## Symmetries in Scattering of Slow Neutrons\*

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Reciprocity, detailed balance, and other symmetry laws for slow-neutron scattering are discussed for the case of anisotropic media. While Friedel's law, stating that  $\Sigma(\mathbf{v} \to \mathbf{v}') = \Sigma(-\mathbf{v} \to -\mathbf{v}')$ , may fail for polar absorbing media, reciprocity as a consequence of time-reversal invariance, and of thermal equilibrium of the medium, remains valid. The optical theorem helps to derive a reciprocity relation for the total cross section  $\Sigma(\mathbf{v}) = \Sigma(-\mathbf{v})$ . Similar conclusions are derived for the matrices used to describe scattering of polarized neutrons. The two reciprocity relations lead to a macroscopic reciprocity theorem, expressing a symmetry property of Green's functions of the linearized Boltzmann equation.

#### I. INTRODUCTION

HE neutron scattering law for any medium in I thermal equilibrium obeys a reciprocity relation,<sup>1</sup> which in terms of the macroscopic differential scattering cross section (per unit velocity space) reads as

$$v e^{-mv^2/2kT} \Sigma(\mathbf{v} \to \mathbf{v}') = v' e^{-mv'^2/2kT} \Sigma(-\mathbf{v}' \to -\mathbf{v}).$$
(1)

In most cases Friedel's law<sup>2</sup> also holds, stating that

$$\Sigma(\mathbf{v} \to \mathbf{v}') = \Sigma(-\mathbf{v} \to -\mathbf{v}'). \tag{2}$$

A combination of Eqs. (1) and (2) gives the detailed balance relation<sup>1,3-5</sup>

$$v e^{-mv^2/2kT} \Sigma(\mathbf{v} \to \mathbf{v}') = v' e^{-mv'^2/2kT} \Sigma(\mathbf{v}' \to \mathbf{v}). \quad (3)$$

In Van Hove's formalism,  $^{4,5}$  Eqs. (1)-(3) are expressed as

$$S(\mathbf{\kappa},\omega) = e^{\hbar\omega/kT} S(\mathbf{\kappa},-\omega), \qquad (1')$$

$$S(\mathbf{k},\omega) = S(-\mathbf{k},\omega), \qquad (2')$$

$$S(\mathbf{k},\omega) = e^{\hbar\omega/kT} S(-\mathbf{k}, -\omega), \qquad (3')$$

where  $\hbar \kappa = m(\mathbf{v} - \mathbf{v}')$  and  $\hbar \omega = \frac{1}{2}m(v^2 - v'^2)$ . In an obvious way these relations are reflected in certain symmetries of the correlation functions  $\chi(\mathbf{k},t)$  and  $G(\mathbf{r},t)$ .

Violations of Friedel's law have been observed in neutron scattering by absorbing polar crystals, such as CdS.<sup>6</sup> Cases of this kind are certainly rare and of no practical importance. Nevertheless, they represent an incentive to retrace the reasoning behind reciprocity, detailed balance, and other symmetries in slow-neutron scattering, and to review the connections with the underlying basic principles.

#### **II. RECIPROCITY**

The subsequent derivation follows that of Hurwitz et al.,3 with a minor generalization to account for a possible polar structure of the medium. The concept of the transition operator for a bound target will be used,7

$$\mathcal{T} = V + V(E - H + i\epsilon)^{-1}V$$

where V is the neutron-target interaction Hamiltonian, E the total energy, H the total Hamiltonian, and  $\epsilon \rightarrow 0$ ,  $\epsilon > 0$ . The target has a volume  $\mathcal{V}$  and is small compared to the neutron mean free path, but large compared to  $\lambda_{\rm th} = \hbar/(mkT)^{1/2}$ .

The cross section is expressed by a canonical average of squared T-matrix elements<sup>7</sup>

$$\Sigma(\mathbf{v} \to \mathbf{v}') = \frac{m^3}{\Im v} \left(\frac{2\pi}{\hbar}\right)^4 \sum_{i,f} Z^{-1} e^{-E_i/kT} \delta(\hbar\omega + E_i - E_f) \\ \times \frac{1}{2} \sum_{\mathbf{s},\mathbf{s}'} |\langle s', \mathbf{v}', f| \mathcal{T} |i, \mathbf{v}, s \rangle|^2.$$
(4)

Here, i and f refer to the initial and final states of the target, and s and s' to the spin states of the neutron, whereas  $|v\rangle$  stands for  $(2\pi)^{-3/2}e^{imv\cdot r/\hbar}$ . Equation (4) represents a shorthand statement, and should properly be written with the left-hand side multiplied by a nottoo-small  $d^3v'$ , and the right-hand side integrated over the same range.

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<sup>1</sup> The terminology, with respect to Eqs. (1) and (3), is that of J. Blatt and V. F. Weisskopf,</sup> *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), Sec. X 2.
<sup>2</sup> R. W. James, *The Optical Principles of the Diffraction of X-Rays* (G. Bell and Sons, London, 1954).
<sup>3</sup> H. Hurwitz, Jr., M. S. Nelkin, and G. J. Habetler, Nucl. Sci. Eng. 1, 280 (1956).
<sup>4</sup> V. F. Turchin, *Medlennye Neitrony* (Moscow, 1963) [English transl.: *Slow Neutrons* (Davey and Co., New York, 1965)].

transl.: Slow Neutrons (Davey and Co., New York, 1965)]. <sup>6</sup> D. E. Parks, M. S. Nelkin, N. F. Wikner, and J. R. Beyster

<sup>(</sup>unpublished).

<sup>&</sup>lt;sup>6</sup>S. W. Peterson and H. G. Smith, Phys. Rev. Letters 6, 7 (1961); J. Phys. Soc. Japan 17, Suppl. B-II, 335 (1962); J. Phys. (Paris) 25, 615 (1964).

<sup>&</sup>lt;sup>7</sup> M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964). See p. 682, Eq. (15a); p. 171, Eq. (235); p. 55, Eq. (130); and p. 183, Eq. (39).

$$|\langle s', \mathbf{v}', f| \mathcal{T} | i, \mathbf{v}, s \rangle |$$
  
= |\langle - s, - \mathbf{v}, i^T | \mathcal{T} | f^T, - \mathbf{v}', -s' \rangle | \langle 5

(for  $\hbar\omega + E_i - E_f = 0$ ), where  $i^T$  and  $f^T$  refer to the timereversed states of the target. Since  $E_i = E_i^T$  and  $E_f = E_f^T$ , expression (4), with the right-hand side of (5) substituted, again represents a canonical average, but with the time-reversed states as a basis. We then substitute  $E_i = E_{f^T} - \hbar \omega$ , and carry out a relabeling:  $i^T$ ,  $f^T$ , -s,  $-s' \rightarrow f$ , *i*, *s'*, *s*. Thereupon, the right-hand side is recognized as  $(v'/v)e^{\hbar\omega/kT}\Sigma(-v'\to -v)$ , so that reciprocity, Eq. (1), is established. This is seen to represent an exact and perfectly general consequence of timereversal invariance of the neutron-target interaction, and of the thermal equilibrium of the target.

So far, we have neglected the possibility of nuclear or atomic magnetization. Time-reversal implies that magnetization is switched. We then have  $E_i(\mathbf{B})$  $=E_{i}r(-\mathbf{B})$ , so that the cross sections in Eq. (1) should be written as  $\Sigma(\mathbf{v} \rightarrow \mathbf{v}'; \mathbf{B})$  and  $\Sigma(-\mathbf{v}' \rightarrow -\mathbf{v}; -\mathbf{B})$ . We shall not insist upon this complication in notation. but rather let the  $\pm \mathbf{B}$  be understood in every reciprocity relation [Eqs. (9), (13), (20)-(22), and (24) below].

## **III. DETAILED BALANCE**

Any element of the point symmetry group of the target structure is, of course, reflected in a corresponding symmetry of the T matrix and of the cross sections. In particular, if the structure has a center of symmetry, Friedel's law, Eq. (2), is a trivial consequence.

Usually<sup>4</sup> detailed balance, Eq. (3), is not derived as a consequence of reciprocity and Friedel's law, but by an independent argument relying upon the first Born approximation, where T = V. The only essential point is that in this approximation  $\mathcal{T}$  is self-adjoint if V is real, which obviously is a necessary condition.

After switching to the complex-conjugate matrix element  $\langle s, \mathbf{v}, i | \mathcal{T} | f, \mathbf{v}', s' \rangle$  in Eq. (4), and substituting  $E_i = E_f - \hbar \omega$ , we carry out a relabeling  $i, f \to f, i$ . The resulting expression is recognized as  $(v'/v)e^{\hbar\omega/kT}$  $\times \Sigma(\mathbf{v}' \rightarrow \mathbf{v})$ , so that detailed balance, Eq. (3), is proven. By the way, no switching of magnetization is implied in this manipulation.

For scattering of slow neutrons by nuclei the first Born approximation, with Fermi's pseudopotential,

$$V = \frac{2\pi\hbar^2}{m} \sum_{n} \mathbf{a}_n \delta(\mathbf{r} - \mathbf{r}_n),$$
  
$$\mathbf{a}_n = a_n^{\text{coh}} + \frac{\mathbf{\sigma} \cdot \mathbf{J}_n}{[J_n(J_n+1)]^{1/2}} a_n^{\text{inc}},$$

is known to be highly accurate.8 If absorption is absent

or weak, the scattering lengths  $a_n^{\rm coh}$  and  $a_n^{\rm inc}$  can be taken as real.<sup>9</sup> Detailed balance is, therefore, approximately valid. Friedel's law then follows from a combination with reciprocity, regardless of any asymmetry in the structure of the target.

Thus, we have verified that with purely nuclear scattering violations of Friedel's law and of detailed balance can be expected only for media with polar structure, if either neutron absorbing nuclei are present or second-order effects become noticeable.

## IV. SYMMETRIES IN SCATTERING OF POLARIZED NEUTRONS

It is interesting to generalize the above considerations to cross sections referring to polarized incident neutron beams and to polarizing detectors for the scattered neutrons. Two representations can be used for this purpose: density matrices and the Stokes-Poincaré representation. The latter has the advantage of avoiding complex quantities and will, therefore, be preferred here. It has been invented for describing polarization of light,10-12 but it applies equally to nonrelativistic spin-<sup>1</sup>/<sub>2</sub> particles.<sup>13,14</sup>

The intensity of a neutron beam is described by a combination of a scalar and a vector:  $\mathbf{n} = (n_0; n_1, n_2, n_3)$ . Herein  $n_0$  represents the number density, and  $\frac{1}{2}(n_1, n_2, n_3)$ the spin density of the neutrons, so that  $(n_1, n_2, n_3)/n_0$ measures the degree and orientation of their polarization. In other words, this ratio is the average (quantummechanical and statistical) of the Pauli-spin vector,

$$n_{\mu}/n_0 = \langle \sigma_{\mu} \rangle, \quad \mu = 1, 2, 3.$$

It will be convenient to include also the scalar component ( $\mu = 0$ ) by using  $\sigma_0$  to denote the unit matrix.

The determination of, say,  $n_0$  and  $n_3$ , requires two measurements, with the polarizing device oriented along +z and -z. The sum of the readings (or a reading without polarizer) gives  $n_0$ , and the difference  $n_3$ . Four independent observations are required for the four values  $n_{\mu}, \mu = 0, 1, 2, 3$ .

Let a parallel neutron beam of velocity v be scattered by a target of volume  $\mathcal{V}$ . The components  $N_{\nu}(\mathbf{v}')$ describing the intensity of the scattered beam (per unit  $d^3v'$  and at some distance r) depend linearly upon  $n_{\mu}$ . Hence,

$$v'N_{\nu}(\mathbf{v}') = \frac{\upsilon}{r^2} \sum_{\mu=0}^{3} vn_{\mu}\Sigma_{\mu\nu}(\mathbf{v}\to\mathbf{v}'), \quad \nu=0,\,1,\,2,\,3. \quad (6)$$

This defines 16 components of the cross-section matrix, corresponding to 16 possible independent observations.

<sup>&</sup>lt;sup>8</sup> J. P. Plummer and G. C. Summerfield, Phys. Rev. **131**, 1153 (1963); G. C. Summerfield, Ann. Phys. (N. Y.) **26**, 72 (1964).

<sup>&</sup>lt;sup>9</sup> R. J. Glauber, Lectures Theoret. Phys. 4, 571 (1962).

<sup>&</sup>lt;sup>10</sup> S. Chandrasekhar, Radiative Transfer (Oxford University Press, New York, 1950).

<sup>&</sup>lt;sup>11</sup> H. C. van de Hulst, *Light Scattering by Small Particles* (John Wiley & Sons, Inc., New York, 1957).
<sup>12</sup> I. Kuščer and M. Ribarič, Opt. Acta 6, 42 (1959).
<sup>13</sup> U. Fano, Rev. Mod. Phys. 29, 74 (1957).
<sup>14</sup> W. H. McMaster, Rev. Mod. Phys., 33, 8 (1961).

The cross-section matrix is seen to be composed of one tensor (components with  $\mu$ ,  $\nu = 1, 2, 3$ ), two axial vectors  $(\Sigma_{01}, \Sigma_{02}, \Sigma_{03})$  and  $(\Sigma_{10}, \Sigma_{20}, \Sigma_{30})$ , and one scalar  $(\Sigma_{00})$ . The latter is just the ordinary cross section  $\Sigma(\mathbf{v} \rightarrow \mathbf{v}')$ , as measured with an unpolarized incident beam and a nonpolarizing detector.

An expression for the cross-section matrix, in terms of the  $\mathcal{T}$  matrix, can be derived along with Eq. (4). We first notice that the spin state of the neutron scattered in the transition  $|i, \mathbf{v}\rangle \rightarrow |f, \mathbf{v}'\rangle$  is described by  $\sum_{s'} |s'\rangle$  $\times \langle s', \mathbf{v}', f | \mathcal{T} | i, \mathbf{v}, \mathbf{X} \rangle$ , where  $|\mathbf{X}\rangle$  denotes the arbitrary initial spin state. The Stokes-Poincaré parameters after scattering are then determined from

$$\langle \sigma_{\mathbf{v}} \rangle_f \propto \operatorname{Tr}(\langle \mathbf{v}, i | \mathcal{T}^{\dagger} | f, \mathbf{v}' \rangle \sigma_{\mathbf{v}} \langle \mathbf{v}', f | \mathcal{T} | i, \mathbf{v} \rangle \rho).$$
 (7)

Here  $\langle \mathbf{v}', f | \mathcal{T} | i, \mathbf{v} \rangle$  is a 2×2 matrix, with elements as in Eq. (4), whereas  $\rho$  represents the initial neutron-spin density matrix,  $\rho = |\chi\rangle\langle\chi|$  in the present case. Any such matrix is a linear combination of the  $\sigma_{\mu}$ ; in fact,<sup>13</sup>

$$\rho = \frac{1}{2} \sum_{\mu=0}^{3} \langle \sigma_{\mu} \rangle_{i} \sigma_{\mu}.$$

The coefficients relating the  $\langle \sigma_{\nu} \rangle_{f}$  to the  $\langle \sigma_{\mu} \rangle_{i}$  are therefore proportional to expressions like (7), with  $\rho$  replaced by  $\sigma_{\mu}$ . With all the proportionality factors inserted, the final result for the cross-section matrix is

$$\Sigma_{\mu\nu}(\mathbf{v} \to \mathbf{v}') = \frac{m^3}{v \mathcal{O}} \left(\frac{2\pi}{\hbar}\right)^4 \sum_{i,f} Z^{-1} e^{-E_i/kT} \delta(\hbar\omega + E_i - E_f)$$
$$\times \frac{1}{2} \operatorname{Tr}(\langle \mathbf{v}, i | \mathcal{T}^{\dagger} | f, \mathbf{v}' \rangle \sigma_{\nu} \langle \mathbf{v}', f | \mathcal{T} | i, \mathbf{v} \rangle \sigma_{\mu}). \quad (8)$$

For  $\mu = 0$ ,  $\nu = 0$ , this equation is the same as (4).

When applying time-reversal invariance to Eq. (8), phase factors for the neutron-spin states must be taken into account. They are given by<sup>7</sup>

$$\left|\frac{1}{2}\right\rangle^{T} = -\left|-\frac{1}{2}\right\rangle, \quad \left|-\frac{1}{2}\right\rangle^{T} = \left|\frac{1}{2}\right\rangle.$$

Otherwise, the procedure is the same as before, and leads to the following reciprocity relation:

$$ve^{-mv^2/2kT}\Sigma_{\mu\nu}(\mathbf{v}\to\mathbf{v}')$$
  
=  $(-1)^{\Delta}v'e^{-mv'^2/2kT}\Sigma_{\nu\mu}(-\mathbf{v}'\to-\mathbf{v}), \quad (9)$ 

where  $\Delta = \delta_{0\mu} + \delta_{0\nu}$ . That is, minus signs are found with the vector components of the cross-section matrix. This must be so, since they belong to axial vectors of the same kind as angular momentum.<sup>13</sup>

When  $\mathcal{T}$  is self-adjoint, as in the Fermi approximation with real scattering lengths, we may switch to complexconjugate matrix elements in Eq. (8). In the same way as before, a detailed balance relation follows:

$$v e^{-mv^2/2kT} \Sigma_{\mu\nu} (\mathbf{v} \to \mathbf{v}') = v' e^{-mv'^2/2kT} \Sigma_{\nu\mu} (\mathbf{v}' \to \mathbf{v}). \quad (10)$$

No minus signs appear here.

If the target structure has a center of symmetry (which implies that there is no magnetization), we consider mirrored states to derive a generalization of Friedel's law:

$$\Sigma_{\mu\nu}(\mathbf{v}\to\mathbf{v}') = \Sigma_{\mu\nu}(-\mathbf{v}\to-\mathbf{v}'). \tag{11}$$

Again there are no minus signs, since axial vectors are invariant under such transformation.

Because of the factor  $(-1)^{\Delta}$  in Eq. (9), Friedel's law and detailed balance no longer follow from each other in combination with reciprocity, as was the case with the scalar component  $\Sigma_{00}$ . Rather, if all three laws are valid, we derive that the vector components  $\Sigma_{01}$ , etc., must vanish, as we should have expected.

The Fermi approximation implies the further simplification that the neutron spin enters only through a  $\sigma \cdot \mathbf{J}$  term ( $\sigma \cdot \mathbf{L}$  coupling is noticeable only at higher energies). This allows us the liberty of representing neutron and nuclear spins in a coordinate system different from the one used for neutron velocities. If the nuclei are in no way polarized, the cross-section matrix must be invariant against rotation of the spin-coordinate system. This is only possible if the vector components  $\Sigma_{01}$ , etc., vanish, and if the tensor part of the matrix is isotropic,

$$\Sigma_{\mu\nu}(\mathbf{v} \to \mathbf{v}') = \Sigma'(\mathbf{v} \to \mathbf{v}')\delta_{\mu\nu}, \quad \mu = 1, 2, 3.$$
(12)

There are then all together only two independent differential cross sections,  $\Sigma(\mathbf{v} \rightarrow \mathbf{v}')$  and  $\Sigma'(\mathbf{v} \rightarrow \mathbf{v}')$ .<sup>16</sup> In this most common and most simple case, the orientation of the polarization vector  $\langle \boldsymbol{\sigma} \rangle$  is never changed in scattering. The degree of polarization  $|\langle \boldsymbol{\sigma} \rangle|$  remains unchanged if  $\Sigma = \Sigma'$ , or it diminishes if  $\Sigma' < \Sigma$ . The difference  $\Sigma - \Sigma'$  is known as the depolarization or spin-flip cross section.<sup>4</sup>

# V. RECIPROCITY FOR TOTAL CROSS SECTION

Whenever Friedel's law, Eq. (2), holds, integration over  $d^3\mathbf{v}'$  leads to a corresponding symmetry relation for the integrated scattering cross section  $\Sigma_s(\mathbf{v})$ . In such case, the same symmetry is expected to apply for the absorption cross section  $\Sigma_a(\mathbf{v})$ , and therefore also for the total cross section.

$$\Sigma(\mathbf{v}) = \Sigma(-\mathbf{v}). \tag{13}$$

It turns out that this reciprocity relation is always valid, even for polar absorbing media where Friedel's law fails to hold, and where it may happen that  $\Sigma_s(\mathbf{v})$ 

<sup>&</sup>lt;sup>15</sup> S. Watanabe, Rev. Mod. Phys. 27, 26 (1955).

<sup>&</sup>lt;sup>16</sup> It may be mentioned that the indicated reduction of the cross-section matrix to two scalars can be interpreted in terms of a broader mathematical theorem. We have to use the density-matrix representation, where the cross sections form a  $2\times2\times2\times2$  matrix, i.e., a fourth-order tensor in spin space. According to that theorem a general symmetric isotropic fourth-order tensor is described by two scalars. The elasticity tensor furnishes a well-known three-dimensional example. See H. and B. S. Jeffreys, New York, 1956), Chap. 3.

 $\neq \Sigma_s(-\mathbf{v})$  and  $\Sigma_a(\mathbf{v}) \neq \Sigma_a(-\mathbf{v})$ . The proof is based upon time-reversal invariance and upon the optical theorem. According to this theorem,<sup>7</sup>

$$\Sigma(\mathbf{v}) = -\left(8\pi^{3}/\mathcal{O}\hbar v\right)\sum_{i} Z^{-1}e^{-E_{i}/kT} \times \sum_{s} \operatorname{Im}\left(\langle s, \mathbf{v}, i \mid \mathcal{T} \mid i, \mathbf{v}, s \rangle\right). \quad (14)$$

In view of time-reversal invariance, the matrix element here equals  $\langle -s, -\mathbf{v}, i^T | \mathcal{T} | i^T, -\mathbf{v}, -s \rangle$ . Any phase factors cancel, because both states are the same. After a relabeling, -s,  $i^T \rightarrow s$ , i, the right-hand side of Eq. (14) is seen to represent  $\Sigma(-\mathbf{v})$ .

A macroscopic analogy will help to understand the reciprocity property of the total cross section and the possible dissymmetry in  $\Sigma_s(\mathbf{v})$  and  $\Sigma_a(\mathbf{v})$ . Consider an asymmetric object painted white on one side and black on the other. We place the object into sunlight, with the white side on top. The total cross section, as measured by the size of the shadow, is predominantly due to scattering, and less to absorption. When the object is turned upside down, the size of the shadow is again the same, but absorption then dominates over scattering.

If polarization effects are to be described, a scalar  $\Sigma(\mathbf{v})$  will suffice only if the attenuation rate of a neutron beam is known to be independent of the polarization state. Although this is the common case, a well-known exception is provided by ferromagnetic crystals, where an effect analogous to dichroism is observed. In such cases, we need a tensor  $\Sigma_{\mu\nu}(\mathbf{v})$ , and the attenuation of a parallel monochromatic neutron beam is described by

$$dn_{\nu} = -\sum_{\mu=0}^{3} n_{\mu} \Sigma_{\mu\nu}(\mathbf{v}) ds , \quad \nu = 0, 1, 2, 3.$$
 (15)

In order to investigate symmetries of this tensor, we try to express its components by aid of the optical theorem, as this was done for the component  $\Sigma_{00}(\mathbf{v})$  $=\Sigma(\mathbf{v})$  [Eq. (14)]. We notice that the four components of the matrix  $\operatorname{Im}(\langle \mathbf{v}, i | \mathcal{T} | i, v \rangle)$  can give no more than four of the components  $\Sigma_{\mu\nu}(\mathbf{v})$ . This is understandable, because the optical theorem originates from a particlecurrent argument. It can therefore yield only the components  $\Sigma_{\mu 0}(\mathbf{v})$ , determining the attenuation of the density of the beam.

The rest of the matrix  $\Sigma_{\mu\nu}(\mathbf{v})$  is derived from an extension of the optical theorem based upon spin currents. For a state  $|\Psi^+\rangle$  of the system, the four neutron currents are

$$\mathbf{j}_{\boldsymbol{\nu}} = -\left(i\hbar/m\right) \langle \Psi^+ | \sigma_{\boldsymbol{\nu}} \nabla | \Psi^+ \rangle, \quad \boldsymbol{\nu} = 0, 1, 2, 3.$$

We insert  $|\Psi^{\dagger}\rangle = |i, \mathbf{v}, \chi\rangle + \text{scattered waves, expressing}$ the amplitudes in terms of the T matrix elements, and then integrate over a large sphere. The term of first order in T describes the (negative) total attenuation of the incident neutron currents. This term is evaluated

as

$$(2/\hbar) \operatorname{Im}[\operatorname{Tr}(\sigma_{\nu} \langle \mathbf{v}, i | \mathcal{T} | i, \mathbf{v} \rangle \rho)].$$

With the same substitution for  $\rho$  and the same arguments as in Sec. IV we then have, for a target in thermal equilibrium,

$$\Sigma_{\mu\nu}(\mathbf{v}) = -\left(8\pi^{3}/\mho\hbar v\right)\sum_{i} Z^{-1}e^{-E_{i}/kT}$$
$$\times \mathrm{Im}[\mathrm{Tr}(\sigma_{\nu}\langle\mathbf{v},i|\mathcal{T}|i,\mathbf{v}\rangle\sigma_{\mu})]. \quad (16)$$

For  $\mu = \nu = 0$ , this is the same as Eq. (14).

After cyclic permutation of the matrices in Eq. (16), we carry out the multiplication  $\sigma_{\mu}\sigma_{\nu}$ . It becomes obvious that all diagonal components of the total cross-section matrix are equal,

$$\Sigma_{\mu\mu}(\mathbf{v}) = \Sigma(\mathbf{v}), \quad \mu = 0, 1, 2, 3$$
 (17)

that both vectors are the same,

$$\Sigma_{0\mu}(\mathbf{v}) = \Sigma_{\mu 0}(\mathbf{v}), \quad \mu = 1, 2, 3$$
 (18)

and that the off-diagonal part of the tensor is antisymmetric, thus again representing an axial vector:

$$-\Sigma_{23}(\mathbf{v}) = \Sigma_{32}(\mathbf{v}) \equiv \Omega_1 / v, \quad \text{etc.}$$
(19)

We see that this matrix contains at most seven independent parameters: one scalar ( $\Sigma_{00}$ ), and two vectors. One of them  $(\Sigma_{01}, \Sigma_{02}, \Sigma_{03})$  obviously describes selective attenuation of polarized neutrons (dichroism). The meaning of the other vector  $(\Omega)$  becomes clear if Eq. (15) is rewritten in vector notation.  $\Omega$  is seen to represent a precession frequency. [For a magnetic field in a vacuum, Eq. (16), with  $T = V = -\mu_n \boldsymbol{\sigma} \cdot \boldsymbol{B}$ , indeed gives the correct value for the Larmor precession.] Time reversal leads to

$$\Sigma_{\mu\nu}(\mathbf{v}) = (-1)^{\Delta} \Sigma_{\nu\mu}(-\mathbf{v}), \qquad (20)$$

which is an obvious generalization of Eq. (13).

In the Fermi approximation, and if magnetization and nuclear polarization are absent, we apply the same symmetry reasoning as in Sec. IV. Clearly, all but the diagonal components  $\Sigma_{\mu\mu}(\mathbf{v}) = \Sigma(\mathbf{v})$  must vanish, so that the matrix becomes equivalent to a scalar.

## VI. MACROSCOPIC RECIPROCITY

The reciprocity relation (1) and Eq. (13) are necessary and sufficient for the derivation of a reciprocity theorem<sup>17-20</sup> for the Green's function of the Boltzmann equation. According to this theorem, the average

<sup>&</sup>lt;sup>17</sup> K. M. Case, Rev. Mod. Phys. 29, 651 (1957)

<sup>&</sup>lt;sup>18</sup> B. B. Kadomtsev, Dokl. Akad. Nauk SSSR 113, 541 (1957) English transl.: Soviet Phys.—Doklady 2, 139 (1958)]. <sup>19</sup> L. M. Biberman and B. A. Veklenko, Zh. Eksperim. i Teor. Fiz. 39, 88 (1960) [English transl.: Soviet Phys.—JETP 12, 64

<sup>(1961)].</sup> <sup>20</sup> I. Kuščer and N. J. McCormick, Nucl. Sci. Eng. 26, 522 (1966); I. Kuščer, Kernenergie 10, 265 (1968).

neutron distribution due to an instantaneous monokinetic unit point source in a nonmultiplying medium with uniform temperature and time-independent properties obeys the relation

$$e^{-m\mathbf{v}_0^2/2kT}G(\mathbf{r}_0, \mathbf{v}_0 \to \mathbf{r}, \mathbf{v}; t)$$
  
=  $e^{-m\mathbf{v}^2/2kT}G(\mathbf{r}, -\mathbf{v}, \to \mathbf{r}_0, -\mathbf{v}_0; t).$  (21)

This may be regarded as a generalization of relation (1) to macroscopic systems which are no longer small with respect to the neutron mean free path. The essential distinction is that G in Eq. (21) describes probabilities for transitions in phase space of the neutron, whereas Eq. (1) concerns only transition rates in velocity space.

The theorem (21) can be specialized in many ways. Integration over t gives the corresponding relation for time-independent neutron distributions. As a special example, we may quote the reciprocity property for the reflectivity of a flat layer. By the substitution  $G(\mathbf{v} \rightarrow \mathbf{v}')$  $= P(\mathbf{v} \rightarrow \mathbf{v}')/v_1'$ , we introduce the probability density  $P(\mathbf{v} \rightarrow \mathbf{v}')$  for a neutron of initial velocity  $\mathbf{v}$  to be reflected with a velocity around  $\mathbf{v}'$ . (The vectors  $\mathbf{v}$  and  $\mathbf{v}'$  are directed towards the layer and away from it, respectively, and  $v_1$  and  $v_1'$  denote the magnitudes of the normal components.) We find

$$v_{\perp}e^{-mv^{2}/2kT}P(\mathbf{v}\rightarrow\mathbf{v}') = v_{\perp}'e^{-mv'^{2}/2kT}P(-\mathbf{v}'\rightarrow-\mathbf{v}). \quad (22)$$

There is actually no need to derive Eq. (22) from the Boltzmann equation, because it also follows directly from time-reversal arguments. Indeed, the reasoning used in Sec. II applies equally well to targets of any size. We notice that  $A(v_1/v)P(\mathbf{v} \rightarrow \mathbf{v}')$  represents the differential cross section of a macroscopic flat layer of an area A. This is expressed in terms of the  $\mathcal{T}$  matrix, and time reversal is invoked. Equation (22) immediately follows.

Such a direct derivation also appears feasible for the more general relation (21). A prerequisite would be a quantum-mechanical definition of the neutron phasespace density, presumably by a Wigner distribution function.

The reciprocity theorem (21) can be generalized to include polarization effects. Equations (6) and (15)

show how to write the appropriate Boltzmann equation :

$$\begin{pmatrix} \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \end{pmatrix} G_{\mathbf{r}_0 \to \mathbf{r}}(\mathbf{r}_0, \mathbf{v}_0 \to \mathbf{r}, \mathbf{v}; t)$$

$$= -\sum_{\mu=0}^3 v G_{\mathbf{r}_0 \to \mu}(\mathbf{r}_0, \mathbf{v}_0 \to \mathbf{r}, \mathbf{v}; t) \Sigma_{\mu\nu}(\mathbf{v})$$

$$+ \sum_{\mu=0}^3 \int v' G_{\mathbf{r}_0 \to \mu}(\mathbf{r}_0, \mathbf{v}_0 \to \mathbf{r}, \mathbf{v}'; t) \Sigma_{\mu\nu}(\mathbf{v}' \to \mathbf{v}) d^3 v'$$

$$+ \delta_{\nu\nu_0} \delta(\mathbf{r} - \mathbf{r}_0) \delta(\mathbf{v} - \mathbf{v}_0) \delta(t).$$
(23)

We assume that there are no neutrons incident from the outside.

Proceeding as in the proof of Eq. (21),<sup>20</sup> we consider the function

$$(-1)^{\delta_0 \nu} e^{m(\nu^2 - \nu_1^2)/2kT} G_{\nu_1 \to \nu}(\mathbf{r}_1, \mathbf{v}_1 \to \mathbf{r}, -\mathbf{v}; t_1 - t),$$

and show that it satisfies an equation adjoint to (23). We then multiply Eq. (23) by this latter function, and the adjoint equation by  $G_{\nu_0 \rightarrow \nu}$  from Eq. (23), integrate over all variables and also sum over  $\nu$ , and substract. The result is immediate:

$$= {}^{-mv_0^2/2kT} G_{\mu \to \nu}(\mathbf{r}_0, \mathbf{v}_0 \to \mathbf{r}, \mathbf{v}; t)$$

$$= (-1)^{\Delta} e^{-mv^2/2kT} G_{\nu \to \mu}(\mathbf{r}, -\mathbf{v} \to \mathbf{r}_0, -\mathbf{v}_0; t).$$
(24)

Most of what has been said so far is not specific for neutrons, but applies equally well, or with little modification, to scattering of any particles by systems in thermal equilibrium. For instance, Eq. (22) also applies for the reflection of monatomic gas molecules by a wall.<sup>21</sup> We should notice, however, that here the reflection process cannot be described by any Boltzmann equation. Therefore, in this case, we can use only the direct derivation of Eq. (22) from the symmetry (5) of the  $\tau$  matrix.

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<sup>21</sup> C. Cercignani, Mathematical Methods in Kinetic Theory (Plenum Publishing Corp., New York, 1969).