Dispersion Theory of the Kondo Effect

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According to recent work by Kondo, the scattering cross section of an electron in exchange interaction with a paramagnetic impurity immersed in a Fermi sea of electrons has a logarithmic infinity as the electron energy approaches the Fermi energy. We examine this problem by means of the Chew-Low method first devised for meson-nucleon scattering. It is found that the singularity is replaced by a resonant scattering close to the Fermi level.

1. INTRODUCTION

As recently demonstrated by Kondo[1] in a paper treating the resistance minimum observed in certain paramagnetic alloys, a diffculty arises in the perturbation theory of a noninteracting electron gas exchange-coupled to the spin of a paramagnetic impurity. Kondo showed that the scattering cross section of an electron off the impurity spin, calculated to third order in the exchange coupling, becomes logarithmically infinite as the energy of the electron approaches the Fermi energy. This difficulty arises essentially because the paramagnetic scatterer has an internal degree of freedom: the orientation of the spin. As a result, the exclusion principle (whose effect in the intermediate states cancels out for a structureless scatterer, such as an ordinary imposed potential) does come into play. The summations over intermediate-state energies, instead of ranging freely from zero to infinity, extend only to (or from) the Fermi level, producing the aforementioned singularity.

A divergence of this sort calls into question the stability of the usual Fermi state when there is a finite density of paramagnetic impurities. As an initial step towards tackling this problem it is desirable to determine if the Kondo singularity remains a singlarity in all orders in perturbation theory, or is restricted to a finite-order calculation.

Unfortunately, there is at present no convenient method for evaluating the general term in the perturbation series for a contact interaction of the form

$$H' = J\Omega_0 \mathbf{S}\cdot\mathbf{s}(0). \tag{1}$$

{Here $\mathbf{S}$ is the impurity spin; $\mathbf{s}(0)$, the conduction-electron spin density at the position (0) of the impurity; J, the exchange coupling which, with Kondo we assume to be antiferromagnetic [$J>0$ for the form (1)]; and Ω_0 is some atomic volume.} The usual methods which are so successful for perturbations involving fermion and boson operators fail in the present case, because of the unwieldy commutation relations of the components of S. (See Sec. 5.) For this reason, it is necessary to seek some nonperturbative procedure. In a different context, that of meson theory, a nonperturbative theory particularly designed for scattering problems was introduced some time ago by Wick,[2] and by Chew and Low.[3] We will show that their general method can be applied to advantage in the present problem also. Compared with the original Chew-Low static-source model of pion-nucleon scattering, the present problem has some increased complexity because of the absence of a finite threshold, and because the interaction (1) is bilinear in the fermion field operators, while the static-source model is linear in the boson field. This radically alters the character of the "crossing relations," in the present case, diminishing the powerful role they play in the solution of the Chew-Low model. On the other hand, the present problem is simpler in that there are fewer degrees of freedom of the "target" than in that model.

2. LOW EQUATION

One of the great advantages of the Chew-Low method is that it formally operates with *exact* eigenstates of the target, and with *exact* scattering states of the target +incident particle, and yet achieves results which make no reference to the details of these states. (See, however, Sec. 7.) In applying this method to the present problem we make the following assumptions:

(1) At an infinite distance from the impurity, the electron gas is in the Fermi state.

(2) There are an even number of conduction elec-electrons, and the value of the impurity spin is one-half, so the ground state of the target (impurity spin+electron gas) is doubly degenerate.

(3) The eigenexcitations of the target are of only two kinds: (a) excitations with energies infinitesimally above the ground-state energy, but with wave functions which at infinity look like electron-hole pairs, or (b) excitations whose wave functions decay at infinity, but Whose energies are above that of the ground state by a finite minimum amount. A band of exact eigenstates with energies infinitesimally above the ground-state energy, but with wave functions falling off at infinity would be fatal in our argument. It is plausible that localized states, if they exist at all, correspond to excited bound states and as such require finite excitation energies.

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[1] J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964).
[2] G. C. Wick, Rev. Mod. Phys. **27**, 339 (1955).
[3] G. F. Chew and F. E. Low, Phys. Rev. **101**, 1571 (1956).

Note that these assumptions do not preclude a quite complicated structure of the two exact degenerate ground states. We denote these two ground states by $|\omega,S\rangle$ where S takes two values, but for conciseness we shall usually drop the index S and distinguish the states by primes on the ω. Were there no interaction, the $|\omega,S\rangle$ would simply be the two product states formed from the Fermi state and the up or down state of the impurity spin. Consider now an additional electron, with energy ϵ_k above the Fermi level incident on the target which is in one or the other of the two ground states $|\omega S\rangle$. We proceed to give a derivation of the Low equation, which closely parallels that given in Schweber's book.[4] With $a_k^\dagger$ denoting the creation operator of an electron with wave number k (incorporating spin orientation for brevity), the incident state may be taken to have the form

$$a_k^\dagger|\omega S\rangle,$$

and, because $|\omega\rangle$ at infinity is essentially the Fermi sea, this state is nonzero only if $\epsilon_k>0$ (the Fermi level is taken as the zero of energy). We now seek *exact* outgoing and incoming scattering eigenstates

$$|k,\omega,S\rangle^\pm=a_k^\dagger|\omega,S\rangle+|\chi\rangle^\pm \tag{2}$$

of the total Hamiltonian

$$H=H^0+H'\equiv\sum\epsilon_k a_k^\dagger a_k+H'.$$

The states $|\chi\rangle$ in each case denote the scattered waves. If ω is the ground-state energy of the system, then the energy of this scattering state is $\epsilon_k+\omega$. Schrödinger's equation therefore reads

$$(H-\omega-\epsilon_k)(a_k^\dagger|\omega\rangle+|\chi\rangle)=0, \tag{3}$$

where we have dropped all obvious indices. But

$$H^0a_k^\dagger|\omega\rangle=a_k^\dagger(\epsilon_k+H^0)|\omega\rangle \tag{4}$$

and

$$H'a_k^\dagger|\omega\rangle=j_k|\omega\rangle+a_k^\dagger H'|\omega\rangle, \tag{5}$$

where

$$j_k=(H',a_k^\dagger)_- \tag{6}$$

denotes the commutator of H' with $a_k^\dagger$. From (4) and (5), it follows that

$$(H-\omega-\epsilon_k)a_k^\dagger|\omega\rangle=j_k|\omega\rangle. \tag{7}$$

Substitution in (3) then gives (recalling that $H|\omega\rangle=\omega|\omega\rangle$)

$$(\omega+\epsilon_k-H)|\chi\rangle=j_k|\omega\rangle,$$

whose outgoing solution is

$$|\chi\rangle^+=(\omega+\epsilon_k-H+i\delta)^{-1}j_k|\omega\rangle,$$

where δ is a positive infinitesimal. A similar result holds for the incoming solution $|\chi\rangle^-$ (with the sign of δ reversed). The solution to Schrödinger's equation is thus

$$|k,\omega\rangle^\pm=a_k^\dagger|\omega\rangle+(\omega+\epsilon_k-H\pm i\delta)^{-1}j_k|\omega\rangle. \tag{8}$$

The scattering matrix element from one single-electron scattering state k to another k' (likewise above the Fermi surface) is defined as

$$\mathcal{S}_{k'\omega';k\omega}=-\langle k'\omega'|k\omega\rangle^+,$$

which we re-express in terms of incoming states alone by noting that, from Eq. (8),

$$|k\omega\rangle^+-|k\omega\rangle^-=-2\pi i\delta(\omega+\epsilon_k-H)j_k|\omega\rangle,$$

so that

$$\begin{aligned}\mathcal{S}_{k'\omega';k\omega}&=-\langle k'\omega'|k\omega\rangle^--2\pi i^-\langle k'\omega'|\delta(\omega+\epsilon_k-H)j_k|\omega\rangle\\&=\delta_{kk'}\delta_{\omega\omega'}-2\pi i\delta(\omega+\epsilon_k-\omega'-\epsilon_{k'})\\&\qquad\times^-\langle k'\omega'|j_k|\omega\rangle.\end{aligned} \tag{9}$$

Next, we define a T matrix by [see Eq. (8)]

$$\begin{aligned}T_{k'\omega',k\omega}&=-\langle k'\omega'|j_k|\omega\rangle\\&=\langle\omega'|a_{k'}j_k|\omega\rangle\\&\qquad+\langle\omega'|j_k^\dagger(\omega'+\epsilon_{k'}-H+i\delta)^{-1}j_k|\omega\rangle.\end{aligned} \tag{10}$$

In terms of T, the transition rate for an incident electron in state k to any other state is given by the average of

$$\sum_{k'\omega'}\delta(\epsilon_{k'}+\omega'-\epsilon_k-\omega)|T_{k'\omega',k\omega}|^2$$

over the two indices S. Also, the $\mathcal{S}$ matrix is

$$\mathcal{S}_{k'\omega',k\omega}=\delta_{kk'\omega\omega'}-2\pi i\delta(\omega+\epsilon_k-\omega'-\epsilon_{k'})T_{k'\omega';k\omega}.$$

The normalization of the "in" states has been taken to be unity. This is consistent with unit normalization of the incident state $a_k^\dagger|\omega\rangle$, so long as the density of scatterers is infinitesimal. For finite density, $a_k^\dagger|\omega\rangle$ would have to be renormalized.

It is clear from the definition (10) that by inserting a complete set of scattering states $\sum|\rangle^-\,^-\langle|$ in the center of the second term on the right, some kind of expression for T in terms of itself may be obtained. First, we process the leading term on the right. j_k is the commutator of H' with $a_k^\dagger$ and therefore depends on the components of S, and linearly on all the $a^\dagger$'s. To get rid of the dependence on the $a^\dagger$'s we write

$$\begin{aligned}a_{k'}j_k&=(a_{k'}j_k)_+-j_ka_{k'}\\&\equiv\mu_{k'k}-j_ka_{k'},\end{aligned} \tag{11}$$

where the anticommutator $\mu_{k'k}$ depends on the components of S alone, and not on the fermion operators. To evaluate $\langle\omega'|a_{k'}j_k|\omega\rangle$, we now need to know $a_{k'}|\omega\rangle$. But

$$Ha_{k'}|\omega\rangle=(H,a_{k'})_-|\omega\rangle+a_{k'}\omega|\omega\rangle$$

and

$$(H,a_{k'})_-=-\epsilon_{k'}a_{k'}+j_{k'},$$

[4] S. S. Schweber, *An Introduction to Relativistic Field Theory* (Harper & Row, New York, 1961), Chap. 12.

where

$$\begin{aligned}\tilde{j}_{k'} &= (H'a_{k'})_- \\ &= -(H'a_{k'}{}^\dagger)_-{}^\dagger \\ &= -j_{k'}{}^\dagger .\end{aligned}$$

Hence, we find that

$$(H-\omega+\epsilon_{k'})a_{k'}|\omega\rangle = -j_{k'}{}^\dagger|\omega\rangle .$$

Now the state $j_{k'}{}^\dagger|\omega\rangle$ can be expressed as a superposition of various $(N-1)$ electron states, if $|\omega\rangle$ had N electrons. This means that we can invert this equation, obtaining

$$a_{k'}|\omega\rangle = -(H-\omega+\epsilon_{k'})^{-1}j_{k'}{}^\dagger|\omega\rangle \qquad (12)$$

without ambiguity, provided our assumption (3) of this section is satisfied. For, by that assumption, $j_{k'}{}^\dagger|\omega\rangle$ can be expanded in a complete set of scattering states which, asymptotically, all have the appearance of excited target states with one electron (below the Fermi sea) removed, and arbitrary numbers of hole-electron pairs excited. When acting on any one of these states, H produces a factor

$$-\epsilon_\lambda+\sum\epsilon_p+\omega' ,$$

where ϵ_λ is the energy of the removed electron (always <0), and $\sum\epsilon_p$ the sum of pair excitation energies (all positive). With $\epsilon_{k'}>0$, we then see that

$$H-\omega+\epsilon_{k'}$$

will never attain values less than zero. This may also be inferred from the fact that $a_{k'}|\omega\rangle$, for $\epsilon_{k'}>0$, must be a purely local state; if there are no localized excitations of arbitrary small energy (or more precisely, energies less than $\epsilon_{k'}$), then $(H-\omega+\epsilon_{k'})a_{k'}|\omega\rangle$ must consist of states with only positive coefficients.

From (10), (11), and (12) we find that

$$\begin{aligned}T_{k'\omega';k\omega} &= \langle\omega'|\mu_{k'k}|\omega\rangle \\ &+\sum_n \langle\omega'|j_{k'}{}^\dagger|n\rangle^-{}^-\langle n|j_k|\omega\rangle/(\omega+\epsilon_{k'}-E_n+i\delta) \\ &+\sum_n \langle\omega'|j_k|n\rangle^-{}^-\langle n|j_{k'}{}^\dagger|\omega\rangle/(E_n-\omega+\epsilon_{k'}) , \qquad (13)\end{aligned}$$

where ${}^-\langle n|$ denotes any one of the complete set of in-scattering states, and E_n its energy. Alternatively, we may write

$$\begin{aligned}T_{k'\omega';k\omega} &= \langle\omega'|\mu_{k'k}|\omega\rangle \\ &+\sum_n T_{n;k'\omega'}{}^*T_{n;k\omega}/(\omega'+\epsilon_{k'}-E_n+i\delta) \\ &+\sum_n \tilde{T}_{n;k\omega'}{}^*\tilde{T}_{n,k'\omega}/(E_n-\omega+\epsilon_{k'}) , \qquad (13a)\end{aligned}$$

with $T_{n;k\omega}={}^-\langle n|j_k|\omega\rangle$, $\tilde{T}_{n;k\omega}={}^-\langle n|j_k{}^\dagger|\omega\rangle$, and stars denoting complex conjugates. In contrast to the Chew-Low static source model, the operators T and $\tilde{T}$ are not quite so simply related here. Because in that model the interaction is linear in the field operators, j_k and $j_k{}^\dagger$ are essentially the same. Here this is not the case, and, as a result, it is impossible to solve the present problem entirely without approximations. (Actually difficulties of a minor nature remain in the Chew-Low problem also.[5])

Next we require an equation for $\tilde{T}_{k'\omega';k\omega}$. This we obtain by considering hole-scattering states of the form

$$|k\omega\rangle^\pm = a_k|\omega\rangle+|\chi\rangle^\pm$$

with energy $\omega-\epsilon_k(\epsilon_k<0)$. We will then show that the matrices T and $\tilde{T}$, though themselves defined only for processes above and below the Fermi level, respectively, can be continued into each other by certain equations, which are the "crossing relations" for the present problem. In exactly the same way as before, we find that the S matrix for hole scattering is given by

$$S_{k'\omega';k\omega}=\delta_{kk'}\delta_{\omega\omega'}+2\pi i\delta(\omega-\epsilon_k-\omega'+\epsilon_{k'})\tilde{T}_{k'\omega';k\omega} ,$$

where

$$\begin{aligned}\tilde{T}_{k'\omega';k\omega} &= -\langle k'\omega'|j_k{}^\dagger|\omega\rangle \\ &= \langle\omega'|a_{k'}{}^\dagger j_k{}^\dagger|\omega\rangle \\ &\quad -\langle\omega'|j_{k'}(\omega-\epsilon_{k'}-H+i\delta)^{-1}j_k{}^\dagger|\omega\rangle\end{aligned}$$

and both k' and k are inside the Fermi sphere. Noting that

$$a_{k'}{}^\dagger j_k{}^\dagger = \mu_{k'k}{}^\dagger - j_k{}^\dagger a_{k'}{}^\dagger ,$$

we see that we need $a_{k'}{}^\dagger|\omega\rangle$. In the same way as before, we derive

$$a_{k'}{}^\dagger|\omega\rangle = (H-\epsilon_{k'}-\omega)^{-1}j_{k'}|\omega\rangle ,$$

where the reciprocal once again is well defined, subject to assumption (3). Thus we conclude that

$$\begin{aligned}\tilde{T}_{k'\omega';k\omega} &= \langle\omega'|\mu_{k'k}{}^\dagger|\omega\rangle-\langle\omega'|j_k{}^\dagger(H+|\epsilon_{k'}|-\omega)^{-1}j_{k'}|\omega\rangle \\ &\quad -\langle\omega'|j_{k'}{}^\dagger(\omega'+|\epsilon_{k'}|-H+i\delta)^{-1}j_k|\omega\rangle \\ &= \langle\omega'|\mu_{k'k}{}^\dagger|\omega\rangle \\ &\quad -\sum_n \tilde{T}_{n;k'\omega'}{}^*\tilde{T}_{n;k\omega}/(\omega'+|\epsilon_{k'}|-E_n+i\delta) \\ &\quad -\sum_n T_{n;k\omega'}{}^*T_{n;k'\omega}/(E_n+|\epsilon_{k'}|-\omega) , \qquad (14)\end{aligned}$$

where we have explicitly used the fact that $\epsilon_{k'}$ is negative.

3. CROSSING RELATIONS

We now make the central approximation of this paper: We permit only one-particle intermediate states

$$|n\rangle^- = |k'',\omega''\rangle^- . \qquad (15)$$

[5] It might be supposed that Eq. (13a) (together with a similar equation T) can be regarded as the first in a hierarchy; however, at some higher stage it becomes impossible to perform the inversion corresponding to (12) because of energy-conserving intermediate states. The necessary generalizations which must then be made are described in Ref. 6.

Then (13a) and (14) form a self-contained set of equations, whose solution corresponds to a summation of selected perturbation series terms. The nature of this approximation is discussed in Sec. 5. Here we remark only that, were we dealing with ordinary scattering from a spin-independent potential, such a procedure would actually be exact (see Appendix I).

Let us now examine $\mu_{kk'}$ in more detail. In second-quantized notation, the interaction reads

$$H'=\Omega_0 J\mathbf{S}\cdot\mathbf{s}(0)$$
$$=(J/2N)\sum_{\lambda\mu}[S^+a_{\lambda\downarrow}{}^\dagger a_{\mu\uparrow}+S^-a_{\mu\uparrow}{}^\dagger a_{\lambda\downarrow}+S^z(a_{\lambda\uparrow}{}^\dagger a_{\mu\uparrow}-a_{\lambda\downarrow}{}^\dagger a_{\mu\downarrow})],$$

where N is the number of atoms in the crystal, and where the spin subscripts have been exhibited explicitly. It follows that

$$j_{k\sigma}=(J/2N)\sum_{\lambda}[\delta_{\sigma\uparrow}S^+a_{\lambda\downarrow}{}^\dagger+\delta_{\sigma\downarrow}S^-a_{\lambda\downarrow}{}^\dagger+\delta_{\sigma\uparrow}S^za_{\lambda\uparrow}{}^\dagger-\delta_{\sigma\downarrow}S^za_{\lambda\downarrow}{}^\dagger]$$

and

$$\mu_{k'\sigma';k\sigma}=[J/2N)[\delta_{\sigma'\downarrow}\delta_{\sigma\uparrow}S^+\delta_{\sigma'\uparrow}\delta_{\sigma\downarrow}S^-+(\delta_{\sigma'\uparrow}\delta_{\sigma\uparrow}-\delta_{\sigma'\downarrow}\delta_{\sigma\downarrow})S^z],$$

so that

$$\langle\omega'|\mu_{k'\sigma';k\sigma}|\omega\rangle=(J/2N)\langle\sigma'\omega'|\mathbf{S}\cdot\mathbf{s}|\sigma\omega\rangle, \quad (16)$$

independent of k and k'. This independence is, of course, due to the choice of a contact interaction and leads to great simplifications. Here $\mathbf{s}$ is the ordinary vector matrix corresponding to spin one-half.

On the other hand (and this is crucial),

$$\langle\omega'|\mu^\dagger{}_{k'\sigma';k\sigma}|\omega\rangle=(J/2N)\langle\sigma\omega'|\mathbf{S}\cdot\mathbf{s}|\sigma'\omega\rangle$$
$$=(J/2N)\langle\sigma'\omega'|\mathbf{S}\cdot\tilde{\mathbf{s}}|\sigma\omega\rangle, \quad (17)$$

where the tilde denotes the transpose of the spin matrices.

It is clear from the foregoing that there will be solutions of (13a) and (14) which depend on the momenta only through the energies. Furthermore, if, according to assumption (3), there are no "internal" excitations with arbitrarily small energies, then, if ϵ_k is very close to the Fermi level, $\epsilon_{k'}$ will be equally close. In fact, energy conservation will require $\epsilon_{k'}=\epsilon_k$, so far as the one-particle T's are concerned. As ϵ_k moves away from the Fermi surface, processes in which an electron emerges accompanied by hole-electron pairs also become possible, but to study these, more general $T_{n;k}$'s have to be considered, and it would be necessary to treat these by means of the previously mentioned Norton-Klein extension[6] applied to the present theory. In this paper, we thus assume $\epsilon_{k'}=\epsilon_k$ and $\omega=\omega'$ (but that does not mean $|\omega\rangle=|\omega'\rangle$ because of the silent index S). Furthermore, we note that adding or subtracting $i\delta$ from the nonvanishing denominators of the crossing terms in (13a) and (14) does not alter the result. Finally, we observe that by assumption (3) the intermediate energies are all of the form $\epsilon_{k''}+\omega''$, and we simply denote $\epsilon_{k''}+\omega''-\omega$ by ϵ''. It is now convenient to introduce operators $T(z)$ and $\tilde{T}(z)$ which are functions of the complex variable z and whose matrix elements satisfy the coupled equations

$$T_{k'\omega';k\omega}=\langle\omega'|\mu_{k'k}|\omega\rangle+\sum T_{k''\omega'',k'\omega'}{}^*T_{k''\omega'',k\omega}/(z-\epsilon'')+\sum\tilde{T}_{k''\omega'';k\omega'}{}^*\tilde{T}_{k''\omega'';k'\omega}/(z+\epsilon'') \quad (18)$$

and

$$\tilde{T}_{k'\omega',k\omega}(z)=\langle\omega'|\mu_{k'k}{}^\dagger|\omega\rangle-\sum\tilde{T}_{k''\omega'';k'\omega}{}^*\tilde{T}_{k''\omega'';k\omega}/z-\epsilon''-\sum T_{k''\omega'';k\omega'}{}^*T_{k''\omega'';k'\omega}/z+\epsilon''. \quad (19)$$

In terms of these, we have

$$T(\epsilon_{k'})=T(z)\,|_{\mathrm{L}z\to\epsilon_{k'}+i\delta},$$
$$\tilde{T}(\epsilon_{k'})=T(z)\,|_{\mathrm{L}z\to|\epsilon_{k'}|+i\delta}. \quad (20)$$

Recalling that the μ's depend only on the spin parts of the k's and using Eq. (17), we see immediately from (18) and (19) that

$$T_{k\omega';k'\omega}(-z)=\tilde{T}_{k'\omega';k\omega}(z), \quad (21)$$

which is the "crossing relation" to be used later. Another crossing relation can be found by taking complex conjugates, but we will have no occasion to use it.

4. PARTIAL WAVES

From the form of (18) and from (16), it is evident that T may be regarded as a matrix function of $\mathbf{s}$ and $\mathbf{S}$. From considerations of rotational invariance, it must have the form

$$T=A+B(\mathbf{s}\cdot\mathbf{S}).$$

However, it is physically more appealing to use a decomposition[7] into triplet and singlet projection operators P_1 and P_0:

$$T(z)=t_0(z)P_0+t_1(z)P_1, \quad (22)$$

where

$$P_0=\tfrac{1}{4}-\mathbf{s}\cdot\mathbf{S}\quad P_1=\tfrac{3}{4}+\mathbf{s}\cdot\mathbf{S}. \quad (23)$$

From here on, we explicitly use σ and σ', the spin parts of k and k', since T does not depend on the wave numbers. The index ω or ω' continues to refer to the two degenerate ground states. The crossing relation states that

$$\tilde{T}_{\sigma'\omega';\sigma\omega}(z)=T_{\sigma\omega';\sigma'\omega}(-z).$$

But that means that

$$\tilde{T}=t_0(-z)\tilde{P}_0+t_1(-z)\tilde{P}_1, \quad (24)$$

where the expressions for P_0 and P_1 are the same as (23), but with the s matrices replaced by their transposes. We note that $\tilde{P}_0$ and $\tilde{P}_1$ are no longer projec-

[6] R. E. Norton and A. Klein, Phys. Rev. **109**, 584 (1958).

[7] Note: For an interaction $J(|k-k'|)$ of finite range, it is necessary to consider higher partial waves. For the p wave, there will be three distinct t matrices corresponding to total angular momentum 0, 1, and 2 compounded from orbital angular momentum $l=1$ and from the two spins.

tion operators since $\tilde{P}_0^2 \neq \tilde{P}_0$. However, we still have $\tilde{P}_0+\tilde{P}_1=1$. We now substitute (24) and (23) into (18). Then it is necessary to evaluate terms such as

$$\frac{\sum T_{\sigma''\omega'',\sigma'\omega'}{}^{*} T_{\sigma''\omega'',\sigma\omega}}{(z-\epsilon'')} = \int_0^\infty \frac{\langle \sigma'\omega' | T^\dagger(x) T(x) | \sigma\omega \rangle}{z-x} \rho(x)dx$$

and, similarly,

$$\int \frac{\langle \sigma\omega' | \tilde{T}^\dagger(x) \tilde{T}(x) | \sigma'\omega \rangle}{z+x} \rho(x)dx,$$

where by $T(x)$ we mean $T(x+i\delta)$, etc. Here $\rho(x)$ is the density of intermediate states. By our hypothesis (3), there are no "internal" excitation energies close to zero; therefore $\rho(x)$ for small x is just the density of unperturbed one-electron states. The final results do not depend critically on $\rho(x)$, and we shall therefore not pursue this point any further. Obviously,

$$T^\dagger(x)T(x) = |t_0(x)|^2 P_0 + |t_1(x)|^2 P_1, \qquad (25)$$

since $P_0^2=P_0$, $P_1^2=P_1$ and $P_0P_1=0$. However, $\tilde{T}^\dagger(x)\tilde{T}(x)$ is more complicated. We shall evaluate it as follows: Powers and products of the transposes $\tilde{\mathbf{s}}$ are expressible in terms of $\tilde{\mathbf{s}}$; therefore powers and products of $\tilde{P}_0$, $\tilde{P}_1$ are expressible in terms of $\tilde{P}_0$ and $\tilde{P}_1$, and therefore $\tilde{T}^\dagger\tilde{T}$ is linear in $\tilde{P}_0$, $\tilde{P}_1$. But this is just what is needed, because $\langle \sigma\omega' | \tilde{P} | \sigma'\omega \rangle = \langle \sigma'\omega' | P | \sigma\omega \rangle$, so that the same projection operators will occur on the right-hand side of Eq. (18) as on the left. Noting that each $\tilde{s}^2=\frac{1}{4}$, and $(\mathbf{S}\cdot\tilde{\mathbf{s}})^2=\frac{3}{16}+\frac{1}{2}(\tilde{\mathbf{s}}\cdot\mathbf{S})$ (whereas $(\mathbf{S}\cdot\mathbf{s})^2=\frac{3}{16}-\frac{1}{2}(s\cdot S)$,) we find

$$\tilde{P}_0^2 = (\tfrac{1}{4}-\mathbf{S}\cdot\tilde{\mathbf{s}})^2 = \tfrac{1}{4},$$
$$\tilde{P}_1^2 = \tfrac{3}{4}+2\mathbf{S}\cdot\tilde{\mathbf{s}},$$

and

$$\tilde{P}_0\tilde{P}_1 = \tilde{P}_1\tilde{P}_0 = -(\mathbf{S}\cdot\tilde{\mathbf{s}}).$$

Finally, $(\tilde{\mathbf{s}}\cdot\mathbf{S})=\frac{1}{4}(\tilde{P}_1-3\tilde{P}_0)$. Combining these results, we see that

$$\tilde{T}^\dagger(z)\tilde{T}(z) = \tfrac{1}{4}|t_0(-z)|^2 + |t_1(-z)|^2\{\tfrac{3}{4}+2(\tilde{\mathbf{s}}\cdot\mathbf{S})\} - [t_0^*(-z)t_1(-z)+t_1^*(-z)t_0(-z)](\tilde{\mathbf{s}}\cdot\mathbf{S}).$$

Using also $\tilde{P}_0+\tilde{P}_1=1$, we finally obtain

$$\tilde{T}^\dagger(z)\tilde{T}(z) = [-\tfrac{3}{4}|t_0-t_1|^2+|t_0|^2]\tilde{P}_0 + [\tfrac{1}{4}|t_0-t_1|^2+|t_1|^2]\tilde{P}_1, \qquad (26)$$

the right-hand sides of these equations being taken at $-z$. For use in Eq. (18), we let $z \to x+i\delta$, noting that in the absolute values in Eqs. (25) and (26), the sign of δ is immaterial. Substituting (26) into (18), changing variables from x to $-x$, and regrouping terms slightly, we obtain from (18)

$$t_0(z) = -\frac{3}{4}\frac{J}{N} + \int_{-\infty}^{+\infty} \frac{|t_0(x+i\delta)|^2\rho(|x|)}{z-x}dx - \frac{3}{4}\int_{-\infty}^{0} \frac{|t_0(x+i\delta)-t_1(x+i\delta)|^2\rho(|x|)}{z-x}dx \qquad (27)$$

and

$$t_1(z) = \frac{1}{4}\frac{J}{N} + \int_{-\infty}^{+\infty} \frac{|t_1(x+i\delta)|^2\rho(|x|)}{z-x}dx + \frac{1}{4}\int_{-\infty}^{0} \frac{|t_0(x+i\delta)-t_1(x+i\delta)|^2\rho(|x|)}{z-x}dx. \qquad (28)$$

5. RELATION TO ORDINARY POTENTIAL SCATTERING AND TO PERTURBATION THEORY

The leading terms $-\frac{3}{4}J/N$ and $\frac{1}{4}J/N$ in Eqs. (27) and (28) are simply the Born terms. If we attempt to iterate (27) and (28) with the Born terms as zero-order solutions, we see at once that the terms integrated only up to the Fermi level give a logarithmic singularity at $Rlz=0$ (the Kondo effect). An iterative expansion in powers of J is therefore misleading. Suppose that the last terms on the right of (27) and (28) are neglected. Then the problem reduces to one of ordinary potential scattering in potentials $-\frac{3}{4}J$ and $\frac{1}{4}J$, respectively. For an ordinary scattering potential V, it is an easy matter to derive the equation

$$t(z) = \frac{V}{N} + \int_{-\infty}^{+\infty} \frac{|t(x+i\delta)|^2\rho(|x|)dx}{z-x}$$

as an *exact* equation (see Appendix I). Its solution is trivial. For, we have

$$\mathrm{Im}t(x+i\delta) = -\pi|t(x+i\delta)|^2\rho(|x|)$$

or

$$\mathrm{Im}[1/t(x+i\delta)] = \pi\rho(|x|).$$

The only solution of this equation which goes to $1/V$ at infinity and has no poles is[8]

$$\frac{1}{t(x+i\delta)} = \frac{N}{V} + \int_{-\infty}^{+\infty} \frac{\rho(|x'|)}{x+i\delta-x'}dx',$$

a familiar result, which exhibits resonant behavior (a virtual bound state), if V has a suitable sign and is large enough so that the equation

$$\frac{1}{V} = -P\int \frac{\rho_1(|x'|)dx'}{x-x'}$$

can be satisfied. Here P denotes the principal part, and $\rho_1=\rho/N$ is the density of states per electron. On the other hand, if the middle terms in Eqs. (27) and (28) were discarded, we would have

$$\Delta(z) = J/N + \int_{-\infty}^{0} \frac{|\Delta|^2}{z-x}\rho(|x|)dx,$$

[8] N. I. Muskhelishivili, *Singular Integral Equations*, translated by J. R. M. Radock (P. Noordhoff Ltd., Groningen, The Netherlands, 1953), Chap. 3, Sec. 26.

where $\Delta=t_1-t_0$, whose solution is

$$\frac{1}{\Delta(z)}=\frac{N}{J}+\int_{-\infty}^{0}\frac{\rho(|x|)dx}{x-z}.$$

For $Rlz>0$, the integral has a real part only. Assuming a very slowly varying density of states, we get for $Rlz>0$

$$\frac{1}{\Delta}=\frac{N}{J}+\rho\ln\frac{z}{\epsilon_f},$$

where the infinite limit has been replaced by a cutoff $-\epsilon_f$. Writing $z=z_0+(z-z_0)$, we see that Δ has a pole with residue $\exp(-1/J\rho_1)$ at $z_0=\epsilon_f\exp(-1/J\rho_1)$.[9] For small positive J (antiferromagnetic, as in Kondo's work), this implies a bound state just above the Fermi surface; for small negative J, there is a pole at a very large value of z outside the range of validity of the present assumptions, which can be dismissed as irrelevant. As we shall see in the next section, when the middle term in (27) and (28) are included, there will be (for positive J) two virtual bound states broadened by the inevitable imaginary part of the middle term.

To conclude this section, we consider the relation between this method and perturbation theory. In the usual time-dependent formulation of perturbation theory using the interaction representation, we cannot in the present case use unlabeled Feynmann diagrams, since, in general, each different set of time labels on the vertices gives a different numerical contribution. This is due to the complicated commutation relations of the components of S. The enormous simplification which the Feynman-Dyson symmetrization of the time labels brings about when only boson and fermion field operators are involved is thereby lost. Of course we can still draw diagrams. With crosses denoting the interactions, a possible fifth-order term is shown in Fig. 1. For ordinary potential scattering, we know that unconnected closed loops, such as that in Fig. 1, factor out of the perturbation series, yielding an unimportant unimodular multiplier of the S matrix. Unlinked diagrams with closed loops can therefore be discarded. However, in the case of spin-dependent scattering, the diagram of Fig. 1 is not, in fact, unlinked, since the vertices must not be deprived of their time labels, which now cannot be symmetrized. Consequently, the five-dimensional time integral representing Fig. 1 no longer factors. It is now clear what diagrams are being retained when only single-particle intermediate states are admitted in Eqs. (13a) and (14): all diagrams without closed loops, that is to say, only simple chains. But this does *not* mean that the result becomes identical with that for potential scattering, because the contributions of the chains still depend on the labeling of their vertices. The crossing terms, which lead to the $|t_1-t_0|^2$ integrands, may be regarded as due to this dependence on time label.

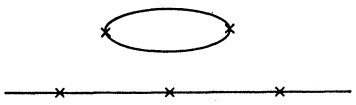

FIG. 1. A fifth-order unlinked diagram which may be factored for potential scattering, but not for the present problem.

[9] This being the case, a single term embodying the contribution from this pole should be included on the right-hand side of the equation for Δ. The term is $A_0/z-z_0$, where A_0 is the aforementioned residue. The solution for $1/\Delta$ remains unchanged.

6. APPROXIMATE SOLUTION OF THE EQUATIONS

We have not succeeded in finding an exact solution to Eqs. (27) and (28). One possible method, which requires a computing machine, is the "N/D" method used in high-energy physics.[10] However, since in the present problem only a qualitative insight is desired and no "bootstrap" solutions are expected (solutions with $J=0$), such an elaborate method is hardly appropriate here. Instead, we use the following iterations scheme: From (27) and (28) we find

$$\operatorname{Im}\frac{1}{t_0}=\pi\rho-\tfrac{3}{4}\pi\rho\left|1-\frac{t_1}{t_0}\right|^2\eta(-x), \tag{29}$$

$$\operatorname{Im}\frac{1}{t_1}=\pi\rho+\tfrac{1}{4}\pi\rho\left|1-\frac{t_0}{t_1}\right|^2\eta(-x), \tag{30}$$

where η is the step function. If t_0-t_1 is nonzero at $x=0$, then t_0 and t_1 will have logarithmic singularities there; if $t_0-t_1\sim x^\alpha$ with $\alpha>0$, no singularity will arise. First, assume that $t_0-t_1\neq0$ at $x=0$. Then (29) and (30) may be "solved" to give

$$\frac{1}{t_0(z)}=-\frac{4N}{3J}+\int_{-\infty}^{+\infty}\frac{\rho dx}{x-z}-\frac{3}{4}\int_{-\infty}^{0}\frac{|1-t_1/t_0|^2\rho dx}{x-z}, \tag{31}$$

$$\frac{1}{t_1(z)}=\frac{4N}{J}+\int_{-\infty}^{+\infty}\frac{\rho dx}{x-z}+\frac{1}{4}\int_{-\infty}^{0}\frac{|1-t_0/t_1|^2\rho dx}{x-z}. \tag{32}$$

Since by hypothesis $|1-t_1/t_0|^2\neq0$, singularities arise; for small z, we may replace the integral

$$\int_{-\infty}^{0}dx\left|1-\frac{t_1}{t_0}\right|^2$$

by

$$|1-t_1(0)/t_0(0)|^2\rho(0)\ln|z|/\epsilon_f,$$

assuming $|1-t_1/t_0|$ and ρ to vary slowly. Very close to $z=0$, the first two terms on the right of (31) and (32)

[10] A simple exposition of this method is found in D. Y. Wong, *Dispersion Relations and Applications, Rendiconti della Suola Internazionale di Fisica "Enrico Fermi," XXIX Convention* (Academic Press Inc., New York, 1964).

may be neglected, and, taking the ratio, we find

$$\frac{t_1}{t_0}=-3\left|1-\frac{t_1}{t_0}\right|^2\Big/\left|1-\frac{t_0}{t_1}\right|^2,$$

all evaluated at $x=0$. Hence $t_1(0)/t_0(0)$ is real, and in fact

$$t_0(0)/t_1(0)=-3.$$

Hence in this approximation,

$$\frac{1}{t_0(x+i\delta)}=-\frac{4N}{3J}+\int_{-\infty}^{+\infty}\frac{\rho dx'}{x'-x-i\delta}-\tfrac{4}{3}\rho\ln\frac{|x|}{\epsilon_f}$$
$$-\tfrac{4}{3}i\pi\rho\eta(-x),$$
$$\frac{1}{t_1(x+i\delta)}=\frac{4N}{J}+\int_{-\infty}^{+\infty}\frac{\rho dx'}{x'-x-i\delta}+4\rho\ln\frac{|x|}{\epsilon_f}+4i\pi\rho\eta(-x).$$

For small J we may now discard the real part of

$$\int_{-\infty}^{+\infty}\rho dx/(x-z)$$

and obtain, finally, for $x>0$,

$$t_0(x+i\delta)=-\frac{3}{4N}\left\{\frac{1}{J}+\rho_1\ln\frac{|x|}{\epsilon_f}-\tfrac{3}{4}i\pi\rho_1\right\}^{-1},$$
$$t_1(x+i\delta)=\frac{1}{4N}\left\{\frac{1}{J}+\rho_1\ln\frac{|x|}{\epsilon_f}+\tfrac{1}{4}i\pi\rho_1\right\}.$$

The two partial-wave resonances occupy the same position, $x_0=\epsilon_f\exp(-1/J\rho_1)$, but have different widths. When $J=0$, the effect disappears for all x other than $x=0$, exactly.[11] (For $x\neq 0$, both the strengths and the widths of the resonances diminish exponentially with J.) On the left-hand cut, we have

$$\frac{t_0}{t_1}=-3\left\{1+J\rho_1\ln\frac{|x|}{\epsilon_f}+\frac{5J}{4}i\pi\rho_1\right\}\Big/$$
$$\left\{1+J\rho_1\ln\frac{|x|}{\epsilon_f}+\frac{J}{4}i\pi\rho_1\right\}$$

so that

$$\frac{1}{4}\left|1-\frac{t_0}{t_1}\right|^2=4\frac{[1+J\rho_1\ln(|x|/\epsilon_f)]^2+\pi^2\rho_1^2J^2}{[1+J\rho_1\ln(|x|/\epsilon_f)]^2+\pi^2\rho_1^2J^2/16}.$$

This ranges from 4 at the Fermi level to 64 at $x=-x_0$, which shows that at least one more iteration should be performed. This must be done numerically; no major qualitative change is likely to result, however. Solutions for which $t_0-t_1\sim x^\alpha$, with $\alpha>0$, cannot be derived as simply as this, because the last integral in (31) and (32) then has no dominant region of integration. Such solutions are, however, so far removed from any resemblance to the perturbation series that they can very likely be ruled out.

Note added in proof. Given t_1 and t_0, it is possible to derive the single particle causal Green's function for the conduction electrons. This is done by expressing the resolvent operator $1/z-H$ in terms of the over-all scattering matrix of the system, and writing the latter as a multiple scattering series. This series is averaged over impurity configurations and impurity spin orientations, and resummed. To lowest order in the concentration ξ, one then finds

$$2\pi G_k(t)=(1-n_k)\int dze^{-izt}[z-\epsilon_k-\xi\{\tfrac{1}{4}t_0(z)+\tfrac{3}{4}t_1(z)\}];\quad t>0$$
$$=-n_k\int dze^{-izt}[z-\epsilon_k-\xi\{\tfrac{1}{4}t_0(-z)+\tfrac{3}{4}t_1(-z)\}];\quad t<0$$

integrated around a contour enclosing the real axis.

7. AMBIGUITIES

The trick of considering $\mathrm{Im}1/t$ instead of $\mathrm{Im}t$ has one obvious pitfall: It does not allow in any simple way for points at which t vanishes. The ambiguities arising from this have been pointed out by Castillejo, Dalitz, and Dyson,[12] who showed that the solution of the original Chew-Low equation was not unique in that an arbitrary number of pole terms could be added to a particular solution $1/t$. In the case of potential scattering, the results of Ref. 8 are that if

$$\mathrm{Im}[1/t(x+i\delta)]=\pi\rho(x)$$

at values of x for which $t\neq 0$, then the general form of $1/t$ is

$$\frac{1}{t}=\int\frac{dR(x')}{x+i\delta-x'},$$

where

$$R(x')=\int^{x'}\rho(y)dy-\sum_i p_i\eta(x-x_i),$$

where the p_i and x_i are arbitrary but subject to certain constraints (see Ref. 8). [The much more special solution which we have used, and which is given in Ref. 6, is restricted to weight functions which satisfy the Holder condition $R'(x_1)-R'(x_2)<(x_1-x_2)^\mu$ along the cut.[8]] It follows that

$$\frac{1}{t}=\frac{1}{t_1}+\sum_i\frac{p_i}{x-x_i},$$

where $1/t_1$ denotes the pole-free solution previously obtained.

[11] A generalization to finite temperatures would presumably remove this exceptional point.

[12] L. Castillejo, R. H. Dalitz, and F. J. Dyson, Phys. Rev. **101**, 453 (1956).

The physical meaning of the extra pole-terms is that the target may have hidden structure in the sense that there may not be a one-to-one correspondence between all the states of the unperturbed Hamiltonian, and the scattering states of the perturbed Hamiltonian. Such structure is missed by the Chew-Low equation. Fairlie and Polkinghorne[13] have demonstrated this explicitly for potential scattering from a Hamiltonian H_0+V, where V is factorizable. In the case, the x_i are the energies of the bound states of H_0 and the p_i are $|u(i)|^2$, where

$$\langle i|V|i'\rangle=u^*(i)u(i').$$

When the incident particle has an energy corresponding to one of these states, the scattering amplitude goes to zero.

In the present case, these considerations may well imply that to obtain the solution of the previous section, we must altogether rule out all localized target states, not just those with infinitesimal excitation energy, as in assumption (3).

8. COMPLEX POLES

In the preceding section, we have diagonalized, not the whole $\mathcal{S}$ matrix, but only a truncated version consisting of single particle to single-particle matrix elements. Unitarity is therefore no longer guaranteed. The possibility that the neglected processes lead to spurious effects cannot be discarded. The lowest iterant to the solution discussed in Sec. 6 does, in fact, show one such spurious effect: a pair of complex conjugate poles with real part below the Fermi surface. Taking $|1-t_1/t_0|^2=16/9$, we find poles in t_0 of the form $x_0(1+i)$ with

$$x_0=-2^{-1/2}\epsilon_f\exp(-1/J\rho_1).$$

Such poles should not occur (causality requires $\mathcal{S}$ to be analytic in the upper half-plane). If these poles survive higher iterations, their nature would have to be tracked down by considering single-particle–single-particle+pair processes also. Even then they may not disappear because the neglect of higher processes amounts to replacing the perturbation H' by PH', where P is the projection operator of the manifold of all the scattering states admitted in the approximation. Since PH' is non-Hermitian, complex poles may appear.

9. CONCLUSIONS

We conclude from these results that the divergence found by Kondo in the scattering cross section of an electron by an impurity spin disappears when a selected class of processes is summed. It remains to establish the connection between the present method, and more conventional ones using Green's functions, as recently investigated by Nagaoka,[14] who likewise found that the divergence disappears. We finally note that the T matrices may be used to calculate some ground-state expectation values, as described in Appendix II.

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APPENDIX I: POTENTIAL SCATTERING

We show here that for a Hamiltonian

$$H=\sum\epsilon_k a_k^\dagger a_k+\sum_{kk'}V_{kk'}a_k^\dagger a_{k'}\equiv H_0+v \qquad \text{(A1)}$$

there are no T-matrix elements from scattering states with one incident particle, to states with one particle and hole-electron pairs. It is sufficient to consider

$$T_{k',p;k}=-\langle k',p|(v,a_k^\dagger)|\omega\rangle,$$

where p denotes one pair. The Hamiltonian (A1) has no "hidden structure" in the sense of Sec. 7. We can change from the fermion operators a_k to a complete set of in-scattering operators A_k. In terms of these,

$$|k'p\rangle^-=A_{k'}^\dagger B_p^\dagger|\omega\rangle,$$

where the operator $B_p^\dagger$ creates the pair p. Also

$$\begin{aligned}(v,a_k^\dagger)&=\sum V_{\lambda\mu}a_\lambda^\dagger\\&=\sum V_{\lambda\mu}\langle\lambda|\nu\rangle^-A_\nu^\dagger\\&=\sum_\nu W_\nu A_\nu^\dagger,\text{ say}.\end{aligned}$$

Hence

$$T_{k'p;k}=\sum_\nu\langle\omega|B_pA_{k'}A_\nu^\dagger|\omega\rangle W_\nu.$$

In evaluating these ground-state averages, the electron operator in B_p must not be contracted with $A_{k'}$, otherwise $A_{k'}^\dagger B_p^\dagger|\omega\rangle$ would again be a one-particle state. We may only contract the hole operator of B_p with $A_\nu^\dagger$. But this leaves averages of the form $A_\lambda^\dagger A_{k'}$, with $\lambda\neq k'$, and these vanish, since $A_\lambda^\dagger A_{k'}$ is an excited eigenstate orthogonal to $|\omega\rangle$. This proves the result.

APPENDIX II: GROUND-STATE EXPECTATION VALUES

As is to be expected, a knowledge of the single-particle T matrices permits one to evaluate ground-state expectation values of various observables. As an example, we quote the shift in the ground-state energy due to H'. By Feynman's theorem, we have, for this shift,

$$\Delta E=\int_0^J\frac{dJ'}{J'}{}_{J'}\langle|H'|\rangle_{J'},$$

where ${}_{J'}\langle|$ denotes the ground state at coupling con-

[13] D. B. Fairlie and J. C. Polkinghorne, Nuovo Cimento 8, 345 and 555 (1958).
[14] Y. Nagaoka (to be published).

stant J'. Some algebra shows that to order $1/N$,

$$j_\uparrow j_\uparrow^\dagger + j_\downarrow j_\downarrow^\dagger = (J'^2/4N)[(3/4N)\sum_{\lambda\lambda'}(a_{\lambda\uparrow}^\dagger a_{\lambda'\uparrow} + a_{\lambda\downarrow}^\dagger a_{\lambda'\downarrow}) - 2\mathbf{S}\cdot\mathbf{s}(0)\Omega_0],$$

$$j_\uparrow^\dagger j_\uparrow + j_\downarrow^\dagger j_\downarrow = (J'^2/4N)[-(3/4N)\sum_{\lambda\lambda'}(a_{\lambda\uparrow}^\dagger a_{\lambda'\uparrow} + a_{\lambda\downarrow}^\dagger a_{\lambda'\downarrow}) - 2\mathbf{S}\cdot\mathbf{s}(0)\Omega_0],$$

where the momentum subscripts of the j have been omitted, since j is the same for all.

Now, for example,

$$\langle | j_\uparrow j_\uparrow^\dagger | \rangle = \sum \langle | j_\uparrow | n \rangle^- {}^- \langle n | j_\uparrow^\dagger | \rangle = \sum_{k'\sigma'} \tilde{T}_{k'\sigma';\uparrow}^* \tilde{T}_{k'\sigma';\uparrow}$$

(where again the k index has been suppressed). Averaging over the two degenerate ground states, we then find

$$\langle | H' | \rangle \sim \frac{1}{2} \int \sum_{S,\sigma} \mathrm{Tr}\{\tilde{T}^\dagger(\epsilon)\tilde{T}(\epsilon) + T^\dagger(\epsilon)T(\epsilon)\}\rho(\epsilon)d\epsilon,$$

which, together with the crossing relation, determines the ground-state shift.

Note added in proof. The ground state shift is thus given in terms of the unknown matrix elements of **S** within the ground manifold. These play a role analogous to the "renormalized" coupling constants, and must be determined from some experiment likewise describable in terms of them.

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Influence of Local Phonon Damping on Mössbauer Spectra

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The contribution of localized-mode phonon emission and absorption to the Mössbauer emission process is evaluated in the presence of damping. *Net*-zero-phonon processes, in which the number of localized phonons (of a given type) emitted is the same as the number absorbed, are shown to contribute to the intensity in the vicinity of the unshifted gamma-ray energy. This contribution is shown to be distributed over a minimum width $\Gamma+2\gamma$ where Γ is the gamma-ray natural width, and γ, the width of the localized phonon, is larger than Γ. The complete Mössbauer spectrum including all multiphonon contributions can be obtained in our approximation by using the continuous spectrum of nonlocalized phonons plus a Lorentz-broadened peak associated with each localized phonon. Optical absorption at impurities in solids may have linewidths $\Gamma >$ the phonon widths γ, thus permitting local phonon enhancement of the zero-phonon transitions in impurity absorption or emission.

1. INTRODUCTION

IN this paper we shall treat the Mössbauer effect in the quasiharmonic approximation which includes frequency shifts and damping due to anharmonicity and other causes. The Mössbauer line is usually described as the emission of a gamma ray with no change in the internal state of the crystal.[1]

The intensity in the vicinity of this line is determined by transitions in which very small changes in vibrational energy occur, e.g., by the simultaneous emission and absorption of the same number of phonons of essentially the same energy. Continuum phonons can contribute to this region but only as part of a smooth background unless the continuum spectrum has sharp peaks. If a phonon localized around the impurity atom[2,3] is present, it contributes a separate sharp peak to the spectrum. If this peak were infinitely narrow, then the emission and absorption of the same number of such phonons ("net-zero-phonon" process) would enhance the intensity of the Mössbauer line in comparison with the usual Debye-Waller factor. This "Bessel-function enhancement" emphasized by Kaufman and Lipkin[4]

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[1] H. Frauenfelder, *The Mössbauer Effect* (W. A. Benjamin, Inc., New York, 1962); Rev. Mod. Phys. **36**, 333–503 (1964), constitute excellent reviews and sources of reference to the literature on "recoilless radiation."

[2] I. M. Lifshitz, Suppl. Nuovo Cimento **3**, 716 (1956), which includes references to earlier Lifshitz work; M. Lax, Phys. Rev. **94**, 1392 (1954); E. W. Montroll and R. B. Potts, *ibid.* **100**, 525 (1955); A. A. Maradudin, P. Mazur, E. W. Montroll, and G. H. Weiss, Rev. Mod. Phys. **30**, 175 (1959); P. G. Dawber and R. J. Elliott, Proc. Roy. Soc. (London) **A273**, 222 (1963); Proc. Phys. Soc. (London) **81**, 453 (1963).

[3] I. Waller, Arkiv Fysik **24**, 495 (1963).

[4] B. Kaufman and H. J. Lipkin, Ann. Phys. (N. Y.) **18**, 294 (1962). See also A. A. Maradudin, Rev. Mod. Phys. **36**, 417 (1964).