What is the correct description of the slow neutron scattering in a gas?

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Abstract

The description of the thermal neutron scattering in a noble gas is discussed. It is shown that the commonly used Placzek's approach is not consistent with the Turchin's formalism which is nicely confirmed by Monte Carlo calculations. A proposal is made concerning more adequate description of thermal motion of gas atoms in diffraction effect under slow neutron scattering by gas atoms.

Last decades a large number of papers was devoted to an investigation of the thermal neutron angular distribution scattered by gases and liquids in order to determine so-called structure factors and to extract a potential of interaction between atoms of the Van der Waals type [see, for example, 1,2,3]. It is strange that in some papers the thermal atom motion even for gases is taken into account according to the Placzek's approach developed in 50s of past century for the description of neutron behavior in solid materials [4,5].

On other hand, starting from the paper by Krohn and Ringo [6] on the measurement of the (n,e)–scattering length in noble gases the perfectly correct consideration of influence of thermal motion of gas atoms is known. This approach is based on pure kinematical description of neutron interaction with moving gas atoms and the formalism was also given in the book by V.F.Turchin [7]. A perplexity arises that in the above mentioned papers this more correct formalism of the gas atom motion consideration of neutron scattering is not used. The aim of our report is to compare these two approaches and to check them with the description of neutron scattering on moving gas atoms by using the Monte Carlo method developed by us in [8].

In paper [1] using the reference to [5] the angular distribution of scattered neutrons by noble gas atoms in the laboratory frame is described by the expression

$$d\sigma(\theta) \sim \frac{\sigma_s}{4\pi}[1+P(\theta)] \quad , \qquad (1)$$

where "Placzek's correction" is taken in the form

$$P(\theta) = \frac{1}{A}[\frac{kT}{2E_o} - 2(1-\cos\theta)] + O(\frac{1}{A})^2 \quad . \qquad (2)$$

Here

σ_s - is the nuclear scattering cross section,

θ - is the scattering angle in the laboratory frame,

E_o - is the initial neutron energy,

k - is the Boltzmann's constant,

T - is the gas temperature (in K),

A - is the atomic weight.

Usually one neglects by the term $O(\frac{1}{A})^2$.

According to [6,7] the differential scattering cross section for moving gas atoms is described by formula

$$d\sigma(\theta) = \frac{\sigma_s}{4\pi} F_s(\vec{V}_o, \vec{V}, A) \,, \tag{3}$$

where

$$F_s(V_0, V, A) = \frac{(A+1)^2}{A^2 \sqrt{\pi} V_0 B_0} \int_0^{\infty} \frac{V^2}{\sqrt{V_0^2 + V^2 - 2V_0 V \cos\theta}} \times$$

$$\times \exp\left\{ - \frac{(V^2 - V_0^2 \frac{A-1}{A+1} - \frac{2V_0 V \cos\theta}{A+1})^2}{4(\frac{A}{A+1})^2 B_0 (V_0^2 + V^2 - 2V_0 V \cos\theta)} \right\} dV \,, \tag{4}$$

$B_0 = \sqrt{\frac{2kT}{mA}} = 128.9\sqrt{\frac{T}{A}}$ [m/s],

V_0 - is the initial neutron velocity,

V - is the neutron velocity after scattering.

At the gas pressure up to 20 atm (at gas density $n < 0.5\, nm^{-3}$) the angular distribution of scattered neutron intensity can be presented, taking into account the (n,e)–interaction and diffraction effects in slow neutron scattering on gas atoms (for the case of single atom noble gases), in the following form

$$\frac{dI(q)}{d\Omega} =$$

$$= \varepsilon \frac{\sigma_s}{4\pi} \{ F_s(V_0, q, A)[1 + \frac{8\pi a_{coh} b_{ne} Z f(q)}{\sigma_s}] +$$

$$+ \frac{nC(q)}{1 - nC(q)} F_s(V_0, q, 2A)[\frac{\sigma_{coh}}{\sigma_s} + \frac{8\pi a_{coh} b_{ne} Z f(q)}{\sigma_s}]\} \,. \tag{5}$$

Here

$\vec{q} = \frac{m}{\hbar}(\vec{V} - \vec{V_0})$ - is the momentum transferred,

ε - is the parameter which takes into account the solid angle and the detector efficiency,

a_{coh} - is the coherent scattering amplitude,

σ_{coh} - is the coherent scattering cross section,

b_{ne} - is the (n,e)–scattering length,

$C(q)$ - is the correlation function related with the structure factor $S(q)$ as

$$S(q) - 1 = \frac{nC(q)}{1 - nC(q)} \,; \tag{6}$$

n - is the gas density.

Let us note that in contradiction to such papers as [1 – 3], where the influence of the thermal motion on the description of diffraction effects is not taken into account, formula (5) contains the effect of thermal motion of atoms in the diffraction term. The second term in the braces of formula (5) just considers the coherent diffraction scattering of neutron on two atoms so the kinematical factor $F_s(V_0,q,2A)$ is calculated with double mass equal to $2A$ [12].

In the formula (5) one introduces terms which contain the contribution of an interaction of neutron with electrons of atomic shell. The (n,e)-interaction is described by the atomic form-factor as

$$f(q) = \frac{1}{\sqrt{1+3(\frac{q}{q_0})^2}}, \qquad (7)$$

constant q_0 is estimated in Hartry-Fok's approach [9].

Our interest in the problem of correct description of neutron interaction with gas atoms has arisen from the task of (n,e)-scattering length b_{ne} definition from experimental data on slow neutron scattering by noble gases [8,10,11,12]. Therefore in the formula (5) the terms depending on the b_{ne} were added. These terms can also be introduced in the formula (1).

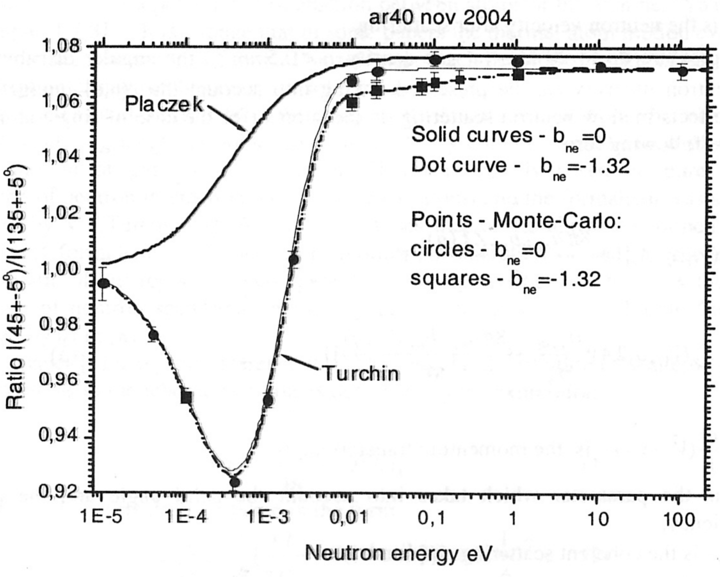

Fig.1. The forward – backward anisotropy of scattered neutrons for different models of thermal motion of gas atoms. The explanations are given in the figure. The bold dashed line corresponds to the calculation by the formula (8).

Let's now shortly discuss the algorithm of the neutron scattering description by the Monte Carlo method which we used in [8]. The algorithm of the Monte Carlo calculation will be presented in more details in the appendix. Here we consider only a main scheme. At first the velocity vector of atom $\vec{W}$ with which the neutron collides is generated taking into account the atomic weight and gas temperature. Then from the initial neutron velocity $\vec{V}_o$ and $\vec{W}$ the relative neutron – atom velocity $\vec{V}_R$ is determined and the transition to the center of mass frame is made, the velocity in this frame V_{cm} is found and the interaction type is defined taking into account a contributions of neutron scattering cross section and capture cross section. If the scattering process takes place then the new neutron velocity $\vec{V}_{cm}$ is generated assuming neutron scattering isotropy in the center of mass frame (if the (n,e)-interaction is neglected) or introducing small anisotropy related to the (n,e)-interaction. After these steps we go back to the laboratory frame and the new neutron velocity $\vec{V}_n^{\,'}$ is determined in this frame.

In order to compare three models of thermal motion consideration (Placzek – Turchin – Monte Carlo) the forward-backward anisotropy was calculated for each variant in the angular intervals $\theta_1 = 45^o \pm 5^o$ and $\theta_2 = 135^o \pm 5^o$. For Placzek's and Turchin's variants an integration of formulas (1) and (3) is made in the limits $\theta_i \pm 5^o$. In the Monte Carlo calculations only those events are chosen which correspond to scattered neutrons in the indicated angular intervals. The results of the calculations are presented in Fig.1.

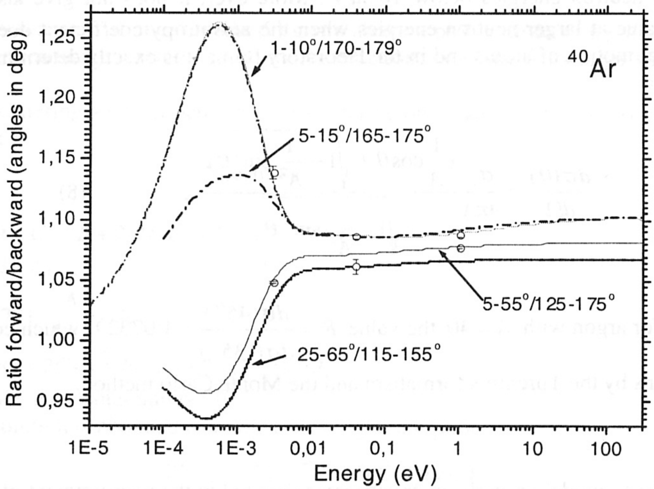

Fig.2. The forward – backward scattering anisotropy for *Ar* depending on the neutron energy as calculated by the formula (4) for different intervals of angles. The points are the results of the Monte – Carlo calculations.

The values for the forward – backward ratios less than unity are obtained when the neutron velocity decreases and it becomes compatible to the atom velocity W_0. Then for atoms moving in directions close to the neutron velocity $\vec{V}_0$, neutron flux (proportional to relative velocity $|\vec{V}_0 - \vec{W}_0|$) is much less than for atoms moving towards neutrons. Therefore the backward scattering probability exceeds the forward scattering probability. In case when $V_0 << W_0$ the neutron is nearly at rest and it is symmetrically bombarded by atoms in front and from behind so the distribution of the scattered neutrons approaches to a symmetric form. Especially one should note that in the interval $W_0 \leq V_0 \leq 2W_0$ (for atoms, which move approximately at an angle of 60^o to the $\vec{V}_0$), the case is realized when the velocity of scattered neutron in the center of mass frame is numerally equal to the velocity of the center of mass. This results in the neutron scattering preferentially into forward hemisphere and the scattering essentially increases in the forward direction. The scattering anisotropy for Ar depending on the neutron energy for different intervals of angles is shown in Fig.2.

From the analysis of the obtained results we can make the following conclusions.

i) The Turchin's formalism and the Monte Carlo calculations give the equivalent description of the scattering anisotropy in the whole diapason of initial investigated neutron energies. Since in our opinion the Monte Carlo procedure is free from any approximations (when the (n,e)-interaction is absent) and includes pure kinematical effects one can confirm that the Turchin's formalism gives the correct consideration of thermal atom motion in processes of slow neutron scattering in gases.
ii) The Placzek's approach, on one hand, provides a completely incorrect behavior of the anisotropy at neutron energies below $10\,meV$. More ever, it does not give also the correct asymptotic value at larger neutron energies when the anisotropy coefficient does not depend on the thermal motion of atoms and in the laboratory frame it is exactly determined according to the formula

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{\sigma_s}{4\pi A} \frac{\left(\frac{1}{A}\cos\theta + \sqrt{1 - \frac{1}{A^2}\sin^2\theta}\right)}{\sqrt{1 - \frac{1}{A^2}\sin^2\theta}}, \qquad (8)$$

which gives for argon with $A = 40$ the value $R = \frac{d\sigma(45^o)}{d\sigma(135^o)} = 1.07329$ which corresponds to the calculations by the Turchin's formalism and the Monte Carlo method.

Appendix

In order to model properly an experiments devoted to the measurement of the b_{ne} from the elastic neutron scattering in single atom noble gases the following algorithm of the description of the angular distribution of scattered neutrons by moving atoms was applied. One assumes that in the center of mass frame the total cross section must have the form

$$\sigma_t. = [4\pi.b_N^2 + 8\pi.b_{ne}b_N f_t(E_R) + \sigma_{SCH}(E_R) + \sigma_\gamma]\frac{V_R}{V_0}, \qquad (9)$$

where

b_N - is the nuclear scattering length,
Z - is the nuclear charge (number of electrons in the atom shell),

f_t - is the total atomic form-factor,

E_R - is the relative neutron-atom energy,

σ_{SCH} -is the Schwinger's total scattering cross section,

V_R - is the relative neutron-atom velocity,

V_0 - is the initial neutron velocity in laboratory frame reference,

E_0 - is the initial neutron energy in laboratory frame reference.

$\sigma_\gamma \frac{V_R}{V_0} = \frac{\sigma_{0\gamma}}{\sqrt{E_0}}$, $\sigma_{0\gamma}$ - is the capture cross section at $1\,eV$.

The factor $\frac{V_R}{V_0}$ in the formula (9) takes into account an influence of thermal atom motion on the total neutron scattering cross in single act of interaction and it is in essence the relative flux of the scattering neutrons. This factor is equivalent to the integration over Maxwell's spectrum of gas atom velocities in the formulas (3) and (4). It is obvious that the factor $\frac{V_R}{V_0}$ influences the Monte Carlo calculations if during generation one chooses only those events which have the path of neutron before scattering much less than the average path of neutrons in a gas.

In accordance with the formula (9) given above a probabilities of the neutron capture, of the nuclear scattering (including the (n,e)-interaction) or of the Schwinger's scattering are generated.

The scattering angle of neutron after scattering on an atom in the center of mass frame is determined as

$$\theta = 2\arcsin\sqrt{x}\ ,$$

where

$$x = D + C^2 / B + 2(D \cdot C^2 / B + C^4 / B + C^2 / B^2)^{1/2}\ ,$$

$$C = 2b_{ne} Z / b_N\ ,$$

$$B = 5791\left(\frac{A}{A+1}\right)^2 E / q_0\ ,$$

$$D = r(1 + 2C\sqrt{1+B} / B) + 2C(1-r) / B\ .$$

r - is the accidental number [0,1].

This solution is obtained from the following assumptions:

$$W(\theta) = C[1 + \frac{2b_{ne}}{b_N} f(E,\theta)]\sin\theta\ ,$$

$$\int_{\theta,\varphi} W(\theta) d\theta d\varphi = 1\ ,$$

$$P(\theta) = 2\pi \int_0^\theta W(t) dt\ .$$

For the Schwinger's interaction the scattering angle is generated using the Neimann's method. The drawing of the atom velocity was done according to the Maxwell's distribution for the room temperature of gas. The transition from the laboratory frame to the center of mass frame and returning (after determination of the velocity of scattered neutron in the center of mass frame) were realized using GAUSIN code and standard routines of the vector algebra from the CERNLIB library.

This work was supported by RFBR, grant 03-02-16883.

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