and 2.
4. A. Steyerl, Springer Tracts Mod. Phys. **80**, 57 (1977).
5. R. Golub, J.M. Pendlebury, Rep. Prog. Phys. **42**, 439 (1979).
6. V.K. Ignatovich, *The Physics of Ultracold Neutrons* (Oxford, Clarendon Press, 1990).
7. R. Golub, D. Richardson, S.K. Lamoreaux, *Ultra-cold Neutrons* (Adam Hilger, Bristol, Philadelphia and New York, IOP Publishing Ltd, 1991).
8. L. Bondarenko, P. Geltenbort, E. Korobkina, V. Morozov, Yu. Panin, A. Steyerl, Pis'ma v ZETP **68**, 663 (1998).
9. V.V. Nesvizhevsky, A.V. Strelkov, P. Geltenbort, P.S. Iadjiev, Eur. Phys. J. AP **6**, 151 (1999).
10. K.M. Watson, Phys. Rev. **105**, 1388 (1957).
11. M.L. Goldberger, K.M. Watson, *Collision Theory* (John Wiley and Sons Inc., New York, London, Sydney, 1964).
12. V.F. Sears, Can. J. Phys. **56**, 1261 (1978).
13. V.F. Sears, Phys. Rep. **82**, 1 (1982).
14. A.L. Barabanov, S.T. Belyaev, Phys. At. Nucl. **62**, 769 (1999).
15. R. Golub, Rev. Mod. Phys. **68**, 329 (1996).
16. A.V. Stepanov, Fiz. Elem. Chastits At. Yadra **7**, 989 (1976) (in Russian).
17. D.I. Blokhintsev, N.M. Plakida, Phys. Status Solidi B **82**, 627 (1977).
18. D. Forster, *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions* (W.A. Benjamin, Inc., Advanced Book Program Reading, Massachusetts, London, Amsterdam, Don Mills, Ontario, Sidney, Tokyo, 1975).
19. J.P. Hansen, I.R. McDonold, *Theory of Simple Liquids*, 2nd edn (Acad. Press, 1986).