The few rigorous results that have been established concerning the properties of this Hamiltonian have been listed by Herring,[6] and the one pertinent to our discussion is that Lieb and Mattis[7] have shown that there can be no ferromagnetism for a linear chain of atoms with $T(1-1')$ nonzero only for nearest neighbors, but with an interaction energy that can be an arbitrary function of $n_{1\uparrow}+n_{1\downarrow}$. Since the Hamiltonian (24) is a particular case of our Hamiltonian (3), our conclusions, which cover more possibilities than those of Lieb and Mattis, apply to it. There is thus not only no ferromagnetism but no antiferromagnetism for both one and two dimensions; also the range of the hopping integral $T(1-1')$ is restricted only by the condition that the expression (19) for a converge. It is a trivial matter to show that our results also apply if the interaction is an arbitrary function of $n_{1\uparrow}+n_{1\downarrow}$, since $[C, n_{1\uparrow}+n_{1\downarrow}]=0$.

Although the above results have some intellectual interest, they are clearly inapplicable to real three-dimensional solids. However, as pointed out by Herring[6] in connection with the Lieb-Mattis theorems, many approximation schemes that have been applied to real solids can equally well be applied to one- and two-dimensional solids. If these approximation schemes predict the occurrence of spontaneous magnetization in one and two dimensions as well as in three dimensions for the Hamiltonian (3), the validity of these predictions in three dimensions should be clearly investigated more fully.

One of the authors (T.W.R.) would like to express his gratitude to the Department of Physics at the University of Toronto, and particularly to Professor J. Van Kranendonk, for their hospitality during his visit.

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[7] E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962).

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Theory of *s-d* Scattering in Dilute Magnetic Alloys with Spin-$\frac{1}{2}$ Impurities*

H. J. SPENCER
Physics Department, Imperial College, London, England

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With the aid of a new Wick theorem for spin-$\frac{1}{2}$ operators, the properties of a single localized paramagnetic impurity in a metal are investigated, using diagrammatic techniques which are completely analogous to those of standard quantum field theory. Attention is directed at the high-temperature magnetic properties of this system. The present results include a new $\ln T$ term in the g shift for the impurity spin and for the electronic susceptibility. In the high-field limit, the former logarithmic result is replaced by the logarithm of the Zeeman energy. A high-order equation is also obtained for the resistivity by a selective resummation of a complete subseries of electron self-energy diagrams. In this approximation, the resistivity exhibits a maximum for both ferro- and antiferromagnetic coupling (but at different temperatures) as the characteristic temperature is approached. The "bound-state" behavior appears in this theory as an anomalous correlation between the two spin systems, and first occurs at the characteristic temperature when the external magnetic field is zero.

1. INTRODUCTION

THE model originally proposed by Kasuya[1] of a contact *s-d* exchange interaction between the conduction electrons and localized magnetic impurities in metals has led to many theoretical papers[2–9] which have gradually exposed several interesting properties lying behind its superficially simple structure. The divergent behavior in the resistivity in the case of isolated impurities was first found by Kondo,[3] who used standard perturbation theory to calculate the effect of the Pauli principle on the second-order intermediate states for the scattering probability of the conduction electrons. The sharpness of the Fermi surface gives rise to a $\ln T$ term in the resistivity; when this is combined with the usual lattice resistivity, the result is a resistance minimum in the case of antiferromagnetic coupling. This logarithmic temperature dependence implied that a divergence would occur in each term of higher order in perturbation theory as the temperature was decreased. Moreover, Nagaoka[5,6] pointed out that, even in third order, the lifetimes of the conduction elec-

* These results have arisen during the preparation of a Ph.D. thesis, submitted to the University of London.
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trons would also go negative at the Fermi surface, below a critical temperature T_k. It is the study of such anomalous behavior which has resulted in the papers concerned with this model over the last three years using both perturbational and nonperturbational techniques. Other authors have concentrated on the magnetic properties of this model.[10–12]

In this paper we present a perturbational treatment of this interesting Hamiltonian, which can be used to make straightforward calculations at all temperatures (and in a magnetic field) to all orders of the perturbation in the interaction between the conduction electrons (characterized by a rectangular band model) and a single, localized magnetic impurity. This latter restriction implies that their collective effects (e.g., permanent magnetism) and interference effects between impurities can be ignored.

In the next section the proof of a Wick theorem[13] for spin-$\frac{1}{2}$ operators is presented which is both simple in form and easy to use; this results in the extension of conventional quantum field theory techniques to all problems involving such localized spin operators. It must be emphasized that the present method uses only Feynman-type diagrams in contrast to many other approaches to this problem.[14] It also has the principal advantage (not immediately apparent in this problem) that there is a normalized correspondence between spin-space averages and averages taken in the representational space. This means that for those problems involving many localized spin operators (for example, the Heisenberg model or the higher-concentration regions of this model) one does *not* have to compensate for on-site coincidences. This must be done for all those methods which do not exhibit a unit correspondence, and this includes the Abrikosov technique[7] for $S=\frac{1}{2}$, even for zero magnetic field.[15]

So in Sec. 3 the problem is reformulated using the drone-fermion representation[16] used in Sec. 2 and the various diagrammatic vertices for this interaction are introduced. We follow Doniach[8] in using an effective potential for the electrons (but now diagonalized differently) which determines the repeated scattering properties of any single impurity. These are then resummed, taking advantage of the unit correspondence of this method, to determine the effects of multiple scattering from several impurities (still in the low-concentration region.)

In Sec. 4, second-order corrections to several self-energy functions are evaluated in both the low- and high-field regimes (relative to the thermal energy kT). We concentrate here on the magnetic properties of the electrons and of the impurity.[17] The static result is compared with the calculations of Yosida and Okiji,[10] who used conventional low-order perturbation theory from the normal ground state. This is also compared with the decoupling treatment of Nagaoka[6] and with the recent work of Fullenbaum and Falk.[11] This result is shown to arise from a $J^2 \ln T$ correction to the impurity g shift, where J is the exchange-coupling constant. This term arises from the effects of the electrons which have been partially polarized by the external field. An analogous result holds for the electrons which now are affected by the partially polarized impurity.

Since this is a Green's-function analysis we can always investigate the complete line shape rather than just the relaxation times which are given as a special case on the energy shell. So the impurity properties can be derived directly from the transverse susceptibility function $\chi^T(\omega)$, which in the low-field region is found to have a Lorentzian form with a damping term proportional to J^2T. In the high-field region the temperature dependence is effectively replaced by the Zeeman energy. The damping term for the electrons is also shown to be proportional to the longitudinal spin fluctuations.

A resummation is made in Sec. 5 by examining the structure of higher-order propagators and exploiting the idea of polarization discussed in Sec. 4. This results in a closed-form expression for the effective potential which does diverge (but not the mass operator) at T_k for $J<0$. However, as the denominator of these expressions is evaluated to $O(J^2)$ [in contrast to other authors, which were to $O(J)$] a new divergence is also introduced for $J>0$, but this is now at a much lower temperature than T_k. Unlike previous perturbational treatments[5–9] for $J<0$, the sign of the lifetime for the electrons is found to be unchanged throughout the whole temperature range. Anomalous behavior, besides maximum scattering, is indicated in the present theory by the appearance at T_k of conjugate poles in the complex, ω plane of the transform of the correlation function of the two spin systems, at the impurity.

In the last section the results of earlier authors[6,7,9] (who have also effectively summed a series of self-energy terms) are reduced to a comparable form and the degree of agreement exhibited. We also include a new manipulation of Nagaoka's[6] second approximation to his high-temperature ($T>T_k$) result into a form closely resembling the present result, which now appears to be an interpolation of several previous and disparate methods in the high-temperature regime.

2. WICK'S THEOREM FOR SPIN-$\frac{1}{2}$ OPERATORS

A simple Wick theorem[13] is presented which enables time-ordered products of spin operators to be rewritten

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as a sum of products of time-ordered pairs of the operators used to represent the actual spin operators.

A representation which is quite straightforward is the drone-fermion representation,[16] where the drones accommodate the Bose-like commutation rules between different localized spin sites. Thus for spin-$\frac{1}{2}$ operators S localized at the positions R_j we have

$$S_j^z = c_j^\dagger c_j - \tfrac{1}{2}, \qquad S_j^+ = c_j^\dagger \phi_j, \qquad \phi_j = d_j + d_j^\dagger, \quad (2.1)$$

where

$$S_j^+ = S_j^x + iS_j^y = (S_j^-)^\dagger, \quad (2.2)$$

as the representation is Hermitian.

Among themselves the fermion fields obey anticommutation rules:

$$[c_j, c_l^\dagger]_+ = [d_j, d_l^\dagger]_+ = \delta_{jl} \quad (2.3)$$

and all the others anticommute.

If we define a "vacuum" state $|0\rangle$ with respect to the C or D fields by the usual condition,

$$c_j |0\rangle = d_j |0\rangle = 0, \quad (2.4)$$

then we have a complete, double representation of the eigenstates of the spin operators. If we denote the spin-up (spin-down) state for each site by $|\frac{1}{2}, +\frac{1}{2}\rangle$ ($|\frac{1}{2}, -\frac{1}{2}\rangle$) (omitting the site index for the moment), then

$$|\tfrac{1}{2}, -\tfrac{1}{2}\rangle = |0\rangle \quad \text{or} \quad d^\dagger |0\rangle;$$
$$|\tfrac{1}{2}, \tfrac{1}{2}\rangle = c^\dagger d^\dagger |0\rangle \quad \text{or} \quad c^\dagger |0\rangle. \quad (2.5)$$

It is shown below that Wick's theorem may be used for traces of operator products in this representation. In perturbation theory, we need to evaluate thermodynamic averages with respect to a diagonalized Hamiltonian H_0 which we will take to be proportional to S^z.

$$H_0 = \omega_0 S^z = \omega_0 (c^\dagger c - \tfrac{1}{2}) \quad (2.6)$$

or

$$[H_0, c^\dagger]_- = \omega_0 c^\dagger; \qquad [H_0, d^\dagger]_- = 0. \quad (2.7)$$

If we let X_j denote a product of spin S_j operators, then a thermal trace over the two spin states gives, with $\beta = (kT)^{-1}$,

$$\mathrm{Tr}_s\{\exp(-\beta H_0) X_j\} = \tfrac{1}{2}\,\mathrm{Tr}_c\{\exp(-\beta H_0) X_j\}, \quad (2.8)$$

where in the right-hand side the trace refers to all four orthogonal C and D states; all spin operators have been replaced by their drone-fermion representations.

In an obvious notation, the equation involving thermal averages becomes

$$\langle X_j(S)\rangle_0^s = \langle X_j(c)\rangle_0^c. \quad (2.9)$$

It is very important to note here that there are no problems involving normalization since $Z_s^0 = \frac{1}{2} Z_c^0$; this is of crucial importance in problems involving many localized spins.

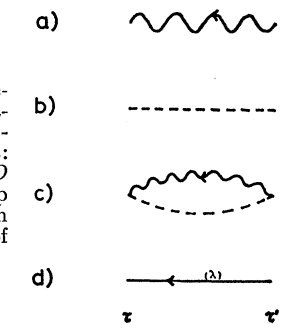

FIG. 1. Diagrammatic representation of the free "field" propagators (the drone-fermions) involving temperature variables: (a) C propagator $C^0(\tau)$. (b) D propagator $D^0(\tau)$. (c) Spin-flip propagator $F^0(\tau)$. (d) Electron (Wannier) propagator $G_\lambda^0(\tau)$ of spin λ.

The final step is now trivial; we can use Gaudin's[18] method for deriving Wick's theorem involving cyclic permutation of the C or D operators under the trace; thus for Wick ordering,

$$\langle T_W\{A_1, A_2, \cdots A_{2n}\}\rangle_0^c = \sum_{\text{all pairs}} (-1)^P \prod_{i,j}^{n} \langle T_W\{A_i, A_j\}\rangle_0^c, \quad (2.10)$$

where P is the signature of the permutation, and A_i is any operator c, $c^\dagger$, ϕ, evaluated in the interaction picture

$$c^\dagger(\tau) = \exp(H_0\tau) c^\dagger \exp(-H_0\tau) = \exp(\omega_0\tau) c^\dagger;$$
$$\phi(\tau) = \phi, \quad (2.11)$$

where $\tau = it$, the usual "temperature variable." Then by Eq. (2.11)

$$\langle c_j^\dagger c_l\rangle_0 = \delta_{jl} f^-; \qquad \langle d_j d_l^\dagger\rangle_0 = \tfrac{1}{2}\delta_{jl} \quad (2.12)$$

with

$$f^- = (\exp(\beta\omega_0) + 1)^{-1} = 1 - f^+.$$

We now define the free (denoted by zero superscript) temperature-ordered C and (symmetrized) D propagators, $C^0(\tau)$ and $D^0(\tau)$, and use Eq. (2.12),

$$C_{jl}^0(\tau) = \langle T_W\{c_j(\tau) c_l^\dagger(0)\}\rangle_0 = \delta_{jl}\exp(-\omega_0\tau)\{\theta(\tau) f^+ - \theta(-\tau) f^-\},$$
$$D_{jl}^0(\tau) = \langle T_W\{\phi_j(\tau)\phi_l(0)\}\rangle_0 = \delta_{jl}\{\theta(\tau) - \theta(-\tau)\}, \quad (2.13)$$

where $\theta(\tau) = 1$ if $\tau > 0$, and zero if $\tau < 0$.

Then the C propagator can be represented diagrammatically by a directed wavy line from the point 0 to the point τ and an undirected checked line between 0 and τ for the D propagator, Figs. 1(a) and 1(b). There is one other propagator of interest, that is the spin-flip propagator $F(\tau)$, which is represented by a parallel pair of C and D lines, Fig. 1(c):

$$F_{jl}^0(\tau) = \langle T_W\{S_j^-(\tau) S_l^+(0)\}\rangle_0^s = \delta_{jl} C^0(\tau) D^0(\tau). \quad (2.14)$$

This well illustrates the nature of the drone propagator,

[18] M. Gaudin, Nucl. Phys. **15**, 84 (1966).

for it converts the C propagator from fermion properties to Bose-like (as one requires for spin waves, for example). These functions also have simple Fourier series transforms for the temperature variable τ $(-\beta<\tau<\beta)$, using the notation

$$\bar{\nu}=(2\nu+1)\pi kT, \qquad \bar{\alpha}=2\alpha\pi kT$$

ν and α taking all integer values, so

$$C^0(\tau)=(1/\beta)\sum_{\bar{\nu}}\exp(-i\bar{\nu}\tau)C^0(\bar{\nu}),$$

with

$$C^0(\bar{\nu})=(\omega_0-i\bar{\nu})^{-1}; \tag{2.15}$$

similarly,

$$D^0(\bar{\nu})=-2/i\bar{\nu}$$

and

$$F^0(\bar{\alpha})=[\tanh(\tfrac{1}{2}\beta\omega_0)]/(\omega_0-i\bar{\alpha}). \tag{2.16}$$

N.B. $F^0(\bar{\alpha})$ is not defined for $\omega_0=0$, unless it can be nonvanishingly renormalized, although $F^0(\tau)$ is well defined (in fact, $\frac{1}{2}$).

We are now ready to proceed to investigate many-body problems involving explicit localized spin operators, using the systematic techniques of quantum field theory.[19]

3. *s-d* HAMILTONIAN

We shall consider the effects of localized impurities interacting with conduction electrons, in the limit of low concentrations ($c\ll 1$). This implies that we need not be concerned with the effects of interference between different impurity sites (as Abrikosov has shown[7]), so that we will initially consider only one impurity (at the origin, for convenience) and then evaluate averages over the ensemble of random impurities.[20]

The unperturbed, diagonal Hamiltonian H_0 for the conduction electrons and the localized impurity in an external static field $\mathfrak{H}^z$ is given by

$$H_0=\sum_{\mathrm{p},\lambda}\xi_{\mathrm{p}\lambda}a_{\mathrm{p}\lambda}{}^{\dagger}a_{\mathrm{p}\lambda}+\omega_0 S^z, \qquad \lambda=\pm 1 \tag{3.1}$$

with

$$\xi_{\mathrm{p}\lambda}=\epsilon_{\mathrm{p}}-\mu+\tfrac{1}{2}\lambda\omega_0; \qquad \omega_0=g\mu_B\mathfrak{H}^z. \tag{3.2}$$

It should be noted that although we have taken $g(\text{electrons})=g(\text{spin})$, this is only for convenience. We will not need the explicit form for ϵ_{p} or the Fermi energy μ, as these will be superseded at the appropriate moment by a suitable choice of band model for the electrons. In fact, we will always use the constant density-of-states model,[10]

$$\rho(\omega)=\pi^{-1}\,\mathrm{Im}G_\lambda{}^0(\omega+is)=\rho \quad \text{if} \quad -D\leq\omega-\tfrac{1}{2}\lambda\omega_0\leq D, \tag{3.3}$$

and zero otherwise, where we have introduced the transform of the Wannier propagator[8] at the origin of spin orientation λ:

$$\alpha_\lambda=N^{-1/2}\sum_{\mathrm{p}}a_{\mathrm{p}\lambda}, \tag{3.4}$$

$$G_\lambda{}^0(\tau)=\langle T_W\{\alpha_\lambda(\tau)\alpha_\lambda{}^{\dagger}(0)\}\rangle_0$$
$$=N^{-1}\sum_{\mathrm{p}}\exp(-\xi_{\mathrm{p}\lambda}\tau)\{\theta(\tau)f_{\mathrm{p}\lambda}{}^{+}-\theta(-\tau)f_{\mathrm{p}\lambda}{}^{-}\}, \tag{3.5}$$

with

$$f_{\mathrm{p}\lambda}{}^{-}=\{\exp(-\beta\xi_{\mathrm{p}\lambda})+1\}^{-1}=1-f_{\mathrm{p}\lambda}{}^{+}$$

and

$$G_\lambda{}^0(\bar{\nu})=N^{-1}\sum_{\mathrm{p}}\{\xi_{\mathrm{p}\lambda}-i\bar{\nu}\}^{-1}. \tag{3.6}$$

Then in terms of the Wannier operators, the δ-function range interaction is given by

$$H_1=-J\mathbf{S}\cdot\sum_{\lambda,\lambda'}\alpha_\lambda{}^{\dagger}\boldsymbol{\sigma}_{\lambda\lambda'}\alpha_{\lambda'}. \tag{3.7}$$

In terms of the drone-fermion representation for $S=\frac{1}{2}$,

$$H_1=-J\{c^{\dagger}\phi\alpha_{\downarrow}{}^{\dagger}\alpha_{\uparrow}+\phi c\alpha_{\uparrow}{}^{\dagger}\alpha_{\downarrow}+\sum_{\lambda}\lambda(c^{\dagger}c-\tfrac{1}{2})\alpha_\lambda{}^{\dagger}\alpha_\lambda\}. \tag{3.8}$$

Using H_1 in the form of Eq. (3.8) as the basis of our perturbation theory and the above-proven Wick theorem for the C and D operators, we can use all the standard results of quantum field theory,[19] especially the Dyson development operator $U(\beta)$ and the linked-cluster theorem. Thus, for exact thermal averages of any Heisenberg operator $\mathbf{A}$ we have, in the interaction picture,

$$\langle\mathbf{A}\rangle=\langle AU(\beta)\rangle_0{}^{L_D};$$
$$U(\beta)=T\exp\left\{-\int_0^\beta d\tau' H_1(\tau')\right\}. \tag{3.9}$$

The superscript L_D denotes the inclusion only of topologically distinct diagrams which are continuous with the "external" operators in A, through any one of the following interaction vertices (see Fig. 2). Equation (3.9) also introduces a crucial property of the drone D field. The transformed interaction Hamiltonian Eq. (3.8) without the D operators would involve only triple products of fermion operators, but the usual

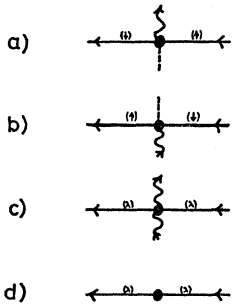

FIG. 2. The simplest interaction vertices for the conduction electrons scattering off the localized spin impurity. The solid lines represent Wannier electron propagators and (a)–(d) correspond to the order of the terms in Eq. (3.8) of the text.

[19] A. A. Abrikosov, L. P. Gor'kov, and D. I. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1963).
[20] S. F. Edwards, Phil. Mag. **3**, 1020 (1958).

substitution of the Wick-ordering operator in the development operator for the Dyson-ordering operator is only valid for even-order products of fermionlike operators. So although we are only dealing with single localized spins, the presence of the drones is of strict mathematical importance.

4. LOW-ORDER CORRECTIONS IN AN EXTERNAL FIELD

The evaluation of the two lowest-order corrections (in powers of J) to the self-energy parts of the previously defined propagators is exhibited in this section. We define an effective potential $V_\lambda^{(n)}(\tau)$ for nth-order scattering of electrons of spin orientation λ off the impurity by the criterion that this part of the graph is irreducible with respect to any one electron line. It should be noted that this differs from Doniach's effective potential where the contributions diagonal in the combined spin of the impurity and of an electron are chosen. This is convenient in the case when no external field is present, as it leaves the Hamiltonian rotationally invariant. However, in a later paper[9] this led to difficulties which will be specified in Sec. 6.

Thus, in Fig. 3, the effective potential will be defined by writing the contribution from the diagram in the form

$$\iint_0^\beta d\tau_1 d\tau_2 G_\lambda^0(\tau-\tau_1) V_\lambda(\tau_1-\tau_2) G_\lambda^0(\tau_2-\tau').$$

Thus the perturbation terms represented by Figs. 3(a) and 3(b) give the total first-order contribution

$$V_\lambda^{(1)}(\tau)=\lambda J\delta(\tau)\{\langle c^\dagger c\rangle_0-\tfrac{1}{2}\}=\lambda J\delta(\tau)\langle S^z\rangle_0. \quad (4.1)$$

Its (odd-periodic) Fourier series transform is therefore

$$V_\lambda^{(1)}(\bar\nu)=\lambda J\langle S^z\rangle_0. \quad (4.2)$$

This is the expected first-order field splitting of the two spin bands which vanishes as the field decreases to zero.

When we consider the second-order effects Fig. 3(c) and 3(d), we can immediately appreciate the dynamics of the situation as the graphs show explicitly which terms in the Hamiltonian are contributing in each case. For example, in Fig. 3(c), we can see that the electron is scattering longitudinally and coherently off the impurity, in contrast to the second-order reducible graph, when the scattering is incoherent, i.e., the two spin averages are quite independent (see later). The contribution of this coherent graph is

$$V_\lambda^{(2l)}(\tau)=-J^2G_\lambda^0(\tau)C^0(\tau)C^0(-\tau)=-J^2f^+f^-G_\lambda^0(\tau). \quad (4.3)$$

Similarly, Fig. 3(d) corresponds to transverse coherent scattering, with the excitation of a spin-flip (or spin-wave, in a lattice) in the intermediate state. Its contribution is

$$V_\lambda^{(2t)}(\tau)=J^2G_{-\lambda}^0(\tau)F^0(\lambda\tau). \quad (4.4)$$

The transform of both contributions becomes

$$V_\lambda^{(2)}(\bar\nu)=\frac{J^2}{N}\sum_{\mathrm{p}}\frac{\{f^+f^-+f^\lambda f_{\mathrm{p}-\lambda}{}^++f^{-\lambda}f_{\mathrm{p}-\lambda}{}^-\}}{\xi_{\mathrm{p}\lambda}-i\bar\nu}. \quad (4.5)$$

This form exhibits the symmetry due to the choice $g_e=g_s$ although the above formalism allows for different g values. Using the constant density-of-states model for the electrons, we can write down the analytic continuation of this expression just above and below the real ω axis (i.e., $i\bar\nu=\omega\pm is$).

$$V_\lambda^{(2)}(\omega\pm is)=\rho J^2\int_{-D}^{D}dE \times\frac{\{f^+f^-+f^\lambda f^+(E-\frac{1}{2}\lambda\omega_0)+f^{-\lambda}f^-(E-\frac{1}{2}\lambda\omega_0)\}}{E+\frac{1}{2}\lambda\omega_0-\omega\mp is}. \quad (4.6)$$

This is still an exact expression for the second-order effective one-electron potential. The absorptive part is given by

$$\mathrm{Im}V_\lambda^{(2)}(\omega\pm is)=\pm\pi\rho J^2 \times\{f^+f^-+f^\lambda f^{-\lambda}(\omega_0-\lambda\omega)+f^{-\lambda}f^\lambda(\omega_0-\lambda\omega)\}, \quad (4.7)$$

where the usual limiting procedure has been used, that is,

$$\lim_{s\to0+}(x\mp is)^{-1}=\mathcal{P}x^{-1}\pm i\pi\delta(x).$$

Now on the energy shell at the Fermi surface ($\omega=0$) we have

$$\mathrm{Im}V_\lambda^{(2)}(0\pm is)=\pm\pi\rho J^2 3f^+f^- =\pm3\pi\rho J^2\{\langle(S^z)^2\rangle_0-\langle S^z\rangle_0^2\} \quad (4.8)$$

or in the limit of zero magnetic field (denoted by a zero subscript, instead of λ)

$$\mathrm{Im}V_0^{(2)}(\omega\pm is)=\pm\tfrac{3}{4}\pi\rho J^2. \quad (4.9)$$

This is essentially Abrikosov's[7] lowest-order result, for $S(S+1)=\frac{3}{4}$ for $S=\frac{1}{2}$, and exhibits the expected rotational invariance as both the transverse and longitudinal terms contribute the same factor in the proportion 2 to 1. The shift in the one-electron energy is given by the real part of Eq. (4.6). It is evaluated in two limits; the first is the high-temperature region $kT\gg\omega_0$ or ω; then each of the three terms in the in-

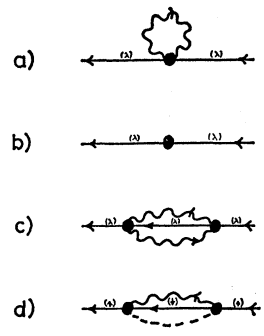

FIG. 3. The lowest-order corrections to the one-electron Wannier propagators. (a) and (b) are first-order corrections $O(J)$, while (c) and (d) are second-order corrections $O(J^2)$.

tegral can be evaluated separately to give

$$\mathrm{Re}V_\lambda^{(2)}(\omega)=\rho J^2\left\{f^+f^-\ln\left|\frac{D-\omega+\frac{1}{2}\lambda\omega_0}{D+\omega-\frac{1}{2}\lambda\omega_0}\right|+f^\lambda\left[\ln\left(\frac{2\gamma\beta D}{\pi}\right)+\ln\left|\frac{D-\omega+\frac{1}{2}\lambda\omega_0}{D+\omega-\lambda\omega_0}\right|\right]\right.$$
$$\left.-f^{-\lambda}\left[\ln\left(\frac{2\gamma\beta D}{\pi}\right)+\ln\left|\frac{D+\omega-\frac{1}{2}\lambda\omega_0}{D+\omega-\lambda\omega_0}\right|\right]\right\}, \quad (4.10)$$

where $\ln\gamma\simeq 0.58$ is Euler's constant. Thus, in a finite external field, neglecting terms of $O(\omega_0/D)$, we have for $\omega\simeq 0$

$$\mathrm{Re}V_\lambda^{(2)}(0)=2\lambda\rho J^2\langle S^z\rangle_0\ln(\pi kT/2\gamma D). \quad (4.11)$$

Again in the zero-field limit, we have (exactly)

$$\mathrm{Re}V_0^{(2)}(\omega)=S(S+1)\rho J^2\ln|\,(D-\omega)/(D+\omega)\,|. \quad (4.12)$$

This could have been anticipated from Eq. (4.5) for

$$V_0^{(2)}(\omega\pm is)=S(S+1)\rho J^2G_\lambda^0(\omega\pm is). \quad (4.13)$$

If we are in the high-temperature regime, that is, far above the Kondo temperature T_k, we can use the low-concentration expression for the electron self-energy $M_{p\lambda}(\omega)$ [anticipating the results of the next section, i.e., Eq. (5.37)]

$$G_{p\lambda}^{(2)}(\omega)=\{\xi_{p\lambda}-cV_\lambda^{(2)}(\omega)-\omega\}^{-1}. \quad (4.14)$$

The value of this expression above the cut on the real ω axis defines the new single-particle energy $E_{p\lambda}$ and the damping coefficient γ by

$$E_{p\lambda}^{(2)}-i\gamma^{(2)}=\epsilon_{p\lambda}-cV_\lambda^{(1+2)}(0+is), \quad (4.15)$$

so that

$$E_{p\lambda}^{(2)}=\epsilon_p+\tfrac{1}{2}\lambda \times\{\omega_0-c2J\langle S^z\rangle_0[1+2\rho J\ln(\pi kT/2\gamma D)]\} \quad (4.16)$$

and

$$\gamma^{(2)}=c3\pi\rho J^2\{\langle(S^z)^2\rangle_0-\langle S^z\rangle_0^2\}. \quad (4.17)$$

It can be seen immediately that the first- and second-order shifts are direct field shifts and vanish as the external field vanishes. As we shall see, the $\ln T$ term occurs in all higher orders and the present result indicates that its introduction is a "polarization" effect as will be confirmed in the next section. The coefficient $\gamma^{(2)}$ is just the electronic relaxation time in the first Born approximation given by Abrikosov[7] for $\mathfrak{H}^z=0$. The present result demonstrates that it originates from fluctuations in the magnetization of the magnetic scatterers—it is the dominant damping mechanism at high temperatures. The energy shift gives a contribution to the electronic relative magnetization, defined by

$$\zeta=\tfrac{1}{2}\sum_\lambda\lambda\langle\alpha_\lambda^\dagger\alpha_\lambda\rangle, \quad (4.18)$$

so that

$$\zeta=-\tfrac{1}{2}\rho\{\omega_0-c2J\langle S^z\rangle_0[1+2\rho J\ln(\pi kT/2\gamma D)]\}. \quad (4.19)$$

In a similar manner, we can calculate the first- and second-order corrections to $C(\tau)$ and $D(\tau)$, whose self-energy parts are denoted by $\Sigma(\tau)$ and $\Lambda(\tau)$, respectively. We will first evaluate Σ which is sufficient to give the corrections to the static susceptibility. The first-order result corresponding to Fig. 4(a) merely reflects the polarization of the impurity spins by the induced electronic magnetization:

$$\Sigma^{(1)}(\omega)=2J\zeta^0=-\rho J\omega_0. \quad (4.20)$$

As expected there are no self-consistent solutions (e.g., molecular-field type) for $\Sigma^{(1)}$ and $V^{(1)}$ when $\mathfrak{H}^z=0$. This is contrary to the case where the impurities interact, when the Curie temperature is finite.

When we evaluate Σ to $O(J^2)$, the first-order corrections on the first-order internal electron "loop" must also be included [see Fig. 4(b) (i and ii)] since these give a large contribution. This cancels exactly with parts of the other second-order graphs, involving the excitation of an electron-hole pair [see Fig. 4(b) (iii and iv)].

So we have

$$\Sigma^{(2i)}(\tau)=-J^2C^0(\tau)\sum_\lambda G_\lambda^0(\tau)G_\lambda^0(-\tau),$$
$$\Sigma^{(2i)}(\tau)=-J^2D^0(\tau)G_\uparrow^0(\tau)G_\downarrow^0(-\tau). \quad (4.21)$$

Thus the analytic continuation of the transforms of these two expressions is

$$\Sigma^{(2)}(\omega)=\left(\frac{J}{N}\right)^2\sum_{pp'}\frac{\{f_{p\uparrow}{}^+f_{p'\downarrow}{}^-+f_{p\uparrow}{}^-f_{p'\downarrow}{}^++\sum_\lambda[f^+f_{p\lambda}{}^+f_{p'\lambda}{}^-+f^-f_{p\lambda}{}^-f_{p'\lambda}{}^+]\}}{\epsilon_p-\epsilon_{p'}+\omega_0-\omega}. \quad (4.22)$$

Again using the constant density-of-states curve, the imaginary part of this function above or below the real ω axis is

$$\mathrm{Im}\Sigma^{(2)}(\omega\pm is)=\pm\pi(\rho J)^2\left\{\omega\coth(\tfrac{1}{2}\beta\omega)+\frac{2(\omega_0-\omega)}{\exp[\beta(\omega_0-\omega)]-1}\left[\frac{1+\exp(-\beta\omega)}{1+\exp(-\beta\omega_0)}\right]\right\}. \quad (4.23)$$

If this exact expression is evaluated in the high-temperature region $kT \gg \omega_0$ in the limit $\omega \to \omega_0$ then

$$\mathrm{Im}\Sigma^{(2)}(\omega_0 \pm is) = \pm 4\pi(\rho J)^2 kT. \tag{4.24}$$

Similarly when $kT \gg \omega_0$ or ω, then

$$\mathrm{Re}\Sigma^{(2)}(\omega) = 4(\rho J)^2\{(\omega - \tfrac{1}{2}\omega_0)[1+\ln(2\gamma\beta D/\pi)] + (\omega_0 - \omega - 2D\langle S^z\rangle_0)\ln 2\}. \tag{4.25}$$

If all the other contributions are included up to $O(J^2)$, the result is

$$\Sigma^{(1+2)}(\omega \pm is) = -\rho J\omega_0 + 4(\rho J)^2 \times\{(\omega - \tfrac{1}{2}\omega_0)[1+\ln(2\gamma\beta D/\pi)] + (\omega_0 - \omega)\ln 2 \pm i\pi kT\}. \tag{4.26}$$

So on the energy shell of the C excitation, i.e., $\omega = \omega_0$,

$$\Sigma^{(1+2)}(\omega_0 \pm is) = 2J\zeta^0\{1+2\rho J\ln(\pi kT/2\gamma D)\} \pm i4\pi(\rho J)^2 kT. \tag{4.27}$$

The other limiting case which can be evaluated from Eq. (4.22) is the very high-field limit $\omega_0, \omega \gg kT$; then

$$\Sigma^{(1+2)}(\omega_0 \pm is) = 2J\zeta^0\{1+2\rho J\ln|\omega_0/D|\} \pm i\pi(\rho J)^2\omega_0. \tag{4.28}$$

If we are interested in the high-temperature static susceptibility of the total system χ^z, we will only be interested in Eq. (4.27).

So Dyson's equation for the C propagator with $\Sigma(\omega)$ evaluated on the energy shell gives

$$C(\omega \pm is) = \{\omega_0 - \Sigma(\omega_0 \pm is) - \omega\}^{-1} = \{\omega_r \mp i\Gamma - \omega\}^{-1}, \tag{4.29}$$

where

$$\omega_r = \omega_0\{1+\rho J[1+2\rho J\ln(\pi kT/2\gamma D)]\}$$

and

$$\Gamma = 4\pi(\rho J)^2 kT. \tag{4.30}$$

The magnetization can be directly evaluated in this approximation, since Γ (the Korringa width) is much smaller than kT. In the usual manner the correlation function $\langle c^\dagger c\rangle$ is obtained by replacing the sum over ν by an integral over ω on the Fermi-Dirac contour C_f, which encircles the whole of the imaginary ω axis, except the origin, in a counterclockwise direction. This contour is then deformed to encircle the damped pole off the real ω axis:

$$\langle c^\dagger c\rangle = (2\pi i)^{-1}\oint_{C_f} d\omega f^-(\omega)C(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f^-(\omega)\frac{\Gamma}{\{(\omega_r-\omega)^2+\Gamma^2\}}. \tag{4.31}$$

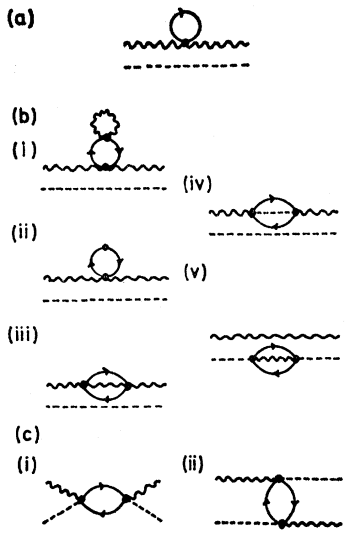

FIG. 4. The lowest-order corrections to $O(J^2)$ for the spin resonance frequency shift. (a)and (b) correspond to all simple corrections to the individual CD lines, while (c) represents their simplest interaction.

This is now approximated by taking

$$\langle c^\dagger c\rangle = f^-(\omega_r)\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\frac{\Gamma}{\{(\omega_r-\omega)^2+\Gamma^2\}}. \tag{4.32}$$

The use of Eq. (2.1) leads directly to the relative magnetization of the impurity spin:

$$\langle S^z\rangle = -\tfrac{1}{2}\tanh(\tfrac{1}{2}\beta\omega_r). \tag{4.33}$$

This can be expanded in the high-temperature approximation to give

$$\langle S^z\rangle \approx \langle S^z\rangle_0\{1+\rho J+2(\rho J)^2[\ln(\pi kT/2\gamma D)-1]\}. \tag{4.34}$$

Apart from the factor of 1 in the $O(J^2)$ term, this has the same structure as the electronic magnetization, that is, using Eq. (4.20),

$$\omega_r \simeq \omega_0 - 2J\zeta^0\{1+2\rho J\ln(\pi kT/2\gamma D)\}. \tag{4.35}$$

This means that the total static susceptibility for a concentration c of impurities has the form

$$\chi^z = \chi_{el}{}^z(0) + c\chi_s{}^z(0)\{1+2\rho J[1+2\rho J\ln(\pi kT/2\gamma D)]\}, \tag{4.36}$$

where the free static susceptibilities of the electrons $\chi_{el}{}^z(0)$ and of one impurity spin $\chi_s{}^z(0)$ are used.

This result exactly agrees with that found by Fullenbaum and Falk[11] (for $g=2$) who used a decoupling scheme similar to Nagaoka's[6] in a finite field, and the total static susceptibility was found from the change in the free energy to $O(J^2)$. It also agrees with the second-order result of Yosida and Okiji[10] (they included

no first-order contribution). However, Nagaoka's calculation differs from the present result by a factor of 2 in the $O(J^2)$ term, as does that of Scalapino[21] using the Anderson model evaluated to second order in $J_{(\text{effective})}$. The discrepancy is not understood but it should be emphasized that in this part of the calculation no diagrams have been omitted to $O(J^2)$ in any of the self-energy terms, V or Σ. The D field self-energy $\Lambda(\omega)$ Fig. 4(b)(v) is only needed for the evaluation of the spin-flip propagator and hence the dynamic g shift, or the localized transverse susceptibility $\chi^T(\omega)$. The latter is the analytic continuation above the real ω axis of the transform of $F(\tau)$, which is equal to the real Fourier transform of the retarded function

$$\chi^T{}_{\text{ret}}(t)=i\theta(t)\langle[S^-(t),S^+(0)]_+\rangle. \tag{4.37}$$

The contributions of Fig. 4(c) do not give a logarithmic temperature shift and cancel exactly in the static limit[17] (minus factor, due to interchange of the fermion like D line) and so in the limit $\beta\omega\ll 1$ are neglected.

This just leaves the self-energy effects on the individual C and D propagators, which then become a convolution to give $F(\tau)$

$$F(\bar{\alpha})=(1/\beta)\sum_{\nu}D(\bar{\nu})C(\bar{\alpha}-\bar{\nu}), \tag{4.38}$$

or

$$F(\omega)=\frac{1}{\pi i}\oint_{C_f}dz\,f^-(z)\times\{[z+2\Lambda(z)][\omega_0-\omega+z-\sum(\omega-z)]\}^{-1}. \tag{4.39}$$

This is deformed around the discontinuities of D and C at $\text{Im}z=0$ and $\text{Im}z=\text{Im}\omega$, respectively.

Writing $z=z_1+iz_2$; $\Lambda(z_1+is)=\Lambda_1(z_1)+i\Lambda_2(z_1)$, etc.,

$$F(\omega)=-2\pi^{-1}\int_{-\infty}^{\infty}dz_1 f^-(z_1)\times\left\{[\omega_0-\omega+z_1-\Sigma]^{-1}\frac{2\Lambda_2(z_1)}{(z_1+2\Lambda_1)^2+(2\Lambda_2)^2}-[z_1+i\omega_2+2\Lambda]^{-1}\frac{\Sigma_2(\omega_1-z_1)}{(\omega_0-\omega_1+z_1-\Sigma)^2+(\Sigma_2)^2}\right\}. \tag{4.40}$$

We have written out Eq. (4.40) to show the nature of the approximation to follow, which can only be done if the widths are small compared to kT; however we cannot be sure of this in higher orders, as we believe that the imaginary parts of the self-energies diverge in the anomalous temperature region (see later). But in simple second-order calculations there is no problem; thus taking into account the form of $\Sigma_1(\omega)$ and noting that

$$\Lambda^{(2)}(\omega\pm is)=2(\rho J)^2\{\omega[\ln(\gamma\beta D/\pi)+1]\pm i\pi kT\}, \tag{4.41}$$

we see that the first square bracket in Eq. (4.40) is strongly peaked around $z_1=0$ while the second peaks at $z_1=\omega_r$. After ensuring a unique analytic continuation,[22] we get

$$F(\omega)=2f^+(\omega_r)\{\omega_r-\omega-2\Lambda(\omega-\omega_r)\}^{-1}-\{\omega_0-\omega-\Sigma(\omega)\}^{-1}, \tag{4.42}$$

but to $O(J^2)$, near ω_r, $\Lambda(\omega-\omega_r+is)=\frac{1}{2}i\Gamma$, so the final result, in this approximation, is

$$F(\omega\pm is)=[\tanh(\tfrac{1}{2}\beta\omega_r)]/\{\omega_r-\omega\mp i\Gamma\}. \tag{4.43}$$

There is an internal check on the correctness of Eq. (4.43) through using the sum rule for $S=\frac{1}{2}$:

$$\langle S^z\rangle=\tfrac{1}{2}-\langle S^-S^+\rangle. \tag{4.44}$$

Thus

$$\langle S^z\rangle=\tfrac{1}{2}-(2\pi i)^{-1}\int_{-\infty}^{\infty}d\omega\{1-\exp(-\beta\omega)\}^{-1}\,\text{disc}F(\omega)\simeq\tfrac{1}{2}-f^-(\omega_r)=-\tfrac{1}{2}\tanh(\tfrac{1}{2}\beta\omega_r) \tag{4.45}$$

[cf. Eq. (4.33)].

The above results can be neatly summarized by stating the the impurity transverse susceptibility has the Lorentzian form

$$\chi^T(\omega)=\tanh(\tfrac{1}{2}\beta\omega_r)\left\{\frac{\omega_r-\omega+i\Gamma}{(\omega_r-\omega)^2+\Gamma^2}\right\}, \tag{4.46}$$

which is illustrated in Fig. 5.

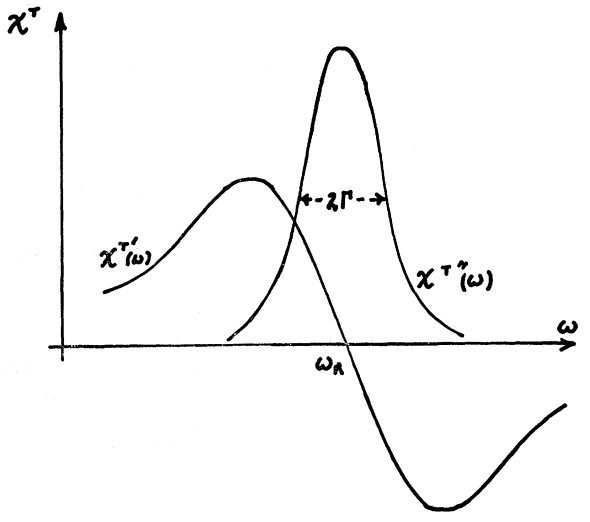

FIG. 5. The real and imaginary parts of the transverse susceptibility evaluated to $O(J^2)$.

[21] D. J. Scalapino, Phys. Rev. Letters **16**, 937 (1966).

[22] G. Baym and N. D. Mermin, J. Math. Phys. **2**, 232 (1961).

5. HIGHER-ORDER EFFECTS

In this section complete subseries of higher-order graphs are summed, which result in expressions evaluated $O(J^2)$ in the (divergent) denominators. This is accomplished by calculating the self-energy parts to $O(J^2)$ of more complex propagators. This extends the work of previous authors whose results were evaluated to $O(J)$ in the denominator and the divergences at the Kondo temperature T_k now enter into certain correlation functions rather than the resistivity, which reaches the unitarity limit of maximum (finite) scattering at T_k. Although various explicit formulas for the self-energies are obtained for finite magnetic fields they are, in fact, evaluated in the zero-field limit, where rotational symmetry introduces several simplifying features. This leads to equations which define a certain critical temperature (T_k for the case of antiferromagnetic coupling, $J<0$) and to a new ferromagnetic resonance ($J>0$) which occurs at a much lower temperature and so is merely of academic interest.

The first $\ln T$ term in the electronic effective potential only appears in second order [$O(J^2)$] for finite fields but in zero external field a nonvanishing $\ln T$ appears in third order, and is the first internal correction to the second-order skeleton graphs (which themselves were seen to exhibit no abnormalities when $\mathfrak{H}^z=0$). This suggests that all higher-order internal corrections to the simple skeleton graphs will be divergent. Thus propagators are constructed from these skeletons and their own self-energy parts are constructed to $O(J^2)$. In fact, a further series of graphs is also included arising from third-order skeleton graphs, which have the same structure as before; this maintains the correct coefficient to $O(J^3)$ in the numerator. By considering those irreducible graphs which occur within an initial and final interaction there will always be a factor of J^2 contributed to the numerator. In practice, this means we look for repeated scatterings of any two internal lines within the second-order skeleton graphs, while

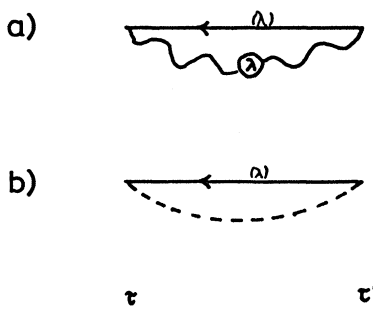

FIG. 6. The skeleton propagators corresponding to the correlated spin polarization of the conduction electrons around the impurity (a) Longitudinal part $\mathcal{S}^{z0}{}_{\lambda\lambda'}(\tau)$. (b) Transverse part $\mathcal{S}^{t0}{}_{\lambda}(\tau)$. Note: The λ in a circle refers to the direction of the C propagator (relative to the electron), for if $\lambda=1$, it propagates from 0 to τ and vice versa for $\lambda=-1$.

FIG. 7. Simplest diagonal element of the scattering matrix $\mathfrak{I}^z{}_{\lambda\lambda}(\tau)$.

the third line remains unaffected from the initial to final vertex (see Figs. 10 and 11).

Physically, this "bare" line effectively maintains the local spin (in the case of the electron self-energy) in a definite orientation with respect to the external electronic spin, i.e., the spin is "polarized" between the initial and final interaction and effectively behaves as if in a magnetic field like the finite-field second-order result (even in the case when there is no external magnetic field, the quantization of the electronic spin direction determines that of the local spin). This agrees with Abrikosov's[7] intuitive choice of cutting only one electron line and two spin lines at any internal point and with Silverstein and Duke.[23]

In all cases we will need the following propagators, illustrated in Fig. 6 [similar to the $\mathcal{G}(\omega)$ of Nagaoka[6] etc.], defined by

$$\mathcal{S}^{z0}{}_{\lambda\lambda'}(\tau)=G_{\lambda}{}^{0}(\tau)C^{0}(\lambda'\tau),$$
$$\mathcal{S}^{t0}{}_{\lambda}(\tau)=G_{-\lambda}{}^{0}(\tau)D^{0}(\lambda\tau). \tag{5.1}$$

The Fourier series transforms (Bose-like as a pair of fermions) are

$$\mathcal{S}^{z0}{}_{\lambda\lambda'}(\bar{\alpha})=\frac{\lambda'}{N}\sum_{\mathrm{p}}\frac{\{f^{\lambda'}f_{\mathrm{p}\lambda}{}^{+}-f^{-\lambda'}f_{\mathrm{p}\lambda}{}^{-}\}}{\xi_{\mathrm{p}\lambda}+\lambda'\omega_0-i\bar{\alpha}};$$
$$\mathcal{S}^{t0}{}_{\lambda}(\bar{\alpha})=\frac{\lambda}{N}\sum_{\mathrm{p}}\frac{\{f_{\mathrm{p}-\lambda}{}^{+}-f_{\mathrm{p}-\lambda}{}^{-}\}}{\xi_{\mathrm{p}-\lambda}-i\bar{\alpha}}. \tag{5.2}$$

We will define a longitudinal scattering matrix by

$$\mathcal{S}^{z}{}_{\lambda\lambda'}=\mathcal{S}^{z0}{}_{\lambda\lambda'}(\tau)$$
$$+\iint_0^{\beta}d\tau_1 d\tau_2\mathcal{S}^{z0}{}_{\lambda\lambda'}(\tau-\tau_1)\mathfrak{I}^{z}{}_{\lambda\lambda'}(\tau_1-\tau_2)\mathcal{S}^{z}{}_{\lambda\lambda'}(\tau_2) \tag{5.3}$$

or

$$\mathcal{S}^{z}{}_{\lambda\lambda'}(\bar{\alpha})=\frac{\mathcal{S}^{z0}{}_{\lambda\lambda'}(\bar{\alpha})}{1-\mathcal{S}^{z0}{}_{\lambda\lambda'}(\bar{\alpha})\mathfrak{I}^{z}{}_{\lambda\lambda}{}'(\bar{\alpha})}. \tag{5.4}$$

On evaluation of the graph in Fig. 7 and using Eqs. (5.3) and (5.4), we have $\mathfrak{I}^{z}{}_{\lambda\lambda}(\tau)=\lambda J\delta(\tau)$, so

$$\mathcal{S}^{z}{}_{\lambda\lambda}(\bar{\alpha})=\mathcal{S}^{z0}{}_{\lambda\lambda}(\bar{\alpha})/[1-\lambda J\mathcal{S}^{z0}{}_{\lambda\lambda}(\bar{\alpha})]. \tag{5.5}$$

For the off-diagonal longitudinal matrix elements, we need both graphs illustrated in Fig. 8, to be accurate

[23] S. D. Silverstein and C. B. Duke, Phys. Rev. **161**, 456 (1967); **161**, 470 (1967).

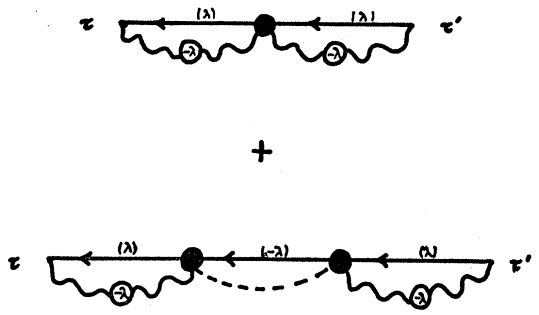

FIG. 8. The two lowest-order off-diagonal elements of $\mathfrak{Z}^z_{\lambda,-\lambda}(\tau)$.

to $O(J^2)$: $\mathfrak{Z}^z_{\lambda-\lambda}(\tau)=\lambda J\delta(\tau)-J^2\mathcal{S}^{t0}_\lambda(\tau)$, so

$$\mathcal{S}^z_{\lambda,-\lambda}(\bar\alpha)=\frac{\mathcal{S}^{z0}_{\lambda,-\lambda}(\bar\alpha)}{1-\lambda J\mathcal{S}^{z0}_{\lambda,-\lambda}(\bar\alpha)\{1-\lambda J\mathcal{S}^{t0}_\lambda(\bar\alpha)\}}. \quad (5.6)$$

The result for $\mathcal{S}^t_\lambda(\tau)$ can be simply obtained by examining Fig. 9 and realizing that the complete series can be obtained by replacing $\mathcal{S}^{z0}_{\lambda,-\lambda}(\bar\alpha)$ in the second term by the complete $\mathcal{S}^z_{\lambda,-\lambda}(\bar\alpha)$; remarkably this results in a form very similar to Eq. (5.6). The equation corresponding to Fig. 9 is

$$\mathcal{S}^{t2}_\lambda(\bar\alpha)=\mathcal{S}^{t0}_\lambda(\bar\alpha)-J^2\mathcal{S}^{t0}_\lambda(\bar\alpha)\mathcal{S}^{z0}_{\lambda,-\lambda}(\bar\alpha)\mathcal{S}^{t0}_\lambda(\bar\alpha).$$

Thus

$$\mathcal{S}^t_\lambda(\bar\alpha)=\frac{\mathcal{S}^{t0}_\lambda(\bar\alpha)\{1-\lambda J\mathcal{S}^{z0}_{\lambda,-\lambda}(\bar\alpha)\}}{1-\lambda J\mathcal{S}^{z0}_{\lambda,-\lambda}(\bar\alpha)\{1-\lambda J\mathcal{S}^{t0}_\lambda(\bar\alpha)\}}. \quad (5.7)$$

We will first use these propagators and their transforms in evaluating the effective potential for the electrons in a systematic way to $O(J^2)$.

We can renormalize the longitudinal scattering potential, Fig. 3(c), by splitting Eq. (4.3) into two equal contributions then renormalizing appropriate pairs of free propagators, thus

$$V_\lambda^{(2l)}(\tau)=-\tfrac{1}{2}J^2\{C^0(\tau)\mathcal{S}^{z0}_{\lambda\downarrow}(\tau)+C^0(-\tau)\mathcal{S}^{z0}_{\lambda\uparrow}(\tau)\}$$
$$=\tfrac{1}{2}\{V_\lambda^{(2la)}(\tau)+V_\lambda^{(2lb)}(\tau)\}. \quad (5.8)$$

Then upon effecting a Fourier series transform,

$$V_\lambda^{(2l)}(\bar\nu)=-(J^2/2\beta)\sum_{\bar\alpha}\{C^0(\bar\nu-\bar\alpha)\mathcal{S}^{z0}_{\lambda\downarrow}(\bar\alpha)$$
$$+C^0(\bar\alpha-\bar\nu)\mathcal{S}^{z0}_{\lambda\uparrow}(\bar\alpha)\}. \quad (5.9)$$

Now each of these parts can scatter independently and repeatedly (i.e., $\mathcal{S}^{z0}\to\mathcal{S}^z$), but this would involve overcounting the first term twice (see Fig. 10). If we now define the renormalized terms corresponding to the correct summation (note absence of brackets around superscript), we have

$$V_\lambda^{2l}(\bar\nu)=V_\lambda^{2la}(\bar\nu)+V_\lambda^{2lb}(\bar\nu)-V_\lambda^{(2l)}(\bar\nu). \quad (5.10)$$

So,

$$V_\lambda^{2l}(\bar\nu)=-(J^2/\beta)\sum_{\bar\alpha,\lambda'}C^0(\lambda'(\bar\alpha-\bar\nu))$$
$$\times\{\mathcal{S}^z_{\lambda\lambda'}(\bar\alpha)-\tfrac{1}{2}\mathcal{S}^{z0}_{\lambda\lambda'}(\bar\alpha)\}. \quad (5.11)$$

Similarly, for the transverse part [Fig. 3(d)], Eq. (4.4) becomes

$$V_\lambda^{(2t)}(\tau)=\tfrac{1}{2}J^2\{D^0(\lambda\tau)\mathcal{S}^{z0}_{-\lambda,\lambda}(\tau)+C^0(\lambda\tau)\mathcal{S}^{t0}_\lambda(\tau)\}, \quad (5.12)$$

which on transforming and renormalizing like Eq. (5.9) becomes

$$V_\lambda^{2t}(\bar\nu)=(J^2/\beta)\sum_{\bar\alpha}\{D^0(\lambda(\bar\nu-\bar\alpha))[\mathcal{S}^z_{-\lambda,\lambda}(\bar\alpha)$$
$$-\tfrac{1}{2}\mathcal{S}^{z0}_{-\lambda,\lambda}(\bar\alpha)]+C^0(\lambda(\bar\nu-\bar\alpha))$$
$$\times[\mathcal{S}^t_\lambda(\bar\alpha)-\tfrac{1}{2}\mathcal{S}^{t0}_\lambda(\bar\alpha)]\}. \quad (5.13)$$

Before proceeding, we must note that this procedure is not quite complete, as we are missing a whole subseries of graphs which have the same structure as those already considered. These are the two third-order skeleton graphs Fig. 11 which are needed when $\mathfrak{H}^z=0$ to preserve rotational symmetry. They give a contribution

$$V_\lambda^{(3t)}(\tau)=\lambda J^3C^0(\lambda\tau)\{R_\lambda^0(\tau)+\tilde R_\lambda^0(\tau)\}, \quad (5.14)$$

where

$$R_\lambda^0(\tau)=\int_0^\beta d\tau_1\mathcal{S}^{t0}_\lambda(\tau-\tau_1)\mathcal{S}^{z0}_{\lambda,-\lambda}(\tau_1);$$

$$\tilde R_\lambda^0(\tau)=\int_0^\beta d\tau_1\mathcal{S}^{z0}_{\lambda,-\lambda}(\tau-\tau_1)\mathcal{S}^{t0}_\lambda(\tau_1) \quad (5.15)$$

or

$$R_\lambda^0(\bar\alpha)=\tilde R_\lambda^0(\bar\alpha)=\mathcal{S}^{t0}_\lambda(\bar\alpha)\mathcal{S}^{z0}_{\lambda,-\lambda}(\bar\alpha). \quad (5.16)$$

So,

$$V_\lambda^{(3t)}(\bar\nu)=2\lambda(J^3/\beta)\sum_{\bar\alpha}C^0(\lambda(\bar\nu-\bar\alpha))R_\lambda^0(\bar\alpha). \quad (5.17)$$

This is simply renormalized by *only* converting $\mathcal{S}^{z0}_{\lambda,-\lambda}\to$

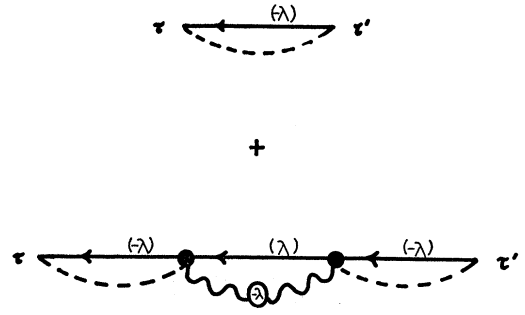

FIG. 9. The diagrammatic equation corresponding to Eq. (60) of the text.

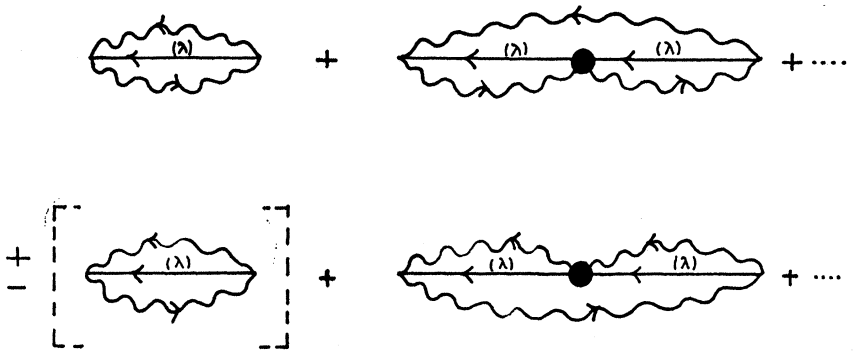

FIG. 10. Renormalization of the (skeleton) second-order effective potential, illustrating the procedure to avoid overcounting the first term twice.

$\mathcal{S}^z_{\lambda,-\lambda}$ in $R_\lambda{}^0(\bar{\alpha})$ [renormalizing $\mathcal{S}^{t0}{}_\lambda(\bar{\alpha})$ also would lead to some overcounting]:

$$V_\lambda{}^{3t}(\bar{\nu}) = 2\lambda \frac{J^3}{\beta} \sum_{\bar{\alpha}} \frac{C^0(\lambda(\bar{\nu}-\bar{\alpha}))\mathcal{S}^{t0}{}_\lambda(\bar{\alpha})\mathcal{S}^{z0}{}_{\lambda,-\lambda}(\bar{\alpha})}{1-\lambda J\mathcal{S}^{z0}{}_{\lambda,-\lambda}(\bar{\alpha})\{1-\lambda J\mathcal{S}^{t0}{}_\lambda(\bar{\alpha})\}}. \tag{5.18}$$

We can now define the complete second-order effective potential, or "polarization potential" $V_\lambda{}^P$ as the sum

$$V_\lambda{}^P = V_\lambda{}^{2l} + V_\lambda{}^{2t} + V_\lambda{}^{3t}. \tag{5.19}$$

The above expressions are somewhat inelegant, so we shall evaluate them in the zero-external-field limit (where many other graphs due only to field splitting also vanish). Thus we have $\lim_{\omega_0\to 0} C^0(\lambda\tau) = \frac{1}{2}D^0(\lambda\tau)$ with $D^0(\lambda\bar{\nu}) = \lambda D^0(\bar{\nu})$, so we can define the zero-field correlation propagator $\mathcal{S}^0(\bar{\alpha})$ by

$$\lambda'\mathcal{S}^0(\bar{\alpha}) = \mathcal{S}^{t0}{}_{\lambda'}(\bar{\alpha}) = 2\mathcal{S}^{z0}{}_{\lambda,\lambda'} = \frac{\lambda'}{N}\sum_{\mathrm{p}} \frac{\{f_{\mathrm{p}}{}^+ - f_{\mathrm{p}}{}^-\}}{\xi_{\mathrm{p}} - i\bar{\alpha}}. \tag{5.20}$$

In this limit Eqs. (5.7–5.9) become

$$\mathcal{S}^z{}_{\lambda,\lambda}(\bar{\alpha}) \to \frac{\frac{1}{2}\lambda\mathcal{S}^0(\bar{\alpha})}{1-\frac{1}{2}J\mathcal{S}^0(\bar{\alpha})};$$

$$\mathcal{S}^z{}_{\lambda,-\lambda}(\bar{\alpha}) \to \frac{-\frac{1}{2}\lambda\mathcal{S}^0(\bar{\alpha})}{\{1-\frac{1}{2}J\mathcal{S}^0(\bar{\alpha})\}\{1+J\mathcal{S}^0(\bar{\alpha})\}};$$

$$\mathcal{S}^t{}_\lambda(\bar{\alpha}) \to \frac{\lambda\mathcal{S}^0(\bar{\alpha})\{1+\frac{1}{2}J\mathcal{S}^0(\bar{\alpha})\}}{\{1-\frac{1}{2}J\mathcal{S}^0(\bar{\alpha})\}\{1+J\mathcal{S}^0(\bar{\alpha})\}}. \tag{5.21}$$

This exhibits the unexpected property of factorizable denominators, as we shall see this leads to ferromagnetic-resonance behavior as well as the usual antiferromagnetic. In fact, if we had only worked to $O(J)$ in the denominator we would only achieve the antiferromagnetic result *but with a factor* $\frac{1}{2}$ *instead of unity*: this factor is important because the Kondo temperature T_k depends exponentially upon it (see Sec. 6).

Before evaluating $V^P(\bar{\nu})$ we will look a little more carefully at $\mathcal{S}^0(\bar{\alpha})$ as this function frequently occurs in the present work (and in superconductivity). We can see that the effect of the spin operators in the interaction Hamiltonian (represented here by fermionlike C and D operators) has converted a bare fermionlike electron line to a Bose-like propagator. This introduces a temperature-dependent factor which changes sign as the momentum passes through the Fermi surface. So from Eq. (5.20) with the constant density of states, the analytically continued form is

$$\mathcal{S}^0(\omega \pm is) = A(\omega) \pm i\pi B(\omega), \tag{5.22}$$

where

$$A(\omega) = \mathcal{P}\int_{-D}^{D} dE\,[\tanh(\tfrac{1}{2}\beta E)]/(E-\omega)$$

and

$$B(\omega) = \tanh(\tfrac{1}{2}\beta\omega), \quad \text{if } |\omega| \le D$$
$$= 0, \quad \text{otherwise.} \tag{5.23}$$

We will also need to use the function $Q(\bar{\alpha})$ defined by

$$Q(\bar{\alpha}) = \frac{1-\frac{1}{2}J\mathcal{S}^0(\bar{\alpha})[1-J\mathcal{S}^0(\bar{\alpha})]}{\{1-\frac{1}{2}J\mathcal{S}^0(\bar{\alpha})\}\{1+J\mathcal{S}^0(\bar{\alpha})\}}, \tag{5.24}$$

or in its analytically continued form to $O(J)$ in the numerator

$$Q(\omega \pm is) = \frac{1 \mp i\pi\rho JB(\omega)}{|\{1-\frac{1}{2}J\mathcal{S}^0(\omega)\}\{1+J\mathcal{S}^0(\omega)\}|^2}. \tag{5.25}$$

We are now in a position to finally evaluate $V^P(\bar{\nu})$ by

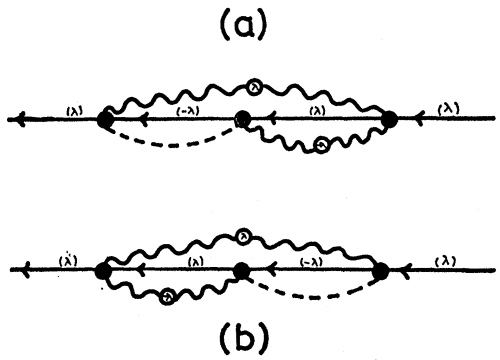

FIG. 11. The two third-order skeleton graphs which must be included to preserve spherical symmetry to $O(J^3)$.

using equations (5.11–5.25):

$$V_0{}^P(\bar{\nu}) = \tfrac{3}{4}(J^2/\beta) \sum_{\bar{\alpha}} D^0(\bar{\nu}-\bar{\alpha}) S^0(\bar{\alpha}) Q(\bar{\alpha}), \tag{5.26}$$

$$V_0{}^P(\omega) = -\frac{3}{2}\frac{J^2}{N} \sum_{\mathrm{p}} \tanh(\tfrac{1}{2}\beta\xi_{\mathrm{p}}) \times \frac{1}{2\pi i} \oint_{C_b} \frac{dz\, Q(z)}{(1-e^{-\beta z})(\omega - z)(\xi_{\mathrm{p}} - z)}. \tag{5.27}$$

The latter form defines the complex integral $I_{\mathrm{p}}(\omega)$ in terms of the Bose-contour C_b, which encircles the whole of the imaginary z axis; we have used the analytic continuations $\omega = i\bar{\nu}$ and $i\bar{\alpha} = z = z_1 + iz_2$. To evaluate $I_{\mathrm{p}}(\omega)$ we see that for $|\omega| \leq D$ discontinuities occur in the complex z plane at $z_2 = 0$ and $z_2 = \omega_2$. However, the discontinuity along the real axis takes in the pole at $z = \xi_{\mathrm{p}}$ as well as the discontinuity from $Q(z)$, i.e.,

$$\mathrm{disc}\left\{\frac{Q(z_1)}{\xi_{\mathrm{p}} - z_1}\right\} = \mathrm{disc}Q(z_1)\, \frac{\mathcal{P}}{\{\xi_{\mathrm{p}} - z_1\}} + 2\pi i \delta(\xi_{\mathrm{p}} - z_1)\, \mathcal{P}Q(z_1). \tag{5.28}$$

This procedure is necessary to pick up the simple second-order result when $Q(z_1) = 1$. Thus deforming C_b around the two mentioned discontinuities we obtain, just above the real ω axis,

$$I_{\mathrm{p}}(\omega + is) = -\tfrac{1}{4}\, \mathrm{disc}Q(\omega)\, \coth(\tfrac{1}{2}\beta\omega)\{\xi_{\mathrm{p}} - \omega\}^{-1} - i\tfrac{1}{2}\pi\delta(\xi_{\mathrm{p}} - \omega) Q(\omega)\, \coth(\tfrac{1}{2}\beta\omega) + \tfrac{1}{2}\{\xi_{\mathrm{p}} - \omega\}^{-1}\left\{Q(\omega) - \frac{\frac{1}{2}Q(\xi_{\mathrm{p}})}{1 - e^{-\beta\xi_{\mathrm{p}}}}\right\} + \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{dz_1\, \mathrm{disc}Q(z_1)}{(1-e^{-\beta z_1})(\xi_{\mathrm{p}} - z_1)(\omega - z_1)}. \tag{5.29}$$

We have used the convention that when the phase is not specified the principal part ($\mathcal{P}$) is understood. Because of the approximations made and the explicit dependence of J in Eq. (5.27), we shall evaluate Eq. (5.29) only to $O(1)$ in the numerator of the real part, and to $O(J)$ in the numerator of the imaginary part:

$$I_{\mathrm{p}}(\omega + is) \simeq \frac{-\{[\coth(\frac{1}{2}\beta\xi_{\mathrm{p}})]/(\xi_{\mathrm{p}} - \omega) + i\pi[\coth(\frac{1}{2}\beta\omega)\, \delta(\xi_{\mathrm{p}} - \omega) - \rho J/(\xi_{\mathrm{p}} - \omega)]\}}{2\,|\,\{1 - \frac{1}{2}JS^0(\omega)\}\{1 + JS^0(\omega)\}\,|^2}. \tag{5.30}$$

Thus by Eq. (5.27) we obtain, in the limit $\omega \ll kT$,

$$V_0{}^P(\omega \pm is) = \frac{\frac{3}{4}\rho J^2\{\ln|(D-\omega)/(D+\omega)| \pm i\pi[1 - \rho JA(\omega)]\}}{|\,\{1 - \frac{1}{2}\rho JA(\omega)\}\{1 + \rho JA(\omega)\}\,|^2}. \tag{5.31}$$

This is the central result of this section, so if we now only consider excitations near the Fermi surface, i.e., $\omega \to 0$ we can use the analytical result [see Eq. (4.10)]

$$A(0) = \int_{-D}^{D} dx[\tanh(\tfrac{1}{2}\beta x)]/x = 2\ln(\zeta\beta D); \qquad \zeta = 2\gamma/\pi \simeq 1.13. \tag{5.32}$$

Thus at the Fermi surface $\omega = 0$, Eq. (5.31) becomes

$$V_0{}^P(0 \pm is) = \frac{\pm i\frac{3}{4}\rho J^2\{1 - 2\rho J \ln(\zeta\beta D)\}}{|\,\{1 - \rho J \ln(\zeta\beta D)\}\{1 + 2\rho J \ln(\zeta\beta D)\}\,|^2}. \tag{5.33}$$

We can immediately see that this diverges under two conditions

$$1 + 2\rho J \ln(\zeta D/kT_{c-}) = 0, \tag{5.34a}$$

$$1 - \rho J \ln(\zeta D/kT_{c+}) = 0. \tag{5.34b}$$

Using Nagaoka's values for the parameters

$$[D \simeq (5\times 10^4)\,^\circ\mathrm{K}, \quad \rho\,|J| = 0.05],$$

Eqs. (5.34) become

$$kT_{c-} = \zeta D \exp(1/2\rho J) = \zeta D \exp\{10\epsilon(J)\}, \tag{5.35a}$$

$$kT_{c+} = \zeta D \exp(-1/\rho J) = \zeta D \exp\{-20\epsilon(J)\}. \tag{5.35b}$$

These only have low-temperature solutions ($kT_c < D$), if in Eq. (5.35a) J is negative giving $T_{c-} \simeq 3^\circ\mathrm{K}$ and if J is positive in Eq. (5.35b) giving $T_{c+} \simeq 2\times 10^{-4}\,^\circ\mathrm{K}$. Thus T_{c-} is the usual antiferromagnetic "transition point" found by Nagaoka,[5] which we will always denote by T_k, while T_{c+} is a new ferromagnetic characteristic temperature. However, this latter is only of academic interest for

$$T_{c+}/T_k = kT_k/\zeta D. \tag{5.36}$$

Before proceeding further we will introduce a comment regarding the stability of this solution, i.e., the sign of the imaginary part of $V^P(\omega + is)$ which in our notation should take the sign of s. This is true for the antiferromagnetic case in the temperature range from zero to the unphysically high value of

$$\zeta D \exp(1/2\rho\,|J|).$$

However, an instability occurs below T_k for the ferromagnetic case, before its own T_{c+} is reached, but the significance of this result is unknown. It seems possible that higher-order terms would counteract this change in sign.

Although the effective potential V diverges at T_k, this is not the quantity of direct physical significance. The single-particle lifetimes τ are determined by the imaginary part of the electron self-energy $M_{p\lambda}(\omega)$. This is given by Edwards's[20] method of taking an ensemble average over all impurity sites in the low concentration limit ($c\to 0$) and this "renormalization" method must be used when V diverges[8]:

$$G_{p\lambda}(\omega)=\{\xi_{p\lambda}-\omega-cM_{p\lambda}(\omega)\}^{-1}, \tag{5.37}$$

where

$$M_{p\lambda}(\omega)=V_\lambda(\omega)/[1-V_\lambda(\omega)G_\lambda^0(\omega)]. \tag{5.38}$$

The quasiparticle lifetime is given by

$$1/\tau_{p\lambda}=\mathrm{Im}cM_{p\lambda}(\xi_{p\lambda}+is). \tag{5.39}$$

From Eqs. (4.9)–(4.13) we know that the real part of $G_\lambda^0(\omega)$ vanishes at the Fermi surface as does the real part of $V^P(\omega)$ in the above approximation, so on using the form of $V^P(0+is)$ valid in the temperature range $1\lesssim T/T_k\lesssim e^{10}$ for $J<0$ we obtain τ_F from Eq. (5.33) and Eqs. (5.38) and (5.39). The restriction ($T>T_k$) anticipates the anomalous results of the remainder of this section:

$$\tau_F^{-1}=c(\pi/\rho)\{\pi^2+6\,|\ln(T/T_k)\,|^2\}^{-1}. \tag{5.40}$$

Equation (5.38) must be used in the temperature range $1\lesssim T/T_k\lesssim 4$ even for small concentrations, as cV^P is diverging as T approaches T_k from above, but outside this range $cV^P(\omega)$ may be used to sufficient accuracy.

Then using the following equation for the resistivity (at temperature T) $\rho_{res}(T)$, we achieve the final result, above the Kondo temperature:

$$\rho_{res}(T)^{-1}=-\frac{2e^2}{3m^2}\int d\xi_p\tau_p p^2\frac{\partial}{\partial\xi_p}f_p\simeq\frac{ze^2}{2m\rho}\tau_F. \tag{5.41}$$

So

$$\rho_{res}(T)=c(2m\pi/ze^2)\{\pi^2+6\,|\ln(T/T_k)\,|^2\}^{-1}, \tag{5.42}$$

where z is the number of conduction electrons (mass m) per atom. A similar analysis for the C self-energy Σ involving pairwise renormalization of the corresponding second-order skeleton graphs leads to the analogous result (for $\mathfrak{H}^z=0$):

$$\Sigma_0^P(\bar\nu)=\frac{J^2}{\beta}\sum_{\bar\alpha}\{G^0(\bar\alpha+\bar\nu)-G^0(\bar\alpha-\bar\nu)\}\mathcal{S}^0(\bar\alpha)Q(\bar\alpha). \tag{5.43}$$

Using the same approximations which were used in evaluating V [see Eq. (5.26)] we find the damping term to be

$$\mathrm{Im}\Sigma_0^P(\omega\pm is)=\frac{\pm 4\pi(\rho J)^2kT\{1-\rho JA(\omega)\}}{|\,\{1-\frac{1}{2}\rho JA(\omega)\}\{1+\rho JA(\omega)\}\,|^2}. \tag{5.44}$$

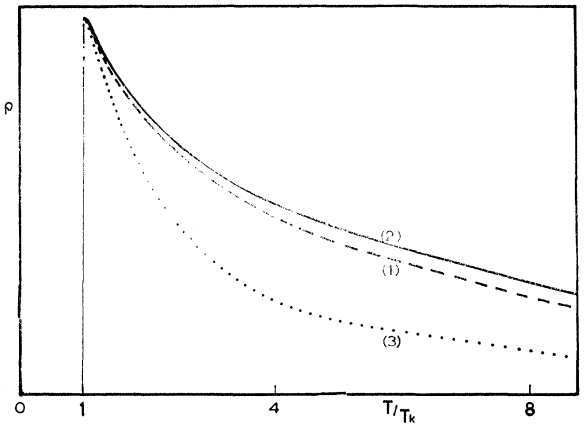

FIG. 12. The one-electron damping at the Fermi surface (or equivalently, the spin-impurity resistivity in arbitrary units) plotted against the reduced temperature T/T_k for antiferromagnetic coupling ($J<0$). No. 1 is our present result [Eq. (5.40)], No. 2 is the modified result of Nagaoka (or Abrikosov), and No. 3 is that of Doniach for $S_i=1$. Only valid for $T\geq T_k$.

So, using Eqs. (4.30) and (5.33), on the C excitation energy shell, in zero external field, we have,

$$\mathrm{Im}\Sigma_0^P(0\pm is)=\frac{\pm\Gamma\{1-2\rho J\ln(\zeta\beta D)\}}{|\,\{1-\rho J\ln(\zeta\beta D)\}\{1+2\rho J\ln(\zeta\beta D)\}\,|^2}. \tag{5.45}$$

In this case damping of the C propagator becomes infinite at the two critical temperatures, again indicating anomalous behavior. Unfortunately we cannot evaluate the real part of the C-field self-energy for general ω, but it is identically zero on the energy shell ($\omega=0$) as can be seen from Eq. (5.43). This means that $\langle S^z\rangle=0$ for all temperatures, when $\mathfrak{H}^z=0$.

However, the divergences in the $\mathcal{S}$ functions [Eq. (5.21)] which enter into the evaluation of the above self-energies do have interesting physical consequences. We can see this by examining the exact propagators $\mathcal{S}^z_{\lambda,-\lambda}(\tau)$ in their Wick-ordered form:

$$\mathcal{S}^z{}_{\uparrow\downarrow}(\tau)=\langle T_W\{\alpha_\uparrow(\tau)c^\dagger(\tau)\alpha_\uparrow{}^\dagger(0)c(0)\}\rangle$$

and

$$\mathcal{S}^z{}_{\downarrow\uparrow}(\tau)=\langle T_W\{\alpha_\downarrow(\tau)c(\tau)c^\dagger(0)\alpha_\downarrow{}^\dagger(0)\}\rangle. \tag{5.46}$$

If we now take the limit of $\tau\to 0^-$ in each case, we have

$$\mathcal{S}^z{}_{\uparrow\downarrow}(0^-)=-\langle\alpha_\uparrow{}^\dagger\alpha_\uparrow cc^\dagger\rangle,$$
$$\mathcal{S}^z{}_{\downarrow\uparrow}(0^-)=\langle\alpha_\downarrow{}^\dagger\alpha_\downarrow c^\dagger c\rangle. \tag{5.47}$$

In order to interpret these expressions we note that the z component of the electronic spin density at the impurity site, written as $\frac{1}{2}\sigma^z$ is defined by

$$\sigma^z=\sum_\lambda\lambda\alpha_\lambda{}^\dagger\alpha_\lambda. \tag{5.48}$$

Now the correlation of this electronic spin density with

the impurity magnetization at the origin is given by

$$\langle\sigma^z S^z\rangle=\sum_\lambda \lambda\langle\alpha_\lambda{}^\dagger\alpha_\lambda S^z\rangle. \tag{5.49}$$

If this sum is written out then we can use the drone-fermion representation for S^z in either of its two equivalent forms, namely

$$S^z=c^\dagger c-\tfrac{1}{2} \quad \text{or} \quad S^z=\tfrac{1}{2}-cc^\dagger. \tag{5.50}$$

So we have

$$\langle\sigma^z S^z\rangle=1+\sum_\lambda \lambda \mathcal{S}^z{}_{\lambda,-\lambda}(0^-). \tag{5.51}$$

Thus, for the noninteracting system,

$$\langle\sigma^z S^z\rangle_0=2\zeta^0\langle S^z\rangle_0, \tag{5.52}$$

and this vanishes at all temperatures when $\tilde{\mathcal{H}}^z=0$. However, a peculiar transformation occurs when all the "polarization" diagrams of the type summed in Eq. (5.3) are considered. For in zero external field we have

$$\lim(\tilde{\mathcal{H}}^z\to 0)\langle\sigma^z S^z\rangle$$
$$=1-\frac{1}{\beta}\sum_{\bar{\alpha}}\frac{\exp(-i\bar{\alpha}0^-)\mathcal{S}^0(\bar{\alpha})}{\{1-\frac{1}{2}J\mathcal{S}^0(\bar{\alpha})\}\{1+J\mathcal{S}^0(\bar{\alpha})\}}. \tag{5.53}$$

If this is converted to a Bose-type contour in the complex z plane, we have

$$\langle\sigma^z S^z\rangle-1$$
$$=\lim_{s\to 0^+}\frac{1}{2\pi i}\oint_{C_b}\frac{dz\, e^{zs}\mathcal{S}^0(z)}{(1-e^{\beta z})\{1-\frac{1}{2}J\mathcal{S}^0(z)\}\{1+J\mathcal{S}^0(z)\}}. \tag{5.54}$$

Apart from the Bose factor, the denominator of the integrand has no zeros above T_k, so deforming the contour will only pick up the poles from $\mathcal{S}^0(z)$ which we have seen [Eq. (5.42)] gives a vanishing result. However, at T_k the expression $1+J\mathcal{S}^0(z)$ has its first zero at $z=0$, indicating the occurrence of anomalous correlations. As the temperature is further lowered, two solutions occur giving rise to two conjugate poles on the imaginary z axis. This is very similar to the behavior of the exact solution to the Nagaoka decoupled equations found by Bloomfield and Hamann.[24] Further discussion of the low-temperature properties of this formalism will not be pursued here, but it might be noted that this anomalous behavior has points in common with the breakdown of the T-matrix approximation in superconductivity for an attractive δ-function potential.[25]

6. DISCUSSION

In this section the results of several authors who have previously investigated this Hamiltonian are compared and contrasted. We only deal with those treatments which have attempted a series summation in the electron self-energy part M. In fact, apart from Doniach,[9] all these authors calculate M directly, without the aid of V, and so include a divergence at T_k for $1/\tau_F$; they then restrict their solutions to the high-temperature region $T>T_k$ [see remarks after Eq. (5.40)].

We shall first analyze Nagaoka's[5,6] results for his high-temperature (perturbation) solution of his truncation scheme for the equations of motion of the Green's functions. If we write Nagaoka's equation for the diagonal element of the electron's Green's function using the same notation as in his first paper[5] (denoted NI), apart from modifying his J (for the purposes of comparison), then Eq. (2.17) of NI becomes

$$2\pi G_{kk}(\omega)=\frac{1}{(\omega-\xi_k)}$$
$$\times\left\{1-\frac{J^2\Gamma(\omega)}{(\omega-\xi_k)[1+2J\mathcal{G}(\omega)+J^2F(\omega)\Gamma(\omega)]}\right\}. \tag{6.1}$$

This is then inverted and expanded to $O(J^2)$ in the numerator to give

$$G_{kk}(\omega)^{-1}=2\pi\left\{\omega-\xi_k+\frac{J^2\Gamma(\omega)}{[1+2J\mathcal{G}(\omega)+J^2F(\omega)\Gamma(\omega)]}\right\}. \tag{6.2}$$

This is the form in Eq. (3.2) of NI apart from the term of $O(J^2)$ in the denominator; however, this must be retained to remove the divergence at T_k. In the limit $\omega+is$, we obtain the damping coefficient:

$$\frac{1}{\tau_k}=\mathrm{Im}\left\{\frac{J^2\Gamma(\omega)}{1+2J\mathcal{G}(\omega)+J^2F(\omega)\Gamma(\omega)}\right\}. \tag{6.3}$$

Now in NI, the zeroth approximation of $n_k=f_k^-$ and $m_k=0$ were used, in our present notation this becomes

$$2\mathcal{G}^0(\omega+is)=\mathcal{S}^0(\omega+is)$$

and

$$\tfrac{4}{3}\Gamma^0(\omega+is)=-F^0(\omega+is)=G^0(\omega+is)$$
$$=\ln|(D-\omega)/(D+\omega)|+i\pi\rho. \tag{6.4}$$

This results, near the Fermi surface, in

$$\frac{1}{\tau_F}=\frac{c\tfrac{3}{4}\pi\rho J^2}{\tfrac{3}{4}(\pi\rho J)^2+1+2\rho J\ln(\zeta\beta D)}$$
$$=c\frac{\pi}{\rho}\left\{\pi^2+\frac{8}{3\rho|J|}\ln\left(\frac{T}{T_k}\right)\right\}^{-1}. \tag{6.5}$$

The initial expansion to $O(J^2)$ was necessary for a meaningful result. Otherwise we would have

$$G_{kk}(\omega+is)^{-1}=2\pi(\omega-\xi_k)^2/\{\omega-\xi_k+\Delta+i/\tau_k\}, \tag{6.6}$$

[24] P. Bloomfield and D. R. Hamann (to be published).
[25] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962), p. 187.

where Δ is the shift. As we can see, this vanishes at the Fermi surface ($\xi_{kf}=0$, $\omega=0$).

In his second paper[6] (NII) Nagaoka starts with the perturbational approximation $n_k=j_k^-$ and $G_{kk}(\omega)=G_{kk}^0(\omega)$, and upon neglecting higher-order effects [Eq. (4.2) of NII], he finds for m_F [see Eq. (4.7) of NII]

$$m_F=\frac{\frac{3}{2}\rho J\ln(\zeta\beta D)}{1+2\rho J\ln(\zeta\beta D)}. \tag{6.7}$$

This can now be used to find

$$\begin{aligned}\mathrm{Im}\Gamma(0+is)&=\mathrm{Im}(1/N)\sum_k(\tfrac{3}{4}-m_k)/(\xi_k-is)\\&=\pi\rho\{\tfrac{3}{4}-m_F\}.\end{aligned} \tag{6.8}$$

Finally, on neglecting the real part of $\Gamma(0)$, the self-consistent result is

$$\begin{aligned}\frac{1}{\tau_F}&=\frac{c_4^3\pi\rho J^2}{\{\frac{3}{4}(\pi\rho J)^2+[1+2\rho J\ln(\zeta\beta D)]^2\}}\\&=c(\pi/\rho)\{\pi^2+\tfrac{16}{3}|\ln(T/T_k)|^2\}^{-1}.\end{aligned} \tag{6.9}$$

On comparing this result[26] with Eq. (5.33) and using Eq. (5.38) we can see that this is in agreement for $J<0$ if we had neglected terms of $O(J)$, which appear apparently to be unimportant near T_k. In fact they do give a numerical contribution of order unity, as we can see by comparing the above result with Eq. (5.40). The difference has been lost somewhere in the decoupling scheme along with the ferromagnetic result. These high-temperature results contrast markedly with the self-consistent solution found at low temperatures (below T_k), which indicates a possible type of condensation. This latter result is found by the use of equations analogous to those in superconductivity and the self-consistent assumption that m_F diverges at absolute zero. However Fischer,[27] who follows Nagaoka in his truncation formulation, adopts a different self-consistent low-temperature assumption and finds that $m_F\simeq\frac{3}{4}$ [see Eq. (6.7)] with the result that the resistivity vanishes as $\ln^{-2}(T)$ at absolute zero, in agreement with Eq. (5.42) if this equation had been used below T_k. The presence of a low-temperature "bound state" is being investigated in the present formalism. Yosida[28] has also found such a possible bound state at 0°K by applying perturbation theory to a singlet-correlated ground-state wave function for the s-d model.

This results in an energy approximately kT_k lower than the corresponding uncorrelated ground state. The present calculations do indicate the presence of anomalous behavior, in this case by correlations arising for $T\leq T_k$ in the spin correlations at the impurity site [Eq. (5.54)]. We mention in passing the work of Takano and Ogawa[29] who use Gor'kov's[30] decoupling method in contrast to that of Zubarev[31] used by Nagaoka. Unfortunately they use the coupled-fermion representation for the spin-$\frac{1}{2}$ operators[32] and are forced to neglect unphysical states with unknown consequences. However, they do find a ferromagnetic resonance, although their parameters differ from all other theories (see later), and they also find a sharp phase transition at T_k, to a possible low-temperature "bound state." Doniach[9] has summed a series of self-energy graphs using his zero-temperature spin-Wick theorem. Although this method results in a resonance rather than a divergence at T_k, two points must be mentioned. Due to an ansatz extension to finite temperatures,[33] the resulting value of T_k is too small and because of his method of averaging, the total spin components ($S=\frac{1}{2}$), $S_t=1$ and $S_t=0$ differ from each other, even in zero magnetic field. This latter separation into S_t channels shows up in an instability in the effective potential for $S_t=0$ but not $S_t=1$. The former having the wrong sign throughout the whole temperature range.

The first successful finite-temperature calculation using a perturbational method and treating the spin operators correctly was that of Abrikosov.[7] He summed a series of "parquet" diagrams which in essence are similar to most of our self-energy terms. His result (in our notation) is

$$1/\tau_F=c(\pi/\rho)\tfrac{3}{16}\{\ln(T/T_k)\}^{-2}. \tag{6.10}$$

This could agree with Nagaoka's second result if the resonant part (π^2) had been included.

Suhl and Wong[34] have also investigated this problem using Chew-Low scattering theory; however, little contact seemed to exist between their theory and previous methods. But very recently Silverstein and Duke[23] have shown an exact agreement between Suhl's approach and that of Abrikosov by imposing the restriction of on-shell energies in the scattering amplitude which also removes any complex poles. They show that the restriction to parquet graphs is valid to third order in the iterative results to logarithmic accuracy—this region is within our own approximation. Finally

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[26] This result was derived by a different method in the last section of Ref. 10, where its validity was also restricted to $T>T_k$. This was based on low-order perturbation results in the calculation of $\langle S^z\rangle$ which appears to diverge at low temperatures.

[27] K. Fischer, Phys. Rev. **158**, 613 (1967).

[28] K. Yosida, Phys. Rev. **147**, 223 (1966).

[29] F. Takano and T. Ogawa, Progr. Theoret. Phys. (Kyoto) **35**, 343 (1966).

[30] L. P. Gor'kev, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **7**, 505 (1958)].

[31] D. N. Zubarev, Usp. Fiz. Nauk **71**, 711 (1960) [English transl.: Soviet Phys.—Usp. **3**, 320 (1960)].

[32] This is identical with the Yolin-Abrikosov pseudofermion technique for $S=\frac{1}{2}$. The unphysical "vacuum" state gives no contribution (apart from overcounting) but this is not true for the two-fermion state, which is compensated correctly in the techniques of the above authors.

[33] Nagaoka (Ref. 6) has reported that Shiba has generalized this method to finite temperatures.

[34] H. Suhl and D. Wong, Physics **3**, 27 (1967).

TABLE I. Coefficient x, defining the Kondo resonance temperature.

x	Source
2	Nagaoka (NII)
$\frac{3}{2}$	Takano, Ogawa[a]
2	Abrikosov
2	Silverstein, Duke
1	Doniach
2	Present work

[a] Their ferromagnetic result is $\frac{1}{2}$ whereas ours is 1 [see Eq. (5.35b) of the text].

Bloomfield and Hamann have solved Nagaoka's decoupled equations exactly, throughout the whole temperature range, giving a smooth behavior of the physical quantities considered, as the temperature is lowered.

As a final summary of the basic results of the above theories we tabulate (in Table I) the parameter x found in each theory which finds an antiferromagnetic resonance condition given by equations like Eq. (5.35) (always in our present notation and band structure):

$$1+x\rho J \ln(\zeta D/kT_k)=0$$

or

$$kT_k=\zeta D \exp(-1/x\rho\,|J|). \quad (6.11)$$

It is the exponential dependence of T_k on x which makes its magnitude important. We also plot the damping term τ_k^{-1} [or equivalently the spin-impurity resistivity Eq. (5.42)] against the reduced temperature T/T_k for $J<0$. This is contrasted with the modified (high-temperature extension) result of Nagaoka [Eq. (6.9)] and one of Doniach's results, that for total spin one.

As can be seen the ascent to the maximum is not very steep (this was anticipated by Abrikosov) of width about $2T_k$. The behavior below T_k is not exhibited in the present theory due to the possible correlation between the spin systems below T_k. It is possible that the resistivity retains its maximum value all the way from T_k to zero.

7. CONCLUSION

The discovery of a simple Wick theorem for spin-$\frac{1}{2}$ operators has enabled the powerful techniques of quantum field theory to be used in the present problem which is one of some dynamical complexity. The extension of the Feynman diagram method to represent spin propagators has enabled us to systematically investigate the magnetic properties of this model. In the present paper we have calculated the self-energies of the various propagators to $O(J^2)$ for the case of low concentration of impurities. We have found that the electronic energy levels are split by a $J^2 \ln T$ term giving rise to such an expression in the electronic g factor. This shift is a polarization effect of the localized impurity spin and vanishes as the external field goes to zero. A similar polarization term occurs in the static and dynamic properties of the impurity spin, and leads to another $\ln T$ term in the second-order g shift and dynamic susceptibility of the impurity.

We approached the Kondo temperature T_k from the high-temperature region by a resummation of a complete subseries of self-energy diagrams selected on the basis of the idea of mutual "polarization" of the two spin systems, even in zero external field where the resulting expressions were evaluated. As the calculation was carried out to $O(J^2)$ in the resulting denominators, two characteristic temperatures appeared. One was the Kondo temperature for $J<0$, while the other one occurred for $J>0$ and was much smaller than T_k. The use of an effective potential indicated that the spin-impurity resistivity reached its maximum (but still finite) value at the characteristic temperature in a $\ln^2 T$ manner. The divergences in the present theory manifested themselves in anomalous behavior in the correlation function between the two spin systems at the impurity site. However the properties of this model were not investigated here in the anomalous low-temperature region.

The present problem ($c \ll 1$) is one of the rarer examples where molecular-field solutions cannot be found. So the standard approximations used to handle spin operators in such theories have to be superceded, as in this paper. However, we have reported elsewhere on applications of this new method to molecular-field type problems like the Heisenberg ferromagnet and the rare-earth model for metals.

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