

Fundamentals of Neutron Optics

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(Received 1 February 1996; accepted 19 March 1996)

It is usually assumed that neutron-optical phenomena are adequately described by a one-body Schrödinger equation containing a complex optical potential that is given by the average value of the Fermi pseudopotential. The main problem with this elementary approach is that it only includes the attenuation of the neutron wave function by absorption, and neglects the often more important contribution from diffuse scattering. We show how this problem is resolved within the rigorous theory of dispersion by taking local-field effects properly into account. We also indicate the importance of corrections for local-field effects and electromagnetic interactions in the accurate determination of coherent scattering lengths by neutron-optical experiments.

KEYWORDS: neutron optics, local-field effects, coherent scattering lengths

§.1. Introduction

The theory of thermal neutron scattering in condensed matter distinguishes four kinds of scattering processes:

- coherent elastic,
- coherent inelastic,
- incoherent elastic,
- incoherent inelastic.

The coherent elastic scattering represents the familiar optical phenomena of reflection, refraction, diffraction, and interference. The other three types of scattering play a secondary role in neutron optics and are referred to collectively as diffuse scattering.

The characteristic property of coherent elastic scattering is that it is not accompanied by any change in the microscopic state of the system and, hence, can be described by a one-body Schrödinger equation,¹⁾

$$\left[-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E \psi(\mathbf{r}), \quad (1.1)$$

in which m is the neutron mass and $V(\mathbf{r})$ the optical potential that represents the effective interaction of the neutron with the system. The neutron wave function $\psi(\mathbf{r})$ is called the coherent wave and provides a formally exact description of the coherent elastic scattering and, hence, all neutron optical phenomena. The optical potential is complex, and its imaginary part describes the attenuation of the coherent wave in the medium by both diffuse scattering and absorption (e.g. radiative capture).

It is important to recognize that the optical potential $V(\mathbf{r})$, and hence the coherent wave $\psi(\mathbf{r})$, are macroscopic thermodynamic quantities. Thus, these quantities depend only on the variables (temperature, pressure, etc.) that define the macroscopic state of the system and are independent of the instantaneous positions of the atoms of which the system is composed. In other words, the system behaves like a continuous macroscopic medium as far as the coherent elastic scattering is concerned. In a homogeneous system (such as a gas, liquid, or amorphous solid) $V(\mathbf{r})$ is constant, independent of \mathbf{r} , while in a crystal $V(\mathbf{r})$ is a periodic function of \mathbf{r} with the same periodicity as the lattice. Outside the system, on the other hand, $V(\mathbf{r})=0$.

Thus, the macroscopic Schrödinger equation (1.1) describes neutron-optical phenomena in terms of the collision of the neutron with a potential barrier.

From a theoretical point of view, neutron optics divides naturally into two parts:

- (1) the theory of dispersion,
- (2) the theory of reflection, refraction, and diffraction.

Part 1 is concerned with the derivation of the macroscopic one-body Schrödinger equation (1.1) from the underlying microscopic many-body Schrödinger equation, and with the calculation of the complex optical potential $V(\mathbf{r})$ for the particular material of interest. Part 2 is concerned with the solution of (1.1) subject to boundary conditions appropriate to the experimental arrangement of interest.

The purpose of this paper is to present a critical analysis of the elementary theory of dispersion, which forms the basis for most work on neutron optics, and a brief non-technical discussion of the rigorous theory of dispersion that must be used in situations where the elementary theory is inadequate. The theory of reflection, refraction, and diffraction is dealt with in Ref. 1 and will not be discussed further here.

§.2. Elementary Theory of Dispersion

§.2.1 Optical potential

In the elementary theory of dispersion it is assumed that the optical potential is given by the equilibrium value of the Fermi pseudopotential:

$$V(\mathbf{r}) = \left\langle \sum_i \frac{2\pi\hbar^2 b_i}{m} \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle. \quad (2.1)$$

Here, \mathbf{r}_i is the position of the i -th atom, b_i is its bound coherent scattering length, and the brackets $\langle \dots \rangle$ denote a thermodynamic average. For a homogeneous system (such as a gas, liquid, or amorphous solid), the optical potential then has a constant value given by

$$V(\mathbf{r}) = \left(\frac{2\pi\hbar^2}{m} \right) \rho b, \quad (2.2)$$

in which ρ is the number of atoms per unit volume and b is the average bound coherent scattering length per atom.

In general, the scattering length is complex,

$$b = b' - ib'' \quad (2.3)$$

Since the imaginary part of the optical potential describes the attenuation of the coherent wave in the medium, it is necessary that $b'' \geq 0$. On the other hand, the real part of the scattering length may be either positive or negative. It is found experimentally that $b' > 0$ for most nuclei, which means that the optical potential is usually repulsive.

§.2.2 Index of refraction

The index of refraction is defined as

$$n = K / k, \quad (2.4)$$

where K is the wave vector in the medium and k the corresponding wave vector in vacuo. Energy conservation then gives

$$E = \frac{(\hbar K)^2}{2m} + V = \frac{(\hbar k)^2}{2m}, \quad (2.5)$$

so that

$$n^2 = 1 - \frac{V}{E}. \quad (2.6)$$

Using the expression (2.2) for the optical potential, we then obtain the familiar result

$$n^2 = 1 - \left(\frac{4\pi}{k^2} \right) \rho b. \quad (2.7)$$

Although the above derivation may seem plausible to those already familiar with the Fermi pseudopotential in the context of Born approximation treatments of thermal neutron scattering in condensed matter, its validity in the present context is by no means obvious. In fact, the expression (2.7) for the index of refraction has some serious defects, which will become clear in the next section.

§.2.3 Optical theorem

Suppose a beam of neutrons with wave vector \mathbf{k} is incident on a slab of material of thickness d . It then follows quite simply from the solution of the Schrödinger equation (1.1) that the fraction of incident neutrons that are transmitted by the slab is given by the expression

$$T = \exp(-\mu d), \quad (2.8)$$

in which the attenuation coefficient is of the form

$$\mu = 2kn'', \quad (2.9)$$

where n'' is the imaginary part of the index of refraction ($n = n' + in''$). On the other hand, we also know that

$$\mu = \rho \sigma_t, \quad (2.10)$$

where σ_t is, by definition, the total collision cross section per atom. A comparison of the above two expressions for μ then gives the optical theorem

$$\sigma_t = \left(\frac{2k}{\rho} \right) n''. \quad (2.11)$$

Using the elementary expression (2.7) for the index of refraction, we find that

$$\sigma_t = \left(\frac{4\pi}{K'} \right) b'', \quad (2.12)$$

where $K' = n'k$ is the real part of the wave vector in the medium. This result is clearly incorrect because the right-hand side of the equation is merely the '1/v law' for the absorption cross section, while σ_t should include contributions from both absorption and diffuse scattering.

Thus, the elementary theory of dispersion violates the optical theorem in the sense that it only includes the attenuation of the coherent wave in the medium by absorption and neglects the often more important contribution from diffuse scattering. In addition, since the elementary theory gives the wrong answer for the imaginary part of the index of refraction, it presumably also gives the wrong answer for the real part. These defects are overcome in the rigorous theory of dispersion which is discussed in the next section.

§.3. Rigorous Theory of Dispersion

§.3.1 Ewald equations

The rigorous theory of dispersion¹⁻⁴⁾ begins by considering the medium from a microscopic point of view as a system of atoms in vacuo. When a neutron with wave vector \mathbf{k} is incident on the system, each atom becomes the source of a spherical scattered wave. Hence, the total wave function at any point inside or outside the system is the sum of the incident plane wave plus the scattered waves from all the atoms. The essential point to note is that the 'local field' that generates the scattered wave from any one atom includes, not only the incident wave, but also the scattered waves from all the other atoms. This represents a problem in the multiple scattering of waves, and is described by a set of coupled equations that are analogous to the Ewald equations in ordinary optics.

§.3.2 Extinction theorem

The central problem in the rigorous theory of dispersion is to prove the extinction theorem which asserts that on average the scattered waves inside the medium interfere with each other in such a way as to extinguish the incident wave and replace it with a new wave that propagates with a different wave vector \mathbf{K} . This new wave is the coherent wave that we introduced earlier, and the fluctuations of the total wave function about this average represent the diffuse scattering.

The extinction theorem is proved by finding an appropriate self-consistent solution of the Ewald equations, and the condition for self-consistency is that the index of refraction is given by the expression

$$n^2 = 1 + \left(\frac{4\pi}{k^2} \right) \rho F, \quad (3.1)$$

where F is the scattering amplitude per atom in the forward direction.

The quantity F is most easily calculated by treating the system as a static configuration of atoms and then taking the appropriate thermodynamic average over all such configurations. Within this static approximation one then finds that for a monatomic system,

$$F = \frac{f}{1-J}, \quad (3.2)$$

where f is the forward scattering amplitude for a single isolated atom and J is the local-field correction,

$$J = \rho f \int \exp(i\mathbf{k} \cdot \mathbf{r}) G(\mathbf{r}) [g(r) - 1] d\mathbf{r} + O(f^2). \quad (3.3)$$

Here, $g(\mathbf{r})$ is the pair correlation function and $G(\mathbf{r})$ the retarded Green function,

$$G(\mathbf{r}) = \frac{e^{ikr}}{r}. \quad (3.4)$$

The integral (3.3) for the local-field correction expresses the interference between the incident plane wave $\exp(i\mathbf{k} \cdot \mathbf{r})$ and the spherical scattered wave $G(\mathbf{r})$, and this interference effect vanishes only in a system such as an ideal gas where the positions of the atoms are statistically independent and $g(\mathbf{r}) = 1$.

§.3.3 Optical theorem

When the rigorous expression (3.1) for the index of refraction is used in the optical theorem (2.11) with $F = F' + iF''$, we get

$$\sigma_t = \left(\frac{4\pi}{K'} \right) F'', \quad (3.5)$$

where $K' = n'k$ is again the real part of the wave vector in the medium. This is now the familiar form of the optical theorem in quantum mechanics.

§.3.4 Scattering amplitude versus scattering length

The neutron scattering community often uses the terms 'scattering amplitude' and 'scattering length' as if they were synonymous. In fact, they are different quantities and, in the present context, we shall see that it is necessary to distinguish very carefully between them.

In general, the scattering amplitude f is defined as the amplitude of the scattered wave (3.4) from a single isolated atom. The scattering length b is then defined in terms of the low-energy limit of f by the relation

$$\lim_{k \rightarrow 0} f = -b. \quad (3.6)$$

It is found experimentally that the real part of f is negative for most nuclei. As a result, it is conventional in neutron physics to include the minus sign in (3.6) so that b' will be predominantly positive.

It can be shown from the partial-wave expansion of the scattering amplitude that for small k ,

$$f = -b + ikb^2 + O(k^2). \quad (3.7)$$

The k^2 term includes the effective-range correction from the s-wave phase shift plus an anisotropic contribution from the p-wave phase shift. With $b = b' - ib''$ and $f = f' + if''$, we then get

$$\begin{aligned} f' &= -b' + k(2b'b'') + O(k^2), \\ f'' &= b'' + k(b'^2 - b''^2) + O(k^2). \end{aligned} \quad (3.8)$$

According to the optical theorem (3.5), the total collision cross section of an isolated atom is given by

$$\sigma_t = \left(\frac{4\pi}{k} \right) f'' = \left(\frac{4\pi}{k} \right) b'' + 4\pi (b'^2 - b''^2) + O(k). \quad (3.9)$$

We also know from quantum mechanics that the scattering cross section is of the form

$$\sigma_s = 4\pi |f|^2 = 4\pi |b|^2 [1 - 2kb'' + O(k^2)]. \quad (3.10)$$

Hence, the absorption cross section is given by

$$\sigma_a = \sigma_t - \sigma_s = \left(\frac{4\pi}{k} \right) b'' [1 - 2kb'' + O(k^2)]. \quad (3.11)$$

Note that, at least to order k^2 , the absorption cross section depends only on b'' , and $\sigma_a = 0$ if $b'' = 0$.

In general, $b' \approx 5$ fm and $k \approx 4 \text{ \AA}^{-1}$ for thermal neutrons. Since $\sigma_a \leq \sigma_s$ for most nuclei, it follows that

$$\begin{aligned} b'' / b' &\leq kb' \approx 2 \times 10^{-4}, \\ kb'' &\leq (kb')^2 \approx 4 \times 10^{-8}. \end{aligned} \quad (3.12)$$

Thus, it is clear that for most practical purposes,

$$\begin{aligned} f' &= -b', \\ f'' &= b'' + kb'^2. \end{aligned} \quad (3.13)$$

and

$$\begin{aligned} \sigma_s &= 4\pi b'^2, \\ \sigma_a &= \left(\frac{4\pi}{k} \right) b''. \end{aligned} \quad (3.14)$$

It is evident that for thermal neutrons the main difference between the scattering amplitude and the scattering length is in their imaginary parts. The quantity b'' only describes the attenuation of the wave function by absorption while f'' describes the attenuation by both absorption and scattering.

In the derivation¹⁾ of the Fermi pseudopotential (2.1) it is assumed that $f = -b$. We now see that this is, in fact, an excellent approximation for f' , the error being typically of the order of 10^{-8} , but it is a very bad approximation for f'' because kb'^2 is usually at least as large as b'' and is often much larger.

§.3.5 Local-field correction

We saw in Sec. 3.2 that, as a result of local-field effects, the scattering amplitude F of an atom in a material medium is different from the scattering amplitude f of an isolated atom. It will be seen later that the local-field correction $J \leq 10^{-4}$. Hence, it follows from (3.2) that, to lowest order,

$$F' = -b'(1 + J'), \quad (3.15)$$

and

$$F'' = b'' + kb'^2 - b'J'', \quad (3.16)$$

in which

$$J = J' + iJ'' = \rho b' \int \exp(ik \cdot \mathbf{r}) G(\mathbf{r}) [1 - g(r)] d\mathbf{r}. \quad (3.17)$$

The imaginary part of J can be expressed in the alternative form⁴⁾

$$J'' = \frac{kb'}{4\pi} \int [1 - S(\mathbf{q})] d\Omega, \quad (3.18)$$

where $S(\mathbf{q})$ is the static structure factor,

$$S(\mathbf{q}) = 1 + \rho \int \exp(i\mathbf{q} \cdot \mathbf{r}) [g(r) - 1] d\mathbf{r}. \quad (3.19)$$

Here, $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}$ is the momentum transfer in units of \hbar in a collision where the incident and scattered wave vectors are \mathbf{k}_0 and \mathbf{k} , and the scattering is elastic ($k_0 = k$). The integral (3.18) is then taken over all directions of \mathbf{k} .

Using the results (3.16) and (3.18), we now find that, to lowest order, the optical theorem (3.5) gives

$$\sigma_t = \left(\frac{4\pi}{k}\right) F'' = \left(\frac{4\pi}{k}\right) b'' + b'^2 \int S(\mathbf{q}) d\Omega. \quad (3.20)$$

Here, the first term on the right-hand side is the absorption cross section, and the second term is the total coherent scattering cross section in the static approximation. When the effect of spin and isotope disorder is taken into account, the right-hand side of (3.20) also includes the incoherent scattering cross section.⁴⁾ Thus, the rigorous expression (3.1) for the index of refraction describes correctly the attenuation of the coherent wave in the medium by both absorption and diffuse scattering.

§.4. Experimental Determination of Neutron Scattering Lengths

§.4.1 Methods of measurement

One of the most important applications of neutron optics is in the experimental determination of the neutron scattering lengths of the elements and their isotopes.^{1,5)} The various methods that have been used are listed in Table I. Most of these methods are based on the phenomena of reflection and refraction at interfaces and, hence, depend mainly on the real part of the index of refraction n' and lead to a determination of the real part of the scattering length b' . Transmission measurements depend on n'' , and hence on σ_t , and allow one to determine both b' and b'' by fitting the data to (3.20), or to a generalized version of this

equation. Powder diffraction (i.e. Bragg scattering in powder samples) and dynamical diffraction in perfect crystals both depend on the absolute value of the unit-cell structure factor,

$$F_{hkl} = \sum b e^{2\pi i(hx - ky - lz)}. \quad (4.1)$$

Here, (hkl) are the Miller indices of the Bragg planes that are used in the measurements, b is the bound coherent scattering length of an atom whose position in the unit cell is (x, y, z) , and the sum runs over all the atoms in the unit cell. It is evident from (3.12) that the measured value of $|F_{hkl}|$ only allows a determination of b' .

Method	Date	Quantity	Acc. (%)
mirror reflection	1946	n'	1
transmission	1947	n''	0.1
powder diffraction	1948	$ F_{hkl} $	1
small-angle scattering	1951	n'	3
gravity refractometry	1965	n'	0.01
dynamical diffraction	1968	$ F_{hkl} $	0.03
Christiansen filter	1969	n'	0.1
prism refraction	1971	n'	0.03
interferometry	1974	n'	0.1

Table I. Neutron-optical methods for the experimental determination of bound coherent scattering lengths. Column 2 gives the dates when these methods were introduced, column 3 the primary quantities that are determined from the measurements, and column 4 the accuracy that can be obtained under favorable conditions.

§.4.2 Local-field correction

To lowest order, the general expression (3.1) for the index of refraction reduces to

$$n^2 = 1 - \left(\frac{4\pi}{k^2}\right) \rho b' (1 + J') + i \left(\frac{\rho \sigma_t}{k}\right). \quad (4.2)$$

In practice, the imaginary term in (4.2) is usually very small and can be calculated using values of σ_t obtained directly from transmission measurements. Thus, as stated in the previous section, neutron reflectometry measurements are normally used to determine b' .

The main difference between (4.2) and the elementary expression (2.7) is the presence of the local-field correction. The correction term is given by (3.17), and at $k = 0$ it can be expressed as

$$J' = b' / r_0, \quad (4.3)$$

where r_0 is of the order of the nearest-neighbor distance when the sample is a solid or liquid, or the mean free path when it is a gas. The value of J' for solids and liquids is typically between 10^{-4} and 10^{-5} . It is therefore evident from Table I that, in practice, the local-field correction is important mainly in gravity refractometry measurements.⁶⁾

§.4.3 Electromagnetic correction

The scattering of thermal neutrons in non-magnetic materials is due almost entirely to the strong (i.e. nuclear) interaction between the neutrons and the nuclei, and the primary role of electromagnetic interactions is in magnetic

materials, where the magnetic dipole interaction between the neutrons and the magnetic electrons gives a contribution to the scattering amplitude of an atom that is normally comparable in magnitude to that from the nuclear interaction. Nevertheless, even in a non-magnetic material, there exist other kinds of electromagnetic interactions between the neutrons and the atoms that give a small but non-negligible q -dependent contribution to the total scattering amplitude.^{7,8)}

Although, strictly speaking, the electromagnetic interactions give a correction to the scattering amplitude f , we shall follow conventional practice and treat it as if it were a correction to the scattering length b . Thus, the effective scattering length for the collision of a neutron with a bound atom of atomic number Z is of the form

$$b(q) = b(0) - b_e Z [1 - \phi(q)], \quad (4.4)$$

where $b(0)$ and b_e are constants, and $\phi(q)$ is the atomic form factor (i.e. the Fourier transform of the electron number density) and is normalized such that $\phi(0) = 1$.

The main contribution to $b(0)$ is from the nuclear interaction between the neutron and the nucleus but there is also a small electrostatic contribution ($\leq 0.5\%$) arising from the neutron electric polarizability. The coefficient b_e is mainly due to the Foldy interaction,⁹⁾ which is a relativistic quantum effect that gives rise to a scalar coupling between the neutron magnetic dipole moment and the electric charge density in the atom. However, there is also a small additional contribution ($\approx 10\%$) to b_e from the intrinsic charge distribution of the neutron.

The quantity b_e is usually called the neutron-electron scattering length because it describes the scattering of a neutron by a single electron. However, this terminology is slightly misleading because b_e is not a property of the neutron-electron interaction per se. Rather, it is entirely a property of the neutron and characterizes its interaction with any electric charge distribution, and not simply that of the electron. Thus, the term $-b_e Z$ in (4.4) represents the electromagnetic interaction of the neutron with the nucleus, while the term $b_e Z \phi(q)$ represents the corresponding interaction with the electrons. The atomic form factor in the latter term describes the screening of the nuclear charge by the electrons. At $q = 0$, where the form factor equals unity, the screening is complete and the electromagnetic contribution to the scattering length (4.4) vanishes. In the limit $q \rightarrow \infty$, on the other hand, $\phi(q) \rightarrow 0$ and the neutron sees the full unscreened nuclear charge so that

$$b(\infty) = b(0) - b_e Z. \quad (4.5)$$

The experimental value of the neutron-electron scattering length b_e is -1.32×10^{-3} fm while $b(0) \approx 5$ fm. Thus, for all but the lightest elements, the correction term in (4.5) is in the range 0.5% to 2%. We see from Table I that this is often one to two orders of magnitude larger than the experimental uncertainty in the scattering length. In this sense, therefore, the electromagnetic correction in (4.4) is a large effect.

According to the exact expression (3.1), the index of refraction is determined by the scattering amplitude in the

forward direction, where $q = 0$. Thus, the scattering length in (4.2) is $b'(0)$. On the other hand, the scattering length in (3.20) is $b'(q)$ and should therefore be put inside the integral when the electromagnetic correction is included. The scattering length in the expression (4.1) for the unit-cell structure factor is also $b'(q)$ where q now equals the magnitude of the reciprocal lattice vector corresponding to the Bragg planes (hkl). The net result is that the methods in Table I that depend on n' determine $b'(0)$ directly. However, the methods that depend on n'' or $|F_{hkl}|$ must be corrected for electromagnetic interactions in order to determine $b'(0)$.

This correction requires a knowledge of the atomic form factor $\phi(q)$. The International Tables for Crystallography¹⁰⁾ list accurate values of this quantity that have been obtained from relativistic Hartree-Fock calculations for all the atoms and chemically important ions in the periodic table. Alternatively, since the correction is small, it is often sufficient to use the approximate analytical expression^{8,11)}

$$\phi(q) = \frac{1}{\sqrt{1 + 3(q/q_0)^2}}, \quad (4.6)$$

with $q_0 = \gamma Z^{1/3}$. The value $\gamma = 1.90 \pm 0.07 \text{ \AA}^{-1}$ provides a good fit to the Hartree-Fock results for $Z \geq 20$.

§.5. Conclusions

The key to resolving the problems with the elementary theory of dispersion that were discussed in Sec. 2 lies in the recognition, firstly, that as a result of local-field effects the scattering amplitude F of an atom in a material medium is different from the scattering amplitude f of an isolated atom and, secondly, that for a finite value of k the scattering amplitude f differs from the scattering length b by more than the conventional minus sign. These differences are ignored in the elementary theory of dispersion where it is tacitly assumed that $F = f = -b$. This is normally a good approximation for F' because $J \leq 10^{-4}$, but it is a bad approximation for F'' because all three terms in (3.16) are usually of about the same order of magnitude.

At present it is only in work of the highest experimental precision, such as in the measurement of neutron scattering lengths by gravity refractometry, that the local-field correction in (3.15) is larger than the experimental uncertainty in b' . It has been shown¹²⁾ that the local-field term could, in principle, produce a non-vanishing Fizeau effect for neutrons. However, the effect is currently too small to observe.

When electromagnetic interactions are taken into account, the effective scattering length of an atom becomes q -dependent and is given by (4.4). The essential point to note here is that it is $b(0)$ that is normally listed in tables of neutron data,^{5,13)} but it is $b(q)$ that determines the coherent scattering of thermal neutrons in condensed matter. To interpret thermal-neutron scattering experiments, where $q > 0$, an explicit correction for the second term in (4.4) should therefore be made. In the past, experimenters have tended to ignore this correction, a practice that was certainly justified in the early days of neutron scattering when the experimental uncertainty in $b(0)$ was much larger

than the value of $b_e Z$. However, for most elements this is no longer true today, and this correction should be made routinely in all experiments where an accurate determination of the scattered-neutron intensity over a wide range of q values is important. Failure to make this correction will introduce systematic errors of 0.5% to 2% in the scattering lengths at large q , and corresponding errors of 1% to 4% in the scattering cross sections.

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