Removing the Divergence at the Kondo Temperature by Means of Self-Consistent Perturbation Theory

C. Y. Cheung
Department of Physics, Collège militaire royal de Saint-Jean, Saint-Jean, Québec, Canada

and

R. D. Mattuck
Physics Laboratory I, H. C. Ørsted Institute, University of Copenhagen, Copenhagen, Denmark
(Received 10 November 1969; revised manuscript received 5 June 1970)

We consider a dilute alloy consisting of conduction s electrons exchange interacting with magnetic impurity d electrons. Perturbation calculations of the s-d scattering amplitude Γ by Abrikosov, Duke, and Silverstein show a divergence at the Kondo temperature T_K; this implies a breakdown of perturbation theory and transition to a bound state. However, Hamann's calculations, utilizing decoupled Green's-function equations of motion, reveal no divergence at T_K. It has been proposed that the disagreement is due to the fact that the perturbation calculations are restricted to a sum over only the leading logarithmic terms ("parquet" diagrams) in each order. To investigate this idea, we have followed a suggestion by Doniach and extended the perturbation sum to include nonparquet diagrams by *self-consistently clothing all s-electron propagators*. We first clothe just the simple ladder parquets, where the sum can be carried out exactly, then extend the argument to include all parquets. In both cases, it is found that the clothing pushes the divergence in Γ down to $T=0$, showing that *perturbation theory is valid for all temperatures greater than zero*. At $T=0$, there is a bound state. The resistance calculated from Γ turns out to have the Hamann form, thus producing agreement between the perturbation-theoretic and decoupled equations-of-motion results.

I. INTRODUCTION

There has been considerable controversy concerning the convergence of the perturbation expansion and the existence of a bound state in a system of conduction s electrons exchange interacting with a localized magnetic impurity d electron ("Kondo problem"). Abrikosov[1] and Silverstein and Duke[2] carried out a sum over the leading logarithmic terms ("parquet" diagrams) in each order of perturbation theory, and found that in this approximation the s-d scattering amplitude or "vertex part" Γ diverged at the "Kondo temperature" T_K. This implies a breakdown of perturbation theory and transition to a bound state under T_K.[3] In addition, ground-state calculations indicate there is a bound state at zero temperature.[4]

Another approach to the problem is based on Nagaoka's decoupled equations of motion for the s-electron propagator.[5] Nagaoka's approximate solution of his equations revealed a divergence at T_K, in agreement with the perturbation theory. On the other hand, Hamann's[6] more accurate solution of Nagaoka's equations showed no indication of any divergence. Hamann's result has also been obtained in a decoupling approximation by Doniach[7] and by Theumann.[8]

Since any decoupling of the Green's-function equation of motion is equivalent to a partial sum in perturbation theory,[9] one is led to suspect that Nagaoka's solution corresponds to Abrikosov's sum over parquet diagrams, while Hamann's solution apparently goes beyond parquet approximation. To investigate this idea, we have followed a proposal of Doniach,[7] and *extended the perturbation sum to include nonparquet diagrams by self-consistently clothing all s-electron propagators.*[10] We first carry this out just for parquets of the ladder type, since the sum here can be done exactly, and then generalize to include all parquets. Both cases yield essentially the same results: Clothing the s propagators pushes the divergence in Γ from $T=T_K$ down to $T=0$. This indicates that *there is no breakdown of perturbation theory at the Kondo temperature T_K and no bound state starting in at T_K*. Instead, in this approximation, *breakdown of perturbation theory and a corresponding bound state occur only at zero temperature*. The resistance calculated from Γ turns out to have the Hamann form, thus producing agreement between the perturbation-theoretic and decoupled equation-of-motion results. Our conclusions agree with the conjectures of Nozières, Gavoret, and Roulet[11] regarding the importance of self-consistent renormalization in the Kondo problem.

The Hamiltonian is discussed in Sec. I. The bare ladder approximation is reviewed in Sec. III, where it is shown that the s-d vertex part Γ, s-electron self-energy, and electrical resistance all diverge at the Kondo temperature. This occurs for both signs of the s-d coupling constant J. Section IV describes the self-consistent perturbation theory in ladder approximation with clothed s propagators. In this approximation Γ diverges (for both signs of J) just at $T=0$. However, the divergence is weak enough so that there is no corresponding divergence in the resistance, which has the Hamann form. Finally, in Sec. V, a heuristic argument is used to generalize the above calculation to include all parquets with self-consistently clothed s electrons. This yields results qualitatively just like those in clothed ladder approximation, except that the $T=0$ divergence occurs only for $J<0$.

II. THE HAMILTONIAN

The Hamiltonian which we will use is the same as that of Kondo,[12] except that Kondo's impurity spin operator is replaced by its second quantized form. It is given by

$$H=\sum_{k,\alpha} \epsilon_k c^\dagger_{k\alpha} c_{k\alpha}+\sum_{\beta} \epsilon_d c^\dagger_{d\beta} c_{d\beta}-\frac{J}{2N} \times \sum_{\alpha\alpha'\beta\beta'kk'} (\vec{\sigma}_{\alpha'\alpha}\cdot\vec{S}_{\beta'\beta}) c^\dagger_{d\beta'} c^\dagger_{k'\alpha'} c_{k\alpha} c_{d\beta}\,, \quad (1)$$

where J is s-d coupling constant, N the number of atoms, ϵ_k, ϵ_d are the bare s,d-electron energies relative to the Fermi energy, $c^\dagger_{k\alpha}$, $c_{k\alpha}$, $c^\dagger_{d\beta}$, $c_{d\beta}$ are the creation and destruction operators for s,d electrons, and $\vec{\sigma}_{\alpha'\alpha}$, $2\vec{S}_{\beta'\beta}$ are the Pauli matrices for s,d electrons. The many-body states for the free d-electron part of the Hamiltonian (i.e., ϵ_d term) are $|0_\uparrow, 0_\downarrow\rangle$, $|1_\uparrow, 0_\downarrow\rangle$, $|0_\uparrow, 1_\downarrow\rangle$, and $|1_\uparrow, 1_\downarrow\rangle$ with associated energies $0, \epsilon_d, \epsilon_d, 2\epsilon_d$, respectively. We have for the average number of $d\uparrow$, root-mean-square d spin, and mean fluctuation in d-electron number, respectively:

$$\langle n_{d\uparrow}\rangle=\langle n_{d\downarrow}\rangle=[\exp(\beta\epsilon_d)+1]^{-1}\,, \quad (2)$$

$$\langle S^2\rangle=(\sqrt{\tfrac{3}{2}})\exp(-\tfrac{1}{2}\beta\epsilon_d)\,[\exp(-\beta\epsilon_d)+1]^{-1}, \quad (3)$$

$$(\langle N_d^2\rangle-\langle N_d\rangle^2)^{1/2}=\sqrt{2}\exp(-\tfrac{1}{2}\beta\epsilon_d)\,[\exp(-\beta\epsilon_d)+1]^{-1}, \quad (4)$$

where $\beta=(k_BT)^{-1}$. The average d spin is zero, but since $\langle S^2\rangle$ is nonzero, there is a free-d magnetic moment.

The Hamiltonian (1) has been employed by Takano and Ogawa (TO),[13] and it is identical with Abrikosov's pseudospin Hamiltonian for a spin-$\frac{1}{2}$ impurity.[1] Unlike the Kondo H,[12] which has *exactly* one d electron in the spin-$\frac{1}{2}$ case, our H also includes states with 0 and 2 d electrons. However, if we follow TO and take $\epsilon_d=0$, then by (2) the *average* number of (unperturbed) d electrons is equal to 1 and, as Abrikosov points out, in calculating such quantities as self-energy, the only effect of the 0 and 2 d-electron states is to introduce a normalization factor of 2. This means that our results for self-energy and resistance should be multiplied by 2 to obtain the corresponding results for the Kondo H.

It should be noted that (1) is for a single impurity spin located at the origin, as in the work of Nagaoka[5] and Hamann.[6] Following these two authors, we will simply multiply our result by cN (c is the concentration of impurity atoms) to get the resistance for a system of noninteracting impurities. However, a more correct procedure requires averaging over a random distribution of impurity positions.[1]

III. BARE LADDER APPROXIMATION

In this section, we will calculate the s-d vertex part, s-electron self-energy, and resistance in bare ladder approximation using Hamiltonian (1) and show that these quantities all diverge at the Kondo temperature. Although similar calculations have been reported before,[14,15] things will be done in some detail here for the following reasons: (i) The details are not available elsewhere; (ii) the formalism here has $\epsilon_d=0$, in contrast to Abrikosov's, which has $\epsilon_d\to\infty$; (iii) to show explicitly that TO's zero resistance above the Kondo temperature[13] is due solely to the fact that their generalized Hartree-Fock approximation is inadequate above T_K; (iv) most of the intermediate results in the bare case may be generalized immediately to the clothed case. Note that the ladder parquet approximation is discussed first, since it is very simple, yet yields almost the same results as the full parquet approximation (Sec. V).

A. s-d Vertex Part

The perturbation expansion for the s-d vertex part in bare ladder approximation is the sum of a particle-particle part Γ and a particle-hole part γ as shown in Fig. 1(a). The integral equations for these quantities, Figs. 1(b) and 1(c), may be translated into functions by associating with each solid line the bare s-electron propagator

$$iG_0(k,\omega_n)=-(i\omega_n-\epsilon_k)^{-1}\,,$$

where

$$\omega_n=\pi(2n+1)\beta^{-1}, \quad n=0,\pm 1,\pm 2,\ldots, \quad \beta=(k_BT)^{-1} \quad (5)$$

with each dotted line the bare d-electron propagator

$$iG_0(d,\omega_m)=-(i\omega_m-\epsilon_d)^{-1} \quad (6)$$

and the value $(J/2N)\,(\vec{\sigma}_{\alpha'\alpha}\cdot\vec{S}_{\beta'\beta})$ with each intersection of a solid and a dotted line. Note that each s-d intersection is simply an abbreviated form for the interaction diagram (b) shown in Fig. 2, which is obtained directly from the interaction term in (1). There is a sum over all intermediate frequencies and s-electron momenta, and a -1 for each s-electron loop and d-electron loop.

Let us examine the particle-particle vertex first. Figure 1(b) yields (note that in the bare case $l=l'$)

$$\Gamma_{\alpha\beta\alpha''\beta''}(q,\omega_n;\,p,\omega_i;\,\omega_m)=\frac{J}{2N}(\vec{\sigma}_{\alpha\alpha''}\cdot\vec{S}_{\beta\beta''})+\frac{J}{2N\beta}\sum_{l,s,\alpha',\beta'}(\vec{\sigma}_{\alpha\alpha'}\cdot\vec{S}_{\beta'\beta})\,iG_0(l,-\omega_s)\times iG_0(d,\omega_s+\omega_m)\,\Gamma_{\alpha'\beta'\alpha''\beta''}(l,\omega_s;\,p\omega_i;\,\omega_m)\,. \quad (7)$$

Writing Γ as the sum of a scalar and a vector part

$$\Gamma_{\alpha\beta\alpha''\beta''}=\Gamma^0\delta_{\alpha\alpha''}\delta_{\beta\beta''}+\Gamma^1\vec{\sigma}_{\alpha\alpha''}\cdot\vec{S}_{\beta\beta''} \quad (8)$$

and utilizing the fact that

$$\sum_{\alpha'\beta'}(\vec{\sigma}_{\alpha\alpha'}\cdot\vec{S}_{\beta\beta'})(\vec{\sigma}_{\alpha'\alpha''}\cdot\vec{S}_{\beta'\beta''})=\tfrac{3}{4}\delta_{\alpha\alpha''}\delta_{\beta\beta''}-\vec{\sigma}_{\alpha\alpha''}\cdot\vec{S}_{\beta\beta''} \quad (9)$$

yields the two coupled equations

$$\Gamma^0(q,\omega_n;\,p,\omega_i;\,\omega_m)=\frac{3J}{8N\beta}\sum_{l's'}iG_0(l',-\omega_s')\,iG_0(d,\omega_s'+\omega_m)\,\Gamma^1(l',\omega_s',p,\omega_i;\,\omega_m) \quad (10)$$

and

$$\Gamma^1(q,\omega_n;\,p,\omega_i;\,\omega_m)=\frac{J}{2N}+\frac{J}{2N\beta}\sum_{l,s}\Gamma^0(l,\omega_s;\,p,\omega_i;\,\omega_n)\,iG_0(l,-\omega_s)\,iG_0(d,\omega_s+\omega_m)-\frac{J}{2N\beta}\sum_{l,s}\Gamma^1(l,\omega_s;p,\omega_i;\omega_m)iG_0(l,-\omega_s)\,iG_0(d,\omega_s+\omega_m)\,. \quad (11)$$

Substituting (11) in (10), and noting that Γ^1 is independent of q, ω_n so that it can be factored out of the sum, leads to

$$\Gamma^1(\omega_m)=\frac{J/2N}{1+K_0-\frac{3}{4}K_0^2}\,, \quad (12)$$

$$\Gamma^0(\omega_m)=\tfrac{3}{4}K_0\Gamma^1(\omega_m)\,, \quad (13)$$

where

$$K_0(\omega_m)=\frac{J}{2N}\sum_l\frac{1}{\beta}\sum_{\omega_s}iG_0(l,-\omega_s)\,iG_0(d,\omega_s+\omega_m)\,. \quad (14)$$

Note that Kondo's approximation[12] is equivalent to taking just the first- and second-order terms in Γ (plus the second-order term in γ), which gives (13) instead of (12):

$$\Gamma^1=(J/2N)(1-K_0);\quad \Gamma^0=\tfrac{3}{4}(J/2N)K_0(1-K_0)\,. \quad (15)$$

The quantity $K(\omega_m)$, which is just one of the s-d "pair bubbles" in Fig. 1(b), may easily be evaluated by means of the following theorem (proved directly from the Poisson sum formula[16]):

$$\frac{1}{\beta}\sum_{s=-\infty}^{+\infty}F(i\omega_s)=\text{sum of the residues of } F(\omega)f(\omega)\text{ at the poles of } F(\omega)\,, \quad (16)$$

where $f(\omega)$ is the Fermi function

$$f(\omega)=(e^{\beta\omega}+1)^{-1}=\tfrac{1}{2}[1-\tanh\tfrac{1}{2}(\beta\omega)] \quad (17)$$

and $F(\omega)\to 0$ at infinity faster than ω^{-1}. Putting (5) and (6) in (14), we have for $F(\omega)$

$$F(\omega)=(\omega+\epsilon_l)^{-1}(\omega+i\omega_m-\epsilon_d)^{-1}\,, \quad (18)$$

so that (16) becomes

$$\frac{1}{\beta}\sum_{\omega_s}F(i\omega_s)=\frac{f(\epsilon_d-i\omega_m)}{\epsilon_l+\epsilon_d-i\omega_m}-\frac{f(-\epsilon_l)}{\epsilon_l+\epsilon_d-i\omega_m}\,. \quad (19)$$

Since, by (5), ω_s and $(\omega_s+\omega_m)$ are both proportional to an odd integer, ω_m is proportional to an even integer, so that

$$f(\epsilon_d-i\omega_m)=f(\epsilon_d)\,. \quad (20)$$

Hence, we find that

$$K_0(\omega)=\frac{J}{4N}\sum_l\frac{\tanh(\frac{1}{2}\beta\epsilon_l)+\tanh(\frac{1}{2}\beta\epsilon_d)}{\epsilon_l+\epsilon_d-i\omega}=\frac{J\rho}{4N}\int_{-D}^{+D}d\epsilon\,\frac{\tanh(\frac{1}{2}\beta\epsilon)}{\epsilon-i\omega}\,. \quad (21)$$

Here we have replaced ω_m by the continuous variable ω, assumed a constant density of states ρ over a band of width $2D$, and we have set $\epsilon_d=0$ as mentioned after (1).

Since the physical scattering amplitude is in the real time domain (and therefore, by Fourier transforming, in the real frequency domain), $K_0(\omega)$ must be analytically continued to just above the real axis, where it has a branch cut. Thus we make the substitution $i\omega\to x+i\delta$, where δ is a positive infinitesimal, in (21). After using the theorem

$$(y+i\delta)^{-1}=Py^{-1}-i\pi\delta(y)\,, \quad (22)$$

where P is the principal part, we obtain

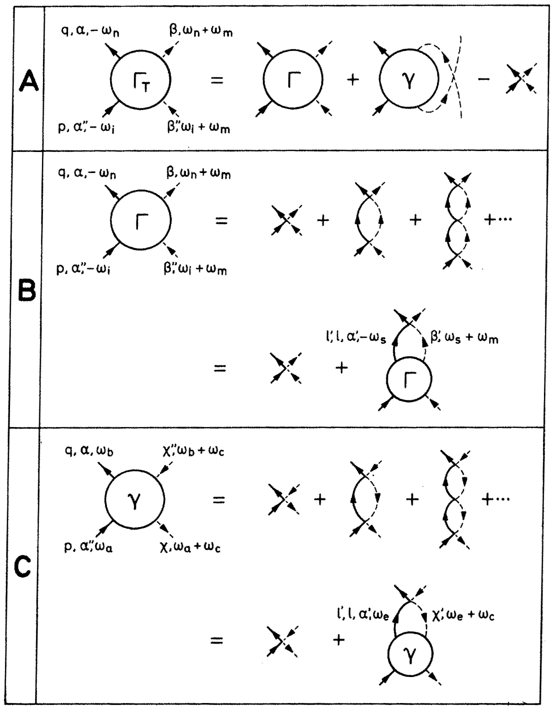

FIG. 1. The s-d scattering amplitude (vertex part) in ladder approximation. (A) shows the total vertex part Γ_T in terms of particle-particle part Γ and particle-hole part γ. (B) and (C) show the ladder sum and integral equation for Γ and γ, respectively. Solid lines: bare or clothed s-electron propagators. Dotted lines: bare d-electron propagators. Intersections: s-d exchange interactions.

$$K_0(x+i\delta)=\frac{J\rho}{4N}\,P\int_{-D}^{+D}d\epsilon\;\frac{\tanh(\frac12\beta\epsilon)}{\epsilon-x}+i\,\frac{J\pi\rho}{4N}\,\tanh\left(\frac{\beta x}{2}\right)$$

$$\approx\frac{J\rho}{4N}\,\ln\left[\frac{D^2}{x^2+(2k_BT)^2}\right]+i\,\frac{J\pi\rho}{4N}\,\tanh\left(\frac{x}{2k_BT}\right)\quad\text{for } D\gg x,\ 2k_BT\ . \tag{23}$$

Examination of (12) shows that Γ^1 diverges when

$$K_0=-\tfrac23+i0\quad\text{or}\quad K_0=2+i0\ . \tag{24}$$

According to (23), we must have $x=0$ for the imaginary part of K_0 to vanish. Hence, the condition for Γ to diverge is

$$K_0(0+i\delta)=\frac{J\rho}{4N}\int_{-D}^{+D}d\epsilon\;\frac{\tanh(\frac12\beta\epsilon)}{\epsilon}=-\tfrac23\ \text{ or }\ +2\ . \tag{25}$$

Using the approximation in (23) yields

$$K_0(0+i\delta)\approx(J\rho/2N)\ln\,(D/2k_BT)\ , \tag{26}$$

so Γ diverges at

$$k_BT_{K_1}=\tfrac12 D\exp(-4N/3|J|\rho)\quad\text{for } J<0\ , \tag{27}$$

$$k_BT_{K_2}=\tfrac12 D\exp(-4N/J\rho)\qquad\text{for } J>0\ , \tag{28}$$

which are just the two critical "Kondo temperatures" found by TO.[13] This result is to be expected since the vertex part must diverge at just the point where the anomalous propagators go to zero.[3] Note that in Kondo's approximation (15), Γ^0 diverges as $\ln^2T$ when $T\to0$, while in ladder approximation, the divergence at T_K is much stronger than $\ln^2T$.

Let us now consider the particle-hole vertex part γ as in Fig. 1(c). This can be evaluated in the same way Γ was, with a couple of slight differences: First, the spin sum which arises in place of (9) is

$$\sum_{\alpha'\chi'}(\vec\sigma_{\alpha'\alpha''}\cdot\vec S_{\chi\chi'})(\vec\sigma_{\alpha\alpha'}\cdot\vec S_{\chi'\chi''})=\tfrac34\delta_{\alpha\alpha''}\delta_{\chi\chi''}+\vec\sigma_{\alpha\alpha''}\cdot\vec S_{\chi\chi''}\ . \tag{29}$$

Second, there is a -1 factor coming from the $+\omega_s$ (instead of $-\omega_s$) in the frequency sum [see (16)–(19)]. The result for γ is

$$\gamma^1(\omega_c)=\Gamma^1(-\omega_c)\ , \tag{30}$$

$$\gamma^0(\omega_c)=-\Gamma^0(-\omega_c)\ . \tag{31}$$

Now we combine (12) and (13) as indicated in Fig. 1(a) to get the total vertex part in ladder approximation

$$\Gamma_T=\Gamma_{\alpha\beta\alpha''\beta''}(\omega_m)+\gamma_{\alpha\beta\alpha''\beta''}(\omega_m+\omega_n+\omega_i)-(J/2N)\,\vec\sigma_{\alpha\alpha''}\cdot\vec S_{\beta\beta''}\ . \tag{32}$$

B. s-Electron Self-Energy and Resistance

The conduction electron self-energy Σ may be obtained from the vertex part as shown in Fig. 3.

Since the s-d interaction in (1) is momentum independent, Σ will be independent of k, k'. (However, if we average over impurity position,[2] a $\delta_{kk'}$ factor appears in Σ.) Furthermore, it is easy to see from Fig. 3 that the outgoing spin α' must always be the same as the incoming spin α. This is because by (8), (30), (31), and (32), Γ_T may be written as the sum of a vector and a scalar part. Hence, using (9), the spin sum for Fig. 3 is

$$\sum_{\beta\beta''\alpha''}(\Gamma_T^0\,\delta_{\alpha'\alpha''}\,\delta_{\beta\beta''}+\Gamma_T^1\,\vec\sigma_{\alpha'\alpha''}\cdot\vec S_{\beta\beta''})$$

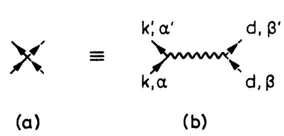

FIG. 2. (a) Abbreviated form for the s-d interaction; (b) long form for the s-d interaction.

$$\times (\vec{\sigma}_{\alpha''\alpha}\cdot\vec{S}_{\beta''\beta}) = \tfrac{3}{2}\Gamma_T^1\,\delta_{\alpha'\alpha}\ . \tag{33}$$

We now evaluate Σ using Fig. 3. (Note that in the bare case, $p'=p$.) Translating Fig. 3 into functions and doing the spin sums yields

$$\Sigma(\omega_n) = \frac{3}{2\beta}\sum_{\omega_n}\frac{K_0(\omega_m)\Gamma_T^1(\omega_m)}{i\omega_n - i\omega_m}\ . \tag{34}$$

Expressing Γ_T^1 with the aid of Fig. 1(a) and Eq. (32), utilizing (30) and (13), and making a change of summation variable in the γ' term, we find, for $\alpha=\alpha'$, that

$$\Sigma(\omega_n) = \frac{1}{\beta}\sum_{\omega_m}\frac{4\Gamma^0(\omega_m) - (3J/4N)K_0(\omega_m)}{i\omega_n - i\omega_m}\ . \tag{35}$$

It is easy to do the frequency sum in (35) if we first express the numerator in spectral form

$$4\Gamma^0(\omega_m) - \frac{3J}{4N}K_0(\omega_m) = \int_{-\infty}^{+\infty} d\omega\,\frac{Q(\omega)}{i\omega_m - \omega}\ , \tag{36}$$

where the spectral density Q is given by

$$Q(\omega) = -(1/\pi)\,\mathrm{Im}[4\Gamma^0(\omega+i\delta) - (3J/4N)K_0(\omega+i\delta)]\ . \tag{37}$$

Then we have

$$\Sigma(\omega_n) = \int_{-\infty}^{+\infty} d\omega\, Q(\omega)\,\frac{1}{\beta}\sum_{\omega_m}\frac{1}{(i\omega_n - i\omega_m)(i\omega_m - \omega)}\ . \tag{38}$$

Since by Fig. 3, ω_m is proportional to an *even* integer, the Poisson sum formula becomes

$$\frac{1}{\beta}\sum_{\omega_m} F(i\omega_m) = -\text{ sum of residues of } F(\omega)g(\omega) \text{ at the poles of } F(\omega)\ , \tag{39}$$

where $g(\omega)$ is the Bose function

$$g(\omega) = [\exp(\beta\omega) - 1]^{-1}\ . \tag{40}$$

Applying this to the sum in (38) yields

$$\Sigma(\omega_n) = -\int_{-\infty}^{+\infty} d\omega\, Q(\omega)\left(\frac{g(\omega)+\frac{1}{2}}{i\omega_n - \omega}\right)\ . \tag{41}$$

Now the resistance may be obtained from the imaginary part of the conduction electron self-energy (inverse lifetime $= -2\,\mathrm{Im}\Sigma$) evaluated at the Fermi surface[5]:

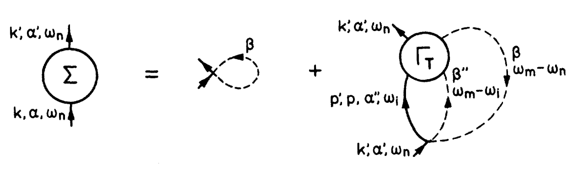

FIG. 3. The s-electron proper self-energy Σ in terms of the total vertex part Γ_T. The s-electron propagator may be bare or clothed.

$$R = 3cN/2e^2\rho v_F^2\tau_F = -(3cN/e^2\rho v_F^2)\,\mathrm{Im}\Sigma(0+i\delta)\ , \tag{42}$$

where $\Sigma(x+i\delta)$ means $\Sigma(\omega_n)$ analytically continued to just above the real axis. Substituting $x+i\delta$ for ω_n in (41) and using (22), (37), (12), and (13) yields

$$\mathrm{Im}\Sigma(x+i\delta) = \pi[g(x)+\tfrac{1}{2}]\,Q(x) \tag{43}$$

$$= -\frac{3J}{4N}\left(g(x)+\frac{1}{2}\right)\mathrm{Im}\left(\frac{2K_0}{1+K_0-\frac{3}{4}K_0^2} - K_0\right)\ . \tag{44}$$

Since $g(0)=\infty$, (44) must be evaluated for small x and the limit taken as $x\to 0$. Breaking up K_0 into real and imaginary parts, and noting from (23) that for small x, $\mathrm{Im}K_0 \ll \mathrm{Re}K_0$, (44) becomes

$$\mathrm{Im}\Sigma(x+i\delta) = -\frac{3J}{4N}\,[g(x)+\tfrac{1}{2}](\mathrm{Im}K_0) \times\left(\frac{2[1+\frac{3}{4}(\mathrm{Re}K_0)^2]}{[1+\mathrm{Re}K_0) - \frac{3}{4}(\mathrm{Re}K_0)^2]^2} - 1\right)\ . \tag{45}$$

From (23) and (40) we have

$$[g(x)+\tfrac{1}{2}]\,\mathrm{Im}K_0 = J\rho\pi/8N\ . \tag{46}$$

Substituting this in (45), using (23) for $\mathrm{Re}K_0$, setting $x=0$, and placing the result in (42) yields for the resistance

$$R = \frac{9\pi J^2 c}{32e^2 v_F^2 N}\left(\frac{2(1+\frac{3}{4}K_0^2)}{(1+K_0-\frac{3}{4}K_0^2)^2} - 1\right)\ , \tag{47}$$

where

$$K_0 = (J\rho/2N)\ln(D/2k_BT). \tag{48}$$

This result should be compared with the resistance obtained by Nagaoka in the high-temperature region[5]:

$$R_{\mathrm{Nagaoka}} = \frac{9\pi J^2 c}{32e^2 v_F^2 N}\left(\frac{1}{1+(J\rho/N)\ln(D/2k_BT)}\right)\ . \tag{49}$$

Qualitatively, (48) and (49) are similar, both increasing monotonically as T is lowered and diverging at a critical temperature. However, the Nagaoka expression diverges only for $J<0$, while (47) diverges for both signs of J.

If we use the second-order approximation for Γ^0 [see (15)], the resistance is

$$R = (9\pi J^2 c/32e^2 v_F^2 N)[1-(J\rho/N)\ln(D/2k_BT)]\ , \tag{50}$$

which is essentially Kondo's result.[12]

IV. LADDER APPROXIMATION WITH SELF-CONSISTENTLY CLOTHED s PROPAGATORS

In Sec. III we saw that in bare ladder approximation all physical quantities diverged at the Kondo temperature. In this section it is shown that self-consistently clothing the s propagators in the ladder pushes the divergence in Γ down to

$T=0$ and that the corresponding resistance has the Hamann form. The calculation here is equivalent to the decoupled equation-of-motion calculation of the singlet and triplet propagators by Doniach.[7] In fact, Doniach pointed out without proof that his method was equivalent to a self-consistent ladder sum. The results in this section constitute the proof of this statement.

We first obtain an integral equation for the vertex part Γ in terms of the pair bubble K. Then K is expressed in terms of the s-electron self-energy Σ, with the aid of the t-matrix equations in Fig. 5. The self-consistent cycle is completed by obtaining Σ in terms of Γ. The argument has the "dog biting its own tail" form pictured in Fig. 4. In this way, a simple and easily solved algebraic equation for K is obtained. When the solution is placed in Γ, we find that Γ diverges as $\ln T$ for $T\to 0$, showing a bound state at zero temperature. Finally, Γ is put into Σ and the resistance is calculated from $\mathrm{Im}\Sigma$.

A. Vertex Part in Terms of Pair Bubble

The vertex part is given by Fig. 1 with solid lines now interpreted as *clothed* s propagators. Following the same procedure as in (7)–(14), we find that (32) holds and

$$\Gamma^1(\omega_m)=\frac{J/2N}{1+K(\omega_m)-(\frac{3}{4})K^2(\omega_m)}\ , \tag{51}$$

$$\Gamma^0(\omega_m)=\tfrac{3}{4}\,K(\omega_m)\Gamma^1(\omega_m)\ , \tag{52}$$

where

$$K(\omega_m)=\frac{J}{2N}\sum_{kk'}\frac{1}{\beta}\sum_{\omega_s} iG(k,k',-\omega_s)\,iG_0(d,\omega_s+\omega_m)\ . \tag{53}$$

Here, $iG(k,k',-\omega_s)$ is the clothed s propagator, as yet unknown. Also

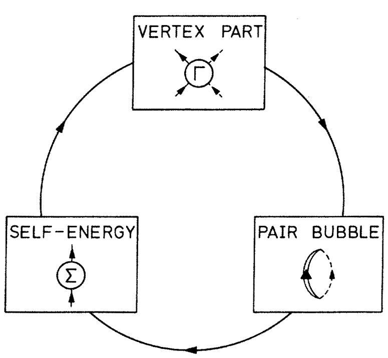

FIG. 4. Schematic view of our self-consistent "dog biting its own tail" argument: The vertex part is expressed in terms of the pair bubble, the pair bubble in terms of the self-energy, and the self-energy in terms of the vertex part. The double line is a clothed s propagator.

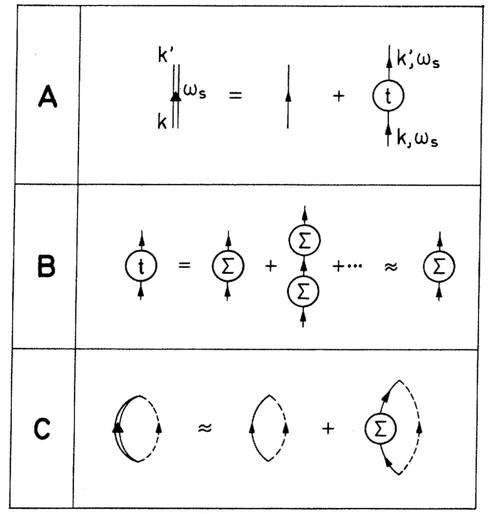

FIG. 5. (A) The s propagator in terms of the t matrix; (B) the t matrix in terms of the proper self-energy Σ; (C) the pair bubble with clothed s propagator. Single solid lines are bare s electrons; double lines are clothed s electrons.

$$\gamma^1(\omega_c)=\Gamma^1(-\omega_c),\quad \gamma^0(\omega_c)=-\Gamma^0(-\omega_c)\ . \tag{54}$$

Equations (51)–(54) express the vertex part in terms of the pair bubble.

B. Pair Bubble in Terms of s-Electron Proper Self-Energy

The expression for the s propagator in terms of the "t matrix" of Nagaoka[5] and Hamann[6] appears in Fig. 5(a). The t matrix is just the *reducible* self-energy, given in Fig. 5(b) in terms of a sum over the repeated *irreducible* (proper) self-energy Σ. The quantity Σ itself is the sum over all irreducible self-energy parts. [Note that Fig. 5(a) may be obtained simply by iterating in the Dyson equation and substituting 5(b).[17]]

To get a simple first approximation to the renormalized s propagator, we set t equal to Σ. Then, using Fig. 5(a) the s-electron propagator may be written as

$$iG(k',k,\omega_s)=iG_0(k,\omega_s)\,\delta_{k'k}+iG_0(k',\omega_s)\times[-\Sigma(\omega_s)]iG_0(k,\omega_s)\ . \tag{55}$$

In (55), we have utilized the fact that Σ is momentum independent [see just before (33)]. Furthermore, Σ is proportional to $\delta_{\alpha\alpha'}$ [see (33)], so that $iG\sim\delta_{\alpha\alpha'}$.

We now evaluate the s-d pair bubble K as given by (53) making use of (55). [The corresponding diagram is Fig. 5(c).] It is easier to do the frequency sum if we introduce the spectral representation of G:

$$iG(k',k,\omega_s)= -\int_{-\infty}^{+\infty} d\omega' \,\frac{A(k',k,\omega')}{i\omega_s-\omega'} , \qquad (56)$$

where the spectral density A is given by

$$A(k',k,\omega')= +(1/\pi)\operatorname{Im}[iG(k',k,\omega'+i\delta)] . \qquad (57)$$

Inserting these in the expression for K yields

$$K(\omega_m)=-\frac{J}{2N\pi}\sum_{k'k}\int_{-\infty}^{+\infty} d\omega' \operatorname{Im}[iG(k',k,\omega'+i\delta)]$$

$$\times\frac{1}{\beta}\sum_{\omega_s}\frac{1}{(i\omega_s-i\omega_m)(i\omega_s-\omega')} . \qquad (58)$$

The sum over ω_s may be carried out with the help of the Poisson formula in a manner similar to (16) –(20) and produces after using (55)

$$K(\omega_m)=K_0(\omega_m)+K_1(\omega_m) , \qquad (59)$$

where K_0 is the bare pair bubble as given by (21), and

$$K_1(\omega_m)=\frac{J}{2N\pi}\sum_{k'k}\int_{-\infty}^{+\infty} d\omega'\left(\frac{f(\omega')-\frac{1}{2}}{\omega'-i\omega_m}\right)$$

$$\times\operatorname{Im}[iG_0(k',\omega'+i\delta)\Sigma(\omega'+i\delta)iG_0(k,\omega'+i\delta)] , \qquad (60)$$

where $f(\omega')$ is the Fermi function, Eq. (17).

Breaking iG_0 and Σ into real and imaginary parts and defining the quantity

$$F(\omega'+i\delta)=\textstyle\sum_k iG_0(k,\omega'+i\delta) , \qquad (61)$$

(which is proportional to Nagaoka's[5] F), we find that

$$\sum_{k'k}\operatorname{Im}[iG_0(k',\omega'+i\delta)\Sigma(\omega'+i\delta)iG_0(k,\omega'+i\delta)]$$

$$=2(\operatorname{Re}F)(\operatorname{Im}F)(\operatorname{Re}\Sigma)+[(\operatorname{Re}F)^2-(\operatorname{Im}F^2)](\operatorname{Im}\Sigma) . \qquad (62)$$

Using (22) in (61) and assuming a constant density of states ρ in a band of width $2D$ yields

$$\operatorname{Re}F(\omega'+i\delta)=\rho P\int_{-D}^{+D}\frac{d\epsilon}{\epsilon-\omega'}=\rho\ln\left|\frac{D-\omega'}{D+\omega'}\right| , \qquad (63)$$

$$\operatorname{Im}F(\omega'+i\delta)=\pi\rho \quad \text{for } |\omega'|<D,$$
$$=0 \quad \text{for } |\omega'|>D . \qquad (64)$$

Making the Nagaoka approximation[5] that $\operatorname{Re}F\approx 0$ and $\operatorname{Im}F\approx\pi\rho$ for *all* ω', (62) becomes $-\pi^2\rho^2\operatorname{Im}\Sigma$. Putting this in (60), we then have from (59)

$$K(\omega_m)=K_0(\omega_m)-\frac{J\rho^2\pi}{2N}\int_{-\infty}^{+\infty} d\omega'\left(\frac{f(\omega')-\frac{1}{2}}{\omega'-i\omega_m}\right)\operatorname{Im}\Sigma(\omega'+i\delta), \qquad (65)$$

which is the pair bubble in terms of the s-electron self-energy.

C. Self-Energy in Terms of Vertex Parts

The "tail" in our self-consistent "dog-biting-tail" argument connects the proper self-energy Σ to the vertex part Γ. The tail is very short; it may be obtained with the aid of Fig. 3 which gives [cf. (34) and (35), and note that Γ^0 is given by (52)]

$$\Sigma(\omega_n)=\frac{1}{\beta}\sum_{\omega_m}\frac{4\Gamma^0(\omega_m)-(3J/4N)K(\omega_m)}{i\omega_n-i\omega_m} . \qquad (66)$$

D. Solution for the Pair Bubble

The procedure now is to solve Eqs. (51), (52), (65), and (66) simultaneously for K, Γ, and Σ. It is easiest to solve for K. First, we express the numerator of the Σ-Γ equation (66) in spectral representation and substitute the result in the K-Σ equation (65). This eliminates Σ and yields an algebraic equation involving Γ and K which may be solved together with the Γ-K equations (51) and (52) to yield K.

The numerator of (66) may be written in terms of a spectral density Q':

$$4\Gamma^0(\omega_m)-\frac{3J}{4N}K(\omega_m)=\int_{-\infty}^{+\infty} d\omega''\,\frac{Q'(\omega'')}{i\omega_m-\omega''} , \qquad (67)$$

where

$$Q'(\omega'')=-\frac{1}{\pi}\operatorname{Im}\left(4\Gamma^0(\omega''+i\delta)-\frac{3J}{4N}K(\omega''+i\delta)\right) . \qquad (68)$$

The pair bubble K in (65) involves $\operatorname{Im}\Sigma(\omega'+i\delta)$. Analogous to (43) this is given by

$$\operatorname{Im}\Sigma(\omega'+i\delta)=\pi Q'(\omega')[g(\omega')+\tfrac{1}{2}] . \qquad (69)$$

Putting this into (65) produces

$$K(\omega_m)=K_0(\omega_m)-\frac{J\rho^2\pi^2}{2N}\int_{-\infty}^{+\infty} d\omega'$$

$$\times\frac{Q'(\omega')[g(\omega')+\frac{1}{2}][f(\omega')-\frac{1}{2}]}{\omega'-i\omega_m} . \qquad (70)$$

At this point a remarkable simplification occurs by noting that

$$[g(\omega')+\tfrac{1}{2}][f(\omega')-\tfrac{1}{2}]=-\tfrac{1}{4} , \qquad (71)$$

so that (70) becomes

$$K(\omega_m)=K_0(\omega_m)+\frac{J\rho^2\pi^2}{8N}\int_{-\infty}^{+\infty} d\omega'\,\frac{Q'(\omega')}{\omega'-i\omega_m} , \qquad (72)$$

and the integral here is just that in (67). Hence, (72) becomes

$$K(\omega_m)=K_0(\omega_m)-\frac{J\rho^2\pi^2}{8N}\left(4\Gamma^0(\omega_m)-\frac{3J}{4N}K(\omega_m)\right) . \qquad (73)$$

Thus on account of (71), the integral equation of (70) reduces to the purely algebraic equation (73)!

Note that the approximations made just after (64) are essential in obtaining this simple result.

Substituting for Γ^0 in terms of K given by (51) and (52), we find that (73) becomes [after dropping the term $\frac{3}{8}(J\rho\pi/2N)^2K\sim 10^{-2}K$]

$$K=K_0-\frac{3}{4}\left(\frac{J\rho\pi}{2N}\right)^2 K\left(\underbrace{\frac{3/4}{1+(3/2)K}}_{A}+\underbrace{\frac{1/4}{1-(1/2)K}}_{B}\right), \tag{74}$$

which is just Doniach's Eq. (22).[7] We wish to find the solution of (74) at low temperatures. Consider first the case $J<0$. Let us look for a moment at the second term on the right-hand side of (74) as a correction to the first term K_0, and evaluate it by substituting K_0 for K. Using (23), we see that for $J<0$ the A term in the bracket will dominate the B term. Let us therefore assume the B term is negligible, evaluate the resulting quadratic equation for K, and then check to confirm that it is indeed $\ll A$ at low T. We find that

$$K=-\tfrac{2}{3}-\tfrac{1}{2}X+\tfrac{1}{2}[X^2+(J\rho\pi/2N)^2]^{1/2}, \tag{75}$$

where

$$X(\omega_m)=-K_0(\omega_m)-\tfrac{2}{3}+\tfrac{3}{8}(J\rho\pi/2N)^2. \tag{76}$$

We have chosen that branch of the square root which is consistent with the fact that $K(i\omega_m)\to 0$ as $i\omega_m\to\infty$ as can be seen from (58).

It is easy to check that indeed $A\gg B$ as $T\to 0$. In the low T limit, $K_0(x+i\delta)$ is given by (23), so that for $x<k_BT$, X becomes very large as $T\to 0$. Hence, we have from (75)

$$K_{T\to 0}(x+i\delta)\to -\tfrac{2}{3}+\tfrac{1}{4}(J\rho\pi/2N)^2X^{-1}. \tag{77}$$

Substituting this in A and B shows that $A/B\to\infty$ as $T\to 0$.

A similar treatment for the case $J>0$, where $B\gg A$, yields

$$\tilde{K}=2-\tfrac{1}{2}\tilde{X}-\tfrac{1}{2}[\tilde{X}^2+3(J\rho\pi/2N)^2]^{1/2}, \tag{78}$$

where

$$\tilde{X}(\omega_m)=-K_0(\omega_m)+2-\tfrac{3}{8}(J\rho\pi/2N)^2. \tag{79}$$

E. Divergence of Vertex Part at $T=0$

The scalar and vector vertex parts Γ^1, Γ^0 are obtained immediately by substituting (75) and (78) into (51) and (52).

Remember that for $K=K_0$, Γ^1 and Γ^0 diverged at the Kondo temperatures (27) and (28). However, when we use the self-consistent K given by (75) and (76), this is no longer true.

Consider first the $J<0$ case. For low T, (77) may be substituted in (51) yielding

$$\Gamma^1(x+i\delta)=(J/2N)[\tfrac{3}{4}(1+\tfrac{3}{2}K)^{-1}+\tfrac{1}{4}(1-\tfrac{1}{2}K)^{-1}]$$
$$\to(4N/J\rho^2\pi^2)X(x+i\delta)$$
$$\sim(1/\rho\pi^2)\ln\{D^2/[x^2+(2k_BT)^2]\}. \tag{80}$$

For $x=0$, we see that Γ^1 (and Γ^0) no longer diverges at T_K, but instead diverges logarithmically as $T\to 0$. This shows that there is a breakdown of perturbation theory and thus a bound state at $T=0$. The same result is obtained using (78) and (79) in (51) and (52) showing that the $T=0$ bound state exists for *either* sign of J, in this approximation.

The reason the divergence in Γ is pushed from $T=T_K$ down to $T=0$ when the s propagator is clothed may be seen as follows: If we look at (74) and approximate K in the second term on the right by K_0, we see that as T decreases, the second term will grow faster than the first. Since its sign is opposite to that of the first term, it will inhibit the growth of K. What we have here is "negative feedback" in the self-consistency loop: When Γ tends to become large, so does Σ, which reduces the s propagator, diminishing K, and thus Γ.[11, 18]

F. Calculation of Resistance

The resistance due to scattering by the impurity may be obtained from the imaginary part of the conduction electron self-energy by means of (42). $\mathrm{Im}\Sigma$ is found with the aid of (68), (69), (73), (75), and (76):

$$\mathrm{Im}\Sigma(\omega'+i\delta)=-[g(\omega')+\tfrac{1}{2}]\,\mathrm{Im}[4\Gamma^0-(3J/4N)K] \tag{81}$$

$$=(8N/J\rho^2\pi^2)[g(\omega')+\tfrac{1}{2}]\,\mathrm{Im}(K-K_0) \tag{82}$$

$$=\frac{4N}{J\rho^2\pi^2}[g(\omega')+\tfrac{1}{2}]\times\mathrm{Im}\left\{X+\left[X^2+\left(\frac{J\rho\pi}{2N}\right)^2\right]^{1/2}\right\}. \tag{83}$$

Since $g(0)=\infty$, we must evaluate (83) for small ω' and then take the limit as $\omega'\to 0$. Breaking up X into real and imaginary parts and noting that by (76) and (23) $\mathrm{Re}X\gg\mathrm{Im}X$ for small ω' yields immediately

$$\mathrm{Im}\Sigma(\omega'+i\delta)=\frac{4N}{J\rho^2\pi}[g(\omega')+\tfrac{1}{2}](\mathrm{Im}X)\times\left(1+\frac{\mathrm{Re}X}{[(\mathrm{Re}X)^2+(J\rho\pi/2N)^2]^{1/2}}\right). \tag{84}$$

Now, since $\mathrm{Im}X=-\mathrm{Im}K_0$, we have, by (46), that

$$[g(\omega')+\tfrac{1}{2}]\,\mathrm{Im}X=-J\rho\pi/8N, \tag{85}$$

so that after substituting this in (84), the limit $\omega'\to 0$ may be taken. Writing $\mathrm{Re}X(0+i\delta)$ in the form

$$\mathrm{Re}X(0+i\delta)=-(|J|\rho/2N)\ln(T/T_K'), \tag{86}$$

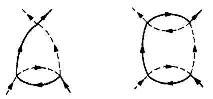

FIG. 6. Some examples of nonladder parquet diagrams contributing to the s-d vertex part.

where T_K' (a parameter nearly equal to T_K) is defined by the equation

$$(|J|\rho/2N)\ln(D/2k_BT_K')=\tfrac{2}{3}-\tfrac{3}{8}(J\rho\pi/2N)^2\ , \qquad (87)$$

and substituting (84) into (42) yields for the resistance

$$R=\frac{3cN}{2e^2\rho^2v_F^2\pi}\left(1-\frac{\ln(T/T_K')}{[\ln^2(T/T_K')+\pi^2]^{1/2}}\right)\ . \qquad (88)$$

This is just Hamann's result,[6] aside from the fact that for spin $\frac{1}{2}$, he has $\frac{3}{4}\pi^2$ instead of π^2 raised to the $\frac{1}{2}$ power.

Note that in Kondo's calculation, Γ^0 [which enters into Σ in (35)] diverges as $\ln^2 T$ as $T\to 0$, which is strong enough to make the resistance diverge as $\ln T$. But in the present calculation, Γ^0 [which enters into Σ in (66)] diverges only as $\ln T$ [see just after (80)] which is too weak to cause a divergence in R at $T=0$. However, the divergence of Γ at zero temperature and the corresponding breakdown of perturbation theory and a bound state at zero temperature do show up in R in the following way: For any given *finite* T, as $J\to 0$, $T_K'\to 0$. Hence $\ln T/T_K'\to\infty$, so the bracketed term in (88) goes to zero and $R\to 0$. That is, $R\to 0$ for $J\to 0$, indicating that perturbation theory is valid. But for $T=0$ and any finite J (no matter how small), $\ln T/T_K' = -\infty$, and the bracketed term in (88) goes to 2. This means that at $T=0$, R is independent of J, which is a nonperturbative result and indicates that a bound state has formed.

V. FULL PARQUET APPROXIMATION

The above calculations contained only parquet diagrams of the ladder type. However, nonladder parquets (see Fig. 6) are equally important and must be included in any realistic calculation.[1] Surprisingly enough, for $J<0$, the full parquet sum appears to yield essentially the same results as the simple ladder sum, as we will show now. It should be emphasized that the argument here is very rough. It is based on a generalization of Silverstein and Duke (SD)[2] and we will adhere quite closely to their notation.

We start with SD's *non*linear equations for the s-d vertex part Γ (this is not our Γ, but is rather our Γ_T generalized to include nonladder parquets). In SD I (3.1) we have the integral equation for Γ

$$\Gamma=\Gamma_0+\Lambda_1+\Lambda_2,\quad \Gamma_0=J\vec{\sigma}\cdot\vec{S} \qquad (89)$$

where Λ_1, Λ_2 are given in terms of Γ in SD I (3.2a) and (3.2b). These equations may be generalized to the clothed s-propagator case by replacing G^0 by G. Using (56) to express G in spectral form, SD I (3.2a) becomes

$$\begin{aligned}\langle\alpha\beta|\,\Lambda_1|\,\alpha'\beta'\rangle=&\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3q'}{(2\pi)^3}\int d\chi A(\vec{q},\vec{q}',\chi)\,\frac{1}{\beta}\sum_{\omega_n}\frac{-1}{(i\epsilon+i\omega_1-i\omega_n-\chi)}\,\frac{-1}{(i\omega_n-\epsilon_d)}\\ &\times\langle\alpha\beta|\,\Gamma[\vec{p},i\epsilon;i\omega_1|\vec{q},i(\epsilon+\omega_1-\omega_n);i\omega_n]|\,\alpha''\beta''\rangle\\ &\times\langle\alpha''\beta''|\,\Gamma[\vec{q}',i(\epsilon+\omega_1-\omega_n);i\omega_n|\vec{p}',i(\epsilon+\omega_1-\omega_2);i\omega_2]|\,\alpha'\beta'\rangle\ ,\end{aligned} \qquad (90)$$

with a similar expression for the generalized $\langle\Lambda_2\rangle$, corresponding to SD I (3.2b). In the bare s-electron case we have

$$A(\vec{q},\vec{q}',\chi)=\delta_{qq'}\,\delta(\chi-\epsilon_q) \qquad (91)$$

and (90) reduces to SD's expression.

Now in carrying out the sum over ω_n in the bare case, the contributions from the singularities of Γ may be neglected. (In SD's method, these contributions are reduced to zero when the $\epsilon_d/T\to\infty$ limit is taken, indicating that they come from "spurious" states, which in the present spin-$\frac{1}{2}$ case is the state $|1_\uparrow,1_\downarrow\rangle$. However, as Abrikosov points out,[1] for spin $\frac{1}{2}$, this limit is unnecessary, the contribution from $|1_\uparrow,1_\downarrow\rangle$ being automatically zero.) It will be assumed that these contributions may also be neglected in the clothed case. Carrying out the ω_n sum in (90) with the aid of (16), putting $\epsilon_d=0$, $\omega_1=\omega_2=0$, and analytically continuing from $i\epsilon\to\epsilon+i\delta$ as in SD I yields

$$\langle\alpha\beta|\,\Lambda_1|\,\alpha'\beta'\rangle=-\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3q'}{(2\pi)^3}\int d\chi\,\frac{A(\vec{q},\vec{q}',\chi)}{\epsilon-\chi+i\delta}\{f(-\chi)\langle\alpha\beta|\,\Gamma[\vec{p},\epsilon;0|\vec{q},\chi;\epsilon-\chi]|\,\alpha''\beta''\rangle$$

$$\times \langle\alpha''\beta''|\Gamma[\vec{q}',\chi;\,\epsilon-\chi|\vec{p}',\epsilon;\,0]|\alpha'\beta'\rangle+\tfrac{1}{2}\langle\alpha\beta|\Gamma[\vec{p},\epsilon;0|\vec{q},\epsilon;0]|\alpha''\beta''\rangle$$
$$\times\langle\alpha''\beta''|\Gamma[\vec{q}',\epsilon;\,0|\vec{p}',\epsilon;0]|\alpha'\beta'\rangle\}\,. \tag{92}$$

The $f(-\chi)$ term comes from the pole at $i\omega_n = i\epsilon + i\omega_1 - \chi$, while the term with factor $\frac{1}{2}$ comes from the pole at $i\omega_n = \epsilon_d$. This is the generalization of SD I (3.4a), with a similar expression for $\langle\Lambda_2\rangle$.

The linear analog of (92) is [cf. SD II (2.2a)]

$$\langle\alpha\beta|\Lambda_1|\alpha'\beta'\rangle=\frac{1}{2}\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3q'}{(2\pi)^3}\int d\chi\,\frac{A(\vec{q},\vec{q}',\chi)}{\epsilon-\chi+i\delta}\,\{-f(-\chi)\langle\alpha\beta|\Gamma_0|\alpha''\beta''\rangle$$
$$\times\langle\alpha''\beta''|\Gamma[\vec{q}',\chi;\,\epsilon-\chi|\vec{p}',\epsilon;0]|\alpha'\beta'\rangle-f(-\chi)\langle\alpha\beta|\Gamma[\vec{p},\epsilon;0|\vec{q},\chi;\epsilon-\chi]|\alpha''\beta''\rangle$$
$$\times\langle\alpha''\beta''|\Gamma_0|\alpha'\beta'\rangle+\tfrac{1}{2}\langle\alpha\beta|\Gamma_0|\alpha''\beta''\rangle\langle\alpha''\beta''|\Gamma[\vec{q}',\epsilon;0|\vec{p}'\epsilon;0]|\alpha'\beta'\rangle$$
$$+\tfrac{1}{2}\langle\alpha\beta|\Gamma[\vec{p},\epsilon;0|\vec{q},\epsilon;0]|\alpha''\beta''\rangle\langle\alpha''\beta''|\Gamma_0|\alpha'\beta'\rangle\}\,, \tag{93}$$

with a similar expression for $\langle\Lambda_2\rangle$ corresponding to SD II (2.2b). For small J, $A(\vec{q},\vec{q}',\chi)$ will be peaked around $\chi=\epsilon_q$ [cf. (91)]. Hence we may approximate the Γ's in (93) by setting $\chi=\epsilon_q$ in each Γ. Then we assume that as in the bare case, the fact that (93) counts diagrams incorrectly[2] may be remedied by the substitution $\epsilon_q\to\epsilon$. After making these changes in (93) and in the corresponding equation for $\langle\Lambda_2\rangle$, placing the results in (89), and abbreviating $\Gamma(l,\epsilon;\,0|m,\epsilon;0)$ by Γ_{lm}, we find that

$$\langle\alpha\beta|\Gamma_{pp'}|\alpha'\beta'\rangle=\frac{J}{2N}\vec{\sigma}_{\alpha\alpha'}\cdot\vec{S}_{\beta\beta'}-\frac{J}{4N}\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3q'}{(2\pi)^3}\{D\vec{\sigma}_{\alpha\alpha''}\cdot\vec{S}_{\beta\beta''}\langle\alpha''\beta''|\Gamma_{q'p'}|\alpha'\beta'\rangle+D\langle\alpha\beta|\Gamma_{pq}|\alpha''\beta''\rangle$$
$$\times\vec{\sigma}_{\alpha''\alpha'}\cdot\vec{S}_{\beta''\beta'}+E\vec{\sigma}_{\alpha\alpha''}\cdot\vec{S}_{\beta''\beta'}\langle\alpha''\beta|\Gamma_{qp'}|\alpha'\beta''\rangle+E\langle\alpha\beta''|\Gamma_{pq'}|\alpha''\beta'\rangle\vec{\sigma}_{\alpha''\alpha'}\cdot\vec{S}_{\beta\beta''}\}\,, \tag{94}$$

where

$$D=\int d\chi\,A(\vec{q},\vec{q}',\chi)\{[f(-\chi)-\tfrac{1}{2}]/(\epsilon-\chi+i\delta)\},$$
$$E=\int d\chi\,A(\vec{q},\vec{q}',\chi)\{[f(\chi)-\tfrac{1}{2}]/(\epsilon-\chi+i\delta)\}. \tag{95}$$

Substituting $\Gamma_{lm}=\Gamma^S_{lm}+\vec{\sigma}\cdot\vec{S}\Gamma^V_{lm}$ in (95) yields two coupled integral equations which have the following momentum-independent solution for Γ:

$$\Gamma^V=\left(\frac{J}{2N}\right)\left\{1+\frac{J}{2N}\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3q'}{(2\pi)^3}(D-E)\right\}^{-1}, \tag{96}$$

$$\Gamma^S=\tfrac{3}{4}\left(\frac{-J}{4N}\right)\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3q'}{(2\pi)^3}\,2\Gamma^V(D+E), \tag{97}$$

where we have omitted a term $\sim J^2$ in (96). Substituting (95) in (96) and using the expression for K obtained from (53) and (56), we find for the vertex part in clothed parquet approximation

$$\Gamma^V(\epsilon+i\delta)=(J/2N)[1+2K(\epsilon+i\delta)]^{-1}. \tag{98}$$

Let us first apply this to the bare case, when $K=K_0$. Using (26), we see that Γ^V diverges at

$$kT_K=\tfrac{1}{2}D\exp(-N/|J|\rho)\ \text{ for } J<0\,, \tag{99}$$

in contrast to the bare ladder result, (27) and (28), where there was a divergence for both signs of J. To find the self-energy and resistance, (34) may be used, with Γ^1 replaced by Γ^V, and also (43) holds, with

$$Q(x)=-\pi^{-1}\,\mathrm{Im}(\tfrac{3}{2}K_0\Gamma^V)\,. \tag{100}$$

Following the same procedure as that after (44) yields immediately

$$R=\frac{9\pi J^2c}{32e^2v_F^2N}\left(1+\frac{J\rho}{N}\ln\frac{D}{2k_BT}\right)^{-2} \tag{101}$$

which has just the form found by Abrikosov.[1]

In the clothed case, we may again use (43), this time with $Q(x)$ as in (100) but with K_0 replaced by K. Equation (23) is valid if we replace the expression in brackets by $\frac{3}{2}K\Gamma^V$. Solving for K and following the same procedure as in (81)–(88) yields for $J<0$

$$R=\frac{3cN}{2e^2\rho^2v_F^2\pi}\left\{1-\frac{\ln(T/T_K'')}{[\ln^2(T/T_K'')+(3/8)\pi^2]^{1/2}}\right\}, \tag{102}$$

where

$$\frac{|J|\rho}{2N}\ln\left(\frac{D}{2k_BT_K''}\right)=\frac{1}{2}-\frac{3}{16}\left(\frac{J\rho\pi}{2N}\right)^2. \tag{103}$$

This differs from Hamann's result by the factor $\frac{3}{8}$ instead of $\frac{3}{4}$ multiplying π^2.

VI. CONCLUSIONS

We have shown that self-consistently clothing the s propagator removes the divergence at the Kondo temperature and produces agreement between the perturbation-theoretic and decoupled equations-of-motion results in the Kondo problem. In fact, the resistance in the clothed parquet case is close enough to that of Hamann to lead us to suspect that Nagaoka's decoupling is equivalent to a parquet sum with self-consistently clothed s electrons. (*Note added in proof.* We have just completed an investigation which shows that clothing the d electrons has essentially no influence on the results reported here. Recently, Theumann has given a short direct proof that Nagaoka's decoupling is equivalent to the linearized parquet sum with self-consistently clothed s and d propagators, thus confirming the conclusions in the present paper.)

Further, we have shown that for $J<0$, the simple ladder approximation gives essentially the same results as the far more complicated parquet approximation, so it may be used for qualitative work. For $J>0$, its results appear to be spurious.

ACKNOWLEDGMENTS

The authors wish to thank Professor O. E. Cerceau, University of Carabobo, Valencia, Venezuela, for his participation during the early stages of this research. We would also like to thank Lars Hansen, Civ. Ing. Ulf Larsen, and Professor S. Doniach for valuable discussions. One of us (C. Y. C.) also wishes to acknowledge a research grant from the Defense Research Board of Canada.

---

[1]A. A. Abrikosov, Physics 2, 5 (1965); Zh. Eksperim. i Teor. Fiz. 53, 2109 (1967) [Soviet Phys. JETP 26, 1192 (1968)]; Usp. Fiz. Nauk 97, 403 (1969) [Soviet Phys. Usp. 12, 168 (1969)].

[2]S. D. Silverstein and C. B. Duke, Phys. Rev. 161, 456 (1967); 161, 470 (1967), hereafter referred to as SD I and SD II, respectively.

[3]R. D. Mattuck and B. Johansson, Advan. Phys. 17, 509 (1968).

[4]See J. Kondo [in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1969), Vol. 23, p. 184] for a detailed review of the Kondo problem.

[5]Y. Nagaoka, Phys. Rev. 138, A1112 (1965); Progr. Theoret. Phys. (Kyoto) 37, 13 (1967).

[6]D. R. Hamann, Phys. Rev. 158, 570 (1967).

[7]S. Doniach, Phys. Rev. 173, 599 (1968).

[8]A. Theumann, Phys. Rev. 178, 978 (1969).

[9]A. Theumann and R. D. Mattuck (unpublished).

[10]A brief report on this work appeared by C. Y. Cheung and R. D. Mattuck, Phys. Letters 30A, 166 (1969).

[11]P. Nozières, J. Gavoret, and B. Roulet, Phys. Rev. 178, 1084 (1969).

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

[13]F. Takano and T. Ogawa, Progr. Theoret. Phys. (Kyoto) 35, 343 (1966); A. P. Klein, Phys. Rev. 172, 520 (1968). For a simple derivation of the TO Hamiltonian and a discussion of exchange Hamiltonians, in general, see Ulf Larsen (unpublished).

[14]J. Sólyom, Phys. Letters 23, 305 (1966).

[15]R. D. Mattuck, Phys. Letters 27A, 210 (1968).

[16]J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964), p. 197.

[17]See, for example, R. D. Mattuck, *A Guide to Feynman Diagrams in the Many-Body Problem* (McGraw-Hill, London, 1967), p. 155.

[18]H. Suhl, Phys. Rev. Letters 19, 442 (1967).