Quasielastic scattering of slow particles by thin films

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The cross section for scattering of slow particles by thin films is obtained in the framework of the quantum theory of multiple scattering by systems of bound particles in the quasielastic approximation. The results are discussed, and in particular, it is shown that if the wavelength χ of the incident particles becomes much greater than the thickness d of the target and at the same time the cross section for scattering by one nucleus, σ_0 , satisfies the inequality $\pi (nd)^2 \sigma_0 \chi^2 > 1$ (n is the number density of nuclei in the target), the total cross section for scattering by the complete target becomes universal and does not depend on σ_0 . © 1996 American Institute of Physics. [S1063-7761(96)01603-9]

1. INTRODUCTION

Extensive monographs (see, for example, Ref. 1) have been devoted to the physics and optics of slow and ultracold neutrons. There have been detailed investigations of the reflection and refraction of neutron waves in matter, and the details of their dispersion law have been studied (see, for example, Ref. 2). In general, the eikonal approximation has been used to study the passage of ultracold neutrons through matter. However, when the wavelength χ of the particle becomes comparable with or greater than the diameter of the scatterer then, as Goldberger and Watson showed,³ the eikonal approximation may be invalid. It is therefore of interest to consider the scattering of ultracold neutrons by thin films ($\chi \ge d$, where d is the film thickness) without using the eikonal approximation.

It should be mentioned that an analogous problem of the passage of resonance gamma rays through matter was considered in Ref. 4. In time-dependent quantum mechanics, it was shown in this study that the eikonal approximation holds only when certain conditions are satisfied. First, the wavelength of the gamma ray must be much less than the thickness of the target $[d/(2\lambda) \gg 1]$ and, second, the medium must be sufficiently tenuous $(\pi n \lambda^3 \ll 1)$. If these conditions are satisfied, the quantum-mechanical treatment is identical to the classical description of the passage of electromagnetic waves through matter that is characterized by an ordinary refractive index. If the conditions are not satisfied, the quantum-mechanical treatment may differ appreciably from the classical one.

2. THE STATIONARY CASE. STATEMENT AND SOLUTION OF THE PROBLEM

Let a stationary flux of particles (neutrons) be incident on a target in the form of a thin plate. Our problem is to find the amplitude for scattering of the particles by this target and, therefore, the cross section. We shall use the method of multiple scattering. It was developed and justified by Goldberger and Watson (Ref. 3, Chap. 11, §3), and the following approximations were used: $I \ge R$, $I \ge \hbar/p$, $I \ge R_c$. Here $I = 1/(n\sigma_0)$ is the mean free path of a particle in the scattering medium (*n* is the number density of the nuclei of the target, and σ_0 is the mean cross section for scattering by a free particle of the target), *R* is the radius of the scatterer, *p* is the momentum of the scattered particle, and R_c is the correlation radius.³ As is shown in Ref. 3, the amplitude for scattering by a system of *N* centers with allowance for multiple scattering can be represented in the stationary case for the quasielastic approximation in the form (see Ref. 3, Eq. (305)),

$$f^{(N)} = \sum_{i} f_{i} \exp(-i\mathbf{k}\mathbf{r}_{i}) \bigg| \exp(i\mathbf{p}\mathbf{r}_{i}) + \sum_{j \neq i} \frac{\exp(ip|\mathbf{r}_{i} - \mathbf{r}_{j}|)}{|\mathbf{r}_{i} - \mathbf{r}_{j}|} Q(\mathbf{r}_{j}) \bigg|, \qquad (1)$$

where \mathbf{r}_i is the position vector of scattering center *i*, f_i is the amplitude for scattering by center *i* (for simplicity, we assume that the scattering amplitude does not depend on the scattering angle or on the spin variables), \mathbf{p} and \mathbf{k} are the initial and final momenta of the particle, and $Q(\mathbf{r}_j)$ is the function determined by the equation (see Ref. 3, Eq. (303)),

$$Q(\mathbf{r}_i) = f_i \exp(i\mathbf{p}\mathbf{r}_i) + \sum_{j \neq i} \frac{\exp(ip|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|} Q(\mathbf{r}_j).$$
(2)

The system of equations (1) and (2) completely determines the scattering cross section in the quasielastic approximation for a target consisting of N scattering centers. For slow particles, when the wavelength $\chi = \hbar/p$ is much greater than the separation *a* between centers, it is possible to go over in Eqs. (1) and (2) from a sum over centers to integration over the coordinates. If we introduce the number density $n(\mathbf{r})$ of the target nuclei, then from (2) we obtain

$$Q(\mathbf{r}) = f \exp(i\mathbf{p}\mathbf{r}) + \int \frac{n(\mathbf{r}')d\mathbf{r}' \exp(ip|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} Q(\mathbf{r}').$$
(2')

For definiteness, we direct the z axis along the normal into the target. Then we write $n(\mathbf{r})=n$ for all x and y when 0 < z < d, where d is the thickness of the target, and $n(\mathbf{r})=0$ for all remaining points of space. Note that the number density of the nuclei can be regarded as constant only if $pd \ll 1$ and $|\mathbf{p}-\mathbf{k}|a \ll 1$. Obviously, $Q(\mathbf{r})$ cannot depend on x or y. Integrating Eq. (2') over x and y, we obtain

$$Q(z) = f \exp(ip_{z}z) + \frac{2\pi ni}{p} \int_{0}^{d} \exp(ip|z-z'|)Q(z')dz'.$$
(2'')

Similarly, for $f^{(N)}$ we can obtain the expression

$$f^{(N)} = \frac{N}{d} \int_0^d dz \, \exp(-ik_z z) \mathcal{Q}(z). \tag{3}$$

To find Q(z), it is convenient to go over from the integral equation (2'') to a differential equation. Differentiating (2'') twice with respect to z, we obtain

$$Q''(z) + (p^2 + 4\pi nf)Q = (p^2 - p_z^2)f \exp(ip_z z).$$
(4)

The solution of Eq. (4) has the form

$$Q(z) = f \exp(ip_{z}z) \frac{\sin^{2} \theta}{\sin^{2} \theta + 4\pi nf/p^{2}} + A \exp(i\alpha_{1}z)$$
$$+ B \exp(i\alpha_{2}z).$$
(5)

Here θ is the angle between the momentum **p** and the *z* axis, and

$$\alpha_{1,2} = \pm p \sqrt{1 + 4\pi n f/p^2}.$$
 (6)

The coefficients A and B are determined by substituting the expression (5) for Q(z) in Eq. (4) for z=0 and z=d. The differential scattering cross section can be obtained from (3):

$$d\sigma/d\Omega = |f^{(N)}|^2. \tag{7}$$

The total scattering cross section is readily obtained from the optical theorem:

$$\sigma = \frac{4\pi}{p} \operatorname{Im}[f^{(N)}(0)], \qquad (8)$$

where $f^{(N)}(0)$ is taken at $\mathbf{k} = \mathbf{p}$.

The expressions (3)-(8) completely determine the multiple scattering cross section in the quasielastic approximation. However, in the general case the expressions for the coefficients A and B are extremely cumbersome, and we therefore consider two limiting cases. In the first case, we impose on d the conditions $|\text{Re } \alpha| d \ll 1$ and $|\text{Im } \alpha| d \ll 1$. These conditions can be satisfied for ultracold neutrons. If for the target nuclei we have

$$4\pi n |\operatorname{Re} f|/p^2 \gg 1, \tag{9}$$

then, bearing in mind that $|\text{Re } f| \ge \text{Im } f$,¹⁾ we obtain

$$\alpha_{1,2} = \pm \sqrt{\pi n |\operatorname{Re} f|} (2 + i\beta), \qquad (10)$$

where $\beta = \text{Im } f/\text{Re } f$.

For $p \sim 10^5$ cm⁻¹ and $|\text{Re } f| \sim 10^{-12}$ cm, the condition (9) is satisfied: $4\pi n |\text{Re } f|/p^2 \sim 10 \ll 1$. Then the condition for a thin target can be written as

$$4\pi n |\operatorname{Re} f| d^2 \ll 1. \tag{11}$$

For a target of thickness $d \sim 10^{-6}$ cm, this condition is satisfied: $4\pi n |\text{Re } f| d^2 \sim 0.1$. In this case, we obtain for $f^{(N)}$ the expression

$$f^{(N)} = fN \left[\frac{1}{1 - 2\pi i n f d/p} - \frac{\sin^2 \theta}{\sin^2 \theta + 4\pi n f/p^2} \right].$$
(12)

For normal incidence of the particles $(p=p_z)$, using (8) and the optical theorem for the amplitude f, we find the total cross section:

$$\sigma = \frac{4\pi}{p} \operatorname{Im} f^{(N)}(0) = \frac{N\sigma_0(1 + 2\pi nd/p^2)}{1 + nd\sigma_0(1 + \pi nd/p^2)}, \quad (13)$$

where σ_0 is the total cross section for scattering of a neutron by a nucleus of the target. Taking into account the orders of magnitude of *n*, *d*, and *p* found above, we conclude that $\pi nd/p^2 \leq 1$, and therefore

$$\sigma = 2\pi n N d\sigma_0 / [p^2 + \pi (nd)^2 \sigma_0]. \tag{13'}$$

Since $\sigma_0 = 4\pi |f|^2 \sim 10^{-23} \text{ cm}^2$, the two terms in the denominator have the same order of magnitude. If σ_0 is somewhat smaller, then

$$\sigma \approx 2\pi n N d\sigma_0 / p^2 \quad \text{for } \sigma_0 < p^2 / [\pi(nd)^2], \tag{14}$$

while if σ_0 is somewhat larger,

$$\sigma \approx 2N/nd = 2S \quad \text{for } \sigma_0 > p^2 / [\pi(nd)^2], \qquad (14')$$

where S is the area of the target. In this case, the cross section does not depend on the cross section for neutron scattering by a nucleus and is twice the geometrical area of the target!

It can be shown that in the case of a thick target, i.e., when $|\text{Re } \alpha_{1,2}| d \ge 1$, for normal incidence $(p=p_z)$ and forward scattering $(\mathbf{k}=\mathbf{p})$ the total scattering cross section to accuracy $[\text{Re}(\alpha)d]^{-2} \ll 1$ is

$$f^{(N)} = Nf[1 - \exp(-\mu d)]/(\mu d), \qquad (15)$$

where

$$\mu = \frac{2\pi n \, \operatorname{Im} f}{p} = \frac{n\sigma_0}{2}$$

is the linear absorption coefficient. Thus, in the approximation of a thick target the solution of the equation for the total scattering amplitude is identical to the expression obtained in the usual eikonal approximation and differs significantly, at least functionally, from the solution for the case of a thin target (see Eq. (12)).

3. TRANSMISSION COEFFICIENT AS A FUNCTION OF TIME

Before we turn to a discussion of the results obtained in the thin-target approximation for resonant scattering of slow particles, we obtain an expression for the transmission coefficient as a function of time. In the resonance approximation, the wave function of the neutron-target system can be written in the form

$$\Psi(t) = A(t)\phi_{\mathbf{p}}^{*}\Phi_{N} + B_{\mathbf{p}}(t)\phi^{0}\Phi_{N} + \sum_{l} C_{\mathbf{p}l}(t)\phi_{0}\Phi_{N}^{*}.$$
(16)

Here A(t) is the amplitude of the state of the system in which the source is in an excited state with energy ε_0 and the target nuclei are in the ground state; $B_p(t)$ is the amplitude of the state in which the source is in the ground state and there is one neutron with momentum **p** and energy ε_p ; $C_{pl}(t)$ is the amplitude of the state in which nucleus *l* of the target is in an excited state and the source is in the ground state. Using Heitler's method for the Fourier transforms of the amplitudes, we can write down the system of equations

$$(\omega - \omega_0 + i\gamma_c/2)A(\omega) = 1 + \sum_{\mathbf{k}} {}^{\prime}H_{\mathbf{k}}B_{\mathbf{k}}(\omega),$$

$$(\omega - \omega_{\mathbf{k}} + i\varepsilon)B_{\mathbf{k}}(\omega) = H_{\mathbf{k}}^* \bigg[A(\omega) + \sum_{l} \exp(-i\mathbf{p}\mathbf{x}_l)C_l(\omega) \bigg],$$

(17)

$$(\omega - \omega'_0 + i\gamma_c/2)C_l(\omega) = \sum_{\mathbf{p}} H_{\mathbf{p}} \exp(i\mathbf{p}\mathbf{x}_l)B_{\mathbf{p}}(\omega),$$

where H_k is the matrix element for interaction of a nucleus with the neutron, and γ_c is the partial width of the excited state of the nucleus not associated with emission of a neutron. We set the thickness of the target equal to d and take the area of the target to be $S=L^2$. If the neutron source is sufficiently far from the target, neutrons incident on the target can be described by plane waves propagating in the positive z direction. In this approximation,

$$(\omega - \omega_{\mathbf{p}} + i\varepsilon)B_{\mathbf{p}}(\omega) = H_{\mathbf{p}}^{*} \left[\frac{\omega_{0}L\,\delta(p_{x})\,\delta(p_{y})\,\theta(p_{z})}{\omega - \omega_{0} + i\Gamma/2} + \sum_{l} \exp(-i\mathbf{p}\mathbf{x}_{l})C_{l}(\omega) \right], \quad (18)$$

where $\Gamma = \gamma_c + \gamma_n$ is the total width of the nuclear level from which the resonant neutron is emitted. Substituting the expression (17) for $B_k(\omega)$ in the equation for $C_l(\omega)$, we obtain

$$\left(\omega - \omega_0' + \frac{i\Gamma}{2}\right) C_l(\omega) = -i\pi\gamma_n \frac{\exp(ipz_l)}{\omega_0 L(\omega - \omega_0 + i\Gamma/2)} - \frac{\gamma_n}{2} \sum_{j \neq i} C_j(\omega) \frac{\exp(ip|z_j - z_l|)}{p|z_j - z_l|}.$$
(19)

As we did above, we can obtain for $C(z, \omega)$ the expression

$$\left(\omega - \omega_0' + \frac{i\Gamma}{2}\right) C(z,\omega) = -i\pi\gamma_n \frac{\exp(ipz)}{\omega_0 L(\omega - \omega_0 + i\Gamma/2)} - \frac{i\pi\gamma_n n}{\omega_0^2} \int_0^d \exp(i|z - z'|p) \times C(z',\omega) dz'.$$
 (20)

In the thin target approximation, when $pd \ll 1$, we obtain a solution of the equation for $C(z, \omega)$ in the form

$$C(z,\omega) = i\pi\gamma_n / [\omega_0 L(\omega - \omega_0 + i\Gamma/2)(\omega - \omega'_0 + i\Gamma/2 + iD)],$$
(21)

where

Substituting the resulting expression into (18), we find $B_k(\omega)$:

$$B_k(\omega)$$

$$= -\frac{i\omega_0 DH_k^*}{(\omega - \omega_k + i\varepsilon)(\omega - \omega_0 + i\Gamma/2)(\omega - \omega_0' + i\Gamma/2 + iD)}.$$
(23)

From (16), (17), (21), and (23), we obtain for the wave function the expression

$$\Psi(z,t) = \frac{\omega_0 \sqrt{L}}{4\pi^2} \int_0^\infty dk \int d\omega \times \frac{H_k^* \exp[i(kz - \omega_k t)]}{(\omega - \omega_k + i\varepsilon)(\omega - \omega_0 + i\Gamma/2)(\omega - \omega_0' + i\Gamma/2 + iD)}.$$
(24)

The integrals are calculated in the same way as in Ref. 4 (see Eqs. (39)-(41)). At the same time, we take into account the fact that

$$k \simeq p + \frac{dk}{d\omega_k} \left(\omega_k - \frac{p^2}{2m} \right) = p + \frac{1}{v_0} \left(\omega_k - \frac{p^2}{2m} \right),$$

where m, v_0 , and p are, respectively, the mass, velocity, and momentum of the incident neutron.⁵ As a result, we obtain

$$\Psi(z,t) = \omega_0 \sqrt{L} \frac{H_{\omega_0}^* D}{\Delta \omega + iD} \exp\left[-\left(i\omega_0' + \frac{\Gamma}{2}\right)\tau\right] \\ \times \{\exp(-D\tau) - \exp(-i\Delta\omega\tau)\},$$
(25)

where

$$\tau = t - z/v_0, \quad \Delta \omega = \omega_0 - \omega'_0.$$

Finally, the ratio of the flux transmitted through the film to the density of the incident neutron flux can be written in the form

$$T(\tau) = \frac{\Gamma}{\pi \gamma_n} L^2 |\Psi|^2 = \frac{\Gamma \exp(-\Gamma \tau) (D/v_0)^2}{(\Delta \omega)^2 + D^2} \times [1 + \exp(-2D\tau) - 2\exp(-D\tau)\cos(\Delta \omega \tau)]. \quad (26)$$

4. CONCLUSIONS AND DISCUSSION

In conclusion, we discuss the results. As our calculations show, for any finite thickness of the target, multiple scattering within the target gives rise to two waves with complex wave vectors α_1 and α_2 . The + sign of the real part of the wave vector α_1 corresponds to a wave propagating along the z component of the wave vector of the incident wave, and, accordingly, the wave with wave vector α_2 propagates in the opposite direction. The amplitudes of these waves depend heavily on the values of the parameters $|\alpha_1|d$ and $|\alpha_2|d$.

For $|\alpha_{12}| d \ll 1$, the amplitudes of the two waves have the same order of magnitude, and in this case, as was shown in (12)-(14'), the quasielastic scattering cross section becomes universal, given a certain relationship between the amplitude for scattering by an individual center, the number density of the target nuclei, and the wavelength of the incident particles, i.e., it does not depend on the amplitude for scattering by an individual target nucleus. This effect, which was first obtained by Foldy for the two-center problem, can, in our view, explain the reduction in storage time of ultracold neutrons in traps made of different materials. Since thin films of oxides, carbides, etc., are essentially always formed on internal walls of traps, it follows that if (9), (11), and (14') are satisfied, the scattering cross section will be universal and will not depend on the material of which the trap walls are made. An indirect confirmation of this conclusion may be provided by experiments on the determination of the coefficient of transmission of ultracold neutrons through films of frozen heavy water,⁶ which showed that the transmission coefficient changes abruptly when the thickness of the film is increased from a value comparable with the neutron wavelength to a value much greater than the wavelength.

For $|\alpha_{1,2}|d \ge 1$, the amplitude of the wave with wave vector α_1 becomes much greater than the amplitude of the wave with wave vector α_2 , and therefore to accuracy $|\alpha_1 d|^{-2}$, the macroscopic scattering cross section is essentially always described by the usual expressions with the complex wave vector α_1 . However, in experiments on the change in phase of the wave function of neutrons after passage through films of finite thickness, it is necessary to take

into account the two waves, with α_1 and α_2 , and there are then corrections to the phase shift determined for just the wave with α_1 . Phenomenologically, these corrections can reduce to corrections to the refractive index, allowance being made for different approximations (see, for example, Ref. 7). Indeed, the physics is such that, as follows from the resulting solution, two waves are formed in the medium, and these are responsible for the correct relationships between the phases of the particle incident on the target and leaving the target. In the general case, errors will arise if these phase relationships are described by a refractive index.

Finally, as is shown by calculations of the transmission coefficient as a function of the time, for sufficiently thin targets $(|\alpha_{1,2}|d<1)$ a universal expression also arises, and it differs strongly from the expression for thick targets.

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¹⁾This inequality follows from the optical theorem for the isotropic amplitude f: Im $f = p|f|^2 \sim 10^5 \cdot 10^{-24}$ cm = 10^{-19} cm, whereas |Re $f| \simeq |f| \sim 10^{-12}$ cm.

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