Interaction of Ultra-Cold Neutrons with Condensed Matter

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Abstract

General theory of neutron scattering (elastic and inelastic) is presented. It is applicable for the whole domain of slow neutrons and includes as limiting cases existing theories for thermal and cold neutrons and for elastic scattering of UCN. New expression for inelastic scattering cross section for UCN is proposed. It differs from the usually used by proper account of re-scattering processes. Evidence for small heating and cooling of UCN is given.

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1 Introduction

Thermal and cold neutrons with wave length $0.03 \text{ nm} \leq \lambda \leq 1 \text{ nm}$ is an important tool for investigation of condensed matter. Theory of their interaction with substance is well established (see, e.g., [1,2]). It is based on the use of Fermi pseudopotential. For thermal and cold neutrons re-scattering of secondary waves is unimportant and one may use Born approximation that gives for double differential cross-section the following expression

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{2\pi k} \sum_{\nu \nu'} b_\nu b_{\nu'} \chi_{\nu \nu'}(\kappa, \omega).$$

(1)

Here $\kappa = k' - k$, $\omega = \varepsilon - \varepsilon'$, where $k$ and $\varepsilon$ are momentum and energy of incident neutron, $k'$ and $\varepsilon'$ are the same quantities for scattered neutron, and
is a scattering amplitude on bound $\nu$-th nucleus. A Fourier transform
\begin{equation}
\chi_{\nu\nu'}(\kappa, \omega) = \int_{-\infty}^{+\infty} \chi_{\nu\nu'}(\kappa, t) e^{i\omega t} dt
\end{equation}
of diagonal matrix element of an operator of nuclear position correlation
\begin{equation}
\chi_{\nu\nu'}(\kappa, t) = \langle i | e^{i\kappa \hat{R}_\nu(t)} e^{-i\kappa \hat{R}_{\nu'}(0)} | i \rangle
\end{equation}
between the initial eigenfunctions $|i\rangle$ of target Hamiltonian, that determines the target response on the scattered neutron wave.

For ultra-cold neutrons (UCN), when $\lambda \geq 10$ nm, re-scattering of neutron wave in media is very essential, and when $k^2 < 4\pi b n$ re-scattering becomes the dominant process and results in the total reflection from the surface of the target (of cause, for positive $b$). Thus, Born approximation in general, and the cross-section (1) in particular, can not be used for UCN. To describe an elastic scattering of UCN by matter one uses a multiple scattering wave approach for fixed (unmovable) nuclei (see, e.g., [3,4]). It gives an effective repulsive (optical) potential for neutron inside a condensed matter, so the neutron wave with the energy below the threshold is exponentially decreasing deep into target. However, UCN escape from vessels, that attracts attention of experimenters for many years, as well as small heating and cooling observed recently [5], belong to inelastic processes. In this paper we present the basic features of a general theory for elastic and inelastic scattering equally applicable for thermal and cold as well as ultra-cold neutrons, and which, when neutron wave-length decreases, smoothly transforms into the usual scattering theory giving the cross-section (1).

\section{2 General expressions}

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. It is, of cause, impossible to solve the many-body problem of neutron – target interaction without any approximations. In our problem there are two main small parameters: short-range of neutron-nuclei interaction (as compared with interatomic distance and wave length), and small neutron energy (as compared with depth of interaction potential).

The first condition allows to consider only s-wave part of the wave function of neutron – nucleus center-of-mass motion, when their interaction is evaluated. And the second condition allows in this evaluation to neglect energy of relative neutron – nucleus motion inside the interaction potential area. No specific
model for neutron–nucleus interaction potential is needed. Its specific features described above (short range and large depth) allows to use scattering length approximation.

From these considerations we obtain a general expression for double differential cross section

\[
\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{2\pi k} \sum_{jj'\nu\nu'} \phi_j^{*} \phi_{j'} \chi_{\nu\nu'}^{jj'}(\kappa, \omega + E_i - E_j).
\]  

(4)

It contains neutron amplitudes \( \phi_j \) and Fourier transform of nondiagonal matrix element of the correlation operator

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

(5)

between the eigenfunctions \( |j\rangle \) and \( |j'\rangle \) of target Hamiltonian. Note, that \( E_i \) is the energy of the initial target state \( |i\rangle \), and \( E_j \) corresponds to a state \( |j\rangle \).

A set of linear algebraic equations for neutron amplitudes \( \phi_j \) is also found. Neglecting in these equations terms that describe re-scattering we get for the amplitudes

\[
\phi_j = \delta_{ij} \beta_\nu \left( 1 - i\alpha_\nu \langle i | \sqrt{k_\nu^2} | i \rangle \right),
\]  

(6)

where \( \alpha_\nu \) and \( \beta_\nu \) are scattering lengths on isolated and bound nucleus, respectively, and \( \hat{k_\nu} \) is an operator of impact momentum in the center-of-mass system for neutron and nucleus. Thus, for thermal and cold neutrons Eq. (4) really transforms into Eq. (1), and the usual relation between \( \beta_\nu \) and \( b_\nu \) arises.

Into a condensed matter we have \( \hat{R}_\nu = \rho_\nu + u_\nu \), where \( \rho_\nu \) is the equilibrium position of the \( \nu \)-th nucleus, and \( u_\nu \) is its shift from the equilibrium. Thus, the factors \( e^{-i\kappa \rho_\nu} \) and \( e^{i\kappa \rho_\nu} \) may be extracted in the matrix element (3) and combined with the amplitudes \( \phi_j^{*} \) and \( \phi_{j'} \) in (4). Equations for new amplitudes \( \psi_j(\nu) = (\phi_j / \beta_\nu) e^{i\kappa \rho_\nu} \) are of the form

\[
\psi_j(\nu) = \delta_{ij} e^{i\kappa \rho_\nu} - \sum_{j'\nu'} \beta_{\nu'} G^{jj'}_{\nu\nu'} \psi_{j'}(\nu').
\]  

(7)

The coefficients \( G^{jj'}_{\nu\nu'} \) are expressed in terms of matrix elements (3).

Then we use an expansion over \( ku \) for functions \( \chi_{\nu\nu'}^{jj'}(\kappa, \omega) \), coefficients \( G^{jj'}_{\nu\nu'} \), and amplitudes \( \psi_j(\nu) \) (or \( \phi_j \)). Zero-order approximation (\( u = 0 \)) corresponds to fixed nuclei and, therefore, results in only elastic scattering. Equations for zero-order amplitudes \( \psi_{(0)j}(\nu) = \delta_{ij} \psi_k(\nu) \)

\[
\psi_k(\nu) = e^{i\kappa \rho_\nu} - \sum_{\nu'} \beta_{\nu'} G^{ii}(\nu\nu') \psi_k(\nu'), \quad G^{ii}(\nu\nu') = \frac{e^{i\kappa |\rho_\nu - \rho_{\nu'}|}}{|\rho_\nu - \rho_{\nu'}|}.
\]  

(8)
coincide with the multiple scattering wave equations usually used to describe UCN elastic scattering.

3 Inelastic scattering

Inelastic scattering arises in the second-order approximation in $k u$. Analysis shows that there are four second-order terms in inelastic cross section (4)

$$
\sum_{jj'} \phi_{j'\nu}^{(0)} \phi_{j\nu}^{(0)i} \chi_{j\nu}^{(2)i} + \phi_{j'\nu}^{(0)} \phi_{j\nu}^{(1)f} \chi_{j\nu}^{(1)f} + \\
+ \phi_{j'\nu}^{(1)f} \phi_{j\nu}^{(0)i} \chi_{j\nu}^{(1)f} + \phi_{j'\nu}^{(1)f} \phi_{j\nu}^{(1)f} \chi_{j\nu}^{(0)f}.
$$

(9)

Four terms in the right-hand side of (9) are illustrated by Fig.1. To disclose physical meaning of these terms, it is instructive to compare our result with that based on the improvement of (1) by replacement of Born amplitudes $b_\nu$ by the neutron amplitudes in optical potential $\phi_\nu^{(0)}$ (see, e.g., [6]). In such an approach expansion similar to (9) would evidently result in only the first term (Fig.1a), where re-scattering is taken into account only for incident neutron wave (already included in $\phi_\nu^{(0)}$).

Three other terms in (9) describe rescattering of out-going waves (in inelastic channels). They are directly and indirectly generated by nondiagonal matrix element $\chi_{jj'}^{\nu\nu'}$. The first-order term for diagonal matrix element ($j = j'$) is absent.

Final expression for the second order inelastic cross section is of the form

$$
\frac{d\sigma^{(2)}}{d\omega} = \frac{1}{2\pi mk} \int d^3k' \delta(\varepsilon' + \omega - \varepsilon) \int \frac{d^3q}{(2\pi)^3} B_\alpha(q) B_\beta(q) \Omega_{\alpha\beta}(q, \omega),
$$

(10)

$$
B(q) = \sum_\nu \beta_\nu e^{-i\mathbf{q}\cdot\mathbf{\rho}_\nu} \nabla_\nu (\psi_{-k'}(\nu) \psi_k(\nu)),
$$

(11)

where $\Omega_{\alpha\beta}(q, \omega)$ is related with Fourier transform of correlation function by the equation

$$
\langle i | \hat{u}_{\nu\alpha}(t) \hat{u}_{\nu'\beta}(0) | i \rangle = \int \frac{d^3q d\omega}{(2\pi)^4} e^{i\mathbf{q}(\mathbf{\rho}_\nu - \mathbf{\rho}_{\nu'}) - i\omega t} \Omega_{\alpha\beta}(\mathbf{q}, \omega).
$$

(12)

Note, that (11) contains symmetrically the functions of the elastic and inelastic neutron channels. In the Born approximation, i.e., neglecting by re-scattering both in the elastic and inelastic channels, we have from (8): $\psi_k(\nu) \rightarrow e^{ik\mathbf{\rho}_\nu}$ and $\psi_{-k'}(\nu) \rightarrow e^{-ik\mathbf{\rho}_{\nu'}}$. Thus,

$$
B(q) \rightarrow -i\kappa \sum_\nu \beta_\nu e^{-i(q+K)} \mathbf{\rho}_\nu,
$$

(13)
and the usually used formula for inelastic cross section arises (see, e.g., [4]). In [6] an attempt was made to improve this approach by replacing the plane wave \( e^{i k \rho} \) in (12) by the damping function \( \psi_k(\nu) \). This attempt is clearly inconsistent as such replacement should be made in (11) before differentiation with respect to \( \rho \).

4 Results

To illustrate the possibilities of our approach we studied small heating and cooling of UCN in a simplest model. Let us consider UCN that fall normally to a thick layer of uniform matter with an energy \( \epsilon \) below a threshold \( U \). Taking the correlation function in phonon model we obtain for the probabilities of inelastic scattering per one bounce the following expressions

\[
\frac{d\omega^{(2)}_{ie}}{d\epsilon'} \bigg|_{\epsilon' \leq U} = \frac{2k\beta}{\pi U} \frac{T}{Ms^2} \frac{\nu'}{s}, \quad \frac{d\omega^{(2)}_{ic}}{d\epsilon'} \bigg|_{\epsilon' > U} = \frac{k\beta}{\pi \epsilon'} \frac{T}{Ms^2} \frac{\nu'}{s} \left( 1 - \left( \frac{\nu' \epsilon'}{2s} \right)^2 \right),
\]

where \( T \) is a target temperature, \( M \) is a mass of target nuclei, \( s \) is a speed of sound, and \( \nu' = \sqrt{2\epsilon' m} \) is a velocity of a scattered neutron. Note, that the second formula is not valid in a small region just above the barrier, where oscillations governed by narrow resonances in transmission and reflection are of importance. However, these oscillations damp rapidly when \( \epsilon' \) increases. A half of neutrons with the energy \( \epsilon' > U \) reflects from the target, while the other half transmits through it.

Spectrum of inelastically scattered neutrons in the model considered has a maximum at \( \epsilon' \simeq U \). Indeed, it increases as \( \sim \nu' \) below the barrier and falls off as \( \sim 1/\nu' \) above the barrier. Thus, qualitatively it is just of the form needed to explain small heating and cooling of UCN into vessels. However, the magnitude of the effect in the phonon model is low, as \( k\beta \sim 10^{-6} \) and \( \nu'/s \sim 10^{-3} \). Nevertheless, it should be noted that an evaluation of the inelastic scattering probability in the Born approximation, i.e., with \( B(q) \) (13), gives

\[
\frac{d\omega^{B}_{ie}}{d\epsilon'} \sim \frac{k\beta}{ms^2} \frac{T}{Ms^2} \frac{\nu'}{s}.
\]

This spectrum, first, has no maximum in low energy region and, second, is additionally suppressed by the factor \( \sim U/ms^2 \) as compared with Eqs.(14). This results from the direct proportionality of \( B(q) \) (13) to \( \kappa \) vanishing for low energy transfer from neutron to target or vice versa.

One should expect that the low energy transfer processes are governed not by phonons but rather by other collective excitations in condensed matter. In
particular, when a propagation speed of the excitation is of the same order as the velocity of UCN, an influence of matter fluctuations on re-scattering processes may be maximal. Our study of UCN interaction with diffusion and thermal wave modes is now in progress.

5 Summary

General theory of neutron scattering (elastic and inelastic) is presented. It is applicable for the whole domain of slow neutrons and includes as limiting cases existing theories for thermal and cold neutrons and for elastic scattering of UCN. The only small parameters used are those for the interaction potential that was assumed a short and relatively deep, what is equivalent to scattering length approximation for the interaction. Evident expression for the inelastic cross section is given. It differs from the usually used by proper account of re-scattering in the inelastic channel. It is shown that in the phonon model our approach qualitatively explains the low energy transfer processes. However, to provide the large observed probabilities of small heating and cooling of UCN into vessels other collective excitations of condensed matter in the limit of small $q$ and $\omega$ should be apparently taken into account.

Acknowledgements

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Fig. 1. Contributions to the second-order inelastic cross section: (a) scattering – scattering interference, (b) scattering – re-scattering interference, (c) re-scattering – re-scattering interference. Solid and dash lines represent neutrons in the elastic and inelastic channels, respectively. Open and crossed circles correspond to elastic and inelastic scattering, respectively.
Figure 1