ON THE SCATTERING OF NEUTRONS BY MOLECULES

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In the treatment of problems involving the thermalization of neutrons an important factor is the choice of scattering functions. The accuracy of these functions and the possibilities of their refinement thus constitute a very significant problem. The scattering functions for neutrons scattered by molecules should take into account the thermal motion of the atoms of the scatterer molecules as well as their chemical bond. Posed in this manner, the problem appears rather complex even for the simplest systems. In this case, as a rule, one must resort to the "monatomic" approximation; this means actually that the molecule is replaced by a hypothetic free particle whose mass \( M(\delta) \) depends on the rotational properties of the molecule but not on the orientation of the molecule relative to the scattered neutron. The characteristics of such a consideration are studied in the present paper in the example of the simplest rotators: spherical and linear. This case, which illustrates the influence of a rigid molecular bond on the neutron scattering process, can be subjected to rigorous treatment within the framework of classical mechanics without invoking any of the above-mentioned simplifications.

In the "monatomic" approximation the differential cross section for the scattering of neutrons by the rotators can be written in the form (see, e.g., [1])

\[
d\sigma^* / d\Omega = a^2 k / k_0 \left( \frac{M(\theta)}{2\pi k_B T x^2} \right)^{1/2} \times \exp \left[ -\frac{M(\theta)}{2k_B T x^2} \left( \frac{1}{2} \right)^2 \right],
\]

where \( a \) is the scattering length of the fixed nucleus (assumed independent of energy), \( k_0 = k = k_0 - x \) are the momenta of the neutron before and after scattering, \( \varepsilon = k_0^2 - k^2 / 2m \), \( m \) is the neutron mass, \( k_B \) is the Boltzmann constant, \( T \) is the temperature of the medium, \( [M(\delta)]^{-1} = \frac{1}{3}(r_1 + r_2) \). The parameters \( r_1 \) and \( r_2 \) are expressed in terms of the principal components of the tensor of inertia [2]. For linear and spherical rotators \( r_1 = r_2 = I^{-1} b^2 \), \( M(\delta) = \gamma_0 b^{-2} \), where \( I \) is the moment of inertia, \( b \) is the radius vector of the scattering nucleus.

It should be noted that Eq. (1) can be used only to obtain the integral scattering characteristics. For example, in [1] there is poor agreement with experiment in the case of \( d\sigma^* / d\Omega = \int d\varepsilon / d\Omega \cdot d\varepsilon \), but the angular moments of the function (1) are still of considerable interest. For the zero moment we have the well known equation [3]

\[
\frac{d\sigma^*(p_0 \rightarrow p)}{dp} = a_\infty \frac{M(\theta)}{4} \frac{p}{p_0} \left\{ \exp (\theta p - \pi p_0) \right\}
\]

(2)

where the upper sign is for \( p_0 > p \), the lower sign for \( p_0 < p \); \( p_0, p \) are the momenta of the neutrons in the units \( \sqrt{2mk_B T} \); \( \theta = \frac{M(\theta)}{2 V M(\theta)} \); \( \pi = \frac{M(\theta) - 1}{2 V M(\theta)} \); \( M(\theta) \) is in units of the neutron mass; \( a_\infty = 4\pi a^2 \).

Equations of the type (2) are used in many thermalization problems. The main inaccuracies of the "monatomic" approximation are caused by incorrect averaging of the scattering effect over the molecular orientations.

In the present article a rigorous and systematic scheme of averaging over rotational orientations is worked out for the simplest rotators within the tenets of classical mechanics. The expressions for the differential cross-section and its moments are obtained in the form of integrals which can be computed numerically:
\[\frac{d^3\sigma}{d\Omega dE} = \frac{\sigma_\infty k}{4\pi} \left( \frac{M}{2\pi k_B T} \right)^{1/2} \exp \left\{ -\frac{M}{2k_BT} \left[ \frac{e^{-x^2}}{(2M)^{1/2}} \right]^2 \right\} \frac{dx}{\kappa \sqrt{\kappa^2 - x^2}},\]

\[\frac{d\sigma (p_0 \rightarrow p)}{dp} = \frac{\sigma_\infty}{4\pi} \left( \frac{M}{p_0^2} \right)^{1/2} \left\{ \exp \left\{ -\frac{1}{4} \left( \frac{M}{m} \right) \frac{1}{x^2} \left[ \frac{M}{m} \left( p_0^2 - p^2 \right) - x^2 \right]^2 \right\} \right\} \frac{dx}{\ln \frac{p_0 + p + \sqrt{(p_0 + p)^2 - x^2}}{|p_0 - p|} \ln \frac{p_0 + p + \sqrt{(p_0 - p)^2 - x^2}}{|p_0 - p|} \ln \frac{p_0 + p + \sqrt{(p_0 + p)^2 - x^2}}{|p_0 - p|} \frac{x}{|p_0 - p|},\]

Comparison of Eqs. (2) and (4) for the case \(M = m\): a) \(p_0 = 1\); b) \(p_0 = 2\); c) \(p_0 = 3\); d) \(p_0 \gg 1\); 1) constructed from Eq. (2) ("monatomic" approximation); 2) constructed from Eq. (4) (Rigorous classical treatment for scattering).

In Eq. (4), as in (2), \(p_0\) and \(p\) are expressed in the units \(\sqrt{2mk_BT}\); \(M = 1b^{-2}\). We have made some comparative calculations on the basis of Eqs. (5) and (4) for the case \(M = m \left(M^{(1)} = \frac{3}{8}\right)\) (scattering by a proton of an HCl-type molecule). The results are given in the figure for \(p_0 = 1, 2, 3\) and \(p_0 \gg 1\). Our attention is drawn to the substantial difference in Curves 1 and 2 in the elastic part of the scattering characteristic, as well as the generally increasing divergence of the curves with increasing momentum (energy) of the incident neutrons.

The values calculated from the curves shown in the figures for the zero and first energy moments are given in Tables 1 and 2.

It follows from a comparison of the moments that, in spite of the reduction in general scattering effect (total cross section \(\sigma^{(1)}\)), the "monatomic" approximation makes the general "slowing-down" properties of the rotator (moment \(\sigma^{(1)}\)) about 10\% too large.