THEORY OF RESONANCE SCATTERING BY ATOMIC SYSTEMS

I. DERIVATION OF GENERAL FORMULAS

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The probability for resonance scattering is expressed in terms of the correlation function for the coordinates of particles of the scattering system at four different times, just as the probability for scattering in the Born approximation is expressed in terms of the Van Hove [1] pair correlation function. The probability for scattering as a result of interference of resonant and potential scattering is treated similarly.

1. Van Hove [1] developed a method for analysis of scattering in the Born approximation, using a pair correlation function which depends only on the properties of the scattering system and the energy and momentum transferred by the incident particles (or light quanta) during the scattering. Then all the information concerning the interactions of the incident particle with the individual atoms of the system is contained in a factor which is independent of the mutual interaction of the atoms and, consequently, is independent of the state of the system. In Van Hove's paper and in later work, [2-6] many important properties of the pair correlation function were studied, and it was shown that this function contains extremely profound information on the dynamics of the atoms in the scattering system. In particular, if the atoms of the system carry out oscillations (not necessarily harmonic) around their equilibrium position, this function can be expressed in terms of the Green's function of the phonon field. [5]

The reason for so much interest in this subject is that, in principle, the experimental investigation of potential scattering of slow neutrons with present techniques already enables us to determine the pair correlation function.

With the discovery of the Mössbauer effect [7] it became possible to study the properties of atomic systems using resonance absorption and emission of γ quanta as well as neutrons by atomic nuclei (cf., for example, [8-10]). In a series of papers [4,5,11,12] it was shown that the probabilities for such processes can also be expressed in terms of the Van Hove pair correlation function. The reason for this is that, although these processes occur in the second order of perturbation theory, summation over final states in the case of absorption and averaging over initial states in the case of emission allows one to write the expression for the transition probability in a form which is analogous to the Born approximation for absorption or emission processes.

The situation is different for resonance scattering, where one must determine the probability of scattering into a given energy and angular range. In this case the expression for the differential cross section is essentially defined in the second order of perturbation theory, taking into account the damping of the intermediate state. In an earlier paper [10] concerning resonance scattering of neutrons by systems of interacting atoms, only the elastic scattering by crystals was calculated and it was implicitly assumed that the crystal consists of identical spinless nuclei. Including the effects of spins and the presence of a mixture of isotopes is quite trivial. More complicated is the generalization to the case of an arbitrary system of interacting atoms and the treatment of scattering with transfer of arbitrary amounts of energy and momentum to the scattering system (and not just pure elastic scattering).

This problem is treated in the present paper. We first restrict ourselves to the case where the potential scattering is negligibly small compared to the resonance scattering, and only later treat the interference between potential and resonance scattering. Just as in Van Hove's work on potential scattering, the expression for the probability will be represented as an average over initial states of Heisenberg operators* at different times.

*Time dependent operators have already been used previously in the problem of scattering of slow neutrons, for example in the papers of Akhiezer and Pomeranchuk, [13] Wick, [14] Zemach and Glauber. [15]

Whereas for potential scattering such an averaging leads to a correlation function for positions of particles of the scattering system at two different times, for pure resonance scattering the averaging gives a time integral of the correlation function for particle positions at four different times, while in the case of interference of potential and resonance scattering we get integrals of the correlation function for particle positions at three different times.*

In the present paper we shall give the derivation and discussion of the general formulas for the probability of resonance and interference scattering. In later papers we shall consider special cases of resonance scattering for various simple models of the scattering materials.

2. In second-order perturbation theory, including damping,† the transition probability per unit time from the initial state i to the final state f is

$$W_i^f = 2\pi \left| \sum_\lambda \frac{\langle f | H_{int} | \lambda \rangle \langle \lambda | H_{int} | i \rangle}{E_i - E_\lambda + i\Gamma_\lambda (E_i)/2} \right|^2 \delta (E_f - E_i),$$

where the index λ denotes the intermediate (resonant) states (with width $\Gamma_\lambda(E)$). In our case the initial and final wave functions are products of the wave functions‡ of the incident, $|\mu_s^{(i)}, \mathbf{p}_i\rangle$, or scattered, $|\mu_s^{(f)}, \mathbf{p}_f\rangle$, particles with spin s (where $\mathbf{p}_i$ and $\mathbf{p}_f$ are the momenta and $\mu_s^{(i)}$ and $\mu_s^{(f)}$ are quantum numbers which determine the spin state of the particle or the polarization of the γ quantum, respectively, in states i and f) with the wave function for the scattering system in states i and f, respectively. The latter can be written as a product of "internal" wave functions $|\nu, \mu_j^{(i,f)}\rangle$, corresponding to the ground states of the resonantly scattering isotopes (where $\mu_j^{(i)}$ and $\mu_j^{(f)}$ are the projections of the spin (j) of the ν-th nucleus in states i and f, respectively), multiplied by the wave function $|m_{i,f}\rangle$ for the motion of the centers of mass $\mathbf{R}_\nu$ of the atoms of the scattering system, which is characterized by a set of quantum numbers which we shall, for simplicity, denote by one symbol $m_{i,f}$.

The intermediate states are states where one of the nuclei (ν_λ) is excited (for the case of absorption of γ quanta) or a compound nucleus is formed (for the case of neutron capture). We shall refer to both of these as excited states.

For simplicity we shall assume that the excitation does not change the part of the Hamiltonian which determines the motion of the centers of mass of the atoms of the scattering system.* Then the wave functions for the intermediate state can be written as

$$|m_\lambda\rangle |\nu_\lambda, M_J^{(\lambda)}\rangle \prod_{\nu \neq \nu_\lambda} |\nu, \mu_j^{(\lambda)}\rangle,$$

where $|\nu_\lambda, M_J^{(\lambda)}\rangle$ is the wave function of the ν-th excited nucleus with projection $M_J^{(\lambda)}$ of its spin J. In addition we assume that the energy and width of the excited state do not depend on the label of the excited nucleus or on its spin projection, and that the width is also independent of the state of motion of the centers of mass of the atoms of the scattering system [$\Gamma_\lambda(E) = \text{const} = \Gamma$]. Then the total probability for resonance scattering of a particle with momentum $\mathbf{p}_i$ into unit interval of momentum around $\mathbf{p}_f$, averaged over the initial states of the system (on the assumption that the nuclear spins are statistically independent) and over the spin projections for the incident particles, will be

$$W(\mathbf{p}_i, \mathbf{p}_f) = 2\pi A \sum_\nu w_{\nu\nu}(\mathbf{p}_i, \mathbf{p}_f) + 2\pi B \sum_{\nu \neq \nu'} w_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f), \quad (1)$$

$$w_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f) = \sum_{m_i} \sum_{m_f} g_{m_i} \sum_{m_\lambda} \sum_{m'_\lambda} (E_i - E_0 - E_{m_\lambda} + \tfrac{1}{2} i\Gamma)^{-1}$$
$$\times (E_i - E_0 - E_{m'_\lambda} - \tfrac{1}{2} i\Gamma)^{-1} \langle m_f | \exp(-i\mathbf{p}_f \mathbf{R}_\nu) | m_\lambda \rangle$$
$$\times \langle m_\lambda | \exp(i\mathbf{p}_i \mathbf{R}_\nu) | m_i \rangle \langle m_f | \exp(-i\mathbf{p}_f \mathbf{R}_{\nu'}) | m'_\lambda \rangle^*$$
$$\times \langle m'_\lambda | \exp(i\mathbf{p}_i \mathbf{R}_{\nu'}) | m_i \rangle^* \delta (E_i - E_f), \quad (2)$$

$$A = \Big(\sum_{\mu_j^{(f)}} \sum_{\mu_s^{(f)}} \Big| \sum_{M_J} \langle \mu_s^{(f)}, \mathbf{p}_f; \mu_j^{(f)}, \nu | H_\nu | \nu, M_J \rangle$$
$$\times \langle M_J, \nu | H_\nu | \nu, \mu_j^{(i)}; \mu_s^{(i)}, \mathbf{p}_i \rangle \Big|^2 \Big)_{av}, \quad (3)$$

$$B = \Big(\sum_{\mu_s^{(f)}} \Big[\sum_{M_J} \langle \mu_s^{(f)}, \mathbf{p}_f; \mu_j^{(i)}, \nu | H_\nu | \nu, M_J \rangle$$
$$\times \langle M_J, \nu | H_\nu | \nu, \mu_j^{(i)}; \mu_s^{(i)}, \mathbf{p}_i \rangle \Big]$$
$$\times \Big[\sum_{M'_J} \langle \mu_s^{(f)}, \mathbf{p}_f; \mu_j^{(i)\prime}, \nu' | H_{\nu'} | \nu', M'_J \rangle$$
$$\times \langle M'_J, \nu' | H_{\nu'} | \nu', \mu_j^{(i)\prime}; \mu_s^{(i)}, \mathbf{p}'_i \rangle \Big]^* \Big)_{av}, \quad (4)$$

*The reason for this is that the resonance scattering amplitude depends on the difference between the times of absorption and emission of particles, which is zero for the case of potential scattering.

†For example, see[16]. From now on we use the system of units with T = 1, k = 1 (where k is the Boltzmann constant).

‡The wave function of the scattering system with momentum p (energy E_p) is written in the form $|\mathbf{p}\rangle = (2\pi)^{-3/2} e^{i\mathbf{p}\cdot\mathbf{r}}$. Then we get the scattering cross section by multiplying the probability by the factor $(2\pi)^3/(dE_{p_i}/dp_i)$.

*For the case of neutrons this approximation is valid if the masses of the nuclei of the scattering system are large compared to the neutron mass.[17] For γ quanta it is always correct, except for those cases where delicate relativistic effects become important, like those discovered by Pound and Rebka[18] in measuring the red shift on the Earth's surface.

where g_{m_i} is the probability that the scattering system is initially in state m_i:

$$g_{m_i} = \left(\sum_m \exp\left[-E_m/T\right]\right)^{-1} \exp\left[-E_{m_i}/T\right] \quad (5)$$

(T is the temperature of the system); H_ν is the part of the Hamiltonian for the interaction of the ν-th nucleus with the scattered particle which depends on the internal coordinates of the nucleus and on the spin variables; E_0 is the energy of the resonance level of the nucleus and E_{m_λ} is the energy of the motion of the centers of mass of the atoms of the scattering system in the state m_λ. The subscript "av" denotes an average over initial states.

3. The quantities A and B depend only on the parameters for the interaction of the scattered particle with a single free nucleus, and can be expressed in terms of the characteristics of the resonance level. The corresponding expressions are calculated in the Appendix.

The main purpose of this paper is to investigate the quantity $w_{\nu\nu'}(\mathbf{p_i}, \mathbf{p_f})$ for arbitrary systems. Following Zemach and Glauber [15] and Van Hove, [1] we go over to a time-dependent representation of this function. To do this we use formula (5) and

$$\delta(E_i - E_f) = (2\pi)^{-1} \int_{-\infty}^{\infty} d\mu \exp\{i\left[E_{p_i} + E_{m_i} - E_{p_f} - E_{m_f}\right]\mu\}, \quad (6)$$

$$(E_{p_i} + E_{m_i} - E_0 - E_{m_\lambda} + \tfrac{1}{2} i\Gamma)^{-1} = -i\int_0^\infty dt \exp\{it\left[E_{p_i} + E_{m_i} - E_0 - E_{m_\lambda} + \tfrac{1}{2} i\Gamma\right]\}, \quad (7)$$

where E_{p_i} and E_{p_f} are the energies of the incident and scattered particles. We then get

$$\begin{aligned} w_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f) &= (2\pi)^{-1} \int_{-\infty}^{\infty} d\mu \int_0^\infty dt \int_0^\infty dt' Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, t') \\ &\times \exp\{i\mu(E_{p_i} - E_{p_f}) + it(E_{p_i} - E_0 + \tfrac{1}{2} i\Gamma) \\ &- it'(E_{p_i} - E_0 - \tfrac{1}{2} i\Gamma)\}, \end{aligned} \quad (8)$$

$$\begin{aligned} Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, t') &= \left\{\sum_m \langle m|\exp(-H/T)|m\rangle\right\}^{-1} \\ &\times \sum_{m_i}\sum_{m_\lambda}\sum_{m'_\lambda}\sum_{m_f} \langle m_i|\exp\left[-H/T + iH(\mu + t - t')\right] \\ &\times \exp(-i\mathbf{p}_i\mathbf{R}_\nu)|m'_\lambda\rangle\langle m'_\lambda|\exp(iHt')\exp(i\mathbf{p}_f\mathbf{R}_{\nu'})|m_f\rangle \\ &\times \langle m_f|\exp(-i\mu H)\exp(-i\mathbf{p}_f\mathbf{R}_\nu)|m_\lambda\rangle \\ &\times \langle m_\lambda|\exp(-iHt)\exp(i\mathbf{p}_i\mathbf{R}_\nu)|m_i\rangle. \end{aligned} \quad (9)$$

Carrying out the summation in (9) over all the quantum numbers and going over to the Heisenberg representation (introducing the notation $\hat{a}(t) = e^{iHt}\hat{a}e^{-iHt}$, where $\hat{a}$ is the Schrödinger operator), we finally get

$$Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, t') = \{\mathrm{Sp}\, e^{-H/T}\}^{-1} \mathrm{Sp}\left[e^{-H/T}\hat{Z}_{\nu\nu'}\right]; \quad (10)$$

$$\begin{aligned} \hat{Z}_{\nu\nu'} &= \exp\{-i\mathbf{p}_i\hat{\mathbf{R}}_{\nu'}(\mu + t - t')\}\exp\{i\mathbf{p}_f\hat{\mathbf{R}}_{\nu'}(\mu + t)\} \\ &\times \exp\{-i\mathbf{p}_f\hat{\mathbf{R}}_\nu(t)\}\exp\{i\mathbf{p}_i\hat{\mathbf{R}}_\nu(0)\}. \end{aligned} \quad (11)$$

We note that (10) is equivalent to the assertion that $Z_{\nu\nu'}$ is the (quantum mechanical and statistical) average of the operator $\hat{Z}_{\nu\nu'}$.

4. In order to understand the physical meaning of the function $Z_{\nu\nu'}$, we consider its Fourier component with respect to the initial and final momenta:

$$\begin{aligned} &\Gamma_{\nu\nu'}(\mathbf{R}_1, \mathbf{R}_2, \mu, t, t') \\ &= (2\pi)^{-6}\int d\mathbf{p}_i\, d\mathbf{p}_f\, Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, t')\, e^{i\mathbf{R}_1\mathbf{p}_i - i\mathbf{R}_2\mathbf{p}_f}, \end{aligned} \quad (12)$$

$$Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, t') = \int d\mathbf{R}_1 d\mathbf{R}_2 \Gamma_{\nu\nu'}(\mathbf{R}_1, \mathbf{R}_2, \mu, t, t')\, e^{i\mathbf{R}_2\mathbf{p}_f - i\mathbf{R}_1\mathbf{p}_i}. \quad (13)$$

Substituting (10) and (11) in (12), we find

$$\begin{aligned} \Gamma_{\nu\nu'}(\mathbf{R}_1, \mathbf{R}_2, \mu, t, t') &= (2\pi)^{-12}\int d\mathbf{p}_i\, d\mathbf{p}_f\, d\mathbf{p}'_i\, d\mathbf{p}'_f\, d\mathbf{R}'_1\, d\mathbf{R}'_2 \\ &\times \exp\left[i\mathbf{R}_1\mathbf{p}_i - i\mathbf{R}_2\mathbf{p}_f + i(\mathbf{p}_i - \mathbf{p}'_i)\mathbf{R}'_1 + i(\mathbf{p}_f - \mathbf{p}'_f)\mathbf{R}'_2\right] \\ &\times \left(\exp(-i\mathbf{p}_i\hat{\mathbf{R}}_{\nu'}(\mu + t - t'))\exp(i\mathbf{p}_f\hat{\mathbf{R}}_{\nu'}(\mu + t))\right. \\ &\times \left.\exp(-i\mathbf{p}'_f\hat{\mathbf{R}}_\nu(t))\exp(i\mathbf{p}'_i\hat{\mathbf{R}}_\nu(0))\right)_{\mathrm{av}} \\ &= \int d\mathbf{R}'_1\, d\mathbf{R}'_2 \left(\delta\left[\mathbf{R}'_1 + \mathbf{R}_1 - \hat{\mathbf{R}}_{\nu'}(\mu + t - t')\right]\right. \\ &\times \left.\delta\left[\mathbf{R}'_2 + \mathbf{R}_2 - \hat{\mathbf{R}}_{\nu'}(\mu + t)\right]\delta\left[\hat{\mathbf{R}}_\nu(t) - \mathbf{R}'_2\right]\right. \\ &\times \left.\delta\left[\hat{\mathbf{R}}_\nu(0) - \mathbf{R}'_1\right]\right)_{\mathrm{av}}. \end{aligned} \quad (14)$$

Thus the function $\Gamma_{\nu\nu'}$ determines the correlation of the positions of the ν-th and ν'-th particles at four different times, in the same way as Van Hove's function determines the pair correlations.

We can get another picture of the physical meaning of the functions $Z_{\nu\nu'}$ and $\Gamma_{\nu\nu'}$ by considering their classical limits. To do this, as in the case of potential scattering, [1] we disregard the noncommutativity of the Heisenberg operators at different times. Then

$$\begin{aligned} \Gamma_{\nu\nu'}(\mathbf{R}_1, \mathbf{R}_2, \mu, t, t') &= \left(\delta\left[\mathbf{R}_1 + \mathbf{R}_\nu(0) - \mathbf{R}_{\nu'}(\mu + t - t')\right]\right. \\ &\times \left.\delta\left[\mathbf{R}_2 + \mathbf{R}_\nu(t) - \mathbf{R}_{\nu'}(\mu + t)\right]\right)_{\mathrm{av}}. \end{aligned} \quad (15)$$

We use the symbol $D(\mathbf{R}_\nu, \mathbf{R}'_\nu, \mathbf{R}_{\nu'} - \mathbf{R}_\nu, \mathbf{R}'_{\nu'} - \mathbf{R}'_\nu, \mu, t, t')$ for the probability that initially ($\tau = 0$) the ν-th particle was in unit volume around the point $\mathbf{R}_\nu$, while at $\tau = t$ it was in unit volume around $\mathbf{R}'_\nu$, while the ν'-th particle was in unit volume around $\mathbf{R}_{\nu'}$ at the time $\tau = \mu + t - t'$, and in unit volume around $\mathbf{R}'_{\nu'}$ at time $\tau = \mu + t$. This definition still holds if the ν-th and ν'-th particles coincide. Then we can write (15) in the form

$$\Gamma_{\nu\nu'}(\mathbf{R}_1, \mathbf{R}_2, \mu, t, t') = \int d\mathbf{R}_\nu\, d\mathbf{R}'_\nu\, D(\mathbf{R}_\nu, \mathbf{R}'_\nu, \mathbf{R}_1, \mathbf{R}_2, \mu, t, t'). \quad (16)$$

Thus in the classical limit the function $\Gamma_{\nu\nu'}(\mathbf{R}_1, \mathbf{R}_2, \mu, t, t')$ can be interpreted as the probability that, at time $\tau = \mu + t - t'$, the ν'-th particle was in unit volume at distance $\mathbf{R}_1$ from the position of the ν-th particle at the initial time, and that at time $\tau = \mu + t$ it was in unit volume at distance $\mathbf{R}_2$ from the position of the ν-th particle at time $\tau = t$.

Just as for Van Hove's function, in the general quantum mechanical case, the interpretation of the functions $\Gamma_{\nu\nu'}$ is more complicated.[1] These functions can no longer be interpreted as probabilities and in the general case are complex quantities. Various authors[3,4,6] have shown that replacing Van Hove's function by its classical analog leads to a violation of the principle of detailed balancing for the potential scattering cross section. Something similar also occurs for the functions $\Gamma_{\nu\nu'}$. But because of the great complexity of the functions $Z_{\nu\nu'}$ themselves, as well as the fact that the resonance scattering cross section depends on them (the cross section is proportional to the integral of $Z_{\nu\nu'}$ over μ, t, and t'), the requirements which the function $Z_{\nu\nu'}$ must satisfy in order to satisfy the principle of detailed balancing become complicated.

The following are important special cases of the functions $Z_{\nu\nu'}$.

a) The limit of $Z_{\nu\nu'}$ for $\mu \to \infty$ corresponds to elastic scattering. Then $Z_{\nu\nu'}$ can be written in the form

$$Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \infty, t, t') = \{\mathrm{Sp}\, e^{-H/T}\}^{-1} \times \sum_{m_i} \langle m_i | e^{-H/T} \exp[-i\mathbf{p}_i \hat{\mathbf{R}}_{\nu'}(0)] \exp[i\mathbf{p}_f \hat{\mathbf{R}}_{\nu'}(t')] | m_i \rangle \times \langle m_i | \exp[-i\mathbf{p}_f \hat{\mathbf{R}}_\nu(t)] \exp[i\mathbf{p}_i \hat{\mathbf{R}}_\nu(0)] | m_i \rangle. \quad (17)$$

In the most interesting case of crystals, the corresponding expression was found and discussed earlier.[10]

b) For $t = t' = 0$,

$$Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, 0, 0) = (\exp[i(\mathbf{p}_f - \mathbf{p}_i)\hat{\mathbf{R}}_{\nu'}(\mu)] \exp[i(\mathbf{p}_i - \mathbf{p}_f)\hat{\mathbf{R}}_\nu(0)])_{\mathrm{av}}. \quad (18)$$

This expression is easy to understand if we consider that we can set $t = t' = 0$ in $Z_{\nu\nu'}$ in Eq. (8) if the level width Γ is large ($\Gamma \to \infty$). Then the scattering loses its resonant character and becomes essentially potential scattering. We can therefore describe it by means of the Born approximation, in the framework of which Van Hove's formalism was developed.[1] It is easily verified that, if we let Γ in (8) tend to infinity and substitute (18) for $Z_{\nu\nu'}$, we get Van Hove's results.

c) If $t' = 0$ (or $t = 0$),

$$Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, 0) = \{\mathrm{Sp}\, e^{-H/T}\}^{-1} \times \mathrm{Sp}\{e^{-H/T} \exp[i(\mathbf{p}_f - \mathbf{p}_i)\hat{\mathbf{R}}_{\nu'}(\mu + t)] \times \exp[-i\mathbf{p}_f \hat{\mathbf{R}}_\nu(t)] \exp[i\mathbf{p}_i \hat{\mathbf{R}}_\nu(0)]\}, \quad (19)$$

i.e., $Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, 0)$ determines the correlations between positions of atoms of the scattering system at three different times.

As we shall see later (cf. Sec. 5), expression (19) corresponds to the contribution to the cross section from interference between potential and resonance scattering.

d) The case of $\mu = 0$.

$$Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, 0, t, t') = \{\mathrm{Sp}\, e^{-H/T}\}^{-1}\ \mathrm{Sp}\{e^{-H/T} \exp[-i\mathbf{p}_i \hat{\mathbf{R}}_{\nu'}(-t')] \times \exp[i\mathbf{p}_f(\hat{\mathbf{R}}_{\nu'}(0) - \hat{\mathbf{R}}_\nu(0))] \exp[i\mathbf{p}_i \hat{\mathbf{R}}_\nu(-t)]\}. \quad (20)$$

In particular, if $\nu = \nu'$,

$$Z_{\nu\nu}(\mathbf{p}_i, \mathbf{p}_f, 0, t, t') = \{\mathrm{Sp}\, e^{-H/T}\}^{-1} \mathrm{Sp}\{e^{-H/T} e^{-i\mathbf{p}_i \hat{\mathbf{R}}_\nu(t - t')} e^{i\mathbf{p}_i \hat{\mathbf{R}}_\nu(0)}\}. \quad (21)$$

We note that this expression is identical with the Fourier component of the Van Hove function for a single particle (if we replace $\mathbf{p}_i - \mathbf{p}_f$ by $\mathbf{p}_i$).

This case is important for the computation of the total probability (integrated over energy) for resonance scattering of γ quanta.

e) If the width Γ of the resonance level is small compared to the energy of the motion of the atoms of the scattering system, the scattering probability, according to (8), is given by the function $Z_{\nu\nu'}$ for $t \to \infty$, $t' \to \infty$:

$$Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, \infty, \infty) = \{\mathrm{Sp}\, e^{-H/T}\}^{-1} \times \sum_{m_i} \langle m_i | \exp(i\mathbf{p}_i \hat{\mathbf{R}}_\nu(0)) | m_i \rangle \langle m_i | \exp(-i\mathbf{p}_i \hat{\mathbf{R}}_{\nu'}(0)) | m_i \rangle \times \langle m_i | e^{-H/T} \exp(i\mathbf{p}_f \hat{\mathbf{R}}_{\nu'}(\mu)) \exp(-i\mathbf{p}_f \hat{\mathbf{R}}_\nu(0)) | m_i \rangle. \quad (22)$$

5. In the preceding computation, we neglected the interference between resonance and potential scattering. As is easily verified, including it results in adding to the probability for resonance scattering, $W(\mathbf{p}_i, \mathbf{p}_f)$, a term of the form

$$W_{int}(\mathbf{p}_i, \mathbf{p}_f) = 4\pi\, \mathrm{Re}\left\{A' \sum_\nu v_{\nu\nu}(\mathbf{p}_i, \mathbf{p}_f) + B' \sum_{\nu \neq \nu'} v_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f)\right\},$$

$$v_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f) = \sum_{m_i} \sum_{m_f} g_{m_i} \sum_{m_\lambda} \delta(E_i - E_f)(E_i - E_0 - E_{m_\lambda} + \tfrac{1}{2} i\Gamma)^{-1} \times \langle m_f | \exp(-i\mathbf{p}_f \mathbf{R}_\nu) | m_\lambda \rangle \langle m_\lambda | \exp(i\mathbf{p}_i \mathbf{R}_\nu) | m_i \rangle \langle m_f | \times \exp(i(\mathbf{p}_i - \mathbf{p}_f)\mathbf{R}_{\nu'}) | m_i \rangle^*. \quad (23)$$

The real constants A′ and B′ can be calculated in exactly the same way as the previously introduced A and B.

In precisely this same way we can represent the function $v_{\nu\nu'}(\mathbf{p_i}, \mathbf{p_f})$ as

$$v_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f) = -i(2\pi)^{-1}\int_{-\infty}^{\infty} d\mu \int_0^{\infty} dt Z_{\nu\nu'}(\mathbf{p}_i, \mathbf{p}_f, \mu, t, 0) \times \exp\{i\mu(E_{p_i} - E_{p_f}) + it(E_{p_i} - E_0 + \tfrac{1}{2}i\Gamma)\}, \quad (24)$$

where $Z_{\nu\nu'}(\mathbf{p_i}, \mathbf{p_f}, \mu, t, 0)$ is defined by formula (19).

6. From experimental cross section data, by varying the concentration of the isotope which gives the resonant scattering, one can determine separately $\bar{w}_{\nu\nu}$ and $\bar{w}_{\nu\nu'}$ (for $\nu \neq \nu'$).* But the fact that the probability for resonance scattering is proportional to an integral of $\bar{Z}_{\nu\nu'}$ has the consequence that, in contrast to the case for potential scattering, it is impossible to construct the function $\bar{Z}_{\nu\nu'}$ from the cross section for resonance scattering. As we see from (8), to determine it we must know $\bar{w}_{\nu\nu'}$ for different values of E_0 and Γ, i.e., we must measure the scattering cross section for a large number of media containing different amounts of the resonant scattering isotope, which is clearly unrealistic. The situation is somewhat better for the case of interference scattering, which is determined by simpler integral expressions [cf. Eq. (24)]. It is, however, hardly possible to separate the interference scattering from resonance scattering in an experiment. Thus there remains the less satisfactory procedure of computing $\bar{Z}_{\nu\nu'}$ on some model of the substance and comparing the theoretical cross sections with experiment. But since the study of the correlations of positions of particles at three and four different times may throw additional light on the dynamics of atomic motions in complex systems, even such a procedure seems useful, since at present one cannot think of any more direct method for studying such correlations.

In a succeeding paper we shall carry out this program for some of the simplest models of the motion of atoms in a scattering medium.

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APPENDIX

Let us express the constants A and B, which are defined by (3) and (4), in terms of the parameters for the interaction of the scattered particle with an isolated nucleus.

We first consider the case of a nonrelativistic particle. We write the wave function for the system consisting of the particle and the ν-th nucleus of the scatterer in its ground state (for simplicity we drop the index ν)

$$|\mu_j; \mathbf{p}, \mu_s\rangle = \sum_{lm_l}\sum_{SM_S}\sum_{JM_J} i^l Y^*_{lm_l}(\mathbf{p})\,(js\mu_j\mu_s|SM_S) \times (SlM_Sm_l|JM_J)|SlJM_J\rangle$$

and denote the matrix element for the transition from the state $|SlJM_J\rangle$, where $\mathbf{S} = \mathbf{s} + \mathbf{j}$, $\mathbf{J} = \mathbf{S} + \mathbf{l}$ (where $\mathbf{l}$ is the orbital angular momentum operator for the incident particle and $\mathbf{S}$ is the channel spin operator) into the state $|JM'_J\rangle$ —the excited state of the nucleus,* by

$$\langle JM'_J|H|SlJM_J\rangle = \delta_{M'_JM_J}C_{Sl}i^{-l}.$$

Then we find that the matrix element in formulas (3) and (4) is

$$\langle M_J|H|\mu_j;\mu_s,\mathbf{p}\rangle = \sum_{lm_l}\sum_{SM_S} Y^*_{lm_l}(\mathbf{p})\,(js\mu_j\mu_s|SM_S)\,(SlM_Sm_l|JM_J)C_{Sl}.$$

By using standard methods,† after computations which are tedious but not difficult, we finally get

$$A = \frac{1}{(2\pi)^2(2s+1)(2j+1)}\sum_{SS'}\sum_{ll'l''l'''} i^{l'+l''-l-l'''} \times C_{Sl}C^*_{S'l'}C^*_{Sl''}C_{S'l'''}K(Jl'l;\ Jl'''l'';\ S'S,\ \theta), \quad (A.1)$$

$$K(Jl'l;\ J'l'''l'';\ S'S,\ \theta) = \tfrac{1}{4}\sum_L P_L(\cos\theta) \times (-1)^{S'-S}Z(lJl''J';\ SL)\,Z(l'Jl'''J';\ S'L), \quad (A.2)$$

$$Z(abcd;\ ef) = i^{f-a+c}[(2a+1)(2b+1)(2c+1)(2d+1)]^{1/2} \times W(abcd;\ ef)\,(ac00|f0),$$

where W(abcd;ef) is a Racah coefficient, and $\cos\theta = \mathbf{p_i}\cdot\mathbf{p_f}/p_ip_f$.

In the case of slow neutrons, $l = l' = l'' = l''' = 0$, $S' = S = J$ and formulas (A.1) and (A.2) simplify:

$$A = \frac{(2J+1)}{32\pi^2(2j+1)}|C|^4. \quad (A.3)$$

In the case of scattering of γ quanta, we know[19] that further discussion is required.

1) In this case it is convenient to express the

*A bar over a symbol means an average over the distribution of atoms of the resonantly scattering isotope.

*It is easy to verify that

$$\sum_{Sl}|C_{Sl}|^2 = (dE_p/dp)\,[\Gamma(E_p)/2\pi p^2],$$

where $\Gamma(E_p)$ is the width for emission of a particle with energy E_p.

†For example, cf.[19,20].

constant A in terms of the amplitudes C_{gp} for transition from states (or into states) with definite total angular momentum $\mathbf{g} = \mathbf{l} + \mathbf{s}$ (s = 1) and definite parity p of the photon. These amplitudes are related to the amplitudes C_{Sl} introduced earlier by the formulas

$$C_{gp} = \sum_{Sl} C_{Sl} \langle S | g \rangle \langle l | p \rangle, \qquad C_{Sl} = \sum_{gp} C_{gp} \langle g | S \rangle \langle p | l \rangle,$$
$$\langle S | g \rangle = \langle g | S \rangle = [(2g+1)(2S+1)]^{1/2} W(lsJj; gS),$$
$$\langle l | p \rangle = \langle p | l \rangle = \sqrt{2}(-1)^{p+1} (g1 - 11 | l0) \delta(l, p), \tag{A.4}$$

$$\delta(l, p) = \begin{cases} 1 \text{ for } l = g \\ 0 \text{ for } l \neq g \end{cases} \text{ for } p = 0 \text{ (magnetic radiation)},$$
$$\delta(l, p) = \begin{cases} 0 \text{ for } l = g \\ 1 \text{ for } l \neq g \end{cases} \text{ for } p = 1 \text{ (electric radiation)}.$$

2) In averaging over the initial states of the system it should be remembered that a photon with a given g has only two states.

We finally get for the case of scattering of photons

$$A = \frac{1}{32\pi^2(2j+1)} \sum_{gg'g''g'''} \sum_{pp'p''p'''} C_{gp} C^*_{g'p'} C^*_{g''p''} C_{g'''p'''} \times \sum_L P_L(\cos\theta) Z_\gamma(gJg''J; jL) Z_\gamma(g'Jg'''J; jL), \tag{A.5}$$

$$Z_\gamma(abcd; ef) = [(2a+1)(2b+1)(2c+1)(2d+1)]^{1/2} \times (ac - 11 | f0) W(abcd; ef).$$

[Only terms for which L + p + g + p″ + g″ is even should be included in the sum in (A.5).]

The constant B is conveniently calculated in a representation in which the total and orbital angular momenta of the scattered particle are sharp, i.e., we express it in terms of the quantities

$$C_{gl} = \sum_S C_{Sl} \langle S | g \rangle.$$

Then, as is easily verified,

$$B = \frac{1}{4\pi^2(2s+1)(2j+1)^2} \sum_{ll'l''l'''} \sum_{gg'} C^*_{l'g} C_{lg} C^*_{l''g'} C_{l'''g'} \times i^{l'+l''-l-l'''} \frac{(2J+1)^2}{(2g+1)(2g'+1)} K(gl'l; g'l'''l''; ss\theta). \tag{A.6}$$

In the case of resonance scattering of slow neutrons

$$B = \tfrac{1}{64}\pi^{-2}(2J+1)^2 (2j+1)^{-2} |C|^4, \tag{A.7}$$

i.e., B = (2J + 1)A/2(2j + 1).

In the case of photon scattering, remembering the remarks made in the calculation of A and the identity [21]

$$\sum_{l_1 l_2} (L_1 1 - 11 | l_1 0)(L_2 1 - 11 | l_2 0) \delta(l_1, p_1) \delta(l_2, p_2) \times (2l_1+1)^{1/2} (2l_2+1)^{1/2} (l_1 l_2 00 | L0) W(l_1 L_1 l_2 L_2; 1L) = \tfrac{1}{2}(-1)^{L-L_1+L_2} (L_1 L_2 1 - 1 | L0),$$

we get

$$B = \frac{1}{32\pi^2} \frac{(2J+1)^2}{(2j+1)^2} \sum_{gg'} \sum_{pp'p''p'''} C_{gp} C^*_{gp'} C^*_{g'p''} C_{g'p'''} \times \sum_L P_L(\cos\theta)(gg'1 - 1 | L0)^2. \tag{A.8}$$

[Only terms for which L + p + g + p″ + g′ is even should be included in the sum in (A.8).] If we assume for simplicity that photons of a definite multipolarity are being scattered, we easily find from (A.5) and (A.8) a relation connecting the constants A and B:

$$B = A \frac{(2J+1)^2}{2j+1} \frac{\sum_L P_L(\cos\theta)(gg1 - 1 | L0)^2}{\sum_L P_L(\cos\theta) Z^2_\gamma(gJgJ; jL)}. \tag{A.9}$$

We note that if the scattering nuclei are spinless, then A = B, as expected.

Note in proof (January 17, 1962). Recently Dzyub and Lubchenko[22] have treated the special case of resonance scattering of γ quanta in crystals by a method analogous to that developed in the present paper.

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