

t Matrix and Phase Shifts in Solid-State Scattering Theory*

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We are concerned with the scattering of an excitation in a solid by a potential of finite range. The appropriate scattering theory is formulated using the t matrix. A general expression for t -matrix elements is obtained involving only finite sums. Phase shifts are introduced and are related to the change in density of states produced by the scattering. The phase shifts satisfy a form of Levinson's theorem. The relation between the phase shifts and the t matrix is examined with the aid of the optical theorem, and it is shown that in the case of the scattering of long-wavelength excitations in a spherical band (subject to certain limitations described in the text), the usual relation between the phase shifts and the scattering amplitude can be recovered. As an application, the change in the density of states and the excitation lifetime are obtained for spin waves in a Heisenberg ferromagnet with a small concentration of magnetic defects.

I. INTRODUCTION

IN a previous publication, an expression for the amplitude for scattering of an excitation in a solid by a potential of finite range was presented.¹ Similar results have also been obtained by Mann.^{2,3} Physically the situation considered is the scattering of an electron, phonon, or spin wave by a single point defect which does not possess any internal degrees of freedom. This is the analog of potential scattering in ordinary quantum mechanics.

Solid-state scattering theory is relevant to several interesting problems. It is obviously of central importance in transport theory.^{3,4} In addition, it furnishes a convenient method of studying bound-state problems involving localized defects.⁵ Virtual states, or scattering resonances, within a band may also be included.⁶ The properties of dilute alloys can be investigated. Moreover, through multiple scattering theory at low temperatures,⁷ and the virial expansion at high temperatures,⁸ it furnishes a practical method of attack on many-body problems in those cases in which a low-density system of particles is of interest.

In I, solid-state scattering theory was described in a form most directly applicable to electrons, leading to a construction of the scattering amplitude. Phase shifts were not introduced (except in a very simple example), and the relation of the theory to the scattering theory of ordinary quantum mechanics was not altogether clear. In the present work, the scattering theory will be formulated more generally and abstractly. This is most conveniently accomplished through the introduction of the t matrix. In Sec. II, general expressions for t -matrix elements are derived, whose evaluation involves

only finite matrices. In Sec. III, scattering phase shifts are introduced. A simple formula relates these phase shifts to the change in density of states produced by the scattering. The phase shifts are shown to satisfy a form of Levinson's theorem. Then we examine the question: Under what circumstances does the relation between the scattering amplitude and the phase shift obtained in elementary quantum mechanics apply in solids? It is found that subject to certain restrictions to be described later, that it will hold for the scattering of long-wavelength excitations in a spherical band. In Sec. IV, the use of phase shifts is illustrated by application to the determination of the change in density of states and the spin-wave lifetime for a simple Heisenberg ferromagnet containing a small concentration of magnetic defects.

We will begin by considering the determination of the t matrix in a general way.⁹ Let us separate the Hamiltonian for the excitations of interest in the presence of the defect into two parts: a part H_0 which describes a supposed perfect crystal in which the defect has been replaced by a normal atom, and a scattering potential V which represents the difference between the real and the perfect crystal:

$$H = H_0 + V. \quad (1)$$

The perfect crystal Hamiltonian H_0 has a set of eigenvectors, representing wave-like states, which are characterized by a wave vector \mathbf{k} and a band or polarization index α , and which we denote by $|\alpha\mathbf{k}\rangle$.

$$H_0 |\alpha\mathbf{k}\rangle = E_\alpha(\mathbf{k}) |\alpha\mathbf{k}\rangle. \quad (2)$$

The band function $E_\alpha(\mathbf{k})$ describes the energy spectrum of the excitations. These states are orthonormal

$$\langle \alpha\mathbf{k} | \beta\mathbf{q} \rangle = \delta_{\alpha\beta} \delta(\mathbf{k} - \mathbf{q}). \quad (3)$$

The scattering process is described by the elements of the t matrix on the basis of the states $|\alpha\mathbf{k}\rangle$. From formal scattering theory,¹⁰ we know that the probability per

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¹ J. Callaway, *J. Math. Phys.* **5**, 783 (1964). This paper will be referred to as I.

² E. Mann, *Phys. Stat. Sol.* **11**, 753, 767 (1965); **13**, 293 (1966).

³ E. Mann, A. Seeger, and G. Thierer, *Z. Physik* **193**, 295 (1966).

⁴ J. M. Luttinger and W. Kohn, *Phys. Rev.* **109**, 1892 (1958).

⁵ G. F. Koster and J. C. Slater, *Phys. Rev.* **96**, 1208 (1959).

⁶ T. Wolfram and J. Callaway, *Phys. Rev.* **130**, 2207 (1963).

⁷ J. Callaway, *Phys. Rev.* **140**, A618 (1965).

⁸ J. Callaway and D. M. Edwards, *Phys. Rev.* **136**, A1333 (1964).

⁹ J. Callaway, in *Lectures in Theoretical Physics* (University of Colorado Press, Boulder, Colorado, 1966), Vol. VIII-A, p. 295.

¹⁰ M. Gell-Mann and M. L. Goldberger, *Phys. Rev.* **91**, 398 (1963).

unit time for a transition in which an excitation in the state $|\beta\mathbf{q}\rangle$ goes to the state $|\alpha\mathbf{k}\rangle$ is given by $W(\beta\mathbf{q}\rightarrow\alpha\mathbf{k})$:

$$W(\beta\mathbf{q}\rightarrow\alpha\mathbf{k})=2\pi\bar{N}^2|\langle\alpha\mathbf{k}|t|\beta\mathbf{q}\rangle|^2G(E_\alpha) \quad (4)$$

in which \bar{N} is a normalization constant [$\bar{N}=8\pi^3$ for states normalized according to Eq. (3), and we will use throughout this paper units in which $\hbar=1$], G is the density of final states, and $\langle\alpha\mathbf{k}|t|\beta\mathbf{q}\rangle$ is the relevant t -matrix element.

The t matrix satisfies the equation

$$t=V+V\mathcal{G}t, \quad (5)$$

in which \mathcal{G} is the operator,

$$\mathcal{G}=1/(E^+-H_0) \quad (6)$$

and is referred to as the Green's function. The superscript (+) on the energy parameter E in Eq. (6) indicates that if E is within the continuous spectrum of H_0 , the Green's function is to be defined by allowing the energy to have an infinitesimal positive imaginary part. This device corresponds to the selection of outgoing wave boundary conditions.¹¹ Equation (5) has the formal solution

$$t=V[1/(1-\mathcal{G}V)]. \quad (7)$$

However, the utility of this result depends on whether the inverse operator can be constructed. We will be concerned with certain potentials V for which this is possible.

In addition to the eigenstates $|\alpha\mathbf{k}\rangle$, it is convenient to introduce another set of basis vectors representing localized states. These states, which are characterized by a band index and a lattice site \mathbf{R}_n , and will be denoted by $|\alpha n\rangle$, are defined by

$$|\alpha n\rangle=\frac{\Omega^{1/2}}{(2\pi)^{3/2}}\int e^{-i\mathbf{k}\cdot\mathbf{R}_n}|\alpha\mathbf{k}\rangle d^3k, \quad (8)$$

in which Ω is the volume of the unit cell, and the integral includes the (first) Brillouin zone. We also have

$$|\alpha\mathbf{k}\rangle=\frac{\Omega^{1/2}}{(2\pi)^{3/2}}\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}|\alpha n\rangle. \quad (9)$$

The localized states are orthonormal

$$\langle\beta m|\alpha n\rangle=\delta_{\alpha\beta}\delta_{mn} \quad (10)$$

and are complete. It should be noted that for electrons, the transformation coefficients $\langle\mathbf{r}|\alpha\mathbf{k}\rangle$ and $\langle\mathbf{r}|\alpha n\rangle$ are Bloch wave functions $\psi_\alpha(\mathbf{k},\mathbf{r})$ and Wannier functions $a_\alpha(\mathbf{r}-\mathbf{R}_n)$, respectively. For magnons, the states $|\mathbf{k}\rangle$ (there is only one band in a simple ferromagnet) represent spin waves and the states $|n\rangle$ are those in which a spin deviation is localized at site \mathbf{R}_n .

We will be concerned here with potentials V which,

¹¹ An exception may occur if the surfaces of constant energy have concave portions (see Ref. 1). This will not concern us here.

when expressed on the localized basis, have only a finite number of nonzero elements. These potentials will be called potentials of finite range. Such potentials arise naturally in certain problems—for instance, the isotopic mass defect in a vibrating crystal lattice, or the magnetic defect in a Heisenberg ferromagnet. In other cases, it may reasonably be supposed that real potentials can be approximated by potentials of finite range. The essential observation of the present theory is that for potentials of finite range, the t matrix can be constructed on the localized basis using ordinary matrix operations with finite matrices. Thereafter, one can obtain the t matrix on the wave-like basis through the transformation of Eq. (9).

II. CONSTRUCTION OF THE t MATRIX

In this section we will derive a general expression for t -matrix elements due to a potential of finite range. Let us suppose that the nonzero portion of the matrix V is $n\times n$ (whereas the full matrix is $\mathfrak{R}\times\mathfrak{R}$, say). The t matrix resembles V in that only a $n\times n$ subset of its elements are nonzero, and it is necessary to consider only the same $n\times n$ portion of the matrix $1-\mathcal{G}V$. Let us write, for this portion (the rest may be ignored)

$$[1-\mathcal{G}V]^{-1}=P/D, \quad (11)$$

where

$$D=\det[1-\mathcal{G}V] \quad (12)$$

and P is the adjoint matrix $\text{adj}(1-\mathcal{G}V)$. The determinant D is of vital importance in the following, so it is convenient to indicate its presence explicitly. We know that a finite matrix always has an inverse unless its determinant vanishes; thus the t matrix will exist except for values of the energy such that $D=0$.

Equation (7), (9), and (11) lead to the following explicit expression for the t matrix elements

$$\langle\alpha\mathbf{k}|t|\beta\mathbf{q}\rangle=\frac{\Omega}{(2\pi)^3D}\sum_{\beta'ijn} e^{i(\mathbf{q}\cdot\mathbf{R}_n-\mathbf{k}\cdot\mathbf{R}_i)} \times (\alpha i|V|\beta'j)(\beta'j|P|\beta n), \quad (13)$$

where we use parentheses to indicate matrix elements on the localized basis. For potentials of finite range, all the sums in Eq. (13) involve only a finite number of terms.

Usually, however, we are concerned with defect potentials which have some symmetry—and frequently, this is that of the point group of the crystal. In such a case, Eq. (13) can be simplified if we introduce functions which transform according to specific irreducible representations of the symmetry group. We will denote these representations by an index s ; and denote the degeneracy of representation s by g_s . The introduction of symmetrized functions can be performed mathematically with the aid of a unitary transformation. We define symmetrized combinations of plane waves

belonging to representation *s* by¹

$$C_{s\nu}(k, R_m) = \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \sum_m U(s_\nu; \mathbf{R}_m) e^{i\mathbf{k} \cdot \mathbf{R}_m}. \quad (14)$$

The sum in Eq. (14) includes lattice vectors of a given type; that is, starting from some given lattice vector, we include all those which can be formed from that one by a rotation in the symmetry group. The index ν designates the row of the representation. The resulting function still depends on the "type" of lattice vector, and for this reason, we retain the R_m in the designation of the symmetrized function.

One property of the functions $C_{s\nu}$ which will be important to us later is the following: Let the function $C_{s\nu}$ be expanded in powers of k . Then the terms in the expansion are proportional to functions of k times Kubic harmonics belonging to the particular representation and row.^{12,13} In particular, let us consider only the leading term in this expansion, and write

$$C_{s\nu}(k, R_m) = \lambda_s k^\sigma K_{s\nu}(\theta, \varphi), \quad (15)$$

in which λ_s is a constant containing the lattice parameter, etc., σ is an exponent depending on s , $K_{s\nu}$ is the relevant Kubic harmonic for row ν of representation s , and the angles θ , φ specify the orientation of \mathbf{k} with respect to the crystal axes. Note that λ_s and σ are independent of ν . In order to simplify some of the subsequent formulas, we will adopt the convention that the Kubic harmonics are to be normalized to 4π . Thus, the $K_{s\nu}$ (which may be taken to be real) satisfy

$$\int K_{s\nu}(\theta, \varphi) K_{s\nu'}(\theta, \varphi) d\Omega = 4\pi \delta_{s\nu} \delta_{\nu\nu'}. \quad (16)$$

The introduction of the symmetrized functions causes the determinant D to factor into a product of subdeterminants coming from the representations.

$$D = \Pi_s (D_s)^{\nu_s}. \quad (17)$$

Each subdeterminant appears a number of times equal to the degeneracy of the representation. The potential-energy matrix V which appears in Eq. (13) becomes block-diagonal, as does the Green's function matrix \mathcal{G} . In consequence, the adjoint matrix P is also block diagonal, and the diagonal blocks contain subdeterminants as factors. Specifically we can write

$$\sum_{n,l} U(s_\nu, \mathbf{R}_n) (\alpha n | V | \beta l) U^\dagger(\mathbf{R}_l, s_{\nu'}) = \delta_{s\nu} \delta_{\nu\nu'} V_{s, \alpha n, \beta l}, \quad (18)$$

where $V_{s, \alpha n, \beta l}$ does not depend on the row of representation s . Also we write

$$\sum_{n,l} U(s_\nu, \mathbf{R}_n) (\alpha n | P | \beta l) U^\dagger(\mathbf{R}_l, s_{\nu'}) = \delta_{s\nu} \delta_{\nu\nu'} \frac{D}{D_s} P_{s, \alpha n, \beta l}. \quad (19)$$

¹² M. Flower, N. H. March, and A. M. Murray, Phys. Rev. **119**, 1885 (1960).

¹³ F. C. Von der Lage and H. A. Bethe, Phys. Rev. **71**, 612 (1947).

With the use of these results, we can express the t matrix as a sum of contributions from the different representations.

$$\langle \alpha \mathbf{k} | t | \beta \mathbf{q} \rangle = \sum_s \langle \alpha \mathbf{k} | t_s | \beta \mathbf{q} \rangle, \quad (20)$$

in which the "partial-wave" t matrices are given by

$$\langle \alpha \mathbf{k} | t_s | \beta \mathbf{q} \rangle = \frac{1}{D_s} \sum_{\beta' l j n} V_{s, \alpha n, \beta' j} P_{s, \beta' j, \beta n} \times \sum_\nu C_{s\nu\alpha}^*(k, R_l) C_{s\nu\beta}(q, R_n). \quad (21)$$

Equation (21) is the general partial wave formula for solid-state scattering theory.

The band index α or β on the symmetrized functions C_s indicates that the wave vector appearing in the argument of C is related to energy through the band function for that particular band. Comparison with Eq. (98) of I indicates that the scattering amplitude is proportional to the t -matrix element. Suppose that a wave with wave vector \mathbf{q} in band β is incident upon a scattering center. Then a scattered wave will appear in each band in which conservation conditions can be satisfied. The excitation wave function describing the scattering will have the asymptotic form in the localized representation¹⁴

$$B_\alpha(\mathbf{R}_n) = \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \left[e^{i\mathbf{q} \cdot \mathbf{R}_n} \delta_{\alpha\beta} - f_{\alpha\beta}(\mathbf{k}, \mathbf{q}) \frac{e^{i\mathbf{k} \cdot \mathbf{R}_n}}{R_n} \right] \quad (22)$$

and the $\alpha\beta$ element of the scattering amplitude, which is a matrix in the bands, is related to the t matrix by

$$f_{\alpha\beta}(\mathbf{k}, \mathbf{q}) = -\frac{2\pi^2}{\gamma_\alpha} \langle \alpha \mathbf{k} | t | \beta \mathbf{q} \rangle, \quad (23)$$

in which γ_α is a constant which depends on the energy surfaces in band α , which in the limit of a spherical band is just the reciprocal effective mass ($E_\alpha(k) = \gamma_\alpha k^2$ in that case).

III. PHASE SHIFTS

Let us recall the usual expression for the scattering amplitude in ordinary quantum mechanics. It is

$$f(\Theta) = -\frac{1}{k} \sum_l (2l+1) e^{i\delta_l} \sin \delta_l P_l(\cos \Theta), \quad (24)$$

in which Θ is the angle between the wave vector of the incoming wave and a vector to the point of observation, P_l is a Legendre polynomial, and δ_l is the phase shift of the l th partial wave. This result has quite a different

¹⁴ See I. We have made a few simplifying approximations. All surfaces of constant energy are assumed to be convex. The quantity we here call γ_α [see Eq. (23) below] would be designated $g_\alpha(k)$ in I and is given by Eq. (28) of that paper.

form from the result obtained by substituting Eqs. (20) and (21) into Eq. (23). Yet a connection must exist at least in the long-wavelength low-energy limit in which we frequently have spherical energy surfaces and details of the crystal structure should not be important. To obtain a relation, it is first necessary to introduce phase shifts. This will be done by the definition

$$\tan\delta_s = \frac{-\text{Im}D_s}{\text{Re}D_s}. \quad (25)$$

This definition of the phase shift corresponds to that given by Baker.¹⁵

Introduction of the phase shifts simplifies many of the calculations of solid-state scattering theory. From Eq. (77) of I, we see that the contribution to the change in density of states produced by scattering in representation s is given by

$$\Delta N_s = -\frac{g_s}{\pi} \text{Im} \frac{1}{D_s} \frac{dD_s}{dE}. \quad (26)$$

Use of Eq. (25) allows us to express Eq. (26) in the form:

$$\Delta N_s = \frac{g_s}{\pi} \frac{d\delta_s}{dE}. \quad (27)$$

This elegant relation, which is valid at any energy within the continuum, connects scattering theory with the calculation of bulk properties of a dilute alloy. We note that Eqs. (26) and (27) give the change in the density of states relative to the entire crystal volume, so that if a finite concentration c , of defects is present we merely multiply Eq. (27) by c . We will apply this result subsequently.

It has been observed previously that a scattering resonance may occur in representation s at an energy close to that at which the real part of D_s vanishes.¹ Let this energy be denoted by $E_0^{(s)}$. For energies close to $E_0^{(s)}$, we may expand D_s , retaining only the leading terms. Then in this region we can write

$$\tan\delta_s = \frac{-\Gamma_s}{2(E - E_0^{(s)})}, \quad (28)$$

where we have defined

$$\Gamma_s = \frac{2 \text{Im}D_s(E_0^{(s)})}{[d(\text{Re}D_s)/dE]E_0}. \quad (29)$$

Equation (28) shows that for positive Γ the phase shift increases through $\pi/2$ as the energy E goes through $E_0^{(s)}$ from below. This behavior is typical of scattering resonances. We can combine Eqs. (27) and (28) to obtain the change in density of states near a resonance

$$\Delta N_s = \frac{g_s \Gamma_s}{2\pi} \frac{1}{(E - E_0^{(s)})^2 + \Gamma_s^2/4}. \quad (30)$$

¹⁵ M. Baker, Ann. Phys. (N. Y.) 4, 271 (1958).

This expression has the characteristic Breit-Wigner form and indicates that Γ_s is the width of the resonance.

Let us now suppose that the defects introduced into the crystal are such that the total number of states is unchanged, and let us also suppose for the moment that we are considering a situation in which a single band (or group of bands) is isolated from all others. The lowest energy in the band is E_0 , and the highest is E_m . Then if we integrate Eq. (27) with respect to energy from E_0 to E_m , the result must be minus the number of states forced out of the band by the perturbation, that is, the number of bound states in representations lying either above or below the band. To take degeneracy into account, we denote the number of such bound states by $g_s n_s$ so that we have

$$\delta_s(E_0) - \delta_s(E_m) = \pi n_s. \quad (31)$$

Equation (31) may also be obtained by consideration of the analytic properties of D_s . This result is analogous to Levinson's theorem.

In order to obtain a relation between the phase shift and scattering amplitude which approximates to Eq. (24) we need the optical theorem. The general statement of the optical theorem appropriate to solid state scattering theory has been established in Ref. 9, and the result is quoted without proof here:

$$\text{Im}\langle \alpha \mathbf{k} | t | \alpha \mathbf{k} \rangle = -\pi \sum_{\beta} \int \frac{dS_{\alpha}(E_{\beta})}{|\nabla_{\alpha} E_{\beta}|} |\langle \alpha \mathbf{k} | t | \beta \mathbf{q} \rangle|^2. \quad (32)$$

Equation (32) differs from the optical theorem for free-space scattering in only two respects: (1) a sum over band indices appears, and (2) the surfaces of constant energy, which are indicated explicitly, may be anisotropic.

We would expect that Eq. (24) would apply in a limiting case which approximates that of scattering in free space. This turns out to be true, and we introduce the following assumptions:

- (1) Elements of the t matrix connecting different bands can be neglected. We will therefore drop the band index in Eq. (29), and consider only a single band.
- (2) The energy-band function has the simple form

$$E = \gamma k^2. \quad (33)$$

Surfaces of constant energy are spherically symmetric.

(3) The symmetrized functions $C_{s\nu}(k, R_m)$ which appear in Eq. (21) are to be expanded in powers of k . Our result is obtained when only the lowest term in this expansion is retained.

We now proceed as follows: From Eq. (25) it follows that we can write

$$\frac{1}{D_s} = -\frac{\sin\delta_s e^{-i\delta_s}}{\text{Im}D_s}. \quad (34)$$

Then, with the use of Eq. (15), we can write the leading

term in the low energy expansion of the t -matrix element as

$$\langle \mathbf{k} | t_s | \mathbf{q} \rangle = -\frac{\sin \delta_s e^{-i\delta_s}}{\text{Im} D_s} \Lambda_s k^{2\sigma} \sum_{\nu} K_{s\nu}(\theta, \varphi) K_{s\nu}(\theta', \varphi'), \quad (35)$$

in which Λ_s is a constant containing the potential, the P matrix and factors of λ_s from Eq. (15). We are not interested in the precise expression for Λ_s at this point, since it depends on the particular scattering problem under consideration. It is of some importance that Λ_s depends only on the representation being independent of the rows. Λ_s may be complex: We write it in the form

$$\Lambda_s = |\Lambda_s| e^{i\rho_s}. \quad (36)$$

The angles θ , φ and θ' , φ' specify respectively the orientation of the vectors \mathbf{k} and \mathbf{q} with respect to the crystal axes. We must now substitute Eq. (35) into Eq. (32). As a consequence of the orthogonality of Kubic harmonics belonging to different representations, there are no cross terms in Eq. (32) connecting different representations. Equation (32) holds for each t_s separately, and this result is true in general, not merely in the low-energy approximation. After the substitution, the left-hand side of Eq. (32) gives

$$\begin{aligned} \text{Im} \langle \mathbf{k} | t_s | \mathbf{k} \rangle \\ = -|\Lambda_s| \frac{\sin \delta_s \sin(\delta_s + \rho_s)}{\text{Im} D_s} k^{2\sigma} \sum_{\nu} K_{s\nu}^2(\theta, \varphi). \end{aligned} \quad (37)$$

The right side of Eq. (29) is correspondingly, with the use of Eq. (33)

$$\begin{aligned} -\pi \int \frac{dS_q(E)}{|\nabla_q E|} |\langle \mathbf{k} | t_s | \mathbf{q} \rangle|^2 \\ = -\frac{\pi q \sin^2 \delta_s |\Lambda_s|^2}{2\gamma (\text{Im} D_s)^2} k^{2\sigma} q^{2\sigma} \int d\Omega' \sum_{\nu\mu} K_{s\nu}(\theta, \varphi) K_{s\nu}(\theta', \varphi') \\ \times K_{s\mu}(\theta, \varphi) K_{s\mu}(\theta', \varphi'). \end{aligned} \quad (38)$$

The integral is performed with the aid of Eq. (16). We also observe that $|\mathbf{k}| = |\mathbf{q}|$ as a consequence of conservation of energy. Then Eq. (38) gives

$$-\frac{2\pi^2 k^{4\sigma+1} \sin^2 \delta_s}{\gamma (\text{Im} D_s)^2} |\Lambda_s|^2 \sum_{\nu} K_{s\nu}^2(\theta, \varphi). \quad (39)$$

We solve the reduced form of Eq. (32) for

$$\text{Im} D_s = \frac{2\pi^2}{\gamma} |\Lambda_s| \frac{\sin \delta_s k^{2\sigma+1}}{\sin(\delta_s + \rho_s)}. \quad (40)$$

We can now substitute this expression for $\text{Im} D_s$ back

into Eq. (35)

$$\begin{aligned} \langle \mathbf{k} | t_s | \mathbf{q} \rangle = -\frac{\gamma}{2\pi^2 k} e^{i(\delta_s + \rho_s)} \sin(\delta_s + \rho_s) \\ \times \sum_{\nu} K_{s\nu}(\theta, \varphi) K_{s\nu}(\theta', \varphi'). \end{aligned} \quad (41a)$$

From Eq. (23), we then obtain the portion of the scattering amplitude coming from representation s :

$$f_s = \frac{1}{k} e^{i(\delta_s + \rho_s)} \sin(\delta_s + \rho_s) \sum_{\nu} K_{s\nu}(\theta, \varphi) K_{s\nu}(\theta', \varphi'). \quad (41b)$$

This result is to be compared with Eq. (24). There are both similarities and differences.

(1) If we add the contributions f_s from the different representations, there are only a finite number of terms in contrast to the infinite number of terms which appear in Eq. (24). This is a general feature of solid-state scattering theory which results from the fact that the scattering potential (and the energies) as invariant under only a finite group. Each phase shift δ_s must contain contributions from an infinite number of spherical partial wave phase shifts in the limit of complete spherical symmetry.

The relation between the phase shifts δ_s defined in Eq. (25) and those of ordinary scattering theory is the following. In the solid, only the phase shifts appropriate to the finite symmetry group of the defect potential are defined. If we imagine a limiting process in which the lattice constant becomes infinite and the scattering potential acquires spherical symmetry, the δ_s must become combinations of spherical wave phase shifts δ_l . In this limit, the determinant D is still well defined, although our methods of calculating it would not be useful. The subdeterminants D_s would then factor still further into a product of terms coming from each of the partial waves which, in the solid, are possible bases for representation s . From this, we see that each δ_s would become in the limit equal to the sum of the phase shifts for all those waves which go into representation s .

(2) The angular dependence of the scattering amplitude as given by Eq. (41) is different from that of Eq. (24). In Eq. (41) both sets of angles θ , φ and θ' , φ' appear and in general the t matrix does not depend simply on the angle between the vectors \mathbf{k} and \mathbf{q} . However, there are some important special cases in which further reduction is possible. In particular, if the representation s has as basis functions all of the spherical harmonics of a given l then the sum over ν can be performed. This happens only for the s -like representation Γ_1 for which the K 's are equal to 1, and the p -like representation Γ_{15} . In the latter case, we can choose a basis in the representation such that

$$K_{p1}(\theta, \varphi) = \sqrt{3} \frac{k_x}{k} = \sqrt{3} \sin \theta \cos \varphi,$$

etc., and the sum over ν gives immediately

$$3\mathbf{k} \cdot \mathbf{q}/kq = 3 \cos \Theta$$

in agreement with Eq. (24). These are the only two representations for which reduction to Eq. (24) is always possible. If we consider $l=2$, for instance, the five spherical harmonics are divided between the Γ_{12} and $\Gamma_{25'}$ representations in a cubic crystal. If, however, $\delta_{12} + \rho_{12} = \delta_{25'} + \rho_{25'}$, then the amplitudes from both representations can be combined to yield

$$5P_2(\cos \Theta)$$

in agreement with Eq. (24). This obviously can only be true for restricted classes of potentials. Higher spherical harmonics are divided in more complicated ways.

(3) Next, we observe that there is an additional contribution to the phase in Eq. (41). We could of course have defined our scattering phase shifts δ_s to include ρ_s as well, but then our definition of the phases would not agree with Eq. (25), and we would not have Eq. (27) either. However, although I know of no general theorem which requires that Λ_s be real, there are some rather important cases in which this happens. These include:

(a) The Koster-Slater model in which there is only one band and one nonzero matrix element of the potential. In this case there is only s -wave scattering.

(b) In cubic lattices with one band, and nearest-neighbor interactions, the p - and d -wave scattering will have $\rho_s = 0$. This need not be true for the s representation Γ_1 , but it does hold for that representation in at least one interesting case, which is

(c) The Heisenberg model of a ferromagnet with nearest neighbor interactions only. We will examine that case in more detail below.

Actually, cases (a) and (b) above have the following in common: Whenever there is only a single term in the interaction potential after symmetrization, then $P=1$, and from the reality of the potential (in this case, the matrix element is required by Hermiticity to be real), it follows that $\rho=0$.

IV. APPLICATION TO SPIN WAVES

In this section, we will apply the preceding general theory to spin waves in a Heisenberg ferromagnet containing defects. This theory has certain features which make it very attractive for the purposes of illustrating scattering theory: (1) there is only one band, (2) matrix elements on the basis of localized states can be obtained readily, and (3) it is nontrivial—the interaction involves nearest-neighbor couplings, and so (unlike the simple Koster-Slater model) analysis of the scattering in terms of irreducible representations is useful. In previous publications, the energies of bound states and the locations and widths of resonances have

been determined.^{6,16-18} The cross section for spin-wave impurity scattering has also been obtained by a process which amounts to direct evaluation of Eq. (21).^{19,20} The present objective is to introduce the phase shifts in order to simplify the calculation of the cross section, and also to apply Eq. (27) to determine the change in the density of states produced by a small concentration of imperfections. This result can be used to obtain the changes in the low-temperature thermodynamic properties of an insulating ferromagnet.

Our discussion will be based on Ref. 20, and we will use much of the notation of that paper. We consider only simple ferromagnets and assume that the exchange interaction couples only nearest neighbors. Let us recall that a magnetic defect in a Heisenberg ferromagnet is an atom characterized by a different spin (S') and/or a different exchange coupling (J') than those of the host crystal (S and J , respectively). The impurity is assumed to couple ferromagnetically: J' is positive.

In cubic crystals (which are the only ones we shall consider) the low-energy spin-wave scattering is dominated by the s and p waves as described in the previous sections. Scattering will exist in other representations depending on the particular lattice, but the phase shifts for these representations are of order k^5 or higher, and will be neglected here.

We begin with the s -like representation Γ_1 ; and for this we have from Eq. (37) of Ref. 20

$$D_s = 1 + \frac{z}{2}(g_1 - g_0) \left(1 - \frac{J'}{J}\right) + \frac{Eg_1}{4JS} \left(1 - \frac{J'S'}{JS}\right), \quad (42)$$

in which z is the number of nearest neighbors. The quantities g_0 and g_1 are dimensionless measures of the central cell and first-neighbor Green's function:

$$g_0 = -\frac{4JS\Omega}{(2\pi)^3} \int d^3q \frac{1}{E^+ - E(\mathbf{q})}, \quad (43)$$

$$g_1 = -\frac{4JS\Omega}{(2\pi)^3} \int d^3q \frac{\exp i\mathbf{q} \cdot \Delta}{E^+ - E(\mathbf{q})}, \quad (44)$$

where Δ is a vector from the origin to any one of the first neighbors. We separate the real and imaginary parts, and retain only the leading terms in an expansion in powers of the energy [or of k , through Eq. (33)]. Then we find the phase shift

$$\delta_s = -\frac{\Omega k^3}{4\pi} \left(1 - \frac{S'}{S}\right). \quad (45)$$

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¹⁹ J. Callaway, Phys. Rev. **132**, 2003 (1963).

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For the p -representation Γ_{15} we find

$$D_p = 1 - \rho g_p, \quad (46)$$

where

$$\rho = \frac{1}{2}(1 - J'S'/JS), \quad (47)$$

and g_p is a symmetrized combination of Green's functions appropriate to the Γ_{15} representation whose precise form we will not give here (see Ref. 20). Again we expand for small k and obtain

$$\delta_p = \frac{\Omega k^3}{3\pi} \frac{\rho}{1 - K\rho}, \quad (48)$$

where K is a numerical constant which depends on the lattice in question (it is the $E=0$ limit of the real part of g_p). For the simple cubic lattice, the value of K may be obtained from the tables contained in Ref. 6 to be $K=0.42$. These expressions will always be valid when k is sufficiently small; however, the range of utility of Eq. (45) will not be large if there is a low-energy s -wave resonance, and in such a case the resonance may exert a dominant effect on the thermodynamics.^{21,22} We will assume here that there is no low-energy resonance.

With the aid of Eq. (27), we can deduce the total change in density of states due to a concentration, c , of magnetic impurities. This is, to lowest order,

$$\Delta N = \Delta N_s + \Delta N_p = \frac{c}{\pi} \frac{d}{dE} [\delta_s + 3\delta_p]. \quad (49)$$

We observe that both the s and p -wave phase shifts are proportional to k^3 . Thus their energy derivatives are proportional to k , that is, to $E^{1/2}$. From this we see that the change in the density of states depends on the energy in the same way in the presence of imperfections that it does in the perfect crystal. Then we can write for the total density of states $N(E)$, after performing the differentiations,

$$N(E) = N_0(E) + \Delta N$$

$$= N_0(E) \left[1 - \frac{3c}{2} \left(1 - \frac{S'}{S} - \frac{4\rho}{1 - K\rho} \right) \right]. \quad (50)$$

The density of states for the perfect crystal is

$$N_0(E) = \frac{\Omega E^{1/2}}{4\pi^2 \gamma^{3/2}}, \quad (51)$$

in which γ is the spin-wave reciprocal effective mass:

$$\gamma = 2JSa^2 \quad (52)$$

for any cubic crystal, and a is the cubic-lattice constant.

Equation (50) suggests that we can define a perturbed reciprocal effective mass, γ_p , for the crystal containing imperfections through the formula

$$N(E) = \Omega E^{1/2} / 4\pi^2 \gamma_p^{3/2}. \quad (53)$$

Then γ_p is determined from Eqs. (53) and (50) to be

$$\gamma_p = \gamma \left[1 + c \left(1 - \frac{S'}{S} - \frac{4\rho}{1 - K\rho} \right) \right]. \quad (54)$$

Equation (54) has the following significance: We can use Eq. (33) to relate energy and wave vector in the crystal containing imperfections provided that we replace γ by γ_p through Eq. (54). This replacement will enable us to compute those properties of the ferromagnet which are determined by the spin-wave density of states, such as the dependence of the magnetization and specific heat on temperature for low temperature. These results are, of course, valid only through first order in the concentration. An extension to higher powers of the concentration would be difficult but could, in principle be carried out through the methods of Lifshitz.²³ Our results, Eqs. (50) and (54) are in agreement with calculations by Izyumov²⁴ and Murray²⁵ using different methods.

The calculation of the low-energy spin-wave scattering cross section is very simple once the phase shifts have been determined. To order k^4 , we have the total cross section

$$\sigma = \frac{4\pi}{k^2} [\delta_s^2 + 3\delta_p^2] = \frac{(\Omega k^2)^2}{4\pi} \left[\left(1 - \frac{S'}{S} \right)^2 + \frac{16}{3} \frac{\rho^2}{(1 - K\rho)^2} \right], \quad (55)$$

which agrees with Ref. 20. The lifetime of a spin wave of wave vector \mathbf{k} in the imperfect crystal can be related to the scattering cross section by the formula

$$\tau^{-1}(k) = cV\sigma/\Omega, \quad (56)$$

where v is the spin-wave velocity, $v = 2\gamma k$. This gives

$$\tau^{-1}(k) = \frac{c\Omega k^3 E(k)}{2\pi} \left[\left(1 - \frac{S'}{S} \right)^2 + \frac{16}{3} \frac{\rho^2}{(1 - K\rho)^2} \right]. \quad (57)$$

We see therefore that τ^{-1} is of order k^5 for small k , so that low-energy spin waves are only very weakly damped. This is of the same order as that due to spin-wave-spin interactions in the perfect ferromagnet.^{26,27} Again, it should be noted that these results apply only if there are no low-energy resonances.

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