of $A(\omega)$ in powers of $J\rho$-N. The result of such an expansion is

$$A(\omega)=\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2\omega\left[1-\frac{i\pi}{2}\left(\frac{J\rho}{N}\right)-2\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}\right]+O\left[\left(\frac{J\rho}{N}\right)^4\right]$$
$$=\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2\omega\left[1-2JG_0(\omega)+\frac{i\pi}{2}\left(\frac{J\rho}{N}\right)\right]+O\left[\left(\frac{J\rho}{N}\right)^4\right]. \quad (38)$$

This solution is presumably valid at high temperatures, and we may expect it to be valid as long as the expression in the brackets on the left-hand side of (26) does not vanish. We call this expression $H(\omega)$,

$$H(\omega)=1+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)-\frac{1}{2}}{\omega-\xi+i\epsilon}-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2$$
$$=1+JG_0(\omega+i\epsilon)-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2$$
$$=1+\frac{J\rho}{N}\left[\ln\frac{D}{2\pi T}-\psi\left(\frac{1}{2}-\frac{i\omega}{2\pi T}\right)\right]-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2, \quad (39)$$

where $\psi(z)$ is the digamma function, the logarithmic derivative of the γ function. The zeros of $H(\omega)$ lie on the imaginary ω axis, and for T sufficiently large there are no zeros in the upper half-plane. However, as T is lowered, for $J<0$, one zero moves up into the upper half-plane, thus producing, we may assume, a new behavior in $A(\omega)$ and invalidating (38). The temperature at which this happens we call T_K' and is determined by

$$0=H(0)=1+JG_0(0)-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2. \quad (40)$$

Using (39) we see that

$$T_K'=\frac{2\gamma D}{\pi}\exp\left\{\frac{N}{J\rho}\left[1-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2\right]\right\} \quad (41)$$

or

$$T_K'=T_K e^{-(3\pi/16)(J\rho^2/N)}>T_K \quad (42)$$

since $J<0$.

ACKNOWLEDGMENTS

We should like to thank Dr. Claude Kacser and Martin S. Fullenbaum for helpful discussions, and Dr. Philip Bloomfield and Dr. Robert Paulson for pointing out an error in the original manuscript.

PHYSICAL REVIEW VOLUME 158, NUMBER 3 15 JUNE 1967

New Solution for Exchange Scattering in Dilute Alloys

D. R. HAMANN
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 30 January 1967)

The *s-d* exchange model is treated using equations of motion truncated at the lowest nontrivial order, following Nagaoka. The coupled equations are reduced to a single nonlinear integral equation for the conduction-electron t matrix, which depends only on energy. An approximation to the integral operator which treats the Kondo divergence accurately permits this equation to be transformed to a differential equation which is exactly integrable. The solution agrees with the leading terms of perturbation calculations above the Kondo critical temperature T_K, and passes through this temperature smoothly, reaching the unitarity limit at zero temperature. A different analytic continuation of the t matrix is trivially found which acquires nonphysical singularities below T_K. At low temperatures this form is shown to be identical to Abrikosov's solution and to Suhl's solution prior to analytic continuation. The resistivity of dilute alloys is calculated. Noninteracting impurities are shown to give no contribution to the specific heat. The effective local moment entering the magnetic susceptibility is found to be almost completely canceled at zero temperature for spin-$\frac{1}{2}$ impurities.

I. INTRODUCTION

SINCE Kondo's discovery of the low-temperature divergence in the perturbation series for conduction-electron scattering in dilute magnetic alloys,[1] a great deal of effort has been expended toward a physical understanding and an accurate calculation of the low-temperature properties of these systems. Unfortunately, a unified picture has not yet emerged. This work represents a "second generation" effort, yielding a new solution for the *s-d* exchange model which is simple,

[1] J. Kondo, Progr. Theoret. Phys. (Kyoto) 32, 37 (1964).

valid at all temperatures, and capable of relating the results of several workers.[2]

The *s-d* exchange model has been treated by diverse methods primarily because the spin-operator commutation relations preclude the direct application of the usual Feynman diagrams of many-body perturbation theory. Abrikosov[3] and Doniach[4] have derived two alternative diagrammatic formalisms which permit the summation of selected infinite series. Suhl has applied an adaptation of the Chew-Low method.[5] The point of departure for the present work will be the method first applied by Nagaoka, who used decoupled equations of motion for double-time Green's functions.[6,7]

There were several reasons for the choice of this approach for further study. First, the formalism was familiar and versatile. Second, the key approximation was simply the use of the lowest-order nontrivial decoupling. This is admittedly not a particularly physical rationale, but the physics of this system is not well understood. In addition, we have seen the identity of calculations based on summing leading divergences with those based on lowest-order decoupling (RPA) in the case of the electron-gas correlation energy,[8] so it might not be overly optimistic to hope for the same unity in this problem. Third and most important, the physical content of Nagaoka's decoupling approximation did not appear to be exhausted by the solutions he found. This remark will be expanded in the next paragraph.

It should be stressed that Nagaoka was fully aware of the limitations of his low-temperature solution, and the criticisms we give here are largely his own.[6,7] First, he found separate solutions for low and high temperatures, which say nothing about the important region around the Kondo critical temperature T_K.[1] Second, his ansatz which led to a low-temperature solution is equivalent to finding the best approximation to the one-electron t matrix by a function with a single complex pole. This form is certainly very restrictive. Third, his self-consistency test of this ansatz was satisfied in only a rather limited sense.[6]

The initial step towards a better solution is the reduction of the decoupled equations of motion to a single integral equation for the one-electron t matrix in the non-spin-flip channel, which is a function of energy and temperature only. This reduction is described in Sec. II. The integral operator in this equation is approximated in Sec. III by a form which treats the logarithmic divergence accurately, and the equation converted to a differential equation which is integrable in simple closed form. The solution is compared with those of Abrikosov[3] and Suhl,[5] and all three are found to be closely related. The resistivity, specific heat, and susceptibility are calculated in Sec. IV.

II. REDUCTION OF THE EQUATION OF MOTION

We shall follow Nagaoka's notation as closely as possible, and repeat the key definitions and equations from Sec. II of Ref. 6 here. The Green's functions involved (for a local spin $S=\frac{1}{2}$)are

$$G_{kk'}(\omega)=\langle C_{k'\uparrow}|C_{k\uparrow}^{\dagger}\rangle, \tag{2.1}$$

$$\Gamma_{kk'}(\omega)=\langle C_{k'\uparrow}S_z+C_{k'\downarrow}S_-|C_{k\uparrow}^{\dagger}\rangle. \tag{2.2}$$

The important thermal averages are

$$n_{k'}=\sum_l \langle C_{l\uparrow}^{\dagger}C_{k'\uparrow}\rangle, \tag{2.3}$$

$$m_{k'}=3\sum_l \langle C_{l\uparrow}^{\dagger}C_{k'\downarrow}S_-\rangle. \tag{2.4}$$

The two equations of motion considered are

$$(\omega-\epsilon_{k'})G_{kk'}(\omega)+(J/2N)\sum_l \Gamma_{kl}(\omega)=(1/2\pi)\delta_{kk'}, \tag{2.5}$$

$$(\omega-\epsilon_{k'})\Gamma_{kk'}(\omega)+(J/N)(n_{k'}-\tfrac{1}{2})\sum_l \Gamma_{kl}(\omega)$$
$$+(J/2N)(\tfrac{3}{4}-m_{k'})\sum_l G_{kl}(\omega)=0, \tag{2.6}$$

where ϵ_k is the electron energy measured from the Fermi level and J is the strength of the exchange coupling between the conduction electrons and the local spin **S**. Equation (2.5) is exact, while Eq. (2.6) has been decoupled.

To complete these equations, the thermal averages must be related to the Green's functions. This relation is given by the general expression[9]

$$\langle AB\rangle=i\int_{-\infty}^{\infty} d\omega\, f(\omega)[G_{AB}(\omega+i\delta)-G_{AB}(\omega-i\delta)]$$
$$\equiv \mathfrak{F}_{\omega}[G_{AB}(\omega)], \tag{2.7}$$

where $f(\omega)$ is the Fermi function. It is customary to write $2i\,\mathrm{Im}G_{AB}(\omega+i\delta)$ for the bracketed expression in the integrand in (2.7), but this is generally correct only if the operators A and B are Hermitian adjoints. In addition, the form (2.7) is much easier to use in the reduction procedure described here, and we shall make extensive use of the functional notation $\mathfrak{F}$.

---

[2] A summary of this work has been presented; see D. R. Hamann, Bull. Am. Phys. Soc. **12**, 22 (1967).

[3] A. A. Abrikosov, Zh. Eksperim. i Teor. Fiz. **48**, 990 (1965) [English transl.: Soviet Phys.—JETP **21**, 660 (1965)]; Physics **2**, 5 (1965); **2**, 61 (1965).

[4] S. Doniach, Phys. Rev. **144**, 382 (1966).

[5] H. Suhl, Phys. Rev. **138**, A515 (1965); Physics **2**, 39 (1965); Phys. Rev. **141**, 483 (1966); H. Suhl and D. Wong, Physics **3**, 1 (1967).

[6] Y. Nagaoka, Phys. Rev. **138**, A1112 (1965).

[7] Y. Nagaoka, Progr. Theoret. Phys. (Kyoto) **37**, 13 (1967).

[8] D. Pines, *The Many Body Problem* (W. A. Benjamin, Inc., New York, 1963).

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

Nagaoka has shown that (2.5) and (2.6) have a formal solution which may be written

$$G_{kk'}(\omega)=\frac{1}{2\pi}\left[\frac{\delta_{kk'}}{(\omega-\epsilon_k)}+\frac{t(\omega)}{(\omega-\epsilon_k)(\omega-\epsilon_{k'})}\right], \tag{2.8}$$

$$t(\omega)=-(J^2/4N)\Gamma(\omega)/[1+JG(\omega)+\tfrac{1}{4}J^2F(\omega)\Gamma(\omega)], \tag{2.9}$$

where

$$F(\omega)=\frac{1}{N}\sum_k\frac{1}{\omega-\epsilon_k}, \tag{2.10}$$

$$G(\omega)=\frac{1}{N}\sum_k\frac{n_k-\frac{1}{2}}{\omega-\epsilon_k}, \tag{2.11}$$

$$\Gamma(\omega)=\frac{1}{N}\sum_k\frac{m_k-\frac{3}{4}}{\omega-\epsilon_k}. \tag{2.12}$$

We note that $t(\omega)$ as defined by (2.8) is the t "matrix" for non-spin-flip scattering.[10] Its independence of $\mathbf{k}$ and $\mathbf{k}'$ is a result of the momentum independence of the exchange interaction in the simple s-d exchange model, and not a necessary feature of the physical problem. By setting $k=k'$ in (2.8) and considering the Lehmann spectral representation for $G_{kk}(\omega)$,[9] we can conclude that the discontinuity of $t(\omega)$ across the real axis in the ω plane is pure imaginary, so

$$t(\omega+i\delta)=t^*(\omega-i\delta). \tag{2.13}$$

To obtain an integral equation for t, we must express $G(\omega)$ and $\Gamma(\omega)$, the unknown functions in (2.9), as functionals of t. This is easy for $G(\omega)$. Using (2.3), (2.7), (2.8), and (2.11) we write

$$G(\omega)=\frac{1}{N}\sum_{k'}\frac{1}{\omega-\epsilon_{k'}}\left\{\sum_l \mathfrak{F}_{\omega'}[G_{lk'}(\omega')]-\tfrac{1}{2}\right\}. \tag{2.14}$$

Now $\mathfrak{F}$ is a linear functional, and the relative position of all the singularities in (2.14) is well defined by the $i\delta$'s [G will always be evaluated as $G(\omega+i\delta)$]. Therefore we can interchange the order of $\mathfrak{F}$ and the l and k' sums. The algebra is easily carried to the point

$$G(\omega)=G^0(\omega)+\frac{1}{2\pi}\mathfrak{F}_{\omega'}\left[\sum_{k'}\frac{F(\omega')t(\omega')}{(\omega-\epsilon_{k'})(\omega'-\epsilon_{k'})}\right], \tag{2.15}$$

where

$$G^0(\omega)=\frac{1}{N}\sum_k\frac{f(\epsilon_k)-\frac{1}{2}}{\omega-\epsilon_k}. \tag{2.16}$$

The key step is now to expand the k' summand in partial fractions in $\epsilon_{k'}$ before carrying out the k' sum. This step yields

$$G(\omega)=G^0(\omega)+\frac{N}{2\pi}\mathfrak{F}_{\omega'}\left[\frac{F(\omega')-F(\omega)}{\omega-\omega'}F(\omega')t(\omega')\right]. \tag{2.17}$$

To obtain a similar expression for Γ, a bit of manipulation is necessary. Using the definition (2.4) of $m_{k'}$ and the properties of the trace, we can show

$$m_{k'}=3\sum_l\langle C_{k'\downarrow}{}^\dagger C_{l\uparrow}S_+\rangle^*. \tag{2.18}$$

Using the symmetry of the system under coordinate rotations in spin space [Nagaoka's Eq. (2.13)],[6] this can be expressed as

$$m_{k'}=2\sum_l\{\mathfrak{F}_{\omega'}[\Gamma_{k'l}(\omega')]\}^*$$

$$=2\{\mathfrak{F}_{\omega'}[\sum_l\Gamma_{k'l}(\omega')]\}^*. \tag{2.19}$$

Using the form (2.18) rather than (2.4) is extremely important, because $\Gamma_{k'l}$ summed over the left index cannot be expressed simply, while the sum over the right index is found from (2.5) and (2.8) to be

$$\sum_l\Gamma_{k'l}(\omega)=-\frac{N}{\pi J}\frac{t(\omega)}{\omega-\epsilon_{k'}}. \tag{2.20}$$

Substituting (2.20) in (2.19), it is easy to show from (2.13) that $m_{k'}$ is real, so the complex conjugation may be dropped. $\Gamma(\omega)$ is expressed in terms of t by using (2.12), (2.19), (2.20), and evaluating the k' sum inside $\mathfrak{F}$ as was done in the case of $G(\omega)$. We find

$$\Gamma(\omega)=-\frac{2N}{\pi J}\mathfrak{F}_{\omega'}\left[\frac{F(\omega')-F(\omega)}{\omega-\omega'}t(\omega')\right]-\tfrac{3}{4}F(\omega). \tag{2.21}$$

Up to this point, the reduction procedure has seemed little but an exercise in algebra with no real direction. Now, however, if we substitute (2.17) for $G(\omega)$ and (2.21) for $\Gamma(\omega)$ into (2.9), the formal solution for t, an unexpected simplification occurs in the denominator, and we find

$$t(\omega)=\left\{\frac{3J^2}{16N}F(\omega)+\frac{J}{2\pi}\mathfrak{F}_{\omega'}\left[\frac{F(\omega')-F(\omega)}{\omega-\omega'}t(\omega')\right]\right\}$$

$$\times\left\{1+JG^0(\omega)-\frac{3J^2}{16}F^2(\omega)+\frac{JN}{2\pi}\mathfrak{F}_{\omega'}\left[\frac{[F(\omega')-F(\omega)]^2}{\omega-\omega'}t(\omega')\right]\right\}^{-1}. \tag{2.22}$$

The functionals in the numerator and denominator are very similar, and as we shall see in the remainder of this section, their leading contributions are identical. We

[10] This identification follows from the definition of the t matrix in one-particle scattering theory and a common identity. See, for example, A. Messiah *Quantum Mechanics*, translated by J. Potter (North-Holland Publishing Company, Amsterdam, 1962), Vol. II, p. 830, Eq. (XIX.102a) and p. 827, Eq. (XIX.88a).

stress that (2.22) is identical to Nagaoka's equations. Its advantage is that it will enable us to make all approximations in terms of the function of most direct physical interest, t. Nagaoka has carried out the generalization of his original treatment to arbitrary spin S.[7] This generalization can be applied to (2.22) simply by replacing the number 3 by $4S(S+1)$ in the two places where it appears.

To proceed, it is necessary to study the functionals in (2.22) in detail. Let us write them

$$\varphi_n(\omega)=\mathfrak{F}_{\omega'}\left[\frac{[F(\omega')-F(\omega)]^n}{\omega-\omega'}t(\omega')\right], \qquad (2.23)$$

where $n=1$ or 2. $F(\omega)$, defined by (2.10), will depend on the conduction-band density of states which is chosen. Rather than choosing a square density of states symmetric about the Fermi level immediately as did Nagaoka,[6] we find it convenient to begin with a Lorentzian form. Then

$$F(\omega)=\frac{\pi\rho D/N}{\omega+iD\,\mathrm{sgn}(\mathrm{Im}\omega)}, \qquad (2.24)$$

where ρ is the Fermi surface density of states, and D is the half-width of the conduction band. Examining the definition of $\mathfrak{F}$, Eq. (2.7), we can see that the ω' integration in φ_n will be singular only when ω and ω' are on opposite sides of the real axis [otherwise $F(\omega)-F(\omega')\to 0$ as $\omega'\to\omega$]. It is only the singular terms which can contribute to logarithmic divergences associated with the Kondo effect. In addition, if we assume that $t(\omega')$ can be large only for $|\omega'|<T_K$, where T_K is the Kondo temperature,[1] it is easy to see that the nonsingular terms will be small [of order $T_K/D\sim\exp(N/J\rho)$] as well as being slowly varying functions of ω. [We are interested in the case of antiferromagnetic exchange ($J<0$), and must consider the dimensionless coupling $J\rho/N$ to be small for the truncation of the equations of motion to make sense.] Therefore it is a good approximation to drop the nonsingular terms, and we find

$$\varphi_n(\omega+i\delta)\approx\frac{(2\pi i\rho D^2/N)^n}{i(\omega+iD)^n}\int_{-\infty}^{\infty}d\omega' \times f(\omega')\frac{1}{\omega-\omega'+i\delta}\frac{t(\omega'-i\delta)}{(\omega'-iD)^n}. \qquad (2.25)$$

Let us consider the ω' integration in (2.25). Since $t(\omega')$ is related to $G_{kk'}(\omega')$ by (2.8), it must satisfy the same analyticity requirements as the Green's function, and can have no singularities except a branch cut along the real axis on the physical sheet of the ω' Riemann surface.[9] Therefore if we were to close the ω' contour in the lower half-plane, the only singularities it would contain would be those of $f(\omega')$.[11] Thus we can replace $f(\omega')$ by $f(\omega')-\frac{1}{2}$ without changing $\varphi_n(\omega)$. It is important to make this symmetry of φ explicit before destroying the analytic simplicity of (2.25) as we shall in the next paragraph.

A key assumption necessary at this point is that $t(\omega')$ goes to zero as $\omega'\to\infty$ sufficiently rapidly so that (2.25) will converge *without* the factor $(\omega'-iD)^{-n}$ in the integrand. It will be shown in Sec. III that the $t(\omega')$ found from this treatment does so, proving the consistency of this assumption. Since the range of $t(\omega')$ is of order $T_K\ll D$, we will replace the slowly varying functions $(\omega+iD)^{-n}$ and $(\omega'-iD)^{-n}$ by their values at $\omega=\omega'=0$. Since the factor $(\omega'-iD)^{-n}$ does impose a range of order D on the integrals, we shall restrict the integration to $-D<\omega'<D$. These steps yield

$$\varphi_n(\omega+i\delta)\approx(i)^{n-1}\left(\frac{2\pi\rho}{N}\right)^n\int_{-D}^{D}d\omega' \times\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}t(\omega'-i\delta). \qquad (2.26)$$

We would have obtained essentially this form by starting with the square density of states and neglecting the real part of $F(\omega)$, following Nagaoka.[6] However, we believe that the above development, in treating the analytic properties carefully, is more satisfactory.

Approximations for the remaining terms in (2.22) which are consistent with (2.26) are

$$F(\omega+i\delta)=-i\pi\rho/N, \qquad (2.27)$$

$$G^0(\omega+i\delta)=\frac{\rho}{N}\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}. \qquad (2.28)$$

With all these substitutions, (2.22) becomes

$$t(\omega+i\delta)=\left\{-\frac{3\pi iJ^2\rho}{16N^2}+\frac{J\rho}{N}\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}t^*(\omega'+i\delta)\right\} \times\left\{1+\frac{3J^2\rho^2\pi^2}{16N^2}+\frac{2\pi iJ\rho^2}{N}\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}\left[t^*(\omega'+i\delta)-\frac{i}{2\pi\rho}\right]\right\}^{-1}, \qquad (2.29)$$

where we have exploited our careful choice of the limits in (2.26) to combine $G^0(\omega)$ with the operator term in the denominator, and used (2.13).[12]

[11] If we in fact performed this contour integral, we would obtain a sum over imaginary values of ω' of the type familiar in temperature perturbation theory.

Equation (2.29) still contains some unexploited symmetry, which we can bring out by considering the integral equation for

$$\psi(\omega+i\delta)=1-2\pi i\rho t(\omega+i\delta), \tag{2.30}$$

$$\psi(\omega+i\delta)=\left[1-S(S+1)\left(\frac{\gamma\pi}{2}\right)^2+\gamma\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}\right]\Big/$$

$$\left[1+S(S+1)\left(\frac{\gamma\pi}{2}\right)^2+\gamma\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}\psi^*(\omega'+i\delta)\right], \tag{2.31}$$

where $\gamma=J\rho/N$ is the dimensionless coupling constant, and we have included the generalization to arbitrary spin. The substitution (2.30), which was motivated purely by the desire to eliminate the unknown function from the numerator of (2.29), is in fact the definition of the S matrix in scattering theory. It has the analytic properties of $t(\omega)$, and the symmetry

$$\psi(\omega+i\delta)=\psi^*(-\omega+i\delta), \tag{2.32}$$

which may be proved from (2.31).

III. SOLUTION OF THE INTEGRAL EQUATION

A. Approximate Operator

Equation (2.31) is a great simplification of the starting set of equations. However, it is nonlinear and singular, and the author is not aware of any general method which may be applied to such equations. A straightforward computer iteration does not seem promising either, since there are three energy scale factors in the problem: T, T_K, and D. These may vary orders of magnitude relative to each other, making it extremely difficult to represent $\psi(\omega)$ by its value on a set of points. Therefore we approached the task by making a rather crude approximation to the integral operator in (2.31), which turned out to give a much better solution to this particular equation than we had any right to expect.

The approximation was suggested by Abrikosov's treatment of the integral equation for the vertex function in his solution of the *s-d* exchange model.[3] Let us consider the integral which occurs in the denominator of (2.31).

$$\varphi(\omega+i\delta)=\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}\psi^*(\omega'+i\delta). \tag{3.1}$$

We expect the most important feature of φ to be a logarithmic divergence as ω and T tend to zero, whose coefficient will be proportional to the value of ψ at $\omega=0$. To emphasize this, let us make the variable change $\xi=\omega-\omega'$. Then

$$\varphi(\omega+i\delta)=\int_{\omega-D}^{\omega+D}\frac{d\xi}{\xi+i\delta}[f(\omega-\xi)-\tfrac{1}{2}]\psi^*(\omega-\xi+i\delta). \tag{3.2}$$

Next, let us neglect ω in the integration limits of (3.2). This is equivalent, for $\psi=$ constant and $T=0$, to the approximation

$$\ln\frac{\omega+i\delta}{iD}\approx\tfrac{1}{2}\ln\frac{(\omega+i\delta)^2}{(\omega+D)(\omega-D)}, \tag{3.3}$$

which is universally made in treating this problem. It is, in fact, closer to the physical situation than the original form, since the divergences at $\omega=\pm D$ are not present for any density of states that goes to zero smoothly at the band edges.

Let us now assume that the Fermi function is more rapidly varying for $\omega-\xi\approx 0$ than ψ for any value of its argument. Then $\varphi(\omega)$ "sees" the $\xi=0$ pole of the integrand primarily through the Fermi function. We should be able to simulate this behavior fairly well by making the Fermi function sharp and broadening the pole by T. Thus we will let

$$\frac{f(\omega-\xi,T)-\frac{1}{2}}{\xi+i\delta}\approx\frac{f(\omega-\xi,0)-\frac{1}{2}}{\xi+iT}. \tag{3.4}$$

For $\psi=$ constant, this step replaces the correct φ by $\ln[(\omega+iT)/iD]$. The approximate result has the correct analytic properties. The quality of the approximation can be judged by examining the imaginary parts,

$$-\frac{\pi}{2}\tanh\frac{\omega}{2T}\approx\operatorname{Im}\ln\frac{\omega+iT}{iD}$$

$$=-\tan^{-1}(\omega/T). \tag{3.5}$$

The two sides of (3.5) have the same limits as ω approaches $\pm\infty$, and approximately the same slope at $\omega=0$. The real parts of the exact and approximate expressions must also agree fairly well since both satisfy the Kramers-Kronig relations. Therefore we will call (3.5) a reasonable approximation for the integral equation and, of course, an exact one in the $T=0$ limit.

[12] Since the completion of this work, the author has learned that D. S. Falk and M. Fowler have independently derived essentially the same equation (to be published). Their equation does not retain the particle-hole symmetry of (2.25), which proved important in our subsequent work.

Finally, we must make a rather brutal approximation. Since the logarithmic behavior of φ for $\omega\sim 0$ is of primary interest in this problem, we will set $\omega=0$ in $\psi^*(\omega-\xi+i\delta)$ in (3.2). This step can be tried for a few simple examples, and it is found to reproduce the logarithmic divergence correctly, and to be surprisingly good over a much wider range. Our final approximate form is

$$\varphi(\omega+i\delta)\approx -\frac{1}{2}\int_{-D}^{\omega}\frac{d\xi}{\xi+iT}\psi^*(-\xi+i\delta) -\frac{1}{2}\int_{D}^{\omega}\frac{d\xi}{\xi+iT}\psi^*(-\xi+i\delta). \quad (3.6)$$

From (2.32), we see that we may replace $\psi^*(-\xi+i\delta)$ by $\psi(\xi+i\delta)$ in (3.6). This step, although it looks trivial, is crucial in solving (2.31), reducing it to an equation in ψ alone instead of ψ and ψ^*.

The form of (3.6) suggests the change of variables

$$x=\ln[(\xi+iT)/iD], \quad (3.7)$$

$$y=\ln[(\omega+iT)/iD]. \quad (3.8)$$

Equation (3.7) is a conformal mapping of the ξ plane into the x plane. The mapping of the original integration contour in (3.6) into the x plane is shown in Fig. 1. Since $\psi(\xi+i\delta)$ is analytic in the upper-half ξ plane, we may deform the two pieces of the contour in the x plane anywhere in the cross-hatched region. If we define

$$\Psi(x)=\psi(\xi+i\delta), \quad (3.9)$$

$$\Phi(y)=\varphi(\omega+i\delta), \quad (3.10)$$

then (3.6) becomes

$$\Phi(y)=-\frac{1}{2}\int_{i\pi/2}^{y}dx\,\Psi(x)-\frac{1}{2}\int_{-i\pi/2}^{y}dx\,\Psi(x). \quad (3.11)$$

B. Solution and Its Properties

The same approximation should be applied to the integral in the numerator of (2.31), which is simply $-y$. We may now express (2.31) as

$$\Psi(y)=\frac{1-S(S+1)(\gamma\pi/2)^2-\gamma y}{1+S(S+1)(\gamma\pi/2)^2+\gamma\Phi(y)}. \quad (3.12)$$

Solving (3.12) for Φ,

$$-\Phi(y)=\frac{1+\alpha}{\gamma}-\frac{1-\alpha-\gamma y}{\gamma\Psi}, \quad (3.13)$$

where $\alpha=S(S+1)(\pi\gamma/2)^2$. Taking the derivative of both sides of (3.13) with respect to y,

$$-\frac{d\Phi}{dy}=\Psi(y)=\frac{1}{\Psi(y)}+\frac{1-\alpha-\gamma y}{\gamma\Psi^2(y)}\frac{d\Psi}{dy}, \quad (3.14)$$

$$-\frac{\gamma}{1-\alpha-\gamma y}dy=\frac{1}{\Psi-\Psi^3}d\Psi. \quad (3.15)$$

The differentials in (3.15) are exactly integrable, and we obtain

$$\ln\beta(1-\alpha-\gamma y)=\tfrac{1}{2}\ln\frac{\Psi^2}{\Psi^2-1}, \quad (3.16)$$

where β is the integration constant, which has been taken inside the logarithm. It is simple to solve (3.16) for Ψ, and

$$\Psi(y)=\pm\frac{1-\alpha-\gamma y}{[(1-\alpha-\gamma y)^2-1/\beta^2]^{1/2}}. \quad (3.17)$$

We may determine the sign of the square root and the integration constant β by substituting (3.17) into (3.11) and (3.12), and setting $y=i\pi/2$. The resulting algebraic equation can be solved to obtain

$$-\frac{1}{\beta^2}=4\alpha\left[1+\frac{(\pi\gamma/2)^2}{(1+\alpha)^2}\right]. \quad (3.18)$$

Although the exact form (3.18) is necessary to satisfy the integral equation, the second term in the brackets is always small compared to unity in cases for which any of this theory is valid, and will generally be neglected.

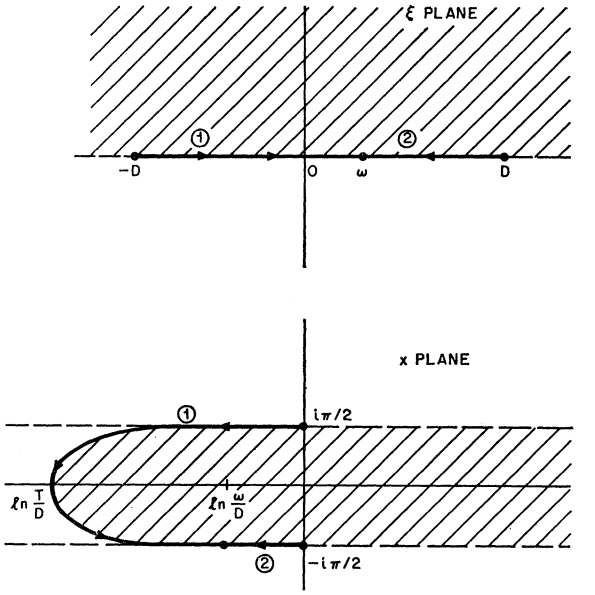

FIG. 1. The conformal mapping generated by Eq. (3.7). The cross-hatched region is the upper-half ξ plane and its x-plane image, and the heavy lines are the integration contours in Eqs. (3.6) and (3.11).

The solution may be simplified by one last change of variables. Let

$$X=-\frac{1}{\gamma}\left[1-S(S+1)(\pi\gamma/2)^2-\gamma\ln\frac{\omega+iT}{iD}\right]$$
$$=\ln[(\omega+iT)/iT_K], \tag{3.19}$$

where T_K is defined by (3.19) and is, explicitly,

$$T_K=D\exp\{[1-S(S+1)(\pi\gamma/2)^2]/\gamma\}. \tag{3.20}$$

This is identical to the usual expression for the Kondo temperature[1] except for the small correction term in the square brackets.

Putting everything together, we arrive at our result for the t matrix:

$$t(\omega)=(1/2\pi i\rho)\{1-X[X^2+S(S+1)\pi^2]^{-1/2}\}. \tag{3.21}$$

In studying its properties, let us also consider the function $\tilde{t}$ obtained from t by bringing the numerator X inside the square root,

$$\tilde{t}(\omega)=(1/2\pi i\rho)\{1-[1+S(S+1)\pi^2/X^2]^{-1/2}\}. \tag{3.22}$$

To begin our analysis of t, let us first consider its analytic properties in the X plane. Both t and $\tilde{t}$ must have two branch cuts because they contain square roots of quadratic functions of X. The branch points are fixed at the poles and zeros of the square root's argument. For both t and $\tilde{t}$, there are poles at $X=\pm i\pi[S(S+1)]^{1/2}$. For t, there is a double zero at $X=\infty$, and for $\tilde{t}$, a double zero at $X=0$. A possible choice of cuts is sketched in Fig. 2 for t and Fig. 3 for $\tilde{t}$. These figures also show the X-plane image of the upper-half (u.h.) ω plane for $T>T_K$ and $T<T_K$. The branch points at $\pm i\pi\times[S(S+1)]^{1/2}$ can never enter this region, since $S\geq\frac{1}{2}$. However, for $T<T_K$, the $X=0$ branch point of $\tilde{t}$ enters the u.h. ω plane.

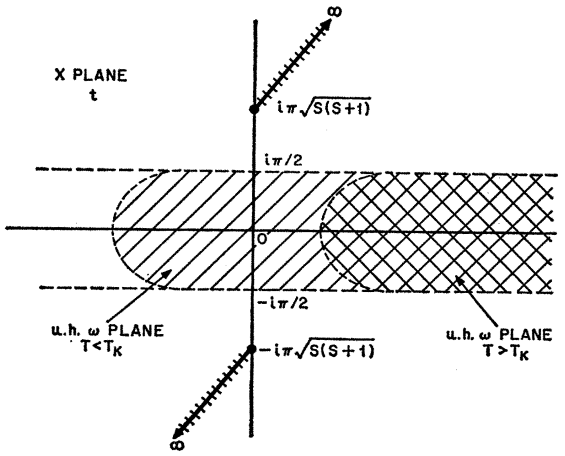

FIG. 2. The analytic structure of t in the X plane. The branch points and cuts are indicated, and the image of the ω plane for high and low temperatures is superimposed.

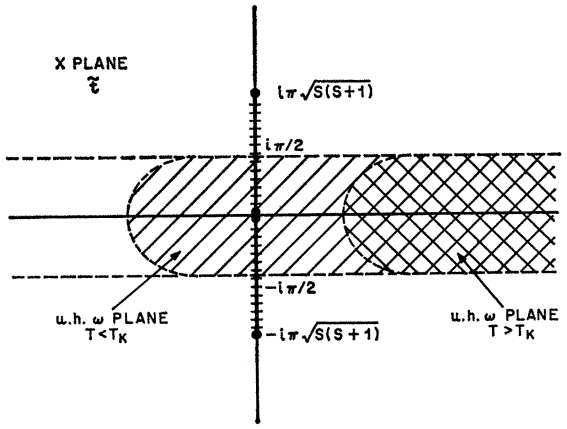

FIG. 3. The analytic structure of $\tilde{t}$ in the X plane. The branch points and cuts are indicated, and the image of the ω plane for high and low temperatures is superimposed.

Both t and $\tilde{t}$ have the same perturbation expansion at high temperatures, which diverges as $T\to T_K$ for $\omega<T_K$. They can be considered analytic continuations of the high-temperature expansion along different paths. For t, the path is in the physical region, while for $\tilde{t}$, it must pass outside $\pm i\pi[S(S+1)]^{1/2}$ in the X plane. Only t is a solution of the integral equation; the incorrect continuation $\tilde{t}$ is not. The fact that $\tilde{t}$ displays nonphysical singularities below T_K clearly does not indicate any instability in the system. The correct solution in our approximation, t, shows that nothing of particular significance happens at $T=T_K$, which simply acts as a parameter setting the energy scale.

Having established the satisfactory analytic behavior of t, let us return to the question of how well it satisfies the original integral equation. First, we note that $t(\omega)\propto\ln^{-2}|\omega/T_K|$ as $\omega\to\infty$. This establishes that the convergence of the integral assumed in going from (2.25) to (2.26) is satisfied (although marginally). Second, let us examine the high-temperature behavior of t by expanding (3.22) for $\tilde{t}$ in this limit. Since $|X|\gg1$ for $T\gg T_K$,

$$t(\omega)=(1/2\pi i\rho)\{\tfrac{1}{2}S(S+1)\pi^2/X^2$$
$$-\tfrac{3}{8}[S(S+1)\pi^2]^2/X^4+\cdots\}. \tag{3.23}$$

To obtain a true perturbation series in γ, we must substitute (3.19) for X, yielding

$$t(\omega)=\frac{1}{2\pi i\rho}\left\{\tfrac{1}{2}S(S+1)\pi^2\gamma^2\right.$$
$$\times\left[1+2\gamma\ln\frac{\omega+iT}{iD}-3\gamma^2\ln^2\frac{\omega+iT}{iD}+\cdots\right]$$
$$-\tfrac{3}{8}[S(S+1)\pi^2\gamma^2]^2$$
$$\left.\times\left[1+4\gamma\ln\frac{\omega+iT}{iD}-\cdots\right]+\cdots\right\}. \tag{3.24}$$

The leading logarithmic terms come from X^{-2}, and go as $\gamma^{n+2}\ln^n|\omega+iT|/D$. The coefficients of these terms agree with perturbation theory through $n=2$,[1,13] which is as far as straightforward perturbation theory has been carried to the author's knowledge. There is also a series of terms proportional to $\gamma^{n+3}\ln^n|\omega+iT|/D$, and these must be given correctly by (3.24) since they arise from the imaginary parts of the logs, which are uniquely related to the real parts by the analytic properties of t. Third, it was feasible to check numerically the most gross assumption of this treatment, that of setting $\omega=0$ in ψ^* in (3.2), at $T=0$. In Table I, we compare our approximate solution Ψ^0 with the first numerical iteration Ψ^1 computed without the aforementioned assumption. The numerical integration is accurate to ± 0.002, and we have chosen $S=0.5$ and $\gamma=-0.1$ to display one of the worst cases that reasonably fits the basic assumptions. It is seen that the approximation is worst at $\omega=T_K$ ($\ln\omega/D=-10$), but rather remarkably good nevertheless. We cannot claim that it should be this good in general, but simply that it is for this particular integral equation. This is not entirely an accident. The approximation treats the logarithmic divergences correctly, and these divergences are the key features of the Kondo problem. Fourth, we note that since our solution is a function of $\ln(\omega+iT)$, the considerations leading to our approximate treatment of temperature, Eq. (3.4), are self-consistently satisfied.

C. Comparison with Other Solutions

Nagaoka's low-temperature solution can be written

$$t_N(\omega)=(1/2\pi i\rho)[2i\Delta/(\omega+i\Delta)], \tag{3.25}$$

where Δ is a function of T, approximately equal to our T_K at $T=0$, and decreasing with increasing T.[6] At the Fermi surface, $t_N(\omega=0)$ is a T-independent constant equal to the unitarity limit for s-wave scattering.[14] Our $t(\omega=0)$ approaches this limit asymptotically as T approaches zero. Nagaoka mentions that a solution with the pole in the u.h. ω plane satisfies his self-consistency condition equally well.[6] It appears that this solution might correspond to our $\tilde{t}$. Beyond a certain rudimentary similarity in analytic structures and agreement at $\omega=T=0$, however, there is little similarity between the two solutions.

TABLE I. Numerical check of key approximation, with $S=0.5$, $\gamma=-0.1$.

$\ln\omega/D$	$\mathrm{Re}\Psi^1$	$\mathrm{Re}\Psi^0$	$\mathrm{Im}\Psi^1$	$\mathrm{Im}\Psi^0$
−40	−0.995	−0.996	0	0
−30	−0.990	−0.991	−0.001	−0.001
−20	−0.965	−0.968	−0.011	−0.010
−15	−0.893	−0.903	−0.062	−0.053
−10	−0.079	−0.120	−0.539	−0.685
−8	0.607	0.690	−0.333	−0.304
−5	0.882	0.892	−0.074	−0.063
−3	0.932	0.936	−0.031	−0.029
−2	0.946	0.949	−0.022	−0.020
−1	0.957	0.958	−0.015	−0.014

Abrikosov's solution may be written[3]

$$t_A(\omega)=(1/2\pi i\rho)\tfrac{1}{2}S(S+1)\pi^2/X^2. \tag{3.26}$$

At high temperatures, this gives the same leading logarithmic terms as our t. However, at low temperatures, it predicts that the scattering goes to zero at the Fermi surface. If we expand our $\tilde{t}$ for $T\ll T_K$, we find that its leading term is equal to t_A. Therefore, we conclude that Abrikosov's theory and ours are equivalent to leading logarithmic order, but that his solution is the wrong analytic continuation at low temperatures.

We can also compare our result to Suhl's, although not quite so directly. From the third paper of Ref. 5, we may extract the relations

$$t_S(\omega)=(1/2\pi i\rho)(1-e^{2i\delta}), \tag{3.27}$$

$$4\,\mathrm{Im}\delta=\ln[1+16S(S+1)\pi^2\rho^2|F|^2], \tag{3.28}$$

$$F(\omega)\approx(4\rho X)^{-1}, \tag{3.29}$$

where we have taken the limit of the ordinary potential scattering going to zero. It is not possible to carry out the Kramers-Kronig integral which gives the real part of the analytic function δ by hand. However, we can easily combine the above equations to find[15]

$$|2\pi i\rho t_S-1|=[1+S(S+1)\pi^2/|X|^2]^{-1/2}. \tag{3.30}$$

From (3.22), we find

$$|2\pi i\rho\tilde{t}-1|=|1+S(S+1)\pi^2/X^2|^{-1/2}. \tag{3.31}$$

Therefore we conclude that t_S and $\tilde{t}$ are almost identical, (3.30) and (3.31) differing only by the appearance of the absolute value sign around X in (3.30). For $T\ll T_K$ or $T\gg T_K$, the results are identical. The difference, of course, makes it impossible to write t_S simply as an analytic function. In the last paper of Ref. 5, Suhl and Wong recognized that the t_S discussed above was the wrong analytic continuation for $T<T_K$, and found the correct one. While we cannot simply compare this result to our t, it is clear that it must be very similar, since the incorrect analytic continuation is so close to our incorrect analytic continuation. Furthermore, they found that the quotient of the S matrices corresponding to the correct and incorrect solutions was a unimodular function. We see from (3.21) and (3.22) that $X/(X^2)^{1/2}$ plays this role in our treatment.

It was pointed out by Suhl[16] that Abrikosov's perturbation-theory approach should yield the same equations as his scattering theory. This was shown to

[13] J. Kondo (private communication).
[14] A. Messiah, Ref. 10, p. 737, Eq. (XVII.52), p. 817, Eqs. (XIX.51) and (XIX.52).
[15] The extraction of this result from Suhl's work was carried out by P. W. Anderson (private communication).
[16] H. Suhl, Lectures presented at the 1966 International School of Physics "Enrico Fermi," Varenna, Italy (unpublished).

be true to leading logarithmic order by Silverstein,[17] and is certainly consistent with the preceding comparisons.

IV. CALCULATION OF MEASURABLE QUANTITIES

A. Resistivity

The conductivity is given by the formula[6]

$$\sigma=-\frac{2e^2}{3}\int\tau(\epsilon)v^2(\epsilon)\frac{\partial f}{\partial\epsilon}\rho(\epsilon)d\epsilon, \tag{4.1}$$

where $v(\epsilon)$ is the velocity at energy ϵ, and

$$[2\tau(\epsilon)]^{-1}=c\,\mathrm{Im}t(\epsilon), \tag{4.2}$$

where c is the impurity concentration. Since the derivative of the Fermi function restricts the ϵ integration to $|\epsilon|<T$, we can expand (4.2) in powers of ϵ. Only the leading term is important, and we find for the resistivity

$$\Delta\rho=\frac{2\pi c}{ne^2k_F}\left\{1-\ln\left(\frac{T}{T_K}\right)\times\left[\ln^2\left(\frac{T}{T_K}\right)+S(S+1)\pi^2\right]^{-1/2}\right\}, \tag{4.3}$$

where n is the electron density and k_F the Fermi wave vector. Since this result is characterized only by a multiplicative constant and T_K, it should be relatively easy to compare this prediction of the theory with experiment. It is qualitatively similar to the numerical results of Suhl and Wong.[5]

B. Specific Heat

The specific heat for one impurity is given by[6]

$$\Delta C_v=\frac{d}{dT}\sum_k\int d\omega\,\omega f(\omega)2\,\mathrm{Im}\Delta G_{kk}(\omega), \tag{4.4}$$

where

$$\Delta G_{kk}(\omega)=t(\omega)/2\pi(\omega-\epsilon_k)^2. \tag{4.5}$$

If we evaluate the k sum using the Lorentzian density of states, and then approximate the resulting function of ω by a sharp cutoff as in Sec. II, we find

$$\Delta C_v=-\frac{\rho}{D}\,\mathrm{Im}\frac{d}{dT}\int_{-D}^{D}d\omega\,\omega[f(\omega)-\tfrac{1}{2}]t(\omega+i\delta). \tag{4.6}$$

There are two contributions to ΔC_v, since d/dT acts on both the Fermi function and t. Considering the latter, we are forced to recognize that our approximate treatment of temperature in Sec. III is not good enough for present purposes. However, the comparisons of our result with others suggest that (3.21) for $t(X)$ may be a more accurate result than Eq. (3.19) for X. Let us take this suggestion, and replace (3.19) by the function it approximates. Then

$$\frac{\partial t}{\partial T}=-\frac{dt}{dX}\int_{-D}^{D}d\omega'\frac{\partial f(\omega')}{\partial T}\frac{1}{\omega-\omega'+i\delta}. \tag{4.7}$$

Substituting in (4.6), interchanging the order of ω and ω' integration, and putting $\omega=\omega-\omega'+\omega'$, we obtain

$$\Delta C_v=-\frac{\rho}{D}\,\mathrm{Im}\left\{\int_{-D}^{D}d\omega\,\omega\frac{\partial f(\omega)}{\partial T}t(\omega+i\delta)-\int_{-D}^{D}d\omega'\,\omega'\frac{\partial f(\omega')}{\partial T}\int_{-D}^{D}d\omega\frac{f(\omega)-\frac{1}{2}}{\omega'-\omega-i\delta}\frac{dt(\omega+i\delta)}{dX(\omega+i\delta)}-\int_{-D}^{D}d\omega\,[f(\omega)-\tfrac{1}{2}]\frac{dt}{dX}\int_{-D}^{D}d\omega'\frac{\partial f(\omega')}{\partial T}\right\}. \tag{4.8}$$

The third term in (4.8) is zero because the ω' integrand is odd. In the second term, the ω integral is exactly the same operator which we approximated in Sec. III. In keeping with our premise that $t(X)$ is more accurate than X, we must regard the replacement of this operator by the integral with respect to X as a better approximation than its derivation indicates. Therefore we obtain

$$\Delta C_v=-\frac{\rho}{D}\,\mathrm{Im}\left\{\int_{-D}^{D}d\omega\,\omega\frac{\partial f(\omega)}{\partial T}t(\omega+i\delta)+\int_{-D}^{D}d\omega'\,\omega'\frac{\partial f(\omega')}{\partial T}t^*(\omega'+i\delta)\right\}. \tag{4.9}$$

Since the quantity in braces is real, we obtain a null result, $\Delta C_v=0$.

This result is difficult to interpret. However, it is consistent with the calculation of Yosida and Miwa, who found that there are no $T^n\ln T$ terms in the free energy to fourth order in J.[18] Insofar as our calculation accurately represents the leading logarithmic terms, we must conclude that they give no contribution to C_v to all orders. As we shall see in the next section, the physical picture of a spin which contracts with temperature—used by Yosida and Miwa to explain their result[18]—is predicted by the present solution. However, this cannot be the complete answer, since real alloys which display straightforward Kondo effects in their resistivity, such as Ag(Mn), do display specific-heat anomalies in the same temperature regions.[19] Explanations of these anomalies have been based on

[17] S. D. Silverstein, J. Appl. Phys. 38, 1150 (1967).

[18] K. Yosida and H. Miwa, Phys. Rev. 144, 375 (1966).

[19] G. J. Van Den Berg, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland Publishing Company, Amsterdam, 1964), Vol. IV, p. 194.

interactions among the impurities, with[20] or without[21] consideration of the anomalous scattering, and on interactions of single impurities with host magnetization.[22] Nagaoka did predict a specific-heat anomaly on the basis of his solution of the one-impurity problem,[6] but the present results force us to question this. It has been suggested by Dworin[23] that C_v may contain logarithmic terms at low temperatures when calculated from the more realistic Anderson model.[24] Therefore we believe that the mechanism of the observed anomalies must remain an open question.

C. Susceptibility

The extent to which the total spin $\mathbf{S}_e$ of the electrons is correlated with the local spin $\mathbf{S}$ should provide a measure of how the susceptibility of the local spin is modified. If we think of $S=\frac{1}{2}$ and an oversimplified model where S interacts with a single electron, we would predict $\langle\mathbf{S}\cdot\mathbf{S}_e\rangle\rightarrow-\frac{3}{4}$ as $T\rightarrow 0$ for antiferromagnetic coupling. Nagaoka has shown that when the g factor of $\mathbf{S}$ and the conduction electrons are equal,[7]

$$\chi=(g^2\mu_B^2/3T)[S(S+1)(1+\gamma/2)+\langle\mathbf{S}\cdot\mathbf{S}_e\rangle], \quad (4.10)$$

where μ_B is the Bohr magneton and we have omitted the temperature-independent Pauli susceptibility. Equation (4.10) is based on a further Green's-function decoupling similar to the basic decoupling used to truncate the equations of motion. However, the preceding simple picture of a two-spin problem leads us to believe that (4.10) is not only correct, but at least qualitatively good for cases in which the g factors differ.

It is easy to show from (2.6) and (2.7) that[7]

$$\langle\mathbf{S}\cdot\mathbf{S}_e\rangle=S(S+1)\gamma/2+\frac{J}{N}\sum_k m_k\frac{dn_k}{d\epsilon_k}, \quad (4.11)$$

where n_k and m_k are defined in (2.3) and (2.4). Using the equations in Sec. II, we can express m_k and n_k as integral operators acting on t. These turn out to be the same operators we usually encounter, and using the Sec. III approximations, we find

$$n_k-\tfrac{1}{2}=(1/2\pi)\,\mathrm{Im}\{[X^2+S(S+1)\pi^2]^{1/2}+X\}, \quad (4.12)$$

$$m_k=(2/\pi^2\gamma)\,\mathrm{Re}\{[X^2+S(S+1)\pi^2]^{1/2}-X\}-(2/\pi^2\gamma)C, \quad (4.13)$$

where X is (3.19) evaluated at ϵ_k. C in (4.13) is the left-hand term evaluated at $|\epsilon|=D$, and is approximately $(\gamma/2)S(S+1)\pi^2$. Substituting these expressions in (4.11), we find

$$\langle\mathbf{S}\cdot\mathbf{S}_e\rangle-S(S+1)\gamma/2=\frac{-1}{\pi^3}\int_{-D}^{D}d\epsilon\times\mathrm{Re}\{[X^2+S(S+1)\pi^2]^{1/2}-X-C\}\times\mathrm{Re}\{[X[X^2+S(S+1)\pi^2]^{-1/2}+1](T-i\epsilon)^{-1}\}. \quad (4.14)$$

This integral is very difficult to handle, since the integrand is not an analytic function of X. We will evaluate it in the high- and low-temperature limits, taking $D/T_K\gg 1$ in both cases. For $T\gg T_K$, we can expand the integrand and use contour integration in the ϵ plane, obtaining

$$\chi=\chi_0[1-\ln^{-1}(2T/T_K)], \quad (4.15)$$

where χ_0 is the susceptibility of the free spin. If we neglect the factor of 2 multiplying T in (4.15), which is consistent with our approximate treatment of temperature, this result agrees with perturbation theory for χ.[25]

In the $T=0$ limit, the X-plane contour for (4.14) is simple, and we have

$$\langle\mathbf{S}\cdot\mathbf{S}_e\rangle-S(S+1)\gamma/2=\frac{2}{\pi^3}\int_{-\infty-i\pi/2}^{+\infty-i\pi/2}dX\times\mathrm{Re}\{[X^2+S(S+1)\pi^2]^{1/2}-X\}\times\mathrm{Im}\{X[X^2+S(S+1)\pi^2]^{-1/2}\}. \quad (4.16)$$

The portion of this integral which is not zero from symmetry can be expressed in terms of complete elliptic integrals by the substitution

$$X=(\pi/2)\{[4S(S+1)]^{1/2}-1\}\tan\varphi-i\pi/2 \quad (4.17)$$

and the use of several identities involving these functions.[26] For T small but nonzero, the contour in (4.16) terminates at $\ln(T/T_K)$ instead of $-\infty$, and the difference can be easily calculated by expanding the integrand. We find

$$\chi=\chi_0[1-(4\kappa/\pi)\mathbf{E}(\kappa)-2\ln^{-1}(T/T_K)+C'], \quad (4.18)$$

where $\mathbf{E}$ is the complete elliptic integral of the second kind, $\kappa=[4S(S+1)]^{-1/2}$, and C' is a constant of order γ.

For the local moment to be canceled at $T=0$, we expect the second term in the brackets in (4.18) to equal -1. [The first terms in (4.18) are only exact consequences of our solution in the limit $\gamma=0$, so C' should be neglected when examining the cancellation.] In fact it equals -0.98 for $S=\frac{1}{2}$, and is smaller in magnitude for larger S. Nagaoka found -0.66 for

[20] J. Kondo, Progr. Theoret. Phys. (Kyoto) **33**, 575 (1965).
[21] M. W. Klein, Phys. Rev. **136**, A1156 (1964); Phys. Rev. Letters **11**, 408 (1963); M. W. Klein and R. Brout, Phys. Rev. **132**, 2412 (1963); W. Marshall, *ibid.* **118**, 1520 (1960).
[22] A. W. Overhauser, Phys. Rev. Letters **3**, 414 (1959).
[23] L. Dworin, Phys. Rev. Letters **16**, 1042 (1966).
[24] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[25] B. Giovannini, R. Paulson, and J. R. Schrieffer, Phys. Letters **23**, 517 (1966); D. J. Scalapino, Phys. Rev. Letters **16**, 937 (1966); K. Yosida and A. Okiji, Progr. Theoret. Phys. (Kyoto) **34**, 505 (1965).
[26] E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, Inc., New York, 1945), p. 56, Sec. V6, line 2; A. Erdelyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 319, bottom line of table.

$S=\frac{1}{2}$.[7] Thus for this case our solution predicts almost complete cancellation, and it is reasonable to suppose that the 0.02 error is a result of our approximations and not physically meaningful. For larger spin, it has been suggested that the simple *s-d* exchange model, in which the momentum dependence of the exchange has been neglected, is inadequate.[27] The present results support this.

Finally, if we assume complete cancellation at $T=0$ and examine the temperature dependence of (4.18), we see that the coefficient of χ_0 does not go to zero sufficiently rapidly to overcome the T^{-1} divergence of χ_0 and predict a finite $T=0$ susceptibility.

V. CONCLUSIONS

The results of this calculation have been examined in detail in the main text, and will only be summarized here. First, we conclude that the approaches of Nagaoka,[6] Suhl,[5] and Abrikosov[3] are all equivalent to leading logarithmic order. The self-energy given by Abrikosov, however, apparently corresponds to an incorrect analytic continuation of the high-temperature perturbation series. Second, we conclude that the properties of the system vary smoothly with temperature. T_K determines the scale of the temperature variation, but does not mark the onset of any instability. Nagaoka's interpretation of his solution as evidence of a quasibound state[6] has engendered a school of thought which would consider Suhl's solution to represent a supercooled state of the system below T_K.[16] Our results indicate that Nagaoka's calculation should not continue to be used to support this view.

This physical picture is also suggested by Yosida's demonstration that a singlet bound state can exist for the *s-d* exchange model.[28] Close examination of his calculation shows that the approximate eigenstate is undamped because sharp Fermi functions keep integrals involving energy denominators away from their singularities by approximately T_K. From (4.12) we see that n_k, which is the average occupation of the state k at the impurity site, is the Fermi function for $T\gg T_K$, but has a width of order T_K for $T\ll T_K$. This suggests that if Yosida had attempted a self-consistent calculation, simultaneously deforming the Fermi sea at the impurity site and calculating the approximate one-particle eigenstates, he would have found damping and a scattering resonance instead of a true bound state.

Experimental susceptibility results, which are most relevant to this question, are usually dominated by impurity interaction at low temperatures. Measurements which seem to be free from this effect have been carried out on Fe in Rh, Ir, and $Rh_{0.5}Ir_{0.5}$, all showing a finite zero-temperature susceptibility.[29] However such measurements of Fe in Cu show a diverging susceptibility with a steadily decreasing moment per Fe far below the T_K inferred from resistivity measurements.[30] The latter is in qualitative agreement with our results, while the former is not. We believe that the *s-d* exchange model may be inadequate for the susceptibility calculation, as we will explain below.

The more realistic dilute alloy model introduced by Anderson[24] can be transformed into the *s-d* exchange model by neglecting the hopping processes which give the level its width.[31] It has been shown that a rather complicated correlation mechanism acts in the Anderson model to make the effective spin lifetime much longer than the hopping time so that a Curie law susceptibility is seen at high temperatures.[32] The Kondo anomaly[1] is also present at these temperatures.[33] However, it has been suggested that below T_K, the Kondo mechanism may act to undo the correlation effect which produced this long spin lifetime, and suppress the impurity moment itself rather than compensating it with a bound cloud of conduction electrons.[34] An accurate low-temperature treatment of the Anderson model should satisfy the self-consistency requirement suggested by Suhl in his criticism of the bound-state result for the *s-d* exchange model.[35]

ACKNOWLEDGMENTS

The author is indebted to P. W. Anderson, J. Kondo, and L. Dworin for many stimulating discussions of this work.

[27] J. R. Schrieffer, J. Appl. Phys. **38**, 1143 (1967).
[28] K. Yosida, Phys. Rev. **147**, 223 (1966).
[29] G. S. Knapp, J. Appl. Phys. **38**, 1267 (1967).
[30] M. D. Daybell and W. A. Steyert, Phys. Rev. Letters **18**, 398 (1967).
[31] J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).
[32] D. R. Hamann, Phys. Rev. Letters **17**, 145 (1966).
[33] D. R. Hammann, Phys. Rev. **154**, 596 (1967).
[34] L. Dworin (private communication).
[35] H. Suhl, Phys. Rev. Letters **17**, 1141 (1966).