Neutron-electron interaction: Transmission and scattering amplitudes and interference corrections

V. K. Ignatovich*
Frank Laboratory of Neutron Physics of Joint Institute for Nuclear Research, 141980, Dubna, Moscow region, Russia

Masahiko Utsuro†
Research Reactor Institute, Kyoto University, Kumatori-cho, Sennan-gun, 590-04 Osaka, Japan

Ph. V. Ignatovich‡
Moscow State University, Physics Faculty, Lenin Hill, Moscow, Russia
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Neutron transmission experiments for neutron-electron interaction are discussed. The contribution of the coherent elastic scattering cross section to the attenuation cross section is reconsidered. Some uncertainties in interference correction to the coherent elastic scattering cross section, which leave some room for doubting the reliability of the number 1.3×10^{-3} fm for *n-e*-scattering amplitude, are pointed out. Some corrections to the real part of the scattering amplitude, which should be taken into account in measurements of the neutron polarizability, are found. [S0556-2813(99)00902-4]

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I. INTRODUCTION

The problem of *n-e* interaction becomes in some respect irritating. It is based on the two experimental results [3] obtained for the *n-e* scattering amplitude[1] b_{ne}:[2]

$$b_{ne}=(1.309\pm0.024)\times10^{-3}\ \text{fm}, \tag{1}$$

$$b_{ne}=(1.577\pm0.034)\times10^{-3}\ \text{fm}. \tag{2}$$

Their difference is considerably larger than the reported uncertainties, and is essential [5] because it gives a different sign for neutron charge radius $\langle r^2\rangle$. The radius is related to b_{ne} via the expression

$$\langle r^2\rangle=-\int\rho_c(r)r^2\,d^3r=-\frac{3\hbar^2}{me^2}(b_{ne}-b_F), \tag{3}$$

where ρ_c is the neutron charge density, m is the neutron mass, e is the electron charge, and b_F is the so-called Foldy term [6], which is the constant: $b_F=1.468\times10^{-3}$ fm. The results (1),(2) give positive and negative values for (3), respectively, and the absolute magnitude of the radius in both cases (≈0.1 fm) is considerably smaller than the Compton wavelength (≈0.2 fm). The image of the neutron as the proton surrounded by a cloud of negatively charged π mesons requires the negative sign. Thus the second result [7] is in better conformity with such a model; nevertheless some scientists [8,9] declare that it is the first result [10] which is the most reliable.

We decided to reconsider the procedure of b_{ne} extraction from transmission experiments, in which the transmission exponent is measured. The exponent contains the coherent elastic scattering cross section, $\sigma_{\rm el}^{\rm coh}$, from which the information about *n-e* interaction is extracted. However this extraction is accompanied by subtractions of many so-called solid state corrections, and reliability of b_{ne} depends on the reliability of knowledge of these corrections.

We investigated here one of them: the interference correction. In the following section we considered the question of when the attenuation cross section contains $\sigma_{\rm el}^{\rm coh}$. We have shown that at low energies and for single crystals the attenuation cross section does not contain $\sigma_{\rm el}^{\rm coh}$.

For polycrystals, amorphous substances, and liquids the attenuation cross section contains $\sigma_{\rm el}^{\rm coh}$ with an interference correction, as calculated in [11]. However we found, that for polycrystals there is an additional term, which was not pointed out in [11].

In the third section we repeated the considerations of [11] in our notations to simplify the comparison of our results with those of [11].

In the fourth section we performed an analysis in the framework of multiple wave scattering theory (MVS), and in the fifth section we discussed some points, which need more investigations to leave no room for doubting the accepted value of b_{ne}.

II. DEFINITION OF TRANSMISSION: RELATION OF TRANSMISSION TO *n-e* SCATTERING

The transmission, T, of a sample of thickness L is represented as

$$T=\exp(-N_0\sigma L), \tag{4}$$

*Electronic address: ignatovi@nf.jinr.ru
†Electronic address: utsuro@rri.kyoto-u.ac.jp
‡Electronic address: phil@femto4.ilc.msu.su

[1]We use all the amplitudes b with negative sign, thus for most nuclei Re $b>0$.

[2]In [4] the new result is reported: from experiments with ^{208}Pb $b_{ne}=(1.33\pm0.027\pm0.03)\times10^{-3}$ fm, and from experiments with Bi: $b_{ne}=(1.44\pm0.033\pm0.06)\times10^{-3}$ fm.

where L is the sample thickness, N_0 is its atomic density, and σ is the attenuation cross section, which is usually taken to be the total scattering cross section σ_t, which includes the elastic coherent scattering cross section $\sigma_{\rm el}^{\rm coh}=4\pi|b|^2$, b being the coherent scattering amplitude. The exponent is obtained because the decrease dI of the neutron intensity I after transmission through the layer of thickness dx is governed by the law: $dI=-dx\,N_0\sigma I$. However this law does not define σ. It only states that σ includes all the processes that take neutrons away from the direct beam. If it includes the coherent elastic scattering cross section $\sigma_{\rm el}^{\rm coh}=4\pi|b|^2$, then it contains information about neutron-electron interaction.

Indeed, at low energies the amplitude b includes the pure nuclear isotropic coherent amplitude b_c[3], and the neutron-electron amplitude b_{ne}, which is characterized by the point-like electrostatic interaction

$$H_{ne}=4\pi b_{ne}\frac{\hbar^2}{2m}[\rho_N-\rho_e], \tag{5}$$

where $\rho_{N,e}$ are the charge distribution (divided by the electronic charge $|e|$) inside the nucleus and the electronic cloud of the atom, respectively.

The interaction (5) gives a slightly anisotropic contribution to scattering, thus the total coherent amplitude is represented by the expression

$$b(q)=b_c+b_{ne}Z[F_N(\boldsymbol{q})-F_e(\boldsymbol{q})],$$

$$F_i(\boldsymbol{q})=\int d^3r\,\rho(\boldsymbol{r})\exp(i\boldsymbol{qr}), \tag{6}$$

where q is the momentum transferred, $F_{N,e}$ are the nuclear and electron form factors, and Z is the charge of the atomic nucleus.

From Eq. (6) it follows that

$$\sigma_{\rm el}^{\rm coh}=4\pi\langle|b|^2\rangle=\int_{4\pi}\{[\mathrm{Re}\,b(\Omega)]^2+[\mathrm{Im}\,b(\Omega)]^2\}d\Omega$$
$$=4\pi[(\mathrm{Re}\,b_c)^2+(\mathrm{Im}\,b_c)^2+2\,\mathrm{Re}\,b_cZb_{ne}(1-\langle F_e(q)\rangle)]. \tag{7}$$

The last equality is obtained by substitution of Eq. (6) under the integral. Here $\langle F(q)\rangle$ is the electron form factor $F_e(\boldsymbol{q})$ averaged over angles, the nuclear form factor $F_N(\boldsymbol{q})$ is replaced by unity, and the term with b_{ne}^2 is neglected.

It is necessary to point out that the suggestion $\sigma=\sigma_t$ in some respect seems paradoxical. Indeed, if we consider transmission of low energy neutrons through a monoatomic, monoisotopic, ordered medium at 0 temperature with heavy (not moving) nonabsorbing atoms then the attenuation is given by $\sigma_t\equiv\sigma_{\rm el}^{\rm coh}$, the intensity I decreases, and the question arises: where do the lost neutrons go? Of course, they can be reflected by the medium, however the reflection coefficient only oscillates with thickness, and does not increase exponentially with it.

[3]Both of potential and resonance scattering.

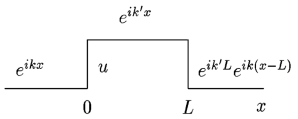

FIG. 1. Transmission of neutrons through a sample of width L with optical potential u.

This consideration shows that we must be careful in defining the attenuation cross section σ in the transmission exponent (4). Quantum mechanics helps us to get this definition without contradictions. Let us look at Fig. 1.

According to the Schrödinger equation, if the incident neutron is described by a plane wave $\exp(ikx)$, where k is the wave number, the wave function inside the medium is

$$\exp(ik'x),\quad \text{where}\quad k'=\sqrt{k^2-u}=kn\approx k(1-u/2k^2), \tag{8}$$

$u=4\pi Nb(q=0)$ is the optical potential of the medium, $n\approx 1-u/2k^2$ is the refractive index, and in the wave function (8) we omitted reflection from the interfaces because for all the neutron energies, $E>25$ meV, considered here, the reflection amplitude has the magnitude $u/4k^2\ll 10^{-5}$.

Since $b(0)$ in general is complex, k' also contains an imaginary part, and the wave function at the exit from the sample becomes proportional to $\exp(-\mathrm{Im}\,k'L)$. Thus the sample transmission is

$$T=|\psi(L)|^2=\exp(-2\,\mathrm{Im}\,k'L)$$
$$=\exp(-4\pi N_0|\mathrm{Im}\,b(0)|L/k), \tag{9}$$

and the amplitude b_{ne} is to be extracted from $-\mathrm{Im}\,b(0)$. If $b(q)$ is the *amplitude* then according to the optical theorem

$$-\mathrm{Im}\,b(0)=k\sigma_t/4\pi, \tag{10}$$

where σ_t is the total cross section containing the elastic coherent scattering cross section $\sigma_{\rm el}^{\rm coh}$ and the *n-e* amplitude b_{ne} in it. After substitution of Eq. (10) into Eq. (9) we get

$$T=\exp(-N_0\sigma_tL). \tag{11}$$

However, if $b(0)$ is the *scattering length*, then

$$-\mathrm{Im}\,b(0)=k[\sigma_t-\sigma_{\rm el}^{\rm coh}]/4\pi, \tag{12}$$

and Eq. (9) is

$$T=\exp(-N_0[\sigma_t-\sigma_{\rm el}^{\rm coh}]L), \tag{13}$$

and it contains no information about b_{ne} (6).

The main question is as follows: what is the magnitude $b(q)$ that enters Eq. (9)? According to [3,12,13] and many others it is the scattering length. Then in Eq. (7) we have $-\mathrm{Im}\,b(q=0)=k[\sigma_t-\sigma_{\rm el}^{\rm coh}]/4\pi$. However in that case the attenuation (9) cannot be represented in the form (11), and b_{ne} cannot be extracted from the transmission experiment.

On the other hand, if b_{ne} is extracted with the help of Eq. (11), then $b(q)$ is not the *length*, but the *scattering amplitude*.

Now we can formulate our results and compare them with the known ones.

(1) We found that for low energy neutrons $b(0)$ is always the scattering length, and $-\mathrm{Im}\, b(0)$ does not contain $\sigma_{\mathrm{el}}^{\mathrm{coh}}$. This result is not surprising.

(2) We proved also that $b(0)$ is the *length* even at higher energies, if the sample is a single crystal. This result was in some respect obtained by Kagan and Afanasiev in 1965 [15,16]. They had shown that the widths of nuclear resonances for neutrons and gamma quanta scattering decreased when nuclei composed an ideal crystalline media. The decrease means that the part of resonance width, which is related to elastic scattering, becomes excluded. Now we see, that this result is a particular case of the more general theorem.

In [11] it was shown that at high energies $\sigma_{\mathrm{el}}^{\mathrm{coh}}$ contributes to σ_t, but it contains the factor $G=1-\pi I/a^2k^2$, in which k is the neutron wave number, a is the interatomic distance, and I is a constant parameter. The factor G implies that the contribution of $\sigma_{\mathrm{el}}^{\mathrm{coh}}$ to σ_t has a correction that decreases with energy decrease.

In [14] it is even stated that at low energies the correction to $\sigma_{\mathrm{el}}^{\mathrm{coh}}$ diverges. In terms of the factor G this statement can be interpreted as an assertion that at low enough energy G becomes zero. We have shown that this is correct for polycrystalline and amorphous media.

(3) For polycrystalline samples, we confirmed the result of [11], however we found that the factor G contains also the term of order $1/ka$, which was not pointed out in [11]. This term can be important, because it decreases with energy slower than the term $1/k^2a^2$ found in [11]. Moreover, this term depends on the dimensions of crystallites and should be studied experimentally for better evaluation of b_{ne}.

(4) For amorphous substances we completely reconfirmed the result of [11] with no extra term, i.e., we found the correction factor G that at high energies behaves as $G=1-\pi I/2k^2a^2$, however we also found its behavior in the full energy range $0<k^2<\infty$.

We calculated the constant I for different models of pair correlation function and found that the broad limits of its variation lead to additional uncertainty for the magnitude of b_{ne}. However the recently published result [4] is based on the experimentally measured pair correlation function and thus it is free from this uncertainty. It is necessary to understand why the measurements with liquid and solid [2] samples perfectly match each other. It is possible that the corrections found for polycrystals appear in liquids via small angle scattering.

In the next section we rewrite the considerations by Placzek *et al.* [11] in our notation to facilitate comparison of our results with those of [11].

III. COHERENT CROSS SECTION IN THE THEORY OF PLACZEK *et al.*

Placzek *et al.* [11] use perturbation theory. They express the scattering amplitude of N identical scatterers via the single atom scattering *amplitude* b in the form

$$b(N)=b\sum_{n=1}^{N}\exp(i\boldsymbol{q}\boldsymbol{r}_n), \tag{14}$$

where $\boldsymbol{q}=\boldsymbol{k}_0-\boldsymbol{k}$ is the scattering vector, $\boldsymbol{k}_0,\boldsymbol{k}$ are the wave vectors of the incident and scattered neutrons, and the nuclei are supposed to be motionless to deal only with the elastic scattering. The cross section attributed to this amplitude is

$$\sigma(N)=\int{}' d\Omega |b(N)|^2, \tag{15}$$

and the cross section related to a single scatterer is

$$\sigma_1=\int{}' d\Omega |b(N)|^2/N, \tag{16}$$

where the prime at the integral means that in the integration the forward angle is excluded, because the neutron moving along the forward direction is not scattered at all.

The magnitude $|b(N)|^2$ is represented in the form

$$|b(N)|^2=|b|^2\left[N+\sum_{n\neq m}\exp(i\boldsymbol{q}\boldsymbol{r}_{mn})\right],$$

$$\text{where}\quad \boldsymbol{r}_{mn}=\boldsymbol{r}_n-\boldsymbol{r}_m. \tag{17}$$

The sum can be replaced by the integral, which gives

$$|b(N)|^2=N|b|^2\left[1+N_0\int w(\boldsymbol{r})\exp(i\boldsymbol{q}\boldsymbol{r})d^3r\right], \tag{18}$$

where $N_0=1/a^3$ is the atomic density of scatterers, a is interatomic distance, and $w(r)$ is the probability to find a second nucleus at a point $\boldsymbol{r}$, if the first one is at $\boldsymbol{r}=0$. The function $w(r)$ can be represented in the form $w(r)=1-\gamma(r)$, where the function $\gamma(r)$ is equal to 1 at $r=0$, and goes to 0 at $r\to\infty$. For definiteness in the following we shall suggest $\gamma(r)=\exp(-r/s)$. The parameter s is determined by the condition

$$N_0\int \gamma(r)d^3r=1\to 8\pi N_0 s^3=1, \tag{19}$$

which gives $s=1/\sqrt[3]{8\pi N_0}=a/2\sqrt[3]{\pi}$.

From Eq. (18) it follows that

$$|b(N)|^2/N=|b|^2\left[1-N_0\int \gamma(\boldsymbol{r})\exp(i\boldsymbol{q}\boldsymbol{r})d^3r\right]. \tag{20}$$

The integral over $w(r)+\gamma(r)=1$ is omitted because it gives $\delta(\boldsymbol{q})$, i.e., the scattering in the forward direction, which, as was mentioned above, represents no scattering at all and should be excluded.

Substitution of Eq. (20) into Eq. (16) gives

$$\sigma=\sigma_{\mathrm{el}}^{\mathrm{coh}}[1-1/(1+4s^2k^2)]\approx\sigma_{\mathrm{el}}^{\mathrm{coh}}(1-2{,}14/k^2a^2), \tag{21}$$

where $\sigma_{\mathrm{el}}^{\mathrm{coh}}=4\pi|b|^2$, and in the last equality $ka\gg 1$ is supposed.

In [11] some more general results were obtained. It was proved that from Eq. (18) for large k it follows

$$\sigma \approx \sigma_{\rm el}^{\rm coh}(1-\pi I/2k^2a^2), \tag{22}$$

and $I<3$. This result was declared to be valid also for crystals, and the magnitude $I\approx 2.8$ for different lattices was calculated. We shall show that this result for crystals is not complete.

IV. OPTICAL POTENTIAL AND SCATTERING AMPLITUDE

The perturbational approach has some deficiency. It is well applicable to a plane of scatterers, however for three dimensional set of nuclei it does not take into account screening of atomic planes by each other. This screening may play a crucial role especially for crystalline arrangement of atoms.

We shall follow a different approach [17,18] based on the multiple wave scattering (MWS) theory. First we consider a single scatterer, and define the scattering length and amplitude, then we consider a crystalline plane, and find how the scattering amplitude is modified. After that we find the propagation of neutrons inside a semi-infinite crystalline medium, and show that the coherent elastic scattering cross section does not contribute to attenuation.

Usually the samples in transmission measurements are not single crystals, and we consider the transmission through a polycrystalline medium. In polycrystals $\sigma_{\rm el}^{\rm coh}$ will be shown to contribute to the transmission exponent but the contribution contains an additional term not obtained in [11].

The next step is a model medium consisting of discrete atomic planes with disordered distribution inside the planes, and the last one is the uniform disordered medium.

A. Definition of the scattering amplitude and length for a single scatterer

The s-scattering by a single nucleus placed at a point 0 is described by the wave function

$$\psi = \exp(i\boldsymbol{kr}) - b\frac{\exp(ikr)}{r}, \tag{23}$$

where b is by definition the scattering amplitude (we define it with negative sign). This amplitude is always representable in the form

$$b = \frac{b_0}{1+ikb_0}, \tag{24}$$

where b_0 (and this is our definition) is the scattering length. If the nucleus has zero absorption and is motionless then b_0 is real, and the expression (24) exactly satisfies the optical theorem: $-\mathrm{Im}\, b = k|b|^2 = k\sigma_{\rm el}^{\rm coh}/4\pi$.

If the nucleus absorbs neutrons, then $b_0 = b_0' - ib_0''$ is complex and

$$-\mathrm{Im}\, b = k|b|^2 + \frac{b_0''}{(1+kb_0'')^2+k^2b_0'^2} = k|b|^2 + k\frac{\sigma_a}{4\pi},$$

$$\text{thus}\quad b_0'' \approx k\sigma_a/4\pi, \tag{25}$$

or, to be precise,

$$b_0'' \approx \frac{k\sigma_a}{4\pi}[1+k^2\sigma_a/2\pi + k^2b_0'^2]. \tag{26}$$

From Eq. (24) it follows that the real part of the amplitude b is

$$\mathrm{Re}\, b = \frac{b_0'}{(1+kb_0'')^2+k^2b_0'^2} \approx b_0'(1-2kb_0''-k^2b_0'^2)$$
$$= b_0'(1-k^2\sigma_a/2\pi - k^2b_0'^2), \tag{27}$$

which shows that at energy 100 eV it contains a correction of the order 5×10^{-4} and at the energy 10 keV the two terms in the brackets give a correction to the real part of the amplitude of order of 10%. This correction may not be very important for extraction of b_{ne}, but it can be important for extraction of the neutron polarizability, which will be considered at the end of this paper.

If the nucleus can move (for instance, oscillate) $-\mathrm{Im}\, b_0$ contains also the inelastic scattering cross section $\sigma_{\rm in}$. Thus, from our definition it follows that $-\mathrm{Im}\, b = k\sigma_t/4\pi$, and $-\mathrm{Im}\, b_0 \approx k(\sigma_a+\sigma_{\rm in})/4\pi$, and

$$\mathrm{Re}\, b = \frac{b_0'}{(1+kb_0'')^2+k^2b_0'^2} \approx b_0'(1-2kb_0''-k^2b_0'^2)$$
$$= b_0'(1-k^2[\sigma_a+\sigma_{ie}]/2\pi - k^2b_0'^2). \tag{28}$$

If the nucleus is inside a set of nuclei, the imaginary part of b changes, because the interference of waves scattered by different scatterers cancels the scattering in some directions and enhances it in some others.

B. The formulation of MWS theory

To find what happens in the collective of nuclei it is necessary to use the MWS theory. In this theory (we shall follow [18,17]) the total wave function is

$$\psi(\boldsymbol{r}) = \exp(i\boldsymbol{kr}) - \sum_n \psi(\boldsymbol{r}_n)\frac{b_n}{|\boldsymbol{r}-\boldsymbol{r}_n|}\exp(ik|\boldsymbol{r}-\boldsymbol{r}_n|), \tag{29}$$

where $\psi(\boldsymbol{r}_n)$ are the so-called ''local fields'' at points $\boldsymbol{r}_n$, which satisfy the system of equations:

$$\psi(\boldsymbol{r}_n) = \exp(i\boldsymbol{kr}_n) - \sum_{j\neq n}\psi(\boldsymbol{r}_j)\frac{b_j}{|\boldsymbol{r}_n-\boldsymbol{r}_j|}\exp(ik|\boldsymbol{r}_n-\boldsymbol{r}_j|). \tag{30}$$

The solution of this system is difficult, and in general is impossible. However in some special cases the solution can be found rigorously or with an arbitrary precision. We shall start with just such a case: the scattering of neutrons from a crystalline plane.

C. Crystalline plane

Let us consider a perfect crystalline plane with a square elementary cell of size d. From symmetry considerations it is

easy to find [18] that a plane wave $\exp(i\boldsymbol{k}\boldsymbol{r})$, incident on a crystalline plane generates the local fields

$$\psi(\boldsymbol{r}_n)=C\exp(i\boldsymbol{k}\boldsymbol{r}_n) \tag{31}$$

with the constant C.

Substituting Eq. (31) into Eq. (29) we obtain

$$\psi(\boldsymbol{r})=\exp(i\boldsymbol{k}\boldsymbol{r})-C\sum_n \exp(i\boldsymbol{k}\boldsymbol{r}_n)\frac{b_n}{|\boldsymbol{r}-\boldsymbol{r}_n|}\exp(ik|\boldsymbol{r}-\boldsymbol{r}_n|). \tag{32}$$

If we use the Fourier expansion of the spherical wave,

$$\frac{\exp(ikr)}{r}=\frac{4\pi}{(2\pi)^3}\int d^3p\frac{\exp(i\boldsymbol{p}\boldsymbol{r})}{p^2-k^2-i\epsilon}$$
$$=\frac{i}{2\pi}\int\frac{d^2p_\parallel}{p_\perp}\exp(i\boldsymbol{p}\boldsymbol{r}_\parallel+ip_\perp|r_\perp|), \tag{33}$$

where $p_\perp=\sqrt{k^2-p_\parallel^2}$ is the component of the wave vector $\boldsymbol{p}$ perpendicular to the plane, and use the relation

$$\sum_n f(n)=\sum_m \int f(x)\exp(2\pi mx)dx, \tag{34}$$

we get the total wave function in the form

$$\psi=\exp(i\boldsymbol{k}\boldsymbol{r})-i\sum_l \frac{\kappa_C}{k_{l\perp}}\exp(i\boldsymbol{k}_l\boldsymbol{r}), \tag{35}$$

where

$$\boldsymbol{k}_l=(\boldsymbol{k}_{l\parallel},k_{l\perp}),\quad \boldsymbol{k}_{l\parallel}=\boldsymbol{k}_\parallel+\boldsymbol{\tau}_l,$$
$$\boldsymbol{\tau}_l=(2\pi n_l/d,2\pi m_l/d),\quad k_{l\perp}=\sqrt{k^2-(\boldsymbol{k}_\parallel+\boldsymbol{\tau}_l)^2}, \tag{36}$$

$\boldsymbol{k}_{l\parallel},k_{l\perp}$ are the components of the lth wave vector parallel and perpendicular to the crystalline plane, respectively; $\boldsymbol{\tau}_l$ are the vectors of the reciprocal lattice of the plane, and n_l,m_l are integers. The expression (35) means that the total wave function consists of the incident wave and many diffracted waves. The amplitudes of the diffracted waves are proportional to

$$\kappa_C=2\pi N_2 b_C,\quad b_C=Cb, \tag{37}$$

where $N_2=1/d^2$ is the two-dimensional density of atoms, and C is the constant to be determined.

Substitution of Eq. (31) into Eq. (30) gives the equation for C

$$C=1-C\sum_{j\neq n}\frac{b_j}{|\boldsymbol{r}_j-\boldsymbol{r}_n|}\exp(ik|\boldsymbol{r}_j-\boldsymbol{r}_n|+i\boldsymbol{k}[\boldsymbol{r}_j-\boldsymbol{r}_n]), \tag{38}$$

from which it follows (for details see [17])

$$C=\frac{1}{1-ikb+i\sum_l \kappa/k_{l\perp}}, \tag{39}$$

where $\kappa=2\pi N_2 b$, and the sum can be extended over all l for which $k_{l\perp}^2>0$.

From Eq. (37) it follows that C renormalizes the amplitude b:

$$b_C=\frac{b_0}{1+i\sum_l \kappa_0/k_{l\perp}},\quad \text{where}\quad \kappa_0=2\pi N_2 b_0. \tag{40}$$

It is seen that the imaginary part of the amplitude has changed, and this change has a very clear physical meaning: the atoms composing the crystalline lattice scatter not isotropically but only in some special diffraction directions, determined by the vectors $\boldsymbol{\tau}_l$, and the leakage of neutrons into diffracted waves contributes to attenuation in the forward direction.

In the case of small $k<2\pi/d$ we have $k_{l\perp}^2<0$ for $|\boldsymbol{l}|\neq 0$, all the diffracted waves exponentially decay away from the plane, and the scattering amplitude becomes

$$b_C(k\to 0)=\frac{b_0}{1+i\kappa_0/k_\perp}. \tag{41}$$

The total wave function is reduced to the form

$$\psi=\exp(i\boldsymbol{k}\boldsymbol{r})-i\frac{\kappa_0}{k+i\kappa_0}\exp(i\boldsymbol{k}_\parallel\boldsymbol{r}_\parallel+ik_\perp|z|), \tag{42}$$

which means that there are only transmitted and reflected waves with the amplitudes

$$t_1=k_\perp/(k_\perp+i\kappa_0),\quad r_1=-i\kappa_0/(k_\perp+i\kappa_0). \tag{43}$$

D. Semi-infinite ideal crystal

To understand what is the b which enters the refractive index, it is sufficient to consider a semi-infinite crystalline medium. For low energy neutrons, when the expression (41) is satisfied, the calculation is straightforward. The transmission through one period for normal incidence according to Eq. (43) is

$$t=t_1\exp(ika)=\frac{k}{k+i\kappa_0}e^{ika}\approx\exp(ik[1-\kappa_0/ak^2]a)$$
$$=\exp(ik[1-u_0/2k^2]a), \tag{44}$$

where a is the distance between the planes, $u_0=4\pi N_0 b_0$, $N_0=1/ad^2$ is the atomic density, and the factor $\exp(ika)$ describes the motion between the crystalline planes. The transmission through the slab of thickness $L=Na$ is

$$\psi(L)=\exp(ik[1-u_0/2k^2]L)=\exp(ik'L),$$
$$\text{where}\quad k'=nk,\quad n\approx 1-\frac{u_0}{2k^2}. \tag{45}$$

We see that the optical potential u_0 contains the scattering length b_0, and not the scattering amplitude b. Thus in this case the transmission experiments do not contain information about b_{ne}. The damping of the transmitted wave is due only to absorption, inelastic and incoherent elastic scattering. (We

do not consider here the case of total reflection, where the wave function is also exponentially decreasing, however the decrease is governed not by the cross sections.) This result is not surprising, because it is related to the neutron energies below the Bragg edge.

Now let us consider higher energies, above the Bragg edge: $k>2\pi/d$, when diffraction on a crystalline plane can take place. In that case the amplitude (41) can be represented in the form

$$b_C=\frac{b_{\rm cr}}{1+i\kappa_{\rm cr}/k_\perp},\quad \kappa_{\rm cr}=2\pi N_2 b_{\rm cr},\quad b_{\rm cr}=\frac{b_0}{1+i\sum_{l\neq 0}\kappa_0/k_{l\perp}}. \tag{46}$$

A comparison with Eq. (41) shows that b_0 becomes $b_{\rm cr}$; i.e., it acquires an imaginary part because of elastic scattering in diffraction directions that become opened in the given geometrical configuration. However it is easy to prove by simple considerations that this imaginary part does not lead to exponentially decaying transmission, i.e.,

$$|\exp(iqL)|^2\neq\exp(-4\pi N_0 L|\mathrm{Im}\, b_1|/k), \tag{47}$$

where q is the Bloch wave number.

Indeed, the diffracted waves are coherent and their number is finite, so they can be rediffracted back into the forward direction till a stationary distribution is established. The wave function inside the crystal is a combination of all the diffracted waves

$$\Psi=\sum_n A_n(x)\exp(i\boldsymbol{k}_n\boldsymbol{r}) \tag{48}$$

with $\boldsymbol{k}_n=(\boldsymbol{k}_{0\parallel}+\boldsymbol{\tau}_\parallel,k_{n\perp})$ being wave vectors of possible diffraction directions, the subscripts $\parallel$ and $\perp$ denoting the vector components parallel and perpendicular to the entrance surface of the crystal, respectively, and $k_{n\perp}=\sqrt{k_0^2-(\boldsymbol{k}_{0\parallel}+\boldsymbol{\tau}_\parallel)^2}$. The main feature of this expression is the coefficients $A_n(x)$. They are oscillating with the depth x inside the crystal (the typical example of it is the ''pandellösung'' phenomenon). Thus the coefficient $A_0(L)$ for transmitted wave in the forward direction also oscillates with L, and does not have the exponentially decaying form. If it were exponentially decaying, the intensity would accumulate in some special directions, which contradicts the principles of thermodynamics.

We can conclude that in the case of ideal crystals the imaginary part of $b_{\rm cr}$ in Eq. (46) does not contribute to the exponential decrease of intensity, which means that $\sigma_{\rm el}^{\rm coh}$ is not contained in the attenuation cross section. In the case of single crystals and neutrons of arbitrary energies the transmission coefficient T is of the form

$$T=A\exp(-N_0L[\sigma_t-\sigma_{\rm el}^{\rm coh}]), \tag{49}$$

where the preexponential factor A can be oscillating with L, and the exponent contains no information about b_{ne}.

E. Small crystallites

All the above is correct for large ideal crystals. The situation for real mosaic crystals is different because different blocks scatter incoherently. In this case the beam damping can be described by the exponent $\exp(-N_{\rm bl}\sigma_{\rm bl}L)$, where $\sigma_{\rm bl}$ and $N_{\rm bl}$ are the scattering cross section of a single block, and the density of blocks, respectively. It is important to investigate how large is the difference between $\sigma_{\rm bl}N_{\rm bl}$ and $N_0\sigma_{\rm el}^{\rm coh}$ where $\sigma_{\rm el}^{\rm coh}=4\pi|b|^2$.

1. The perturbational result

Let us calculate the scattering on a small crystallite with the help of perturbation theory [11]. In this theory the scattering amplitude is

$$f=b\sum\ \exp(i\boldsymbol{q}\boldsymbol{r}_i)=bN_0\sum_\tau\ (2\pi)^3\delta(\boldsymbol{q}-\boldsymbol{\tau}), \tag{50}$$

where $\boldsymbol{q}=\boldsymbol{k}-\boldsymbol{k}_0$ is the momentum transferred, $\boldsymbol{\tau}=(2\pi/a)(m,n,l)$ is the vector of the reciprocal lattice (here we suppose that the crystal has a cubic elementary cell with parameter a), m, n and l are integers, and the sum over scatterers is replaced by the integral over space with the sum over vectors $\boldsymbol{\tau}$ of the reciprocal lattice, in agreement with the formula

$$\sum_n\ G(n)=\sum_m\ \int_n G(n)dn\exp(2\pi imn). \tag{51}$$

The cross section of this set of scatterers integrated over the angles of the scattered wave vectors $\boldsymbol{k}$ is

$$\Sigma=\int|f|^2d\Omega_k=|b|^2N_0^2(2\pi)^6\int\sum_{\tau,\tau'}\delta(\boldsymbol{q}-\boldsymbol{\tau})\,\delta(\boldsymbol{q}-\boldsymbol{\tau}')d\Omega_k. \tag{52}$$

The nondiagonal terms with $\boldsymbol{\tau}\neq\boldsymbol{\tau}'$ are equal to zero, because in this case

$$\delta(\boldsymbol{q}-\boldsymbol{\tau})\,\delta(\boldsymbol{q}-\boldsymbol{\tau}')=\delta(\boldsymbol{q}-\boldsymbol{\tau})\,\delta(\boldsymbol{\tau}-\boldsymbol{\tau}')=0, \tag{53}$$

and we are left only with the diagonal terms with the same τ. For diagonal terms we have

$$\Sigma=|b|^2VN_0^2(2\pi)^3\int\sum_\tau\ \delta(\boldsymbol{q}-\boldsymbol{\tau})d\Omega_k, \tag{54}$$

where we used the relation $\delta^2(\boldsymbol{p})=V\delta(\boldsymbol{p})/(2\pi)^3$. Integration over the angles in Eq. (54) can be transformed as follows:

$$\int\ G(\boldsymbol{k})d\Omega_k=\int(2/k)d^3k\ \delta(k^2-k_0^2)G(\boldsymbol{k}), \tag{55}$$

and as a result we obtain

$$\Sigma=\frac{1}{k_0}N\sigma_0(2\pi)^2N_0\sum_\tau\ \delta([\boldsymbol{k}_0-\boldsymbol{\tau}]^2-k_0^2), \tag{56}$$

where $N=N_0V$ is the total number of particles in the set, and $\sigma_0=4\pi|b|^2$. Averaging this expression over orientations of the vectors $\boldsymbol{\tau}$, we obtain $\langle\Sigma\rangle=N\sigma_0G$, where[4]

$$G=\frac{(2\pi)^2N_0}{k_0}\int\sum_{\tau}\delta([\boldsymbol{k}_0-\boldsymbol{\tau}]^2-k_0^2)\Omega_{\tau}/4\pi$$

$$=2\pi^2\sum_{\tau<2k_0}N_0/2k_0^2\tau=\sum_{|\boldsymbol{n}|=1}^{M=ka/\pi}\frac{\pi}{2(k_0a)^2|\boldsymbol{n}|}. \quad (57)$$

Here $|\boldsymbol{n}|$ is $\sqrt{n^2+m^2+l^2}$, and the upper limit of summation is defined by $|\tau|\leqslant 2k_0$.

The sum in Eq. (57) can be approximated by the integral. For the one-dimensional sum we use the approximation [19]

$$\sum_{n=a}^{b}f(n)=\int_a^b f(n)dn+\frac{1}{2}[f(a)+f(b)]$$

$$-\frac{1}{12}[f'(a)+f'(b)]+\cdots, \quad (58)$$

where $f'(x)=df(x)/dx$. In our three-dimensional case we use the following approximation:

$$\sum_{|\boldsymbol{n}|=1}^{|\boldsymbol{n}|\leqslant M}f(|\boldsymbol{n}|)=\int_1^M f(|\boldsymbol{n}|)d^3n+\frac{6}{2}f(1)-\frac{1}{12}f'(1)+\cdots, \quad (59)$$

where $\boldsymbol{n}$ is a vector with components $\boldsymbol{n}=(n,m,l)$, n, m, and l being integers, and for large M the magnitudes $f(M)$ and $f'(M)$ are negligible.

The calculation gives

$$G=1-\pi I/2k^2a^2, \quad \text{where} \quad I\approx 2\pi-3-0.25\approx 3, \quad (60)$$

which is in good agreement with the result obtained by Placzek *et al.* [11]. We did not have a goal to get the result with the same precision as in [11]. We are quite satisfied to obtain a result (60) very close to that of [11] but in a different way. It proves the reliability of our method.

In the above considerations the nuclei were considered to be infinitely heavy. For finite masses it is necessary to take into account the Debye-Waller factor that diminishes the amplitude b and gives a weight $w(|\boldsymbol{n}|)<1$ to each term in the sum (57). Calculations with this factor will certainly lead to a lower value of the factor G and therefore to a higher coefficient I in Eq. (60), which should increase with increasing temperature.

2. More rigorous theory

The perturbation theory (PT) has a deficiency. It gives the correct positions of the Bragg peaks, however it does not give the widths of the peaks. For large crystallites the width of a peak is infinitesimal, while from dynamical diffraction theory it is found to have a finite magnitude known as the Darwin plateau.

We shall show below that the perturbation theory in fact describes diffraction only outside of the Darwin plateau, and we must use a more rigorous theory to look for corrections related to the Darwin plateau itself.

Let us consider Bragg diffraction on a single small crystal with thickness L and surface area S. The reflection amplitude r_L is [17]

$$r_L=R\frac{1-\exp(2iqL)}{1-R^2\exp(2iqL)}, \quad (61)$$

where R is the reflection amplitude for an infinitely thick crystal and q is the Bloch wave number inside it.

If the component of the incident neutron wave vector perpendicular to the reflecting atomic planes has value in the interval $\tau/2<k_{\perp}<\tau/2+u/\tau$ where $\tau/2$ is the Bragg wave number $\tau/2=\pi n/a$, n is the integer and a is the distance between the reflecting planes, then $R=\exp(-2i\xi)$ with real phase ξ, $\boldsymbol{q}=\boldsymbol{\tau}+i\boldsymbol{\delta q}$, and the expression (61) for sufficiently small L looks like

$$r_L=R\frac{1-\exp(-2\delta qL)}{1-R^2\exp(-2\delta qL)}=2\delta qL\frac{R}{1-R^2}. \quad (62)$$

The interval $\delta k_{\perp}=u/\tau$ is known as the Darwin plateau. The PT cannot give exponentially decaying waves. For sufficiently thick crystal $\delta qL\gg 1$ the reflection at the Darwin plateau is the total, thus $|r_L|^2=1$.

If the reflection and transmission of a single crystalline layer of a period thickness are r and t, respectively, then

$$R=\frac{\sqrt{(1+r)^2-t^2}-\sqrt{(1-r)^2-t^2}}{\sqrt{(1+r)^2-t^2}+\sqrt{(1-r)^2-t^2}}, \quad (63)$$

$$e^{iqa}=\frac{\sqrt{(1+t)^2-r^2}-\sqrt{(1-t)^2-r^2}}{\sqrt{(1+t)^2-r^2}+\sqrt{(1-t)^2-r^2}}. \quad (64)$$

For a cubic monoatomic lattice we have [see Eq. (46)]

$$r=\frac{-i\kappa}{k_{\perp}+i\kappa}e^{2i\phi}, \quad t=\frac{k_{\perp}}{k_{\perp}+i\kappa}e^{2i\phi}, \quad \phi=k_{\perp}a/2,$$

$$\kappa\equiv\kappa_{\mathrm{cr}}=2\pi N_2b_{\mathrm{cr}}, \quad (65)$$

and $k_{\perp}$ is the normal component of the incident wave vector with respect to the crystalline planes. Substituting into R, we obtain

$$R=\frac{\sqrt{k_{\perp}+\kappa\tan\phi}-\sqrt{k_{\perp}-\kappa\cot\phi}}{\sqrt{k_{\perp}+\kappa\tan\phi}+\sqrt{k_{\perp}-\kappa\cot\phi}}$$

$$=\frac{\sqrt{\tan\phi}-\sqrt{\tan(\phi-\alpha)}}{\sqrt{\tan\phi}+\sqrt{\tan(\phi-\alpha)}}, \quad \text{where} \quad \alpha=\arctan(\kappa/k_{\perp}). \quad (66)$$

The same substitution into Eq. (64) for q gives

$$e^{iqa}=\frac{1+i\sqrt{\tan\phi\tan(\phi-\alpha)}}{1-i\sqrt{\tan\phi\tan(\phi-\alpha)}}. \quad (67)$$

[4]In notations of [14] $G=S_{\mathrm{coh}}^{\mathrm{el}}$.

The sign before the square root is defined by the condition: $q=k_\perp$ if $\alpha=0$.

The Bragg reflection takes place when ϕ and $\phi-\alpha$ are on opposite sides of points $n\pi/2$ (integer n), because in that case the reflection amplitude R becomes modulo 1. Indeed, at $\phi-\alpha\leqslant m\pi/2\leqslant\phi$ with even m we have

$$R=\frac{\sqrt{\tan\phi}-i\sqrt{\tan(\alpha-\phi)}}{\sqrt{\tan\phi}+i\sqrt{\tan(\alpha-\phi)}},\quad |R|=1. \tag{68}$$

From Eq. (68) it follows

$$\frac{R}{1-R^2}=\frac{\tan\phi+\tan(\alpha-\phi)}{4i\sqrt{\tan\phi\tan(\alpha-\phi)}}$$

$$\approx\frac{\alpha}{4i\sqrt{(\phi-m\pi/2)(m\pi/2-\phi+\alpha)}}, \tag{69}$$

and Eq. (67) gives

$$\delta q\approx\frac{2}{a}\sqrt{(\phi-m\pi/2)(m\pi/2-\phi+\alpha)}. \tag{70}$$

Substituting into Eq. (62) we obtain that the cross section of a crystallite for the given reflection (for the given τ) can be represented as

$$\Sigma_\tau=S\cos\theta|r_L|^2=4V\cos\theta|\delta q|^2L\frac{|R|^2}{|1-R^2|^2}$$

$$=\cos\theta\frac{VL}{a^2}\alpha^2=VL\cos\theta\frac{u^2}{4k_\perp^2}, \tag{71}$$

where V is the crystallite's volume, and $u=4\pi N_0 b_{\rm cr}$. We must average over orientations of the crystallite, which is the same as averaging over direction of the incident neutron. The averaging gives $\langle\Sigma_\tau\rangle=N\sigma G_\tau$, where N is the total number of atoms in the crystallite, $\sigma=4\pi|b_{\rm cr}|^2$, and

$$G_\tau=\int_0^1\frac{4\pi N_0 L}{4k_\perp^2}\vartheta(\tau^2/4<k_\perp^2<\tau^2/4+2u)\cos\theta\frac{d\Omega}{\pi} \tag{72}$$

is the correction factor for the given reflection (the given vector $\boldsymbol{\tau}$ of the reciprocal lattice). Here $\tau/2=\pi n/a$ with integer n, θ is the angle between the wave vector of the incident neutron and the normal to the Bragg planes, and we introduced the function $\vartheta(x)$, which is equal to unity when inequality of its argument is satisfied, and zero in the opposite case.

A change of variables $\cos\theta=k_\perp/k$, $d\cos\theta=dk_\perp/k\approx u/2kk_\perp$ gives

$$G_\tau\approx\frac{4\pi N_0 L}{\tau^2}\ \frac{u}{2k^2}. \tag{73}$$

For arbitrary position of the Bragg planes τ^2 should be represented as

$$\tau^2=\frac{4\pi^2}{a^2}\boldsymbol{n}^2. \tag{74}$$

Summation over all the Bragg reflections, and approximation of the sum by the integral, as shown in Eq. (59), gives

$$G=\sum_\tau G_\tau=2\frac{N_0 L b_{\rm cr}a}{(ka)^2}\sum_{|\boldsymbol{n}|=1}^{M=ka/\pi}\frac{1}{|\boldsymbol{n}|^2}$$

$$\approx 2\frac{LN_0 b_{\rm cr}a}{(ka)^2}[4\pi(ka/\pi-1)+4]$$

$$=\frac{8}{ka}\ \frac{L}{a}\ \frac{b_{\rm cr}}{a}(1-2.14/ka). \tag{75}$$

We see that the correction to elastic scattering due to diffractions at the Darwin plateau contains terms of order $I(L)/\sqrt{E}$ with a little known parameter L, which characterizes the dimensions of crystallites.

If we shall take into account thermal vibrations of the nuclei, we should renormalize the scattering amplitude by the Debye-Waller factor $b\to b\exp[-\tau^2W(T)/k_D^2]=b\exp[-\tau^2W(T)/k_D^2]$, where at high temperature T we have [14] $W\propto(m/M)T/T_D$, M is nuclear mass, T_D is the Debye temperature: $T_D=\hbar^2k_D^2/2mk_B$, and k_B is the Boltzmann constant. In that case the summation in Eq. (75) will be modified as follows:

$$G=\sum_\tau G_\tau=2\frac{N_0 L b_{\rm cr}a}{(ka)^2}\sum_{|\boldsymbol{n}|=1}^{M=ka/\pi}\frac{\exp(-|\boldsymbol{n}|^2/n_T^2)}{|\boldsymbol{n}|^2}$$

$$=8A\frac{L}{a}\ \frac{b_{\rm cr}}{a}\ \frac{n_T}{(ka)^2}, \tag{76}$$

where $n_T^2\propto(k_Da/\pi)^2(M/m)T_D/T$, and the constant A is of order 1. We see that in this case the dependence of the G factor becomes of $\propto 1/k^2$, though linear dependence on the unknown parameter L is preserved.

Outside of the Bragg peaks

Now let us calculate the probability of reflection outside of the Darwin plateau, i.e., when $|k_\perp^2-\tau^2/4|>u$. In that case the reflection amplitude R in Eq. (61) as it follows from Eq. (66) is approximated by

$$R=\frac{\sin\alpha}{(\sqrt{\sin\phi\cos(\phi-\alpha)}+\sqrt{\cos\phi\sin(\phi-\alpha)})^2}\approx\frac{ua}{2\tau|\sin\xi|}, \tag{77}$$

where $\xi=(k_\perp-\tau/2)a$. The scattering cross section averaged over incidence angles can be represented as follows:

$$\Sigma=\int_0^1 4S|R|^2\sin^2(\xi L/a)\cos\theta\frac{d\Omega}{4\pi}$$

$$=S\int\frac{d\xi}{4k^2a^2}\ \frac{u^2a^3}{\tau}\left|\frac{\sin(\xi L/a)}{\sin\xi}\right|^2=\pi S\frac{L}{a}\frac{u^2a^3}{8k^2a^2\tau}=N\sigma G_\tau, \tag{78}$$

where

$$G_\tau = \frac{\pi}{2}\,\frac{1}{(ka)^2}\,\frac{1}{|\boldsymbol{n}|}, \tag{79}$$

and the ratio $|\sin(\xi L/a)/\sin\xi|^2$ was approximated as $\pi(L/a)\,\delta(\xi)$. Summation over all τ gives the same expression (57), as in perturbation theory, and the final result coincides with Eq. (60), or more precisely, with the result obtained by Placzek *et al.* [11]. However, if we shall take into account the Debye-Waller factor, then

$$G = \sum\nolimits_\tau G_\tau = \frac{\pi}{2}\,\frac{1}{(ka)^2}\sum_\tau \frac{\exp(-|\boldsymbol{n}|^2/n_T^2)}{|\boldsymbol{n}|} \approx \frac{\pi^2 n_T^2}{(ka)^2}\exp(-1/n_T^2), \tag{80}$$

where the upper limit of the integral was extended to infinity.

F. A layered media with disordered atomic planes

Again we split the substance into thin separate layers, and use the MWS equations for the amplitudes ψ_n of the waves illuminating nuclei at the points r_n in a single layer:

$$\psi_n = \exp(i\boldsymbol{k}\boldsymbol{r}_n) - b\sum_{m\neq n}\psi_m\frac{\exp(ikr_{mn})}{r_{mn}}. \tag{81}$$

In the first approximation the solution can be suggested in the form $\psi_n = C\exp(i\boldsymbol{k}\boldsymbol{r}_n)$. After substitution in Eq. (81) we obtain the equation for C:

$$C = 1 - bC\sum_{m\neq n}\exp(i\boldsymbol{k}[\boldsymbol{r}_m - \boldsymbol{r}_n])\frac{\exp(ikr_{mn})}{r_{mn}}. \tag{82}$$

The sum on the right-hand side can be approximated by the integral

$$\sum_{m\neq n}\exp(i\boldsymbol{k}[\boldsymbol{r}_m - \boldsymbol{r}_n])\frac{\exp(ikr_{mn})}{r_{mn}} = \int w(r)N_2\,d^2r\exp(i\boldsymbol{k}\boldsymbol{r}_\parallel)\frac{\exp(ikr)}{r}, \tag{83}$$

where $w(r)$ is the pair correlation function, showing the probability to find a nucleus at the point $\boldsymbol{r}$ if there is a nucleus at the point $r=0$. The function $w(r)$ should be chosen in such a way as to exclude the second atom from being at the point $r=0$. We suggest the form $w(r) = 1 - \exp(-r/s)$. The parameter s is defined by the condition

$$N_2\int^R w(r)d^2r = N_2(\pi R^2 - 2\pi s^2) = N - 1, \quad 2\pi N_2 s^2 = 1, \tag{84}$$

which means that the integral over all the particles should give the number of particles except the one which is at the origin. For simplicity in the following we shall suppose that the neutron enters the bulk matter normally to the surface, so $\boldsymbol{k}_\parallel = 0$.

The integral in Eq. (83) is now easily calculated:

$$I = \int [1 - e^{-r/s}]N_2\,d^2r\frac{\exp(ikr)}{r} = 2\pi N_2\left(\frac{i}{k} - \frac{s}{1-iks}\right). \tag{85}$$

Taking into account Eq. (84) we obtain

$$C = 1 - C\left[\frac{i\kappa}{k} - \frac{ibk}{1+k^2s^2} - \frac{\kappa s}{1+s^2k^2}\right], \quad \kappa = 2\pi N_2 b. \tag{86}$$

The solution of this equation is

$$C = 1/[1 + i\kappa/k - ibk/(1+s^2k^2) - \kappa s/(1+s^2k^2)]. \tag{87}$$

Thus, again, the constant C renormalizes the amplitude b, transforming it into

$$b_C = bC = b_0/[1 + ikb_0 + i\kappa_0/k - ib_0k/(1+s^2k^2) - \kappa_0 s/(1+s^2k^2)], \tag{88}$$

where $\kappa_0 = 2\pi N_3 b_0$. After some evident algebraic manipulations it is reduced to the form

$$b_C = \frac{b_r}{1 + i\kappa_r/k}, \quad \text{where} \quad \kappa_r = 2\pi N_2 b_r, \tag{89}$$

$$b_r = \frac{b_0'}{1 + ikb_0'[1 - 1/(1+k^2s^2)]}, \quad b_0' = \frac{b_0}{1 - \kappa_0 s/(1+s^2k^2)}. \tag{90}$$

Here b_0' is a renormalized length b_0. Renormalization increases it by the amount $\approx 10^{-4}$ even for zero energy, so it can be neglected, and in the following we will take $b_0' = b_0$.

At low energies

$$b_r = \frac{b_0}{1 + ikb_0[1 - 1/(1+s^2k^2)]} \approx \begin{cases} b_0 & \text{for } k\to 0 \\ b & \text{for } k\to\infty. \end{cases} \tag{91}$$

The transmission of an atomic plane is determined by the amplitude of the plane wave in the function:

$$\Psi(\boldsymbol{r}) = \exp(i\boldsymbol{k}\boldsymbol{r}) - b\sum_m \psi_m\frac{\exp(ikr_{mn})}{r_{mn}} = (1 - i\kappa_C/k)\exp(i\boldsymbol{k}\boldsymbol{r}) = \frac{k}{k + i\kappa_r}\exp(i\boldsymbol{k}\boldsymbol{r}), \tag{92}$$

where $\kappa_C = 2\pi N_2 b_C$, and $\kappa_r = 2\pi N_2 b_r$. Thus the transmission of n planes with the gaps between them (their thickness a_i can be different) leads to the wave function

$$\Psi(\boldsymbol{r}) = \exp(ikr[1 - u_r/2k^2]) = \exp(ik'r), \quad \text{where} \quad u_r = 2n\kappa_r \Big/ \sum_{i=1}^n a_i = 2\kappa_r/\langle a\rangle, \tag{93}$$

and $\langle a \rangle$ is the average distance between atomic planes. It follows that $u_r = 4\pi N_0 b_r$.

In the considered model the positions of atoms in neighboring planes are not correlated, and we can suppose that every one layer scatters independently. Then the imaginary part of b_r (90) should be considered on an equal footing with the one created by other scattering processes, and we may conclude that it is the *scattering amplitude* (especially for high energies, where $b_r \approx b$) which enters the refractive index. Its imaginary part contains the coherent elastic scattering cross section

$$\sigma_{\rm el}^{\rm coh} = 4\pi(b'^2 + b''^2), \tag{94}$$

and of course $b'' = k\sigma_t/4\pi$, as it follows from the optical theorem.

However at intermediate energies the coherent cross section has the correction factor: $G = 1 - 1/s^2k^2 = 1 - 2\pi N_2/k^2 \equiv 1 - \pi I/2k^2a^2$, where $I = 4$, and the expression for s^2 from Eq. (84) was used. The correction has the same form $1/k^2$ as in calculations by Placzek *et al.* [11]. However the magnitude of the constant $I = 4$ is larger than 2.8 by 43%. And if the new magnitude of I is used the amplitude $|b_{ne}|$ of *n-e* interaction obtained would be larger than 1.33 nearly by 10%.

G. Amorphous substance

In the case of amorphous media the atoms are distributed uniformly, and we cannot split the medium into well-separated atomic planes. Of course, we always can split it into arbitrary layers; however the approach used above shows that the result becomes nonunique. It depends on the thickness of layers. For that reason we use here a different approach. However we can foresee the result. It will be of the type (91), and in agreement with the one obtained by Placzek *et al.* [11].

1. Refraction in amorphous matter

We start with the MWS equations (29) and (30) for the set of nuclei in a semi-infinite amorphous medium ($z > 0$). The wave function inside the medium is suggested to be $\psi(\boldsymbol{r}) = A\exp(i\boldsymbol{k}\boldsymbol{r}_\parallel + ik'_\perp z)$, where A is a constant, and $k'_\perp \neq k_\perp$. Then the local fields in Eq. (30) are

$$\psi(\boldsymbol{r}_n) = AC(z)\exp(i\boldsymbol{k}\boldsymbol{r}_\parallel + ik'_\perp z_n), \tag{95}$$

where $C(z)$ is an unknown function of z. Substitution of Eq. (95) in Eq. (29) gives the first equation for A and $C(z)$:

$$A\exp(ik'z) = e^{ik_\perp z} - AbN_0 \int C(z') \frac{d^3r' \exp(ik|\boldsymbol{r}' - \boldsymbol{r}|)}{|\boldsymbol{r}' - \boldsymbol{r}|} \times \exp(i\boldsymbol{k}(\boldsymbol{r}' - \boldsymbol{r})_\parallel + ik'_\perp z'). \tag{96}$$

Substitution of Eq. (95) into Eq. (30) gives the second equation for A and $C(z)$:

$$AC(z)e^{ik'z} = e^{ikz} - AbN_0 \times \int C(z')d^3r' \frac{\exp(ik|\boldsymbol{r}' - \boldsymbol{r}|)}{|\boldsymbol{r}' - \boldsymbol{r}|} w(\boldsymbol{r} - \boldsymbol{r}') \times \exp(i\boldsymbol{k}(\boldsymbol{r}' - \boldsymbol{r})_\parallel + ik'_\perp z'), \tag{97}$$

where $w(\boldsymbol{r} - \boldsymbol{r}')$ is the pair correlation function. If we replace it with $1 - \gamma(|\boldsymbol{r}|/s)$, where s is the range of the function, which is of the order of interatomic distance, and use Eq. (96), we reduce Eq. (97) to the form

$$C(z) - 1 = bN_0 \int C(z')d^3r' \frac{\exp(ik|\boldsymbol{r}' - \boldsymbol{r}|)}{|\boldsymbol{r}' - \boldsymbol{r}|} \gamma(|\boldsymbol{r} - \boldsymbol{r}'|/s) \times \exp(i\boldsymbol{k}(\boldsymbol{r}' - \boldsymbol{r})_\parallel + ik'_\perp(z' - z)). \tag{98}$$

In the first approximation we can take C to be a constant C_0. Substitution into Eq. (96) gives

$$Ae^{ik'z} = e^{ik_\perp z} - \frac{iAu_C}{2k_\perp}\left[\frac{e^{ik'_\perp z} - e^{ik_\perp z}}{i(k'_\perp - k_\perp)} - \frac{e^{ik'_\perp z}}{i(k'_\perp + k_\perp)}\right], \tag{99}$$

where we used the Fourier representation for spherical wave and have introduced the potential $u_C = 4\pi N_0 b_C$ with the renormalized amplitude $b_C = bC_0$.

From Eq. (99) it follows

$$k'^2 = k^2 - u_C, \quad \text{and} \quad A = 2k/(k + k'). \tag{100}$$

We see the expected result. The coefficient A plays the role of the transmission amplitude through the interface for the plane wave $\exp(ikz)$ incident on the medium with the optical potential u_C.

To find C_0 we substitute it for $C(z)$ in Eq. (98), and obtain

$$C_0 = \frac{1}{1 - bJ}, \tag{101}$$

where

$$J = J' + iJ'' = \int N_0 d^3r' \frac{\exp(ik|\boldsymbol{r}'|)}{|\boldsymbol{r}'|} \gamma(|\boldsymbol{r}'|/s) \times \exp(i\boldsymbol{k}\boldsymbol{r}'_\parallel + ik'_\perp r' \cos\theta)\,\vartheta(r'\cos\theta > -z). \tag{102}$$

ϑ is the step function equal to 1 or 0 when inequality is satisfied or not.

Now for simplicity we limit ourselves to the case of the normal incidence of neutrons on the interface: $\boldsymbol{k}_\parallel = 0$. Then the integral (102) becomes

$$J=2\pi bN_0\int r'dr'd\cos\theta\exp(ikr'+ik'r'\cos\theta)$$
$$\times\vartheta(r'\cos\theta>-z)\gamma(r'/s)$$
$$=\frac{2\pi bN_0}{ik'}\int_0^\infty dr'\exp(ikr')[e^{ik'r'}-e^{-ik'r'}\vartheta(r'<z)$$
$$-e^{-ik'z}\vartheta(r'>z)]\gamma(r'/s), \tag{103}$$

which can be represented as

$$J=\frac{2\pi bN_0}{ik'}\int_0^\infty dr'\exp(ikr')[e^{ik'r'}-e^{-ik'r'}]\gamma(r'/s)$$
$$+\zeta(z)=J_0+\zeta(z), \tag{104}$$

where

$$\zeta(z)=\frac{2\pi bN_0}{ik'}\int_0^\infty dr'e^{ikr'+i(k-k')z}[e^{-ik'r'}-1]$$
$$\times\gamma([r'+z]/s). \tag{105}$$

We see, that for $z\gg s$ the term $\zeta(z)$ is negligible, the integral $J=J_0$ is constant, and $C_0=1/(1-bJ_0)$.

Now we shall consider several models for the γ function.

No correlation, $\gamma=0$

In that case $J=0$, $C_0=1$ and b is the scattering *amplitude*, i.e., $-\mathrm{Im}\,b=k|b|^2$.

Exponential

$$\gamma(r/s)=\exp(-r/s). \tag{106}$$

Since integration $\int w(r)N_0d^3r$ should give $N-1$, where N is the total number of particles, the integral $\int\gamma(r/s)N_0d^3r$ should give 1. Thus

$$\int N_0\gamma(r/s)d^3r=1,\quad 8\pi N_0s^3=1,\quad s=a/2\pi^{1/3}. \tag{107}$$

Substitution of Eq. (106) into Eq. (104) gives

$$J_0=\frac{2\pi N_0}{ik'}\left[\frac{1}{1/s-ik-ik'}-\frac{1}{1/s-ik+ik'}\right]$$
$$=\frac{4\pi N_0}{(1/s-ik)^2+k'^2}=\frac{4\pi N_0}{(1/s-ik)^2+k^2-C_0u}. \tag{108}$$

Substitution in Eq. (101) gives

$$C_0=\frac{(1/s-ik)^2+k^2-C_0u}{(1/s-ik)^2+k^2-C_0u-u}. \tag{109}$$

Now, for $x\equiv C_0$ we have the equation

$$x^2u-\alpha x+\alpha=0, \tag{110}$$

where $u=4\pi N_0b$ and $\alpha=(1-2iks)/s^2$. The solution of this equation is

$$x=\sqrt{\frac{\alpha}{u}}\frac{\sqrt{\alpha+2\sqrt{u\alpha}}-\sqrt{\alpha-2\sqrt{u\alpha}}}{\sqrt{\alpha+2\sqrt{u\alpha}}+\sqrt{\alpha-2\sqrt{u\alpha}}}$$
$$=\frac{2}{1+\sqrt{1-4us^2/(1-2iks)}}\approx\frac{1}{1-us^2/(1-2iks)}. \tag{111}$$

Thus

$$b_C=bC_0\approx\frac{b_0}{1+ikb_0[1-1/(1+4k^2s^2)]}$$
$$\times\begin{cases}\dfrac{b_0}{1+4ib_0k^3s^2} & \text{for } k\to0\\[2ex] \dfrac{b_0}{1+ikb_0(1-1/4k^2s^2)} & \text{for } k\to\infty.\end{cases} \tag{112}$$

Accounting for the relation (107) we get for large k

$$b_C=\frac{b_0}{1+ikb_0(1-I\pi/2a^2k^2)},\quad \text{where}\quad I=2/\pi^{1/3}=1.37. \tag{113}$$

Similar considerations for other functions $\gamma(r/s)$ give

Lorentz-like dependence

$$\gamma(r)=\frac{1}{(1+r^2/s^2)^2},\quad I=\pi^{1/3}=1.46. \tag{114}$$

Gaussian

$$\gamma(r/s)=\exp(-r^2/s^2),\quad I=2. \tag{115}$$

Constant

$$\gamma(r)=\vartheta(r<s),\quad I=4s/a=4(3/4\pi)^{1/3}=2.48. \tag{116}$$

We see that for more or less realistic correlations the constant I varies from 1.4 up to 2.5, and this range approximately shows the precision with which the interference correction to $\sigma_{\mathrm{el}}^{\mathrm{coh}}$ in amorphous and liquid substances can be estimated.

V. EXTRACTION OF *n-e* AMPLITUDE FROM THE TRANSMISSION

We shall consider three papers [1,2,4], dealing with the measurement of the scattering amplitude. The solid state effects were considered in [11,14,20,21].

The experimental values were fitted to the expression

TABLE I. The magnitude of the form factor used in [1,2].

Energy (eV)	0.1	1.26	2.0	5.19	18.6	100	128
Pb form factor							
[2]	0.545	0.1802	0.144	0.0934	0.0476	0.0205	0.0196
[1]	0.488		0.134			0.0122	

$$\sigma_r=\sigma_{\rm el}^{\rm coh}+\sigma_{ss}=4\pi(\mathrm{Re}\,b)^2[1-KF(E)-\zeta E_0/E] \tag{117}$$

with $E_0=\hbar^2/2ma^2\approx 0.009$ meV, $\zeta=\pi I/2$ was calculated, and $K=2(b_{ne}/b)Z$ was the fitting parameter. For $b_{ne}=1.32\times10^{-3}$ the magnitude of K is 0.0228.

In [2] the analytical expression for $F(E)$ [8] was used:

$$F(E)=\frac{1}{\sqrt{1+3E/E_1}},\quad \text{where}\quad E_1=0.127\ \text{eV}. \tag{118}$$

This expression was obtained from x-ray data. The approximation (118) is valid up to $E=16E_1=2.032$ eV.

In [1] numerical experimental data from x-ray scattering is used. We can compare the numerical value of $F(E)$ for several energies used by [1] and [2]. The data are represented in Table I.

We see that there is always a difference at least of the order 10%. It means that the extracted [2] amplitude b_{ne} has an uncertainty at least of the same order.

If we shall take into account the correction (75) for the elastic scattering cross section in transmission through polycrystalline samples, the relation (118) should look as follows:

$$\sigma_{\rm el}^{\rm coh}=\sigma_0[1+\zeta_1\sqrt{E_0/E}-K\sqrt{E_1/3E}-\zeta E_0/E], \tag{119}$$

where

$$\zeta_1=4\frac{L}{a}\,\frac{b}{a}. \tag{120}$$

Because the constant K in Eq. (119) is determined by fitting to an experimental curve, this fitting determines the magnitude

$$K'=K-\zeta_1\sqrt{3E_0/E_1}=K-4\,\frac{L}{a}\,\frac{b}{a}\,\sqrt{3E_0/E_1}, \tag{121}$$

thus K is the sum $K=K'+4(Lb/a^2)\sqrt{3E_0/E_1}$, which leads to an increase of the scattering amplitude b_{ne}. How large this increase is depends on the dimension L of the crystallites; however it is important to point out that the two terms at the right hand side of Eq. (121) are of the same order when $L/a\approx 200$.

After correcting for the Debye-Waller factor the correction (75) becomes of the type (76), which means that it does not contribute to ζ_1, but can considerably (it depends on L) change the coefficient ζ. With this term the fitting procedure would lead to a larger value of b_{ne}.

In the most recent paper [4] the measurements were performed with liquid Pb and Bi, and the experimental data for pair correlation function were used. For these measurements there are no polycrystalline corrections and pair correlation uncertainties. However in liquids there is multiple small angle scattering on fluctuations, and this scattering could be important in the range of energy up to several eV.

It is also necessary to estimate inelastic scattering. In [8,14,20,21] the inelastic scattering was calculated in the framework of the Debye model, which can be used for estimation purposes only. For a reliable extraction of b_{ne} it is necessary to perform measurements of the inelastic scattering in liquid Pb or Bi. If there is some collective excitation with energy of order 1 eV the cross section of inelastic scattering in the vicinity of incident neutrons energy near 1 eV will be of the type $1/\sqrt{E}$. Accounting for this effect will also increase the absolute value of b_{ne}.

A. A remark on polarizability

The polarizability of the neutron α_n gives the additional contribution $b_p g(E)$ to the real part of the coherent scattering amplitude [22], where $b_p\propto\alpha_n$ is the scattering length at low energy due to the neutron polarizability, and $g(E)$ is the form factor created by the electric field of the nucleus. To find α_n it is possible to use the same procedure as the one used for the extraction of b_{ne}. We write the coherent cross section in the form

$$\sigma^{\rm coh}=4\pi(\mathrm{Re}\,b)^2[1+K\{1-F(E)\}-\zeta E_0/E+2(b_p/b_0)g(E)]+4\pi(\mathrm{Im}\,b)^2. \tag{122}$$

Here it is not correct to neglect $(\mathrm{Im}\,b)^2$ because for polarizability measurements the energies above 10 keV are important, and here this term gives a considerable contribution.

In many papers (see, for instance, [3,22]) the magnitude b is supposed to be the scattering length and $-\mathrm{Im}\,b$ is taken to be $k\sigma_a/4\pi$. However, as it follows from above, at high energies and in disordered substances the refractive index contains the *amplitude*, so $-\mathrm{Im}\,b=k\sigma_t/4\pi$. Thus $(\mathrm{Im}\,b)^2$ gives the contribution $(k^2\sigma_t^2/4\pi)$ which is of the order $10^{-2}\sigma_0$ at 10 keV, where $\sigma_0=4\pi(\mathrm{Re}\,b)^2$. It means that for extraction of the neutron polarizability it is necessary to subtract $(\mathrm{Im}\,b)^2=k^2\sigma_t^2/4\pi$, as was correctly pointed out in [23], i.e., to fit the experimental data to the expression

$$\sigma_t-k^2\sigma_t^2/4\pi-\sigma_{\rm other}=4\pi(\mathrm{Re}\,b)^2[1+K\{1-F(E)\}-\zeta E_0/E+2(b_p/\mathrm{Re}\,b)g(E)]. \tag{123}$$

For higher precision it might be necessary to take into

account also the corrections to $\mathrm{Re}\, b$ shown in Eq. (28), which have the same behavior at high energies as the polarizability amplitude.

VI. CONCLUSION

We can summarize our results as follows.

(1) We have found a method to calculate the interference correction to the coherent elastic scattering cross section $\sigma_{\mathrm{el}}^{\mathrm{coh}}$ for all neutron energies. This method shows when $\sigma_{\mathrm{el}}^{\mathrm{coh}}$ contributes to the attenuation cross section of the transmission exponent and when it does not. It contributes when the refractive index contains the scattering amplitude b, and does not, when the refractive index contains the scattering length b_0.

(2) In the case of ideal crystals and in the case of slow neutrons the transmission exponent does not contain $\sigma_{\mathrm{el}}^{\mathrm{coh}}$.

(3) In the case of polycrystals and amorphous substances transmission exponent contains $\sigma_{\mathrm{el}}^{\mathrm{coh}}$ with the correction factor $G=1-\alpha E_0/E-\beta\sqrt{E_0/E}$, where the term with α coincides with that found by perturbational method in [11], while the term with β results from dynamical diffraction theory and cannot be found with the perturbational approach.

(4) In the case of amorphous substances the correction factor $G=1-\alpha E_0/E$ coincides with that found in [11]. The magnitude of the coefficient α is sensitive to the model of pair correlation function and can vary in range of the order of 100%. However this uncertainty may be reduced if the correction is calculated for experimentally measured structure factor, as is done in [4]. It was shown there that the hard-core model describes well the experimental data on static structure factor, which means that this model should be used for calculation of α. However for liquid samples the multiple small angle scattering on fluctuations should be additionally investigated.

(5) We have proven that for extraction of neutron polarizability at high energy the correct definition of $-\mathrm{Im}\, b$ is $-\mathrm{Im}\, b=k\sigma_t/4\pi$ with the total cross section σ_t, as was correctly shown in [23], instead of the absorption cross section σ_a which was used, for instance, in [3].

(6) It was also shown, that $\mathrm{Re}\, b$ has the correction

$$\frac{\delta \mathrm{Re}\, b}{\mathrm{Re}\, b_0}=-\frac{k^2[\sigma_a+\sigma_{ie}]}{2\pi}+k^2 b_0^2, \tag{124}$$

which can be important in the energy range above 10 keV.

(7) It was pointed out that it is desirable to measure inelastic scattering in liquid Pb and Bi to be sure that there is no appreciable amount of inelastic scattering on collective excitations with energy of the order 1 eV, because, if present, it can give a contribution to the correction factor of the type $1/\sqrt{E}$. Moreover, the liquids give small angle scattering, which can lead to corrections of the same order of magnitude as those obtained for polycrystals.

It seems that some room for doubts about reliability of the result (1) or even 1.33, found in [4], is left, and it is necessary to look how well the transmissions of solid and liquid Pb are matched considering the new interference corrections found here.

We are going to investigate also the corrections on inelastic scattering, and to analyze uncertainties in the diffraction result (2).

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