Anderson Model of Localized Magnetic Moments. I. High-Temperature Behavior

LOWELL DWORIN*
Bell Telephone Laboratories, Murray Hill, New Jersey
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In this, the first of a series of papers on the nondegenerate Anderson model, there is presented a graphical representation of the equations of motion of the d-electron Green's function such that the intra-atomic Coulomb energy $U\hat{n}_+\hat{n}_-$ is treated exactly. In this paper, the high-T behavior of the system is studied. It is found that the magnetic susceptibility is given by

$$\chi=\chi_P+\frac{g^2}{T}\left(1-\frac{2\Delta}{\pi U\xi(1-\xi)}-\left(\frac{2\Delta}{\pi U\xi(1-\xi)}\right)^2\ln\left|\frac{2U(1-2\xi)\gamma}{\pi T}\right|+\cdots\right),$$

where χ_P is the usual temperature-independent Pauli paramagnetism of the host metal; this expression agrees (except for the replacement $W\rightarrow 2U\,|\,1-2\xi\,|\,\gamma/\pi$) with that obtained by Scalapino. The method of derivation makes it clear that the existence of a Curie-law susceptibility at high T is intimately connected with the Kondo anomaly present in this model.

The resistivity is found to be given by

$$\rho=\rho_0\left(1+\frac{9\Delta}{4\pi(\epsilon_F-\epsilon_d)}\ln\left|\frac{2U(1-2\xi)\gamma}{\pi T}\right|+\cdots\right),$$

the coefficient of the logarithmic term differing from the value $3\Delta/\pi(\epsilon_F-\epsilon_d)$ obtained in the *s-d* model. This discrepancy is due to the finite lifetime of the d electron, an important feature of the Anderson model, contrary to the remarks of Schrieffer and Wolf. An even more important lifetime effect (at low T) is the replacement of ln (W/T) by ln $[W/\Gamma(T)]$, where $\Gamma(T)$ is a nonanalytic (in Δ) function of T such that $\Gamma(0)$ is of order T_c and $\Gamma(T)\rightarrow 0$ with increasing T [although $\Gamma(T)\neq 0$ for all T].

I. INTRODUCTION

THIS is the first of three papers on the nondegenerate Anderson model of localized magnetic moments in metals.[1,2] This model was proposed by Anderson in 1961 to explain the magnetic properties of a dilute solution of magnetic atoms in an otherwise nonmagnetic host metal.

The model consists of a gas of independent conduction electrons interacting with localized d electrons. The d electrons, however, interact with each other via an atomic Coulomb exchange energy such that the state of two d electrons on the same atom is energetically unfavorable as compared to the singly occupied state. The Hamiltonian for the system is, in the notation of second quantization,

$$\mathcal{H}=\sum_{k,\sigma}\epsilon_{k\sigma}C_{k\sigma}{}^{\dagger}C_{k\sigma}+\sum_{\sigma}\epsilon_{d\sigma}d_{\sigma}{}^{\dagger}d_{\sigma}+U\hat{n}_+\hat{n}_- +\sum_{k,\sigma}V(d_{\sigma}{}^{\dagger}C_{k\sigma}+C_{k\sigma}{}^{\dagger}d_{\sigma}),\quad(1.1)$$

where $V=V^*$ and $\hat{n}_+=d_+{}^{\dagger}d_+$, etc. The energies $\epsilon_{d\sigma}$ and $\epsilon_{k\sigma}$ are given by (we set $\hbar=\mu_B=1$ throughout)

$$\epsilon_{k\sigma}=\epsilon_k-\sigma H,\quad(1.2)$$

and

$$\epsilon_{d\sigma}=\epsilon_d-g\sigma H,\quad(1.3)$$

where

$$\epsilon_d=\epsilon_F-\xi U,\qquad 0<\xi<1,\quad(1.4)$$

and where

$$\epsilon_k=\epsilon_{-k}.\quad(1.5)$$

According to Anderson, the most favorable value of ξ for the presence of a local moment (that is, for a temperature-dependent magnetic susceptibility approximating a Curie law at high temperatures) is $\xi=\frac{1}{2}$. However, we shall see that the values $\xi=0$, $\frac{1}{2}$, and 1 require special care, and so in this paper it shall be assumed that $\xi\neq 0$, $\frac{1}{2}$, 1.

If, following Anderson, we define the energy Δ by

$$\Delta=\pi V^2\rho(\epsilon_F),\quad(1.6)$$

where $\rho(\epsilon_F)$ is the density of conduction electron states at the Fermi surface, and if we regard ϵ_F to be of order U, the inequality

$$U\gg\Delta\gg T\quad(1.7)$$

shall be assumed throughout.

Despite the fact that the model was constructed so as to yield a Curie law susceptibility for finite U and $\Delta=0$ [making condition (1.7) the interesting regime], a number of authors have studied the model within the Hartree-Fock approximation.[3,4] In this work, however, we shall treat the interaction U exactly. Aside from the importance of such a treatment as regards the

* Present address: Department of Physics, University of Toronto, Toronto, Canada.
[1] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[2] L. Dworin, Phys. Rev. Letters **16**, 1042 (1966). In the present paper, and in two succeeding papers, the analysis leading to the results stated in this letter (in several cases incorrectly) is presented. At the time the letter was written, the existence of the nonanalytic width Γ was not recognized, nor the necessity of going beyond the lowest-order iteration of the integral equation obtained for the Green's function $G_d{}^{\sigma}(\omega)$.
[3] G. Kemeny, Phys. Rev. **150**, 459 (1966).
[4] J. R. Schrieffer and D. C. Mattis, Phys. Rev. **140**, A1412 (1965).

magnetic impurity problem, this approach affords a comparison with the Hartree-Fock approach, which might elucidate both methods in other contexts.

In this paper we shall present a graphical representation of the equations of motion of the Green's function of the d electron in Sec. II. In Secs. III and IV, we shall examine the first few terms in the perturbation expansion in powers of Δ/U of the Green's function as obtained from the graphical representation.

The first few terms of an expansion of the magnetic susceptibility in powers of Δ/U, the interaction U having been treated exactly, have been obtained independently by Suhl and Fredkin,[5] Nagaoka,[6] Scalapino,[7] and Hamann[8] (for the case $\xi\rightarrow 0$, $U\rightarrow\infty$ such that ξU finite) as well as the present author. It is found that the magnetic susceptibility of the system has a perturbation expansion of the form [neglecting terms of order $\exp(-\beta\xi U)$]

$$\chi=\chi_p+\frac{g^2}{T}\left[1+O\left(\frac{\Delta}{U}\right)+O\left(\frac{\Delta}{U}\right)^2\ln\frac{W}{T}+\cdots\right], \quad (1.8)$$

where χ_p is the usual temperature-independent susceptibility of the conduction electrons, and where an arbitrary energy cutoff W (which might be thought of as the bottom of the conduction band) has been introduced for convenience, the density $\rho(\epsilon_F)$ being set equal to a constant ρ.

This result is not trivial and requires a delicate cancellation of terms which would not have been guessed at. We shall derive this result in Sec. III, but our main interest lies in the temperature regime for which the perturbation expansion (1.8) is no longer valid. We see from Eq. (1.8) that Δ/U is not the only parameter in the problem, but rather the parameter $(\Delta/T)\ln(W/T)$ also enters.

From Eq. (1.8) we see that the perturbation expansion "breaks down" for temperatures of order T_c, where

$$T_c=W\exp(-U/\Delta). \quad (1.9)$$

By now the presence of logarithmic terms is not surprising, in view of the discussion of Schrieffer and Wolf[9] concerning the relationship between the Anderson and s-d exchange models.[10] Nevertheless, because of the finite lifetime of the d electron in the Anderson model, we might anticipate a major difference between the two models; namely, we might expect the d lifetime, of order $1/\Delta$, to enter the argument of the logarithmic functions, such that the logarithmic terms are no more singular than $(\Delta/U)\ln(W/\Delta)$, rather than $(\Delta/U)\ln(W/T)$.

We shall show (in Appendices B, C, and D) that whereas all the logarithmic terms are indeed of the form $(\Delta/U)\ln(W/\Delta)$ for the case where both levels ϵ_d and ϵ_{d+U} are greater than the Fermi energy (or both less), for the case considered here, where ϵ_d is less and ϵ_{d+U} greater than the Fermi energy the effect of the finite d lifetime on some of the logarithmic terms is much reduced. That is, because of the finite d lifetime, some of the logarithmic terms are of order $(\Delta/U)\ln\{W/[T+\Gamma(T)]\}$, where $\Gamma(T)$ is a temperature- (and energy-) dependent width of order T_c for $T\rightarrow 0$. Further, $\Gamma(T)$ decreases with increasing T; unlike the $\Delta(T)$ which appears in the work of Nagaoka,[11] $\Gamma(T)$ is finite, though small, for all T and shall be neglected in this paper, where only the high T behavior is discussed. The existence of a nonanalytic (in Δ) width which is finite at all T implies that perturbation theory is essentially invalid at all T. Although the behavior of the system changes (smoothly) for $T\approx T_c$, we find no phase transition, in contrast to the s–d exchange model theories of Yosida,[12] Nagaoka,[11] and Kondo.[13]

We shall discuss the high-temperature magnetic susceptibility in Sec. III and resistivity in Sec. IV. Our result for the resistivity differs somewhat from that obtained by Hamann,[14] in that he did not consider the self-energy effects which are an essential feature of the Anderson model. Our result thus also differs from the high-T resistivity as calculated in the s-d model.[10]

In the second paper of this series we shall make use of the graphical representation to obtain a linear [for the case ξU, $(1-\xi)U\ll W$] integral equation for the d Green's function.

II. MATHEMATICAL PRELIMINARIES

Following Zubarev,[14] we define $\langle\hat{A}\mid\hat{B}\rangle$ by

$$\langle\hat{A}\mid\hat{B}\rangle=i\int_0^\infty dt\exp(i\omega t)\langle[\hat{A}(t),\hat{B}(0)]_+\rangle, \quad (2.1)$$

where $\hat{B}$ has the property

$$\exp(-\beta\epsilon_F\hat{N})\hat{B}\exp(\beta\epsilon_F\hat{N})=\exp(-\beta\epsilon_F)\hat{B}. \quad (2.2)$$

We shall be interested in the functions $G_d^\sigma(\omega)$ and $G_{kk'}^\sigma(\omega)$, defined by

$$G_d^\sigma(\omega)=\langle d_\sigma\mid d_\sigma^\dagger\rangle,$$

and

$$G_{kk'}^\sigma(\omega)=\langle C_{k\sigma}\mid C_{k'\sigma}^\dagger\rangle, \quad (2.3)$$

respectively, because the thermal averages $n_\sigma=\langle d_\sigma^\dagger d_\sigma\rangle$ and $f_k^\sigma=\langle C_{k\sigma}^\dagger C_{k\sigma}\rangle$ may be obtained from these functions

[5] H. Suhl and D. R. Fredkin, Phys. Rev. **131**, 1063 (1963).
[6] Y. Nagaoka (private communication).
[7] D. J. Scalapino, Phys. Rev. Letters **16**, 937 (1966).
[8] D. R. Hamann, Phys. Rev. Letters **17**, 145 (1966).
[9] J. R. Schrieffer and P. A. Wolf, Phys. Rev. **149**, 491 (1966).
[10] J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964).
[11] Y. Nagaoka, Phys. Rev. **138**, A1112 (1965).
[12] K. Yosida and A. Okiji, Progr. Theoret. Phys. (Kyoto) **35**, 204 (1965).
[13] J. Kondo (private communication).
[14] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [English transl.: Soviet Phys.—Usp. **3**, 320 (1960)].

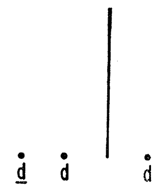

FIG. 1. Representation of the operators $d_{-\sigma}^{\dagger}d_{-\sigma}d_{\sigma}$. In this and all subsequent figures, the operators $d^{\dagger}$, $c_k^{\dagger}$, etc., are written with the bar below the letter, rather than above, as in the text.

by performing an integration over ω:

$$n^{\sigma}=\pi^{-1}\int_{-\infty}^{\infty} d\omega\, f(\omega)\ \mathrm{Im}G_d^{\sigma}(\omega), \qquad (2.4)$$

where $f(\omega)$ is the Fermi function $\{\exp[\beta(\omega-\epsilon_F)]+1\}^{-1}$ and

$$f_k^{\sigma}=\pi^{-1}\int_{-\infty}^{\infty} d\omega\, f(\omega)\ \mathrm{Im}G_{kk}^{\sigma}(\omega). \qquad (2.5)$$

It may readily be seen that

$$G_{k|d}^{\sigma}(\omega)=VD_k^{\sigma}G_d^{\sigma}(\omega), \qquad (2.6)$$

where we have introduced the notation

$$D_k^{r\sigma}=(\omega-\epsilon_k+r\sigma H)^{-1}. \qquad (2.7)$$

From the identities $V=V^*$ and $\epsilon_k=\epsilon_{-k}$, the relationship

$$G_{d|k}^{\sigma}(\omega)=G_{k|d}^{\sigma}(\omega) \qquad (2.8)$$

follows from Eq. (2.1), and hence the relation

$$G_{kk'}^{\sigma}(\omega)=-D_k^{\sigma}\delta_{k,k'}+V^2D_k^{\sigma}D_{k'}^{\sigma}G_d^{\sigma}(\omega) \qquad (2.9)$$

also follows. Equation (2.9) is valid for a single impurity, or if the factor $N_i\delta_{k,k'}$ is added to the second term on the right, for a sufficiently small concentration of fixed, but randomly located, noninteracting impurity atoms.

Using Eqs. (2.8) and (2.9), we find that the thermal averages $f_{kk_1}^{\sigma}=f_{k_1k}^{\sigma}=\langle C_{k\sigma}^{\dagger}C_{k_1\sigma}\rangle$ and $n_{kd}^{\sigma}=n_{dk}^{\sigma}=\langle C_{k\sigma}d_{\sigma}^{\dagger}\rangle$ are given by

$$f_{kk_1}^{\sigma}=f(\epsilon_{k\sigma})\delta_{k,k_1}+\pi^{-1}\int_{-\infty}^{\infty} d\omega\, f(\omega)\, V^2\ \mathrm{Im}\frac{G_d^{\sigma}(\omega)}{(\omega-\epsilon_{k\sigma})(\omega-\epsilon_{k_1\sigma})}, \qquad (2.10)$$

and

$$n_{kd}^{\sigma}=\pi^{-1}\int_{-\infty}^{\infty} d\omega\, f(\omega)\, V\ \mathrm{Im}\frac{G_d^{\sigma}(\omega)}{\omega-\epsilon_{k\sigma}}. \qquad (2.11)$$

In order that the interaction U be treated exactly, it is convenient to introduce the auxiliary functions $G_{\alpha-d}^{\sigma}(\omega)$ defined by[15]

$$G_{\alpha-d}^{\sigma}(\omega)=\langle\hat{n}_{-\sigma}d_{\sigma}\mid d_{\sigma}^{\dagger}\rangle, \qquad \text{for } \alpha=1$$
$$=\langle(1-\hat{n}_{-\sigma})d_{\sigma}\mid d_{\sigma}^{\dagger}\rangle, \qquad \text{for } \alpha=-1. \qquad (2.12)$$

[15] This method, which was originally used by J. Hubbard [Proc. Roy. Soc. (London) **A276**, 238 (1963)] was suggested to the author by D. R. Fredkin.

Thus

$$G_d^{\sigma}(\omega)=G_{+d}^{\sigma}(\omega)+G_{-d}^{\sigma}(\omega). \qquad (2.13)$$

From the equation of motion $i(d\hat{A}/dt)=[\hat{A},\hat{H}]$, we obtain the equation

$$\omega G_{\alpha-d}^{\sigma}(\omega)=-n_{\alpha}^{\sigma}+(\epsilon_{d\sigma}+\eta_{\alpha}U)G_{\alpha-d}^{\sigma}(\omega)+(2\eta_{\alpha}-1)\sum_k V\{G_{(dd)k}^{\sigma}+G_{(dk)d}^{\sigma}-G_{(kd)d}^{\sigma}\}+(1-\eta_{\alpha})\sum_k VG_k^{\sigma}, \qquad (2.14)$$

where we have used the notation

$$G_{(dd)k}^{\sigma}=\langle d_{-\sigma}^{\dagger}d_{-\sigma}C_{k\sigma}\mid d_{\sigma}^{\dagger}\rangle,$$
$$G_{(dk)d}^{\sigma}=\langle d_{-\sigma}^{\dagger}C_{k-\sigma}d_{\sigma}\mid d_{\sigma}^{\dagger}\rangle,$$
$$G_k^{\sigma}=\langle C_{k\sigma}\mid d_{\sigma}^{\dagger}\rangle, \text{ etc.}, \qquad (2.15)$$

where

$$\eta_{\alpha}=1, \qquad \text{for } \alpha=1$$
$$=0, \qquad \text{for } \alpha=-1, \qquad (2.16)$$

and where

$$n_{\alpha}^{-\sigma}=n^{-\sigma}, \qquad \text{for } \alpha=1$$
$$=1-n^{-\sigma}, \qquad \text{for } \alpha=-1. \qquad (2.17)$$

The advantage of using the auxiliary functions $G_{\alpha-d}^{\sigma}$ is seen from the simple way in which U enters the equation of motion of these functions.

From Eq. (2.44) we may at once obtain $G_d^{\sigma(0)}(\omega)$, the value of $G_d^{\sigma}(\omega)$ for the case $V=0$:

$$G_d^{\sigma(0)}(\omega)=-\left\{\frac{n^{-\sigma}}{\omega-\epsilon_{d\sigma}-U}+\frac{1-n^{-\sigma}}{\omega-\epsilon_{d\sigma}}\right\}. \qquad (2.18)$$

The equations of motion for the quantities $G_{(dk)d}^{\sigma}$, G_k^{σ}, etc., may likewise be obtained. If we extend our notation by writing

$$G_{\alpha+(kd)k_1}^{\sigma}=\langle\hat{n}_{\sigma}C_{k-\sigma,d-\sigma}^{\dagger}C_{k_1\sigma}\mid d_{\sigma}^{\dagger}\rangle, \qquad \alpha=+1$$
$$=\langle(1-n_{\sigma})C_{k-\sigma,d-\sigma}^{\dagger}C_{k_1\sigma}\mid d_{\sigma}^{\dagger}\rangle, \qquad \alpha=-1,$$

and

$$G_{(kd)(dk_2)+k_1}^{\sigma}=\langle C_{k-\sigma}^{\dagger}d_{-\sigma}d_{\sigma}^{\dagger}C_{k_2\sigma}C_{k,\sigma}\mid d_{\sigma}^{\dagger}\rangle,$$

etc., then the equations of motion for the higher-order Green's functions from which $G_d^{\sigma}(\omega)$ may be obtained

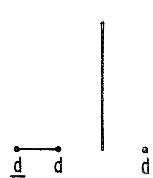

FIG. 2. Representation of $G_d^{\sigma(0)}(\omega)$.

to fourth order in V may be written as

$$\omega G_{(dk)d}{}^{\sigma}=-n_{dk}{}^{-\sigma}+(\epsilon_{k\sigma}+\epsilon_{d\sigma}-\epsilon_{d-\sigma})G_{(dk)d}{}^{\sigma}+\sum_{k_1}V\{G_{(dk)k_1}{}^{\sigma}-G_{(kk)d}{}^{\sigma}\}+VG_{+d}{}^{\sigma}. \quad (2.19)$$

$$G_{(dd)k}{}^{\sigma}=\epsilon_{k\sigma}G_{(dd)k}{}^{\sigma}+\sum_{k_1}V\{G_{(dk_1)k}{}^{\sigma}-G_{(k_1d)k}{}^{\sigma}\}+VG_{+d}{}^{\sigma}. \quad (2.20)$$

$$\omega G_{(kd)d}{}^{\sigma}=-n_{kd}{}^{-\sigma}+(\epsilon_{d\sigma}+\epsilon_{d-\sigma}+U-\epsilon_{k-\sigma})G_{(kd)d}{}^{\sigma}=VG_{+d}{}^{\sigma}+\sum_{k_1}V\{G_{(kd)k_1}{}^{\sigma}+G_{(kk_1)d}{}^{\sigma}\}. \quad (2.21)$$

$$\omega G_{\alpha-(k_1k)d}{}^{\sigma}=-(2\eta_\alpha-1)\langle\hat{n}_{-\sigma}C_{k_1-\sigma}{}^{\dagger}C_{k-\sigma}\rangle-(1-\eta_\alpha)n_{k_1k}{}^{-\sigma}+(\epsilon_{k-\sigma}-\epsilon_{k_1-\sigma}+\epsilon_{d\sigma}+\eta_\alpha U)G_{\alpha(k_1k)d}{}^{\sigma}+(2\eta_\alpha-1)\sum_{k_2}V$$
$$\times\{G_{(k_1k)(dk_2)d}{}^{\sigma}-G_{(k_2d)(k_1k)d}{}^{\sigma}\}+(\eta_\alpha-1)VG_{(dk)d}{}^{\sigma}+(\eta_\alpha-1)+\sum_{k_2}VG_{\alpha-(k_1k)k_2}{}^{\sigma}-(\eta_\alpha-1)VG_{(k_1d)d}{}^{\sigma}. \quad (2.22)$$

$$\omega G_{\alpha+(dk)d_1}{}^{\sigma}=(2\eta_\alpha-1)\langle d_\sigma{}^{\dagger}C_{k_1-\sigma}d_{-\sigma}{}^{\dagger}C_{k-\sigma}\rangle+(\epsilon_{k-\sigma}-\epsilon_{d-\sigma}+\epsilon_{k_1\sigma}-\eta_\alpha U)G_{\alpha+(dk)k_1}+(2\eta_\alpha-1)\sum_{k_2}V$$
$$\times\{G_{(dk)(dk_2)+k_1}{}^{\sigma}-G_{(k_2d)+(dk)k_1}{}^{\sigma}\}-\sum_{k_2}VG_{\alpha+(k_2k)k_1}{}^{\sigma}+(1-\eta_\alpha)VG_{(dk)d}{}^{\sigma}+VG_{\alpha+(dd)k_1}{}^{\sigma}. \quad (2.23)$$

$$\omega G_{\alpha+(kd)k_1}{}^{\sigma}=(2\eta_\alpha-1)\langle d_\sigma{}^{\dagger}C_{k_1\sigma}C_{k-\sigma}d_{-\sigma}{}^{\dagger}\rangle+(\epsilon_{d-\sigma}-\epsilon_{k-\sigma}+\epsilon_{k_1\sigma}+\eta_\alpha U)G_{\alpha+(kd)k_1}-VG_{\alpha+(dd)k_1}{}^{\sigma}+\sum_{k_2}VG_{\alpha+(kk_2)k_1}$$
$$+(2\eta_\alpha-1)\sum_{k_2}V\{G_{(kd)(dk_2)+k_1}{}^{\sigma}-G_{(kd)(k_2d)+k_1}{}^{\sigma}\}+(1-\eta_\alpha)VG_{(kd)d}{}^{\sigma}. \quad (2.24)$$

$$\omega G_{\alpha+(k_2k)k_1}{}^{\sigma}=(2\eta_\alpha-1)\langle C_{k_2-\sigma}{}^{\dagger}C_{k-\sigma}d_\sigma{}^{\dagger}C_{k_1\sigma}\rangle+(\epsilon_{k_1\sigma}-\epsilon_{k-\sigma}-\epsilon_{k_2-\sigma})G_{\alpha+(k_2k)k_1}{}^{\sigma}-VG_{\alpha+(dk)k_1}{}^{\sigma}+VG_{\alpha+(k_2d)k_1}{}^{\sigma}+(1-\eta_\alpha)VG_{(k_2k)d}{}^{\sigma}$$
$$+(2\eta_\alpha-1)\sum_{k_3}V\{G_{(k_2k)(dk_3)+k_1}{}^{\sigma}-G_{(k_2k)(k_3d)+k_1}{}^{\sigma}\}. \quad (2.25)$$

$$\omega G_{\alpha-(k_1k)k_2}{}^{\sigma}=(\epsilon_{k_2\sigma}+\epsilon_{k-\sigma}-\epsilon_{k_1-\sigma})G_{\alpha-(k_1k)k_2}{}^{\sigma}-\eta_\alpha VG_{(dk)k_2}{}^{\sigma}+VG_{\alpha-(k_1k)d}{}^{\sigma}+(1-\eta_\alpha)VG_{(k_1d)k_2}{}^{\sigma}$$
$$+(2\eta_\alpha-1)\sum_{k_3}V\{G_{(dk_3)(k_1k)k_2}{}^{\sigma}-G_{(k_3d)(k_1k)k_2}{}^{\sigma}\}. \quad (2.26)$$

$$\omega G_{\alpha+(dd)k_1}=(2\eta_\alpha-1)\langle d_\sigma{}^{\dagger}C_{k_1\sigma}\hat{n}_\sigma\rangle+\epsilon_{k,\sigma}G_{\alpha+(dd)k_1}+(1-\eta_\alpha)VG_{+d}{}^{\sigma}+\sum_{k_2}V\{G_{\alpha+(dk_2)k_1}{}^{\sigma}-G_{\alpha+(k_2d)k_1}{}^{\sigma}\}$$
$$+(2\eta_\alpha-1)\sum_{k_2}V\{G_{(dd)(dk_2)+k_1}{}^{\sigma}-G_{(dd)(k_2d)+k_1}{}^{\sigma}\}. \quad (2.27)$$

$$\omega G_k{}^{\sigma}=\epsilon_{k\sigma}G_k{}^{\sigma}+V_kG_d{}^{\sigma}. \quad (2.28)$$

Equations (2.14) and (2.19) to (2.28) are clearly the first several in an infinite hierarchy of equations. A few comments might be made about these equations. It should be noted that the inhomogeneous terms of the successive equations are thermal averages of greater and greater complexity. These averages may be evaluated by considering the appropriate Green's function and performing the required integration, as in Eq. (2.4). It is clear that an infinite set of self-consistent equations for the thermal averages would result from such a procedure.

In the next paper we shall show that this procedure may nevertheless be carried out by considering only the lowest-order terms in powers of Δ/U [although all powers of $(\Delta/U)\ln(W/T)$], leading to a single self-consistency equation, namely that for n^σ. In this paper we shall be content with the first few terms of an expansion in Δ/U and hence this procedure poses no difficult problems, although it should be noted that when the interaction U is treated exactly the thermal averages cannot always be approximated by their "natural" truncation (e.g., $\langle d_\sigma{}^{\dagger}C_{k_1\sigma}d_{-\sigma}{}^{\dagger}C_{k-\sigma}\rangle\neq\langle d_\sigma{}^{\dagger}C_{k_1\sigma}\rangle\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}\rangle$, even to lowest order in Δ/U, as shown in Appendix F).

III. A GRAPHICAL REPRESENTATION OF $G_d{}^{\sigma}(\omega)$

It is desirable to represent the equations of motion (2.14) ff. graphically. It is clear that as we start with the Green's function $G_d{}^{\sigma}$ and proceed to an infinite set of equations for more and more complex operators, the graphical structure will be that of a tree with a more and more complex branch structure as one proceeds up the tree. The only novel feature of such a structure is that we must introduce the auxiliary Green's functions (for example, $G_{\alpha-d}{}^{\sigma}$) in order that the interaction U be treated exactly. One such representation is as follows:

I. Represent each creation and destruction operator by a dot labeled by the state (e.g., $-d$) if a destruction operator and by the state with a bar above it (e.g., $-\bar{k}$) if a creation operator. Draw a vertical line and place all dots referring to spin σ on the right; those of spin $-\sigma$ on the left. Each interaction is represented by a vertical wiggly line, and each statistical factor $n_{kd}{}^{\sigma}$, n^{σ}, $f_{kk_1}{}^{\sigma}$, etc., by a solid line. The diagram is ordered in the vertical direction. Since we are interested in $G_{\alpha-d}{}^{\sigma}$ we start by drawing three dots, representing the operators $d_{-\sigma}{}^{\dagger}$, $d_{-\sigma}$, and d_σ (see Fig. 1).

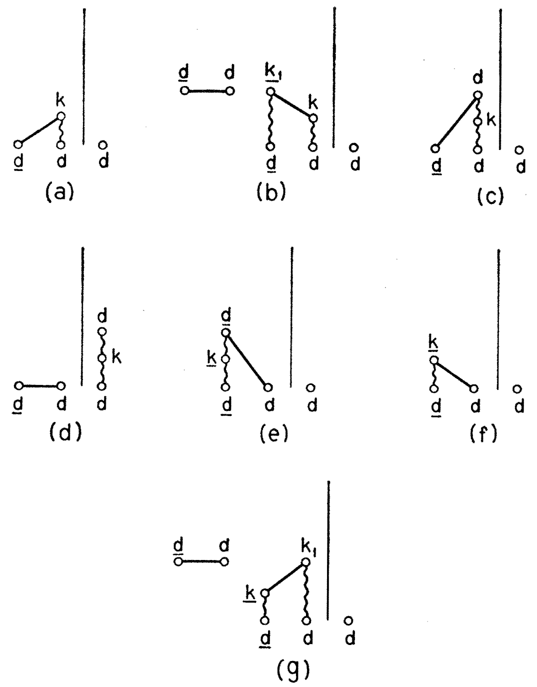

FIG. 3. Representation of $G_d^{\sigma(2)}(\omega)$.

II. Each diagram is terminated by connecting all dots which appear at the top of each wiggly line except for a single dot which must always appear at the top of some wiggly line on the right (although the wiggly line may consist of just a single dot, as in the zeroth-order diagram, Fig. 2). To the figure on the left consisting of two "d" dots connected by a solid line we associate the factor $G_d^{\sigma(0)}$, given by Eq. (2.18). This factor combines both the statistical factor ($n^{-\sigma}$ or $1-n^{-\sigma}$) associated with the solid line and an energy denominator (see below). We note here that to the order considered in this paper, all statistical factors except three (the averages $\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}d_{\sigma}{}^{\dagger}C_{k_1\sigma}\rangle$, $\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}C_{k_1\sigma}{}^{\dagger}d_{\sigma}\rangle$, and $\langle \hat{n}^{\sigma}C_{k\sigma}{}^{\dagger}C_{k_1\sigma}\rangle$) may be factored into the product of lowest-order thermal averages, and as a result we shall terminate almost all diagrams by connecting the upper dots pairwise.

III. To go to higher order in V we must change one of the "d's" to a "k", indicating this by the vertical wiggly line. To such a line from a "d" to a "k" or a "k" to a "d" we associate the factor $-V$; to a line from a "$\bar{d}$" to "$\bar{k}$" or "$\bar{k}$" to "$\bar{d}$" we associate the factor V. The solid line from k to $\bar{k}_1$, on the left, represents the statistical factor $f_{kk_1}{}^{-\sigma}$; on the right, it represents $f_{kk_1}{}^{\sigma}$, where $f_{kk_1}{}^{\sigma}$ is given by Eq. (2.10). Likewise, the solid line on the left from $\bar{k}$ to d represents the factor $-n_{d\bar{k}}{}^{-\sigma}$ and on the right, it represents $-n_{dk}{}^{\sigma}$, while the solid line from $\bar{d}$ to d represents the factor $-n^{-\sigma}$ if on the left and $-n^{\sigma}$ if on the right.

There are two additional sign factors associated with each diagram. There is the factor $(-)^{N_+}$, where N_+ is the number of creation operators at the top corresponding to conduction electron states with spin σ. There is also a sign factor corresponding to the number of permutations required to bring the conduction-electron operators to the order required for the statistical averages from the following order: first, all creation operators with spin $-\sigma$ in the vertical order of appearance (from the bottom), then all destruction operators with spin $-\sigma$ in the reverse order, then the corresponding product of the spin-σ conduction-electron operators (to this end, the d operator in the factor $n_{kd}{}^{\pm\sigma}$ should be imagined to go to a creation operator at the very top).

IV. To each horizontal line we associate the factor $D_{a+b-\bar{c}}{}^{r\sigma}$, etc., where a, b, $\bar{c}$, etc., are the labels of all the highest dots appearing on the wiggly lines up to and including that line. There are, however, two exceptions to this rule, due to our treating U exactly.

(1) We must write $D_{2d+a}{}^{r\sigma}$ as $D_{2d+U+a}{}^{r\sigma}$.

(2) There must always appear more than one "d" dot at the top of the wiggly lines; thus we must add the two dots as shown at the top of Fig. 4(b) and (g). These dots, when they are not connected, and when no single "d" dot appears on any line above them [as in Figs. 8(b), 3(d), 3(c), etc.], correspond to the difference of denominators

$$D_{a+d+U}{}^{r\sigma}-D_{a+d}{}^{r\sigma}.$$

If they are at the top they must be connected by a solid line and the factor $G_d^{\sigma(0)}$ is taken as in Rule II. If a single "d" dot appears on the same side above these dots and the single dot is not connected by a wiggly line to these double dots [as in Fig. 8(b)], we connect these dots with a double line and write the usual denominator $D_{a+d}{}^{r\sigma}$ or $D_{a-d}{}^{r\sigma}$ to the line on which these dots appear. In satisfying the first paragraph of (2), we do not count the dots connected by a double line.

If they are connected by a solid line, but are not at the absolute top [as in Fig. 3(d)] the factor

$$-[D_{a+d+U}{}^{r\sigma}D_{b+d+U}{}^{r\sigma}\cdots(n^{-\sigma})+D_{a+d}{}^{r\sigma}D_{b+d}{}^{r\sigma}\cdots(1-n^{-\sigma})]$$

appears instead of the product $G_d^{\sigma(0)}D_{a+d}{}^{r\sigma}D_{b+d}{}^{r\sigma}\cdots$, etc., where $D_{a+d}{}^{r\sigma}$, $D_{b+d}{}^{r\sigma}$, etc., are the "usual" energy denominators appearing on the even lines above the connected dots.

In the case where one or both of the double dots are connected by a wiggly line to some higher line as in Fig. 3(c), the energy denominator

$$D_{a+d+U}{}^{r\sigma}-D_{a+d}{}^{r\sigma}$$

is to be associated with the line on which the double dots appear, whereas the denominator $D_{b+d+U}{}^{r\sigma}$ is to be associated to all even lines above these dots until (and including) the lowest level to which one of the dots is connected is reached.

All possible diagrams consistent with the above rules are to be drawn. These rules will be made clear by considering the second-order terms given in Fig. 3 and the fourth-order terms in Figs. 4, 5, 7, 8, 10.

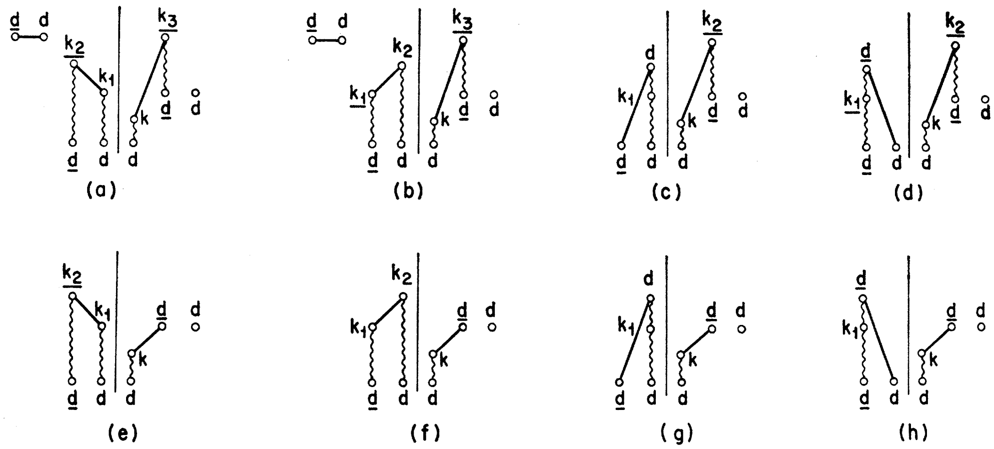

FIG. 4. Representation of those fourth-order singular terms which reduce to second-order ln W/T terms upon self-energy renormalization.

The terms of Fig. 3 yield, in the order in which they appear:

$$\begin{aligned}&\sum_k V(D_{d+U}^{g\sigma}-D_d^{g\sigma})(-n_{dk}^{-\sigma})D_k^{(2g-1)\sigma}\\&\quad-\sum_{k,k_1} V^2(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_k^{(2g-1)\sigma}(f_k^{-\sigma}\delta_{k,k_1})G_d^{\sigma(0)}\\&\quad+\sum_k V^2(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_k^{(2g-1)\sigma}D_{d+U}^{g\sigma}(-n^{-\sigma})\\&\quad-\sum_k V^2[(D_{d+U}^{g\sigma})^2 n^{-\sigma}+(D_d^{g\sigma})^2(1-n^{-\sigma})]D_k^{\sigma}\\&\quad+\sum_k V^2(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_{2d+U-k}^{\sigma}D_{d+U}^{g\sigma}(-n^{-\sigma})\\&\quad-\sum_k V(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_{2d+U-k}^{\sigma}(-n_{kd}^{-\sigma})\\&\quad-\sum V^2(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_{2d+U-k}^{\sigma}(f_k^{-\sigma}\delta_{k,k_1})G_d^{\sigma(0)}.\end{aligned}\qquad(3.1)$$

The first two terms in the above expression are proportional to $\Delta\ln(W/T)$ for $|\omega-\epsilon_F|\ll T$; the next three terms represent self-energy corrections of order Δ, while the last two are of order $(\Delta/U)\ln|W/U(1-2\xi)|$.

If we define the quantity $A_{(\omega)}^{\sigma}$ [represented by Fig. 3(b) and 3(g)] by

$$A_{(\omega)}^{\sigma}=V^2\sum_k f_k^{-\sigma}(D_k^{(2g-1)\sigma}+D_{2d+U-k}^{\sigma})+i\Delta,\qquad(3.2)$$

and $E_{(\omega)}^{\sigma}$ [represented by Figs. 3(a) and 3(f)] by

$$E_{(\omega)}^{\sigma}=V\sum_k n_{dk}^{-\sigma}(D_k^{(2g-1)\sigma}-D_{2d+U-k}^{\sigma}),\qquad(3.3)$$

we may thus write $G_d^{\sigma(2)}(\omega)$ as given by (3.1) as

$$\begin{aligned}UG_{d(\omega)}^{\sigma(2)}=-U^2\bigg\{&n^{-\sigma}+E_{(\omega)}^{\sigma}+\frac{\omega-\epsilon_{d\sigma}-U}{U}+\frac{3i\Delta}{U}\\&-2i\Delta\left(n^{-\sigma}+\frac{\omega-\epsilon_{d\sigma}-U}{U}\right)\frac{(2\omega-2\epsilon_d-U)}{(\omega-\epsilon_{d\sigma}-U)(\omega-\epsilon_{d\sigma})}\\&-\frac{UA_{(\omega)}^{\sigma}[n^{-\sigma}+(\omega-\epsilon_{d\sigma}-U)/U]}{(\omega-\epsilon_{d\sigma}-U)(\omega-\epsilon_{d\sigma})}\bigg\}\\&+\{(\omega-\epsilon_{d\sigma}-U)(\omega-\epsilon_{d\sigma})\}^{-1},\end{aligned}\qquad(3.4)$$

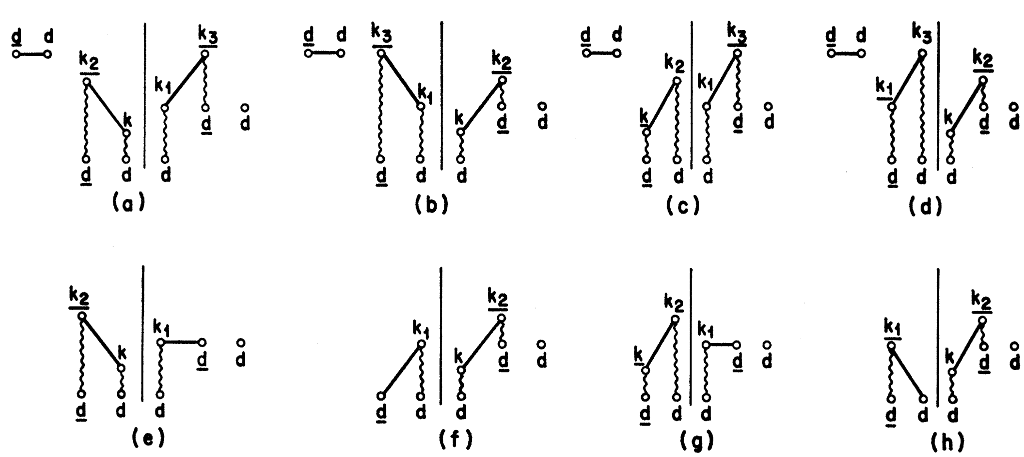

FIG. 5. Representation of fourth-order terms whose real part is of order $(\Delta/U\ln W/T)^2$.

where we have set

$$\sum_k (\omega-\epsilon_{k\sigma})^{-1} = -i\pi\rho.$$

The reader may verify that Eq. (3.4) is the same as would be obtained by truncating the equations of motion by writing

$$G_{(dk)k_1}{}^{\sigma} = G_{(kd)k_1}{}^{\sigma} = G_{(k_2k_3)k_1}{}^{\sigma} = 0, \tag{3.5}$$

and

$$G_{(k_1k)d}{}^{\sigma} = f_k{}^{-\sigma}\delta_{k,k_1}G_d{}^{\sigma}, \tag{3.6}$$

and setting $G_d{}^{\sigma}(\omega) = G_d{}^{\sigma(0)}(\omega)$ in the right-hand side of Eq. (2.14), which may be written, using Eqs. (3.5) and (3.6), as

$$\begin{aligned} G_{\alpha d}{}^{\sigma} = (\omega-\epsilon_{d\sigma}-\eta_\alpha U)^{-1}\{ &-n_\alpha{}^{-\sigma} + (1-\eta_\alpha)\sum_k V^2 G_d{}^{\sigma} D_k{}^{\sigma} \\ &+(2\eta_\alpha-1)\sum_k V^2 G_{+d}{}^{\sigma}(D_k{}^{\sigma}+D_k{}^{(2g-1)\sigma}+D_{2d+U-k}{}^{\sigma}) \\ &-(2\eta_\alpha-1)\sum_k V^2 G_d{}^{\sigma} f_k{}^{-\sigma}(D_k{}^{(2g-1)\sigma}+D_{2d+U-k}{}^{\sigma}) \\ &-(2\eta_\alpha-1)\sum_k V n_{dk}{}^{-\sigma}(D_k{}^{(2g-1)\sigma}-D_{2d+U-k}{}^{\sigma})\}, \end{aligned} \tag{3.7}$$

and adding $G_{+d}{}^{\sigma}+G_{-d}{}^{\sigma}$.

It is clear that if we set $G_d{}^{\sigma(0)}(\omega)$, which appears in the graphical representation equal to $G_d{}^{\sigma}(\omega)$, we would automatically be summing all diagrams which may be obtained by iteration of the lowest-order one (Fig. 3). We would then obtain an expression for $G_d{}^{\sigma}(\omega)$ which would agree completely with Eq. (3.7):

$$G_d{}^{\sigma}(\omega) = -U^{-1}\frac{\{n^{-\sigma}+E_{(\omega)}{}^{\sigma}+(\omega-\epsilon_F)/U-(1-\xi)+3i\Delta/U\}}{\{(\omega-\epsilon_{d\sigma}-U+2i\Delta)(\omega-\epsilon_{d\sigma}+2i\Delta)/U^2+A_{(\omega)}{}^{\sigma}/U\}}. \tag{3.8}$$

It should be noted that $A_{(\omega)}{}^{\sigma} = \tilde{A}_{(-\omega)}{}^{-\sigma*}$ and $E_{(\omega)}{}^{\sigma} = -\tilde{E}_{(-\omega)}{}^{-\sigma*}$ (i.e., $\epsilon_F-\epsilon_{d\sigma}\rightleftarrows\epsilon_{d\sigma}+U-\epsilon_F$, $n^{\sigma}\rightleftarrows 1-n^{-\sigma}$, etc., see Appendix A), so that it may be seen from Eq. (3.7) that $G_{+d(\omega)}{}^{\sigma}\rightleftarrows -G_{-d(\omega)}{}^{-\sigma*}$, as it should (in all our approximations we shall be careful to maintain charge conjugation symmetry).[16]

The function $A_{(\omega)}{}^{\sigma}$ given by Eq. (3.2) is singular in the limit $T\to 0$ for $|\omega-\epsilon_F|\ll T$. To see this, we note that if we change the summation over k to an integration over ϵ_k, assuming a constant density of states ρ, we may write Eq. (3.4) as

$$\begin{aligned} A_{(\omega)}{}^{\sigma} &= \frac{\Delta}{\pi}\left\{\int_{\epsilon_F-W}^{\epsilon_F+W}\frac{f(\lambda)d\lambda}{\omega-\lambda+2g\sigma H}+\int_{\epsilon_F-W}^{\epsilon_F+W}\frac{f(\lambda)d\lambda}{\omega+\lambda-2\epsilon_F-U(1-2\xi)}+i\pi\right\} \\ &= \frac{\Delta}{\pi}\left\{\psi\left[\frac{1}{2}-\frac{i(\omega+2g\sigma H-\epsilon_F)}{2\pi T}\right]-\psi\left[\frac{1}{2}-\frac{i[U(1-2\xi)+\epsilon_F-\omega]}{2\pi T}\right]\right\}, \end{aligned} \tag{3.9}$$

where $\psi(x)$ is the digamma function.[17]

For $|\omega-\epsilon_F+2g\sigma H|\ll T$, $A_{(\omega)}{}^{\sigma}$ has the asymptotic form[18]

$$A^{\sigma} = \frac{\Delta}{\pi}\left\{\ln\left|\frac{2U(1-2\xi)\gamma}{\pi T}\right|+\tfrac{1}{2}(i\pi)+\frac{i\pi g\sigma H}{2T}-i\pi\theta\right\}, \tag{3.10}$$

where we shall use the symbol θ to mean

$$\begin{aligned} \theta &= 0, \quad \xi<\tfrac{1}{2} \\ &= 1, \quad \xi>\tfrac{1}{2} \end{aligned} \tag{3.11}$$

throughout, and where $\ln\gamma$ = Euler's constant $(0.577\cdots)$.

It should be noted that the arbitrary cutoff W has been replaced by $2U\gamma(1-2\xi)/\pi$ in Eq. (3.14) for $A_{(\omega)}{}^{\sigma}$ as a result of our keeping both terms in the sum appearing in Eq. (3.4), a procedure not followed in Scalapino's paper with the consequent appearance of the unphysical parameter W in his expansion (1.8).

Likewise, for $|\omega+2g\sigma H|\gg T$, $A_{(\omega)}{}^{\sigma}$ is given by

$$A_{(\omega)}{}^{\sigma} = \frac{\Delta}{\pi}\left\{\ln\left|\frac{U(1-2\xi)}{\omega-\epsilon_F}\right|+i\pi-i\pi\theta(\epsilon_F-\omega-2g\sigma H)-i\pi\theta\right\}. \tag{3.12}$$

The function $E_{(\omega)}{}^{\sigma}$ is also singular for $\omega\approx\epsilon_F$. However, in order to evaluate $E_{(\omega)}{}^{\sigma}$, we must obtain $n_{dk}{}^{\sigma}$, which is given in terms of $G_{d(\omega)}{}^{\sigma}$ by Eq. (2.11). Because we wish to study the perturbation results in this paper, let us begin by evaluating $E_{(\omega)}{}^{\sigma}$ to lowest order in Δ/U by using the zero-order expression $G_{d(\omega)}{}^{\sigma(0)}$ as given by Eq. (2.18) in Eq. (2.11) for $n_{dk}{}^{\sigma}$. We readily obtain the result

$$\begin{aligned} n_{dk}{}^{\sigma(1)} &= \frac{V}{\pi}\int_{-\infty}^{\infty}d\omega\, f(\omega)\,\mathrm{Im}\frac{G_{d(\omega)}{}^{\sigma(0)}}{\omega-\epsilon_{k\sigma}} \\ &= V\left\{(1-n_{-\sigma})\frac{f_d{}^{\sigma}-f_k{}^{\sigma}}{\epsilon_{d\sigma}-\epsilon_{k\sigma}}+n_{-\sigma}\frac{f_{d+U}{}^{\sigma}-f_k{}^{\sigma}}{\epsilon_{d\sigma}+U-\epsilon_{k\sigma}}\right\}. \end{aligned} \tag{3.13}$$

[16] The importance of examining the charge symmetry of all expressions obtained was pointed out to the author by J. R. Schrieffer.
[17] A. Erdélyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. p. 15.
[18] Reference 17, p. 47, Eq. (7), making use of the fact that $\psi(\frac{1}{2}) = -\ln 4\gamma$.

Using this value for $n_{dk}^{\sigma(1)}$, the real part of $E_{(\omega)}^{\sigma}$ may be found to be

$$\mathrm{Re}E_{(\omega)}^{\sigma(2)}=\{\tfrac{1}{2}(D_{d+U}^{g\sigma}+D_{d}^{g\sigma})\}\,\mathrm{Re}A_{(\omega)}^{\sigma}+\tfrac{1}{2}(D_{d+U}^{g\sigma}-D_{d}^{g\sigma})\,\frac{\Delta}{\pi}\ln\left|\frac{1-\xi}{\xi}\right|$$

$$+\tfrac{1}{2}(n^{\sigma}-n^{-\sigma})(D_{d+U}^{g\sigma}-D_{d}^{g\sigma})\times\left\{\mathrm{Re}A_{(\omega)}^{\sigma}+\frac{\Delta}{\pi}\left(\ln\left|\frac{1-\xi}{1-2\xi}\right|+\ln\left|\frac{\xi}{1-2\xi}\right|\right)\right\},\qquad(3.14)$$

where we have written $f_{d}^{\sigma}=1$ and $f_{d+U}^{\sigma}=0$. We see that the lowest-order perturbation expression for $\mathrm{Re}E_{(\omega)}^{\sigma}$ is singular, as claimed, being proportional to $\mathrm{Re}A_{(\omega)}^{\sigma}$.

The imaginary part of $E_{(\omega)}^{\sigma(2)}$ may likewise be obtained:

$$\mathrm{Im}E_{(\omega)}^{\sigma(2)}=-\Delta\left\{(1-n^{\sigma})\,\frac{[1-f(\omega+2g\sigma H)]}{\epsilon_d-\omega}-n^{\sigma}\frac{f(\omega+2g\sigma H)}{\epsilon_d+U-\omega}\right\}$$

$$+\Delta\left\{\frac{(1-n^{\sigma})(1-\theta)}{(\epsilon_d+\omega-U(1-2\xi)-2\epsilon_F)}-\frac{n^{\sigma}\theta}{(\epsilon_d+\omega+2\xi U-2\epsilon_F)}\right\}.\qquad(3.15)$$

From a study of the equations of motion, Eqs. (2.14 ff.), it might be supposed that Eq. (3.4) is in fact correct to order Δ/U. However, Eq. (3.4) is not quite correct.

To see this, consider the diagrams of Fig. 4(a)–4(d). These terms yield, in the order shown, the expression

$$-\sum_{k\to k_3}(D_{d+U}^{g\sigma}-D_{d}^{g\sigma})(D_{k}^{\sigma})^2(D_{k+k_1-d-U}^{g\sigma}-D_{k+k_1-d}^{g\sigma})g_{k_1}^{-\sigma}\,\delta_{k_1,k_2}f_{k}^{\sigma}\,\delta_{k,k_3}G_d$$

$$-\sum_{k\to k_3}V^4(D_{d+U}^{g\sigma}-D_{d}^{g\sigma})(D_{k}^{\sigma})^2(D_{k-k_1+d+U}^{g\sigma}-D_{k-k_1+d}^{g\sigma})f_{k_1}^{-\sigma}\,\delta_{k_1,k_2}f_{k}^{\sigma}\,\delta_{k,k_3}G_d^{\sigma}$$

$$+\sum_{k\to k_2}V^4(D_{d+U}^{g\sigma}-D_{d}^{g\sigma})(D_{k}^{\sigma})^2(D_{k+k_1-d-U}^{g\sigma}-D_{k+k_1-d}^{g\sigma})f_{k}^{\sigma}\,\delta_{k,k_2}G_{+d}^{\sigma}$$

$$+\sum_{k\to k_2}V^4(D_{d+U}^{g\sigma}-D_{d}^{g\sigma})(D_{k}^{\sigma})^2(D_{k-k_1+d+U}^{g\sigma}-D_{k-k_1+d}^{g\sigma})f_{k}^{\sigma}\,\delta_{k,k_2}G_{+d}^{\sigma}.\qquad(3.16)$$

If we sum over k, we find that only the diagrams (a) and (b) contribute, yielding the expression

$$-V^2\sum_{k}(D_{d+U}^{g\sigma}-D_{d}^{g\sigma})(D_{k}^{\sigma})^2(2i\Delta)f_{k}^{\sigma}G_{d}^{\sigma},\qquad(3.17)$$

where we have set $f_d=1$, $f_{d+U}=0$.

The sum $\sum_k f_k^{\sigma}(D_k^{\sigma})^2$ would, if taken as it stands, yield a term $1/\omega$, so that expression (3.17) would appear to be of order $i(\Delta/U)^2U/\omega$ for $|\omega|\gg T$, and thus although of order $(\Delta/U)^2$, even more singular than $(\Delta/U)\ln(W/\omega)$. We shall see in Appendix C that because of the finite lifetime of the d electron, the factor $2i\Delta(D_k^{\sigma})^2$ gets renormalized:

$$2i\Delta(D_k^{\sigma})^2\to\tfrac{1}{2}\{[\omega-\epsilon_{k\sigma}+i\Gamma(\omega-\epsilon_{k\sigma})]^{-1}-(\omega-\epsilon_{k\sigma}+4i\Delta+\cdots)^{-1}\},\qquad(3.18)$$

where $\Gamma(\omega)$ is a nonanalytic (in Δ) energy and temperature-dependent width of order T_c for $T\to 0$. $\Gamma(\omega)$ decreased with increasing T (and ω) and though finite for all T is small for $T\gg T_c$, and may thus be neglected in this paper (it plays an important role for $T\lesssim T_c$, as will be shown in the succeeding two papers). Thus, because of the renomalization of the denominator $(D_k^{\sigma})^2$, expression (3.17) may be written

$$-\tfrac{1}{2}[\bar{A}(\omega)-\bar{A}(\omega+4i\Delta)]D_{d+U}^{g\sigma}D_{d}^{g\sigma}G_{d}^{\sigma(0)},\qquad(3.19)$$

and hence is seen to be of order Δ/U. The diagrams (e)→(h) of Fig. 4 likewise contribute the term

$$-\tfrac{1}{2}[\bar{E}_{(\omega)}^{-\sigma}-\bar{E}_{(\omega+4i\Delta)}^{-\sigma}]D_{d+U}^{g\sigma}D_{d}^{g\sigma},\qquad(3.20)$$

where we have written $A^{\sigma}(\omega)|_{g=0}$ as $\bar{A}(\omega)$ and $E^{-\sigma}(\omega)|_{g=0}$ as $\bar{E}^{-\sigma}(\omega)$.

If we add these two terms to $G_d^{\sigma(2)}$, as given by Eq. (3.4), we obtain

$$UG_d^{\sigma(2)}(\omega)=-U^2\left\{n^{-\sigma}+E^{\sigma}(\omega)+\tfrac{1}{2}[\bar{E}_{(\omega)}^{-\sigma}-\bar{E}_{(\omega+4i\Delta)}^{-\sigma}]+\frac{3i\Delta}{U}-2i\Delta n^{-\sigma}+\frac{\omega-\epsilon_{d\sigma}-U}{U}\,\frac{(2\omega-2\epsilon_d-U)}{(\omega-\epsilon_{d\sigma}-U)(\omega-\epsilon_{d\sigma})}-U\frac{\{A^{\sigma}(\omega)+\tfrac{1}{2}[\bar{A}(\omega)-\bar{A}(\omega+4i\Delta)]\}(n^{-\sigma}+\omega-\epsilon_{d\sigma}-U)}{(\omega-\epsilon_{d\sigma}-U)(\omega-\epsilon_{d\sigma})}\right\}$$

$$\times\{(\omega-\epsilon_{d\sigma}-U)(\omega-\epsilon_{d\sigma})\}^{-1}.\qquad(3.21)$$

In Appendix B we study the self-energy corrections to the denominators $D_k^{(2g-1)\sigma}$ and D_{2d+U-k}^{σ} which enter into the expressions (3.2) and (3.3) for $A^{\sigma}(\omega)$ and $E^{\sigma}(\omega)$. We show that

$$D_k^{(2g-1)\sigma}\to\{\omega-\epsilon+(2g-1)\sigma H+i\Gamma[\omega-\epsilon_k+(2g-1)\sigma H]\}^{-1},\qquad(3.22)$$

and

$$D_{2d+U-k}^{\sigma} \to [\omega - \epsilon_k + \sigma H - (2\epsilon_d + U) + 2i\Delta]^{-1}, \quad (3.23)$$

where again we may neglect the Γ term for $T \gg T_c$, while the $2i\Delta$ term in D_{2d+U-k} is irrelevent (we have explicitly excluded the case $\xi = \frac{1}{2}$).

From Eq. (3.21) we may obtain the magnetic susceptibility and other interesting physical properties of the system for high T (the resistivity will be discussed in the next section).

From Eq. (2.18) we find that for $H=0$,

$$\mathrm{Re}G_d^{\sigma(0)}(\epsilon_F) = -(1-2\xi)/2U, \quad (3.24)$$

while from Eq. (3.21) we find, for $H=0$,

$$\mathrm{Im}G_d^{\sigma(2)}(\epsilon_F) = \Delta(1-\xi+\xi^2)/[\xi^2(1-\xi)^2U^2], \quad (3.25)$$

where we have made use of Eqs. (3.14) and (3.15).

From Eq. (2.9) we see that the conduction-electron scattering matrix $T_{kk'}(\epsilon_F)$ is given, for $H=0$, by

$$T_{kk'}(\omega) = V^2 G_d(\epsilon_F). \quad (3.26)$$

From Eqs. (3.24) and (3.25) we see that to lowest order in Δ/U the "optical theorem"

$$\mathrm{Im}T_{kk}(\epsilon_F) = \pi \sum_{k'} |T_{kk'}(\epsilon_F)|^2 \delta(\epsilon_k - \epsilon_{k'}) \quad (3.27)$$

is not satisfied;

$$\frac{\pi\rho V^4[1-\xi(1-\xi)]}{U^2\xi^2(1-\xi)^2} \neq \frac{\pi V^4\rho[\frac{1}{4}-\xi(1-\xi)]}{U^2\xi^2(1-\xi)^2}, \quad (3.28)$$

so that the phase shift $\delta(\epsilon_F)$ is complex, unlike the case where V is treated exactly and $U=0$.[19] It is interesting to note that the difference

$$\mathrm{Im}T_{kk}(\epsilon_F) - \pi\rho\, |T_{kk}(\epsilon_F)|^2 = 3\pi\rho V^4/[4\xi^2(1-\xi)^2U^2] \quad (3.29)$$

is just $3\pi\rho\,|\tau_{kk}(\epsilon_F)|^2$, where $\tau_{kk'}(\epsilon_F)$ is the spin-flip amplitude appropriate to the s-d exchange model[20] if we use the lowest-order expression $\tau = J/4$,[21] where

$$J = 2V^2U/[(\epsilon_d - \epsilon_F)(\epsilon_d + U - \epsilon_F)]. \quad (3.30)$$

Thus our $T_{kk'}(\epsilon_F)$ satisfies, to lowest order in Δ/U, the optical theorem appropriate for a spin-$\frac{1}{2}$ impurity[22]

$$\mathrm{Im}T_{kk}(\epsilon_F) = \pi\rho[\,|T_{kk}(\epsilon_F)|^2 + 3\,|\tau_{kk}(\epsilon_F)|^2], \quad (3.31)$$

although there is no intrinsic spin-flip amplitude in the Anderson model (remark we are considering the case $H=0$).

By integrating the imaginary part of $G_{d(\omega)}^{\sigma(2)}$ as given by Eq. (3.21) over ω with the weighting factor $f(\omega)$, the self-consistency equation, Eq. (2.4), for n^σ, E may be obtained.

After much algebra one finds

$$n^\sigma = 1 - n^{-\sigma} + j(\xi)\frac{\Delta}{U} + k(\xi)\frac{\Delta}{U}\tfrac{1}{2}(n^\sigma + n^{-\sigma}) + \left\{\left[\frac{(f_d-1)-f_{d+U}}{2} + M(\xi)\frac{T\Delta}{U^2}\right]\left((n^\sigma - n^{-\sigma}) - \frac{g\sigma H}{T}\right)\right\}, \quad (3.32)$$

where $j(\xi)$, $k(\xi)$ and $M(\xi)$ are functions of ξ of order unity, and where $f_d \equiv f(\epsilon_d)$. Equation (3.32) may be written as the two equations

$$n^\sigma + n^{-\sigma} = (1 + j\Delta/U)(1 - k\Delta/2U), \quad (3.33a)$$

and

$$n^\sigma - n^{-\sigma} = g\sigma H/T, \quad (3.33b)$$

thus showing that the Curie-law susceptibility obtains to first order in Δ/U. For a constant density of states the susceptibility of the conduction electrons may readily be shown to be just the usual Pauli susceptibility.

Although this method of computing the magnetic susceptibility furnishes a zero-order (in Δ/U) term in the susceptibility from a second-order Green's function, it is useful in that it shows that the Curie-law susceptibility arises from the Fermi function $f(\omega + 2g\sigma H)$ appearing in the imaginary part of $A^\sigma(\omega)$ and $E^\sigma(\omega)$, and thus is a consequence of the "Kondo anomaly" [the real part of $A^\sigma(\omega)$ and $E^\sigma(\omega)$ yield in $\ln\omega/T$ term]. Indeed, if we had set[23]

$$G_d^{\sigma(2)} = -\left\{\frac{1-n^{-\sigma}}{\omega - \epsilon_{d\sigma} + U + 2i\Delta} + \frac{n^{-\sigma}}{\omega - \epsilon_{d\sigma} + 2i\Delta}\right\}, \quad (3.34)$$

we would have obtained

$$n^\sigma - n^{-\sigma} = O(g\sigma H/U), \quad (3.35)$$

resulting in a temperature-independent susceptibility.

We may also obtain the second-order term in the suceptibility by noting that the free-energy $F(V)$ may be given by

$$F(V) - F(0) = \int_0^V \frac{dV'}{V'}\langle H_i(V')\rangle, \quad (3.36)$$

where we have defined

$$H_i(V') = V' \sum_{k,\sigma} (d_\sigma^\dagger C_{k\sigma} + C_{k\sigma}^\dagger d_\sigma), \quad (3.37)$$

so that

$$F(V) - F(0) = \int_0^V V'\,dV' \sum_{k,\sigma} \langle d_\sigma^\dagger C_{k\sigma} + C_{k\sigma}^\dagger d_\sigma\rangle_{V'}. \quad (3.38)$$

[19] P. W. Anderson, in *Proceedings of the International Conference on Magnetism, Nottingham, England, 1964* (The Institute of Physics and the Physical Society, London, 1965) p. 17.

[20] H. Suhl, Lectures presented at the 1966 International School of Physics "Enrico Fermi" Varenna, Italy p. 61, Eq. (54) (to be published).

[21] Reference 20, p. 75, Eq. (72b).

[22] Reference 20, p. 82, Eq. (82).

[3] This expression was suggested by B. Kjöllerstrom, D. J. Scalapino, and J. R. Schrieffer, Bull. Am. Phys. Soc. 11, 79 (1966). The authors recognized the inadequacy of the expression as regards the magnetic properties.

Using Eq. (2.12) we may write

$$F(V)-F(0)$$
$$=\pi^{-1}\int_0^{V^2} d(V')^2 \sum_{k,\sigma}\int_{-\infty}^{\infty} d\omega\, f(\omega)\ \mathrm{Im}\,\frac{G_d^{\sigma}(\omega)_{V'}}{\omega-\epsilon_{k\sigma}}$$
$$=-\sum_{\sigma}\int_0^{V^2} \rho d(V')^2 \int_{-\infty}^{\infty} d\omega\, f(\omega)\ \mathrm{Re}G_d^{\sigma}(\omega)_{V'}, \tag{3.39}$$

where we have dropped the principal-value term

$$P\int_{-\infty}^{\infty} d\epsilon[1/(\omega-\epsilon)].$$

If we insert expression (3.21) for $G_d^{\sigma}(\omega)$ into Eq. (3.38), we obtain

$$F(V)-F(0)=\sum_{\sigma}\frac{\Delta}{\pi}\left\{n^{-\sigma(0)}\ln\left|\frac{\epsilon_F-\epsilon_{d\sigma}-U}{W+\epsilon_{d\sigma}-U}\right| +(1-n^{-\sigma(0)})\ln\left|\frac{\epsilon_F-\epsilon_{d\sigma}}{W+\epsilon_{d\sigma}}\right|\right\}$$
$$+\frac{\Delta}{\pi}\sum_{\sigma}\int_{-\infty}^{\infty} d\omega\, f(\omega)\,\frac{U^2\,\mathrm{Re}A_{(\omega)}{}^{\sigma}(n^{\sigma}-n^{-\sigma(0)})}{(\omega-\epsilon_{d\sigma}-U)^2(\omega-\epsilon_{d\sigma})^2}, \tag{3.40}$$

where we have kept all second-order terms but only that fourth-order term proportional to $\mathrm{Re}A^{\sigma}(\omega)$.

It might be noted that no $\ln W/T$ term appears in $\mathrm{Re}G_d^{\sigma(2)}(\omega)$ for $H=0$ [and thus the leading $\ln W/T$ term in $T_{kk}(\omega)$ is of order $(\Delta/U)^3$ for $H=0$, agreeing with the results for the s-d model]. Upon summing over σ, making use of the fact that $\mathrm{Re}A^{\sigma}(\epsilon_F+2g\sigma H)$ is given by $\mathrm{Re}\bar{A}(\epsilon_F)+O[(2g\sigma H/T)^2]$, we find that the last term of (3.40) is just

$$2\left(\frac{\Delta}{U}\right)^2\frac{H^2g^2\ln|2U(1-2\xi)\gamma/\pi T|}{T\xi^2(1-\xi)^2\pi^2}, \tag{3.41}$$

so that the free energy as given by (3.39) may be seen to be the same as obtained by Scalapino.

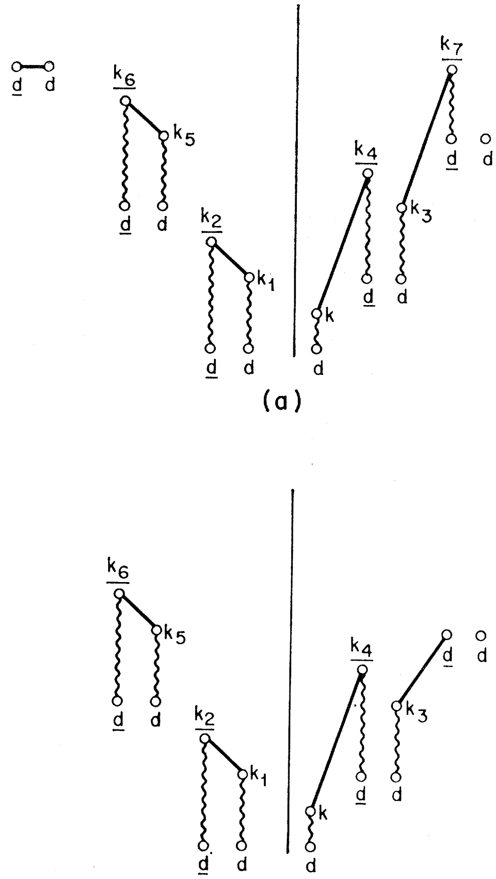

FIG. 6. Representation of those eighth-order singular terms which reduce to order $(\Delta/U\ \ln W/T)^2$ upon self-energy renormalization.

IV. $G_d^{\sigma(4)}(\omega)$ AND THE DC RESISTIVITY

In this section we continue our study of the perturbation series by computing $G_d^{\sigma(4)}(\omega)$. From a knowledge of $\mathrm{Im}G_d^{\sigma(4)}(\epsilon_F)$ we may obtain, using Eq. (3.26), the $J^3\ln(W/T)$ correction to the resistivity.

It is not hard to see that the fourth-order terms represented by Fig. 5 have a real part proportional to $[(\Delta/U)\ln(W/T)]^2$. In the order shown, the terms (a)→(d) yield the expression

$$-\sum_{k,k_1} V^4 f_{k_1}{}^{\sigma} f_k{}^{-\sigma}(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_k{}^{(2g-1)\sigma}(D_{k+k_1-d-U}{}^{g\sigma}-D_{k+k_1-d}{}^{g\sigma})D_{k_1}{}^{\sigma}G_d{}^{\sigma}-\sum_{k,k_1} V^4 f_k{}^{\sigma} f_{k_1}{}^{-\sigma}(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_k{}^{\sigma}$$
$$\times(D_{k+k_1-d-U}{}^{g\sigma}-D_{k+k_1-d}{}^{g\sigma})D_{k_1}{}^{(2g-1)\sigma}G_d{}^{\sigma}$$
$$-\sum_{k\to k_3} V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_{2d+U-k}{}^{\sigma}(D_{d+U+k_1-k}{}^{(2-g)\sigma}-D_{d+k_1-k}{}^{(2-g)\sigma})D_{k_1}{}^{\sigma}f_k{}^{-\sigma}\,\delta_{k,k_2}f_{k_1}{}^{\sigma}\,\delta_{k_1,k_3}G_d{}^{\sigma(0)}(\omega)$$
$$-\sum_{k\to k_3} V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_k{}^{\sigma}(D_{d+U+k-k_1}{}^{(g-2)\sigma}-D_{d+k-k_1}{}^{(g-2)\sigma})D_{2d+U-k_1}{}^{g\sigma}f_k{}^{\sigma}\,\delta_{k,k_2}f_{k_1}{}^{-\sigma}\,\delta_{k_1,k_3}G_d{}^{\sigma(0)}(\omega). \tag{4.1}$$

Upon summing over k and k_1, we obtain

$$-2[A^{\sigma}(\omega)+2i(\theta-\xi)\Delta][\bar{A}(\omega)+i\Delta(\theta-\xi)]\frac{D_{d+U}{}^{g\sigma}D_d{}^{g\sigma}G_d{}^{\sigma}(\omega)}{\xi(1-\xi)U}, \tag{4.2}$$

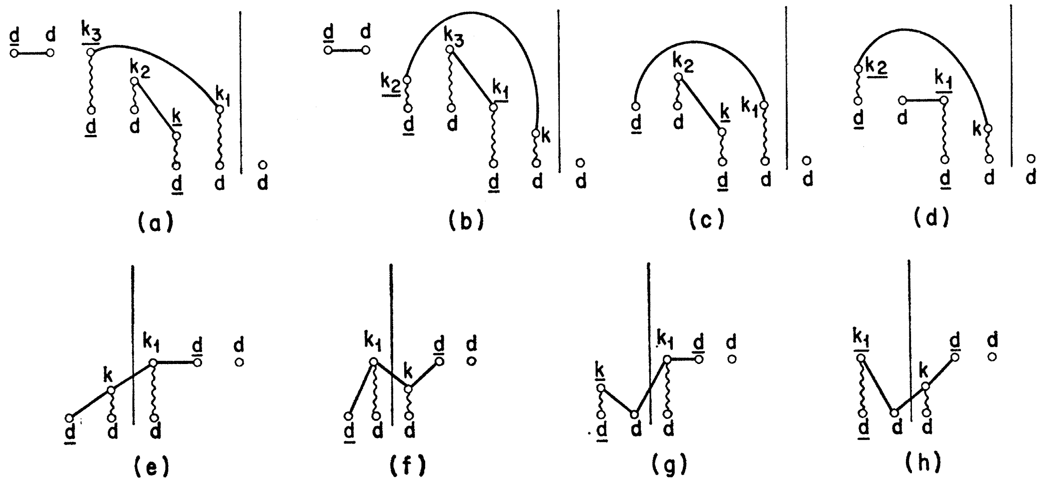

FIG. 7. Representation of fourth-order terms whose imaginary part is of order $\Delta/U(\Delta/U \ln W/T)$.

where we have neglected terms of order $\Delta/U \ln(\xi/1-\xi)$, etc., and have set $\epsilon_k=\epsilon_{k_1}=\epsilon_F$ in the term $(D_{d+U+k_1-k}{}^{(2-g)\sigma}-D_{d+k_1-k}{}^{(2-g)\sigma})$.

The terms of Fig. 5(c)–5(h) are also of order $[\Delta/U)\ln(W/T)]^2$. In the order shown, they yield

$$-\sum_{k,k_1} V^3(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_k{}^{(2g-1)\sigma}(D_{k+k_1-d-U}{}^{g\sigma}-D_{k+k_1-d}{}^{g\sigma})D_{k_1}{}^{\sigma}n_{dk_1}{}^{\sigma}f_k{}^{-\sigma}$$
$$-\sum_{k,k_1} V^3(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_k{}^{\sigma}(D_{k+k_1-d-U}{}^{g\sigma}-D_{k+k_1-d}{}^{g\sigma})D_{k_1}{}^{(2g-1)\sigma}f_k{}^{\sigma}n_{dk_1}{}^{-\sigma}$$
$$+\sum_{k\to k_2} V^3(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_{2d+U-k}{}^{\sigma}(D_{k_1+d+U-k}{}^{(2-g)\sigma}-D_{k_1+d-k}{}^{(2-g)\sigma})D_{k_1}{}^{\sigma}f_k{}^{-\sigma}\,\delta_{k,k_2}(-n_{dk_1}{}^{\sigma})$$
$$+\sum_{k\to k_2} V^3(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_k{}^{\sigma}(D_{k-k_1+d}{}^{(2-g)\sigma})f_k{}^{\sigma}\,\delta_{k,k_2}(-n_{kd}{}^{-\sigma})D_{2d+U-k}{}^{+\sigma}. \quad (4.3)$$

The contribution from these terms may be written

$$-\{[A^{\sigma}(\omega)+2i(\theta-\xi)\Delta][\bar{E}^{-\sigma}(\omega)-i\Delta][(1-n^{-\sigma})\xi\theta$$
$$+n^{-\sigma}(1-\theta)(1-\xi)]+[E^{\sigma}(\omega)-i\Delta/U][\bar{A}(\omega)+i\Delta(\theta-\xi)]\}D_{d+U}{}^{g\sigma}D_d{}^{g\sigma}/[\xi(1-\xi)U]. \quad (4.4)$$

In addition to these "irreducible" terms of order $[(\Delta/U)\ln(W/T)]^2$, there is another set of "irreducible" terms of the same order represented in Fig. 6. These terms are nominally of order $(i\Delta^2/TU)^2$ but because of the self-energy renormalization discussed in Sec. III and Appendix C, they may be shown to be of order $[(\Delta/U)\ln(W/T)]^2$ [just as the $(i\Delta/T)$ term was shown to be of order $\Delta/U \ln W/T$ in Sec. III].

The contribution of Fig. 6(a) (where $k_1\to\bar{k}_1$ and $k_5\to\bar{k}_5$ are also included) is given by

$$\sum_{k,k_1,k_3,k_5} V^8(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(D_k{}^{\sigma})^2(D_{k+k_1-d-U}{}^{g\sigma}-D_{k+k_1-d}{}^{g\sigma})f_{k_1}{}^{-\sigma}$$
$$\times(D_{k+k_3-d-U}{}^{(2-g)\sigma}-D_{k+k_3-d}{}^{(2-g)\sigma})(D_{k_3}{}^{\sigma})^2(D_{k_3+k_5-d-U}{}^{g\sigma}-D_{k_3+k_5-d}{}^{g\sigma})f_{k_5}{}^{-\sigma}f_k{}^{\sigma}f_{k_3}{}^{\sigma}G_d{}^{\sigma}(\omega). \quad (4.5)$$

Upon summing over k_1 and k_5 (and relabeling the variables), we may write expression (4.5) as

$$\sum_{k,k_1} V^4(2i\Delta D_k{}^{\sigma 2})(D_{k+k_1-d-U}{}^{(2-g)\sigma}$$
$$-D_{k+k_1-d}{}^{(2-g)\sigma})(2i\Delta D_{k_1}{}^{\sigma 2})f_k{}^{\sigma}f_{k_1}{}^{\sigma}G_d{}^{\sigma}(\omega), \quad (4.6)$$

so that upon making use of the renormalization Eq. (3.18) we obtain

$$\tfrac{1}{4}[\bar{A}(\omega)-\bar{A}(\omega+4i\Delta)]^2\frac{D_{d+U}{}^{g\sigma}D_d{}^{g\sigma}}{\xi(1-\xi)U}G_d{}^{\sigma}(\omega), \quad (4.7)$$

where we have set $\epsilon_k=\epsilon_{k_1}=\epsilon_F$ in the term

$$(D_{k+k_1-d-U}{}^{(2-g)\sigma}-D_{k+k_1-d}{}^{(2-g)\sigma}).$$

From Fig. 6(b) we likewise obtain

$$\tfrac{1}{4}[\bar{A}(\omega)-\bar{A}(\omega+4i\Delta)][\bar{E}^{-\sigma}(\omega)$$
$$-\bar{E}^{-\sigma}(\omega+4i\Delta)]\frac{D_{d+U}{}^{g\sigma}D_d{}^{g\sigma}}{\xi(1-\xi)U}. \quad (4.8)$$

In Appendix D we show that the self-energy renormalization leads to the replacement

$$\bar{A}(\omega)+i\Delta(\theta-\xi)\rightarrow\tfrac{1}{2}[\bar{A}(\omega)+\bar{A}(\omega+4i\Delta)+2i\Delta(\theta-\xi)], \tag{4.9}$$

and that

$$\begin{aligned}\bar{E}^{-\sigma}(\omega)-i\Delta\{(1-n^{-\sigma})\xi\theta+n^{-\sigma}(1-\theta)(1-\xi)\}\\ \rightarrow\tfrac{1}{2}[\bar{E}^{-\sigma}(\omega)+\bar{E}^{-\sigma}(\omega+4i\Delta)\\ -2i\Delta\{(1-n^{-\sigma}\xi\theta+n^{-\sigma}(1-\theta)(1-\xi)\}],\end{aligned} \tag{4.10}$$

in Eqs. (4.2) and (4.4); we again have neglected the $\Gamma(T)$ term in the argument for $T\gg T_c$.

We have now examined the fourth-order "irreducible" terms having a real part proportional to $[(\Delta/U)\ln(W/T)]^2$. In order to obtain the leading logarithmic term in the resistivity we must also examine the "irreducible" terms of order $i\Delta/U[(\Delta/U)\ln(W/T)]$. These terms are represented in Fig. 7 (only those fourth-order terms yielding a nonzero contribution are shown). In the order shown they yield

$$\begin{aligned}&-\sum_{k,k_1}V^4f_k^{-\sigma}f_{k_1}^{-\sigma}(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_{d+U+k_1-k}^{(2g+1)\sigma}-D_{d+k_1-k}^{(2g+1)\sigma})D_{2d+U-k}^{\sigma}D_{k_1}^{(2g-1)\sigma}D_d^{\sigma}\\
&\quad-\sum_{k,k_1}V^4f_k^{-\sigma}f_{k_1}^{-\sigma}(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_k^{(2g-1)\sigma}D_{2d+U-k_1}^{\sigma}(D_{d+U+k-k_1}^{g\sigma}-D_{d+k-k_1}^{g\sigma})G_d^{\sigma}\\
&\quad-\sum_{k,k_1}V^3(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_{2d+U-k}^{\sigma}(D_{d+U+k_1-k}^{(2g+1)\sigma}-D_{d+k_1-k}^{(2g+1)\sigma})D_{k_1}^{(2g-1)\sigma}n_{dk_1}^{-\sigma}f_k^{-\sigma}\\
&\quad-\sum_{k,k_1}V^3(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_k^{(2g-1)\sigma}D_{2d+U-k_1}^{\sigma}(D_{d+U+k-k_1}^{g\sigma}-D_{d+k-k_1}^{g\sigma})f_k^{-\sigma}n_{k_1d}^{-\sigma}\\
&\quad+\sum_{k,k_1}V^2D_k^{(2g-1)\sigma}(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_{k+k_1-d-U}^{g\sigma}-D_{k+k_1-d}^{g\sigma})\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}d_{\sigma}{}^{\dagger}C_{k_1\sigma}\rangle\\
&\quad+\sum_{k,k_1}V^2(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_k^{\sigma}(D_{k+k_1-d-U}^{g\sigma}-D_{k+k_1-d}^{g\sigma})\langle d_{-\sigma}{}^{\dagger}C_{k_1-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle\\
&\quad-\sum_{k,k_1}V^2(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_{2d+U-k}^{\sigma}(D_{k_1+d-k+U}^{(2-g)\sigma}-D_{k_1+d-k}^{(2-g)\sigma})\langle C_{k-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k_1\sigma}\rangle\\
&\quad-\sum_{k,k_1}V^2(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_k^{\sigma}(D_{k+d+U-k_1}^{(1-2g)\sigma}-D_{k+d-k_1}^{(1-2g)\sigma})\langle C_{k_1-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle.\end{aligned} \tag{4.11}$$

It should be noted that the thermal averages $\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}d_{\sigma}{}^{\dagger}C_{k_1\sigma}\rangle$ and $\langle C_{k_1-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle$ are required. These averages are computed to order Δ, with U treated exactly, by studying the equations of motion of the required Green's functions in Appendixes F and G. We shall see below that the last two terms of Eq. (4.11) do not contribute for $H=0$. If we leave these terms aside for the moment, the contribution from the first two terms is found to be

$$2\Delta i[(1-\theta)/(1-\xi)-\theta/\xi]A^{\sigma}(\omega)D_{d+U}^{g\sigma}D_d^{g\sigma}G_d^{\sigma}(\omega), \tag{4.12}$$

while the contribution from the third through sixth is found to be, taking into account the self-energy renormalization, to the order required,

$$\begin{aligned}&i\left(\frac{\theta}{\xi}-\frac{1-\theta}{1-\xi}\right)\frac{\Delta}{U}D_{d+U}^{g\sigma}D_d^{g\sigma}E^{\sigma}(\omega)\\
&\quad+i(\theta-1)\frac{\Delta}{U}D_{d+U}^{g\sigma}D_d^{g\sigma}[E^{\sigma}(\omega)+\tilde{E}^{-\sigma}(\omega)]\\
&\quad+i\frac{\Delta}{U}D_{d+U}^{g\sigma}D_d^{g\sigma}[E_+^{\sigma}(\omega)+\tilde{E}_+^{-\sigma}(\omega)]\\
&\quad-\frac{i\Delta}{U}\left[\tfrac{1}{3}(n^{\sigma}\theta)+\frac{(1-n^{\sigma})(1-\theta)}{1-\xi}+\xi n^{\sigma}+(1-n^{\sigma})(1-\xi)\right]\\
&\quad\times D_{d+U}^{g\sigma}D_d^{g\sigma}\frac{A^{\sigma}(\omega)}{\xi(1-\xi)}+\frac{i\Delta}{U\xi(1-\xi)}\\
&\quad\times\left[A^{\sigma}(\omega)\left\{n^{\sigma}\left[\frac{\xi(1-\xi)}{1-\xi}-\theta(1-\xi)\right]\right.\right.\\
&\quad+(1-n^{\sigma})\left[\frac{(1-\xi)\theta}{\xi}-\xi(1-\theta)\right]\\
&\quad\left.+n^{-\sigma}\left[\xi-\theta\frac{\theta(1-\xi)}{\xi}\right]+(1-n^{\sigma})\left[\theta-\xi-\frac{\xi(1-\theta)}{(1-\xi)}\right]\right\}\\
&\quad\left.+\tilde{A}(\omega)\{\sigma\rightarrow-\sigma\}\right]D_{d+U}^{g\sigma}D_d^{g\sigma},\end{aligned} \tag{4.13}$$

where we have written

$$E_+^{\sigma}(\omega)=V\sum_k\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}d_{\sigma}{}^{\dagger}d_{\sigma}\rangle(D_k^{(2g-1)\sigma}-D_{2d+U-k}^{\sigma}), \tag{4.14}$$

and

$$\tilde{E}^{-\sigma}(\omega)=\tfrac{1}{2}[\bar{E}^{-}(\omega)+\bar{E}^{-\sigma}(\omega+4i\Delta)], \tag{4.15}$$

and

$$\tilde{E}_+^{-\sigma}(\omega)=\tfrac{1}{2}[\bar{E}_+^{-\sigma}(\omega)+\bar{E}_+^{-\sigma}(\omega+4i\Delta)], \tag{4.16}$$

and

$$\tilde{A}(\omega)=\tfrac{1}{2}[\bar{A}(\omega)+\bar{A}(\omega+4i\Delta)]. \tag{4.17}$$

In addition to the terms of Eq. (4.12) of order $i\Delta/UA(\omega)$, there are two other terms which must be considered represented by Figs. 3(b) and 3(g) for which $k_1\neq k$. These terms are given by

$$+\sum_{k,k_1}{}' V(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_k^{(2g-1)\sigma}[\langle \hat{n}_{-\sigma}C_{k_1-\sigma}^\dagger C_{k-\sigma}\rangle(D_{d+U+k-k_1}^{g\sigma}-D_{d+k-k_1}^{g\sigma})+\langle C_{k_1-\sigma}^\dagger C_{k-\sigma}\rangle D_d^{g\sigma}]$$
$$+\sum_{k,k_1}{}' V(D_{d+U}^{g\sigma}-D_d^{g\sigma})D_{2d+U-k}^{\sigma}[\langle \hat{n}_{-\sigma}C_{k-\sigma}^\dagger C_{k_1-\sigma}\rangle(D_{d+U+k_1-k}^{g\sigma}-D_{d+k_1-k}^{g\sigma})+\langle C_{k-\sigma}^\dagger C_{k_1-\sigma}\rangle D_d^{g\sigma}]. \quad (4.18)$$

In Appendix E we show that only the term proportional to $\langle \hat{n}_{-\sigma}C_{k_1-\sigma}^\dagger C_{k-\sigma}\rangle$ contributes for a constant density of states. [For a density of states of the form $\rho(\epsilon_k)=\rho W^2/(\epsilon_k-\epsilon_F)^2+W^2$, the remaining terms enter with a coefficient $G_d^{(0)}(\epsilon_F+iW)$, so that for $U\xi$ and $(1-\xi)U\ll W$ these terms, which would otherwise result in a nonlinear integral equation for $G_{d(\omega)}^\sigma$, as we shall show in the succeeding paper, may be neglected.] Further, we show in Appendix H that the contribution from the $\langle \hat{n}_{-\sigma}C_{k_1-\sigma}^\dagger C_{k-\sigma}\rangle$ term, which arises from the region $\epsilon_{k_1}\approx\epsilon_d$, just cancels the last two terms of (4.11) for $H=0$.

We have listed all the "irreducible" terms which go into $G_{d(\omega)}^{\sigma(4)}$. If we incorporate these terms into the second-order (iterated) expression, Eq. (3.8), we obtain, for $|\omega-\epsilon_F|\ll T$ and $H=0$,

$$G_{d(\omega)}=U^{-1}\bigg\{n^{-\sigma}-(1-\xi)+\frac{3i\Delta}{U}+\tfrac{3}{2}E(\omega)-\tfrac{1}{2}E(\omega+4i\Delta)+[2\xi(1-\xi)U]^{-1}\{[A(\omega)+2i(\theta-\xi)\Delta][E(\omega)+E(\omega+4i\Delta]$$
$$-i\Delta[\xi\theta+(1-\theta)(1-\xi)]+[E(\omega)-i\Delta/U][A(\omega)+A(\omega+4i\Delta)+2i\Delta(\theta-\xi)]\}$$
$$-[4\xi(1-\xi)U]^{-1}[A(\omega)-A(\omega+4i\Delta)][E(\omega)-E(\omega+4i\Delta)]+\frac{i\Delta R(\xi)A(\omega)}{U^2\xi^2(1-\xi)^2}+\frac{i\Delta S(\xi)E(\omega)}{U\xi(1-\xi)}\bigg\}$$
$$\times\bigg\{-\xi(1-\xi)+\frac{3A(\omega)}{2U}-(2U)^{-1}A(\omega+4i\Delta)-\frac{2i\Delta}{U}(1-2\xi)+[U^2\xi(1-\xi)]^{-1}[A(\omega)+2i\Delta(\theta-\xi)]$$
$$\times[A(\omega)+A(\omega+4i\Delta)+2i\Delta(\theta-\xi)]+\frac{i\Delta T(\xi)A(\omega)}{U^2\xi(1-\xi)}-[4U\xi(1-\xi)]^{-1}[A(\omega)-A(\omega+4i\Delta)]^2\bigg\}^{-1}, \quad (4.19)$$

where $R(\xi)$, $S(\xi)$, and $T(\xi)$ are functions of ξ (S and T being odd under charge conjugation, R even) which go to zero as $U\to\infty$ ($\xi\to 0$). In order to obtain the $(\Delta/U)^2\ln W/T$ contribution to $\mathrm{Im}G_d(\epsilon_F)$, we must expand expression (4.19). In addition, we must remember that $E(\omega)$ has an imaginary part of order

$$i\Delta^2\ln(W/T)/U^2\xi(1-\xi)\quad\text{when}\quad \mathrm{Im}G_d^{(2)}(\omega),$$

as given by Eq. (3.21), is used in Eq. (2.11) for n_{kd}. Thus

$$E^{(4)}(\omega)=\frac{i\Delta^2(1-\xi+\xi^2)}{U^2\pi^2\xi^2(1-\xi)^2}\int_{-\infty}^{\infty}d\omega' f(\omega')\times\{(\omega-\omega')^{-1}+(\omega+\omega'-2\epsilon_d-U)^{-1}\}$$
$$=\frac{i\Delta(1-\xi+\xi^2)}{\pi U^2\xi^2(1-\xi)^2}A(\omega), \quad (4.20)$$

where we have set $\mathrm{Im}G_d^{(2)}(\omega)=\mathrm{Im}G_d^{(2)}(\epsilon_F)$ and added the second term as a convergence factor, a procedure valid to the order required.

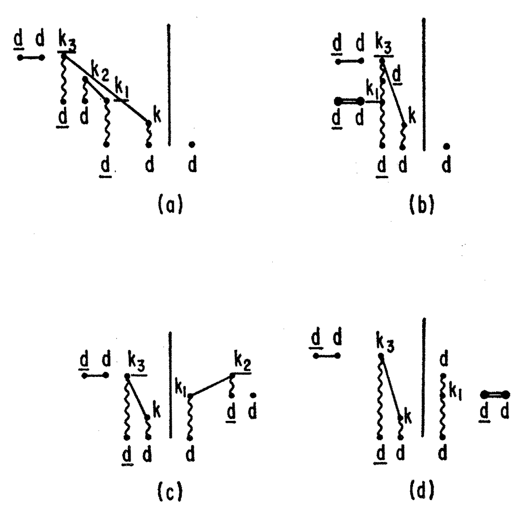

FIG. 8. Second-order self-energy corrections to $D_k^{(2g-1)\sigma}$.

The complete fourth-order contribution to $\mathrm{Im}G_d(\epsilon_F)$ of order $(\Delta/U)^2 \ln W/T$ is thus

$$\mathrm{Im}G_d^{(4)}(\epsilon_F)=\frac{1}{\xi(1-\xi)U}\Bigg\{\tfrac{3}{2}E^{(4)}(\epsilon_F)+\frac{\Delta A(\epsilon_F)}{4\xi^2(1-\xi)^2U^2}\{2(1-2\xi)^2-2(1-2\theta)(1-2\xi)+2\xi(1-\xi)[1+\xi\theta+(1-\theta)(1-\xi)]\}$$
$$+\left[\frac{R(\xi)\Delta A(\epsilon_F)}{\xi^2(1-\xi)^2U^2}+\frac{S(\xi)\Delta(1-2\xi)A(\epsilon_F)}{2\xi^2(1-\xi)^2U^2}-\frac{(1-2\xi)\Delta T(\xi)A(\epsilon_F)}{2\xi^2(1-\xi)^2U^2}\right]$$
$$\times\left[3\xi(1-\xi)+\frac{(1-2\xi)(1-2\theta)}{4}\right]\frac{3\Delta A(\epsilon_F)}{2\xi^2(1-\xi)^2U^2}+[\tfrac{1}{2}(1-2\theta)-2(1-2\xi)]$$
$$\times\frac{3(1-2\xi)\Delta A(\epsilon_F)}{4\xi(1-\xi)U^2}-\frac{\Delta(1-2\xi)A(\epsilon_F)}{2\xi^2(1-\xi)^2U^2}[2(1-2\xi)-\tfrac{1}{2}(1-2\theta)-2\xi(1-\theta)+2\theta(1-\xi)]$$
$$-\frac{3\Delta(1-2\xi)[\frac{1}{2}(1-2\theta)-2(1-2\xi)]A(\epsilon_F)}{2\xi^2(1-\xi)^2U^2}\Bigg\}. \tag{4.21}$$

In the limit $\xi\rightarrow 0$ (with $\xi U=\epsilon_F-\epsilon_d$ finite), we obtain, making use of Eq. (4.20),

$$\lim_{\xi\rightarrow 0}\mathrm{Im}G_d^{(4)}(\epsilon_F)=\frac{\Delta^2\ln|2\gamma U(1-2\xi)/\pi T|}{(\epsilon_F-\epsilon_d)^3\pi}\{\tfrac{3}{2}+0+0+0+0+\tfrac{3}{2}\times\tfrac{1}{4}-\tfrac{3}{2}\times\tfrac{3}{4}-\tfrac{1}{2}\times\tfrac{3}{2}+\tfrac{3}{2}\times\tfrac{3}{2}\}$$
$$=\frac{9\Delta^2\ln|2\gamma U(1-2\xi)/\pi T|}{4(\epsilon_F-\epsilon_d)^3\pi}. \tag{4.22}$$

If we compare our expression for $\mathrm{Im}G_d(\epsilon_F)$ for $\xi\rightarrow 0$ with the expression obtained by Hamann,[24] we see that whereas our $\mathrm{Im}G_d^{(2)}(\epsilon_F)$ agrees with his, our $\mathrm{Im}G_d^{4}(\epsilon_F)$ has the coefficient 9/4 whereas his has the coefficient 3, which is just such as to result in a logarithmic term in the resistivity which agrees with Kondo's result if Eq. (3.30) is used for J and a constant density of states is used in the s–d model. This discrepancy arises from the effects of the self-energy renormalization, Eqs. (3.18), (3.22), (3.23), (4.9), and (4.10) [leading to a factor $\frac{3}{2}$ rather than 2 in each of the expressions in Eq. (4.21) and thus $\frac{3}{2}\times\frac{3}{2}$ rather than $2\times\frac{3}{2}$ in (4.22)]. We thus find that because of the finite "d" lifetime the leading logarithmic term in the resistivity in the Anderson model differs from that obtained in the s–d exchange model. This difference calls into question the argument of Schrieffer and Wolf, which implies that the Anderson and s–d exchange models are essentially the same, at least as far as the logarithmic divergences are concerned. We have already mentioned the nonanalytic width $\Gamma(T)$, which also represents a lifetime effect and will play a major role for $T<T_c$, as will be discussed in the succeeding paper, so that it would appear that the finite d lifetime is an important aspect of the Anderson model.

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[24] D. R. Hamann, Phys. Rev. 154, 596 (1967).

APPENDIX A: CHARGE-CONJUGATION SYMMETRY

If we define the operators D_σ and $E_{k\sigma}$ by

$$d_\sigma{}^\dagger=D_\sigma,$$
$$d_\sigma=D_\sigma{}^\dagger,$$
$$C_{k\sigma}{}^\dagger=E_{k\sigma},$$
$$C_{k\sigma}=E_{k\sigma}{}^\dagger, \tag{A1}$$

it is clear that the D's and E_k's satisfy the usual fermion commutation relations. Further, if

$$\epsilon_F-\epsilon_{d\sigma}\equiv\xi U+g\sigma H\rightleftarrows U+\epsilon_{d\sigma}-\epsilon_F\equiv(1-\xi)U-g\sigma H \tag{A2}$$

and

$$\epsilon_{k\sigma}-\epsilon_F\rightleftarrows\epsilon_F-\epsilon_{k\sigma}, \tag{A3}$$

then the Hamiltonian (1.1) goes into $\mathcal{H}_c$, where

$$\mathcal{H}_c=\mathcal{H}_0+\tilde{\mathcal{H}}(-V), \tag{A4}$$

where $\tilde{\mathcal{H}}(V)$ is given by (1.1) with $D_{-\sigma}$ and $E_{k-\sigma}$ replacing $d\sigma$ and $C_{k\sigma}$, respectively, and where

$$\mathcal{H}_0=2\epsilon_d+U+2\sum_k\epsilon_k-2\epsilon_F N. \tag{A5}$$

It is readily seen that

$$\langle d_{-\sigma}{}^\dagger d_{-\sigma}d_\sigma\,|\,d_\sigma{}^\dagger\rangle_{-V,\omega}\rightarrow\langle(1-D_{-\sigma}{}^\dagger D_{-\sigma})D_\sigma{}^\dagger\,|\,D_\sigma\rangle_{-\tilde{V},\omega}, \tag{A6}$$

the $\mathcal{H}_0$ term being absorbed in the altered free energy. By taking the complex conjugate, and making use of the definition (2.1), we may write

$$\langle(1-\hat{n}_{-\sigma})D_\sigma{}^\dagger\,|\,D_\sigma\rangle_{-\tilde{V},\omega}=-\langle(1-\hat{n}_{-\sigma})D_\sigma\,|\,D_\sigma{}^\dagger\rangle^*{}_{-\tilde{V},-\omega}, \tag{A7}$$

so that

$$G_{-d(\omega)}{}^{-\sigma}\rightleftarrows-\tilde{G}_{+d(-\omega)}{}^{\sigma*},$$

where $\tilde{G}_{\alpha d(\omega)}{}^{\sigma}$ is the d electron Green's function in the charge-conjugate system ($\xi \rightleftarrows 1-\xi$, $n^{\sigma}\to 1-n^{-\sigma}$, etc.).

APPENDIX B: SELF-ENERGY CORRECTIONS

The $\ln W/T$ parts of $A^{\sigma}(\omega)$ and $E^{\sigma}(\omega)$ arise from a sum of the form $\sum_k[f_k/(\omega-\epsilon_k)]$. It is therefore of interest to consider the possible self-energy corrections to the denominator, since $\sum_k[f_k/(\omega-\epsilon_k+i\Delta)]$ is of order $\ln(W/\Delta)$ for $\Delta\gg T$. The $\ln(W/T)$ part of $A^{\sigma}(\omega)$ [Fig. 4(b)] admits the four self-energy correction diagrams shown in Fig. 8. Using the prescription given in Sec. III, we find that these terms yield the expression

$$
\begin{aligned}
&-\sum_{k\to k_3} V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(D_{k-k_1+d+U}{}^{g\sigma}-D_{k-k_1+d}{}^{g\sigma})(f_k{}^{-\sigma}\,\delta_{k,k_3})(D_k{}^{(2g-1)\sigma})^2(f_{k_1}{}^{-\sigma}\,\delta_{k_1,k_2})G_d{}^{\sigma(0)}\\
&\qquad-\sum_{k,k_1,k_3} V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(D_k{}^{(2g-1)\sigma})^2D_{k+d-k_1}{}^{g\sigma}(f_k{}^{-\sigma}\,\delta_{k,k_3})G_d{}^{\sigma(0)}\\
&\qquad-\sum_{k\to k_3} V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(D_{k+k_1-d-U}{}^{g\sigma}-D_{k+k_1-d}{}^{g\sigma})(f_{k_1}{}^{\sigma}\,\delta_{k_1k_2})(D_k{}^{(2g-1)\sigma})^2(f_k{}^{-\sigma}\,\delta_{k,k_3})G_d{}^{\sigma(0)}\\
&\qquad-\sum_{k,k_1,k_3} V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(D_k{}^{(2g-1)\sigma})^2(f_k{}^{-\sigma}\,\delta_{k,k_3})D_{k+k_1-d}{}^{g\sigma}G_d{}^{\sigma(0)}. \qquad (\mathrm{B1})
\end{aligned}
$$

It may be seen that the imaginary parts of (B1) vanish as $\exp(-U/T)$, whereas the real part contributes a term $-2\Delta\sigma Hg/\pi\xi(1-\xi)U$ to the self-energy:

$$
D_k{}^{(2g-1)\sigma}\to\frac{1}{\omega+(2g-1+2\Delta g/\pi\xi(1-\xi)U)\sigma H-\epsilon_k}. \qquad (\mathrm{B2})
$$

This term, proportional to H, is the expected Knight shift of the d electron resonance line due to the interaction of the d and conduction electrons.

It might be noted that the imaginary terms do not vanish (being $2i\Delta$) if both ϵ_d and ϵ_{d+U} are either greater than the Fermi energy or both less (though both within the conduction band), so that in these two (nonmagnetic) cases, the logarithmic terms are of order $\Delta/U\ \ln W/\Delta$.

Let us next consider the Δ^2/U part of the self-energy. The diagrams representing the Δ^2/U self-energy terms are shown in Fig. 9. There are two types of terms—those representing the Δ/U correction to the energy denominators appearing in the lowest-order expression for the self-energy, (C1), and the second-order "irreducible" self-energy terms in which the lowest-order energy denominators appear. The contribution to the from the diagrams of Fig. 9 yields, for $H=0$; in the order shown,

$$
\begin{aligned}
&-\sum_k V^6(D_{d+U}-D_d)D_kf_kG_d{}^{\sigma}\sum_{k_1,k_2}\{[-(D_{k+d+U+k_1}-D_{k+d-k_1})^2D_{k_2+k-k_1}-(D_{k+k_1-d-U}-D_{k+k_1-d})^2\\
&\quad\times D_{k+k_1-k_2}+(D_{k+d+U-k_1}-D_{k+d-k_1})D_{k+2d+U-k_1-k_2}(D_{k+d+U-k_2}-D_{k+d-k_2})+(D_{k+k_1-d-U}-D_{k+k_1-d})D_{k+k_1+k_2-2d-U}\\
&\quad\times(D_{k_2+k-d-U}-D_{k_2+k-d})-(D_{k+d+U-k_1}-D_{k+d-k_1})^2D_{k+2d+U-k_1-k_2}-(D_{k+k_1-d-U}-D_{k+k_1-d})^2D_{k+k_1+k_2-2d-U}]f_{k_1}f_{k_2}\\
&\quad+[(D_{k+d+U-k_1}-D_{k+d-k_1})D_{k_2+k-k_1}D_{k+d+U-k_1}+(D_{k+k_1-d-U}-D_{k+k_1-d})D_{k_1+k-k_2}D_{k+k_1-d-U}\\
&\quad+(D_{k+d+U-k_1}-D_{k+d-k_1})D_{k+k_2-k_1}(D_{k_2+k-d-U}-D_{k_2+k-d})f_{k_2}+(D_{k+k_1-d-U}-D_{k+k_1-d})\\
&\quad\times D_{k_1+k-k_2}(D_{k+d-k_2+U}-D_{k+d-k_2})f_{k_2}+(D_{k-k_1+d+U}-D_{k-k_1+d})D_{k-k_1+2d+U-k_2}\\
&\quad\times D_{k-k_1+d+U}+(D_{k+k_1-d-U}-D_{k+k_1-d})D_{k+k_1+k_2-2d-U}D_{k+k_1-d-U}+(D_{k+k_1-d-U}-D_{k+k_1-d})D_{k+k_1-k_2}\\
&\quad\times D_{k_1+k-d-U}+(D_{k-k_1+d+U}-D_{k-k_1+d})D_{k+k_2-k_1}D_{k-k_1+d+U}+(D_{k-k_1+d+U}-D_{k-k_1+d})D_{k-k_1+d}\\
&\quad\times D_{k+k_2-k_1}+(D_{k+k_1-d-U}-D_{k+k_1-d})D_{k+k_1-d}D_{k+k_1-k_2}]f_{k_1}\}. \qquad (\mathrm{B3})
\end{aligned}
$$

It may be seen that the real part of the self-energy vanishes, while the imaginary part is given by

$$
4\Delta^2T/\pi U^2\xi^2(1-\xi)^2=\pi(J\rho)^2T, \qquad (\mathrm{B4})
$$

where we have used Eq. (3.30) for J. This imaginary self-energy term is the expected Korringa width due to the interaction of the d electron with the conduction electrons.

We have thus found that the imaginary part of the self-energy goes to zero as $T\to 0$ to order Δ^2/U. Let us suppose this to be true for all higher-order terms in Δ/U. It does not follow that the exact imaginary self-energy is zero. To see this, consider the denominators $D_{k-k_1+d+U}{}^{g\sigma}-D_{k-k_1+d}{}^{g\sigma}$ which appear in the first term of (B1). These denominators may be written as $D^{\sigma}(\omega-\epsilon_k+\epsilon_{k_1})^{-1}$, where the exact Green's function $G_d{}^{\sigma}(\omega)$ may be written

$$
G_d{}^{\sigma}(\omega)=N^{\sigma}(\omega)/D^{\sigma}(\omega), \qquad (\mathrm{B5})
$$

and where

$$
UD^{\sigma}(\omega)^{(0)}=(\omega-\epsilon_{d\sigma})(\omega-\epsilon_{d\sigma}-U). \qquad (\mathrm{B6})
$$

From Eq. (3.8) we see that the real part of $D^{\sigma}(\omega)$ vanishes at $|\omega-\epsilon_F|\approx\pi T_c/2\gamma$ (for $T=0$), while the imaginary part is of order $\Delta/U\xi(1-\xi)$, where T_c is

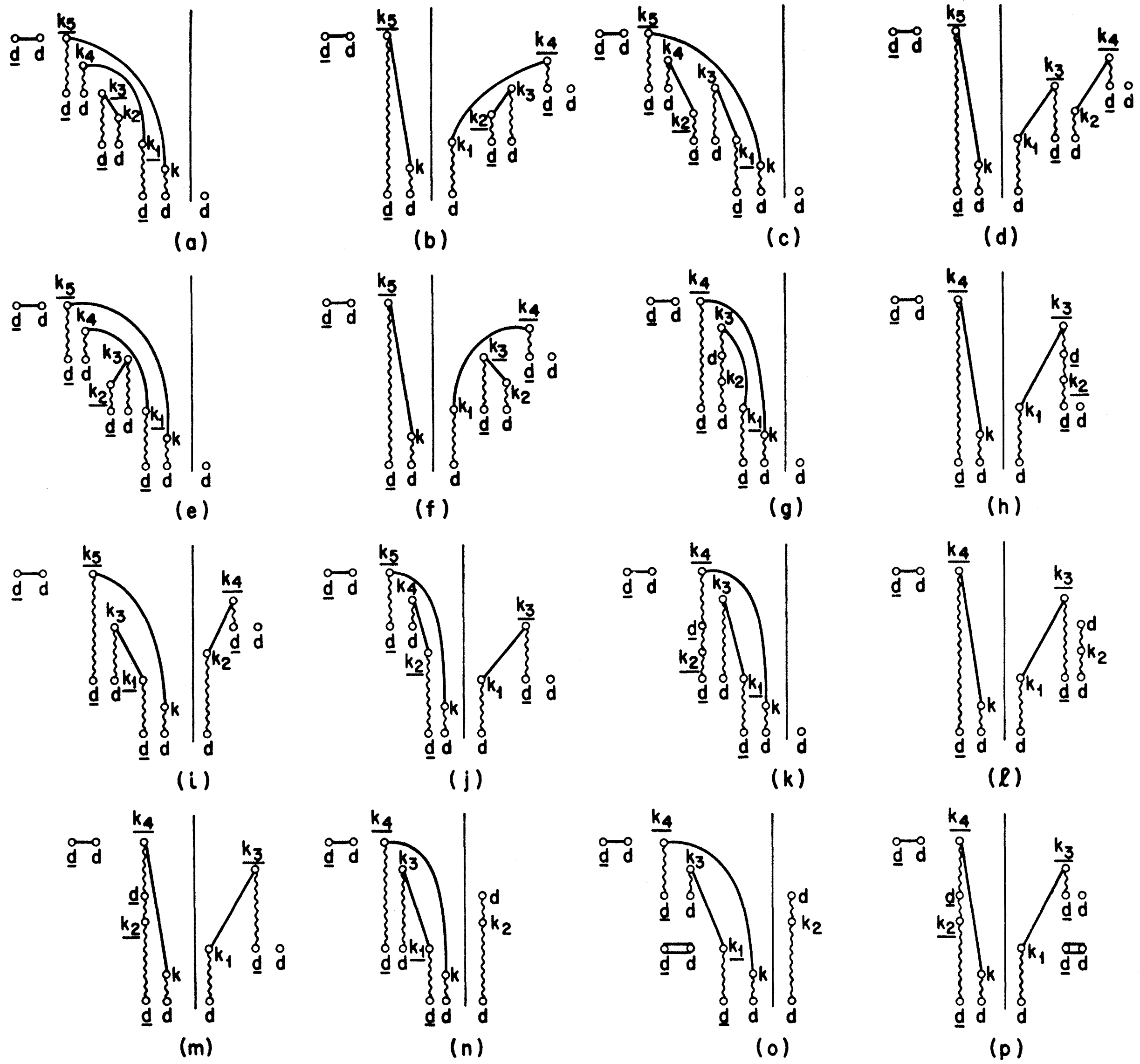

FIG. 9. Fourth-order self-energy corrections to $D_k^{(2g-1)\sigma}$.

given by

$$T_c=(2U\,|\,1-2\xi\,|\,\gamma/\pi)\exp\{-[\xi(1-\xi)\pi U/\Delta]\},\tag{B7}$$

rather than the tentative expression (1.9).

Thus, as a rough approximation, for $T=0$,

$$\begin{aligned}V^2\sum_{k_1}\mathrm{Im}(D_{k-k_1+d+U}-D_{k-k_1+d})f_{k_1}&=-\Delta(f_{d+U+k-\omega}-f_{d+k-\omega})+(\Delta T_c/2\gamma)(1/\Delta)\\&=O(\Delta)+O(\Delta^2/U)+\cdots+O(T_c),\end{aligned}\tag{B8}$$

with a similar result for the other terms in (B1). We have already seen that the terms analytic in Δ go to zero as $T\to 0$ (at least the first two, and we conjecture that all do), so that for $T\to 0$ the imaginary part of the self-energy is just the nonanalytic (in Δ) contribution. More exactly, if we write this term as $\Gamma(\omega-\epsilon_k+i\epsilon)$ (its dependence on T being understood), then $\Gamma(\omega-\epsilon_k+i\epsilon)$ satisfies, to lowest order in T_c, the equation (for $H=0$)

$$\begin{aligned}\Gamma(\omega-\epsilon_k+i\epsilon)=-\mathrm{N.A.P.}\frac{\Delta}{\pi}\int_{-\infty}^{\infty}d\omega'\{&[f(\omega')+(\omega'-\epsilon_F)/U+(\omega-\epsilon_k+i\epsilon)/U-(1-\xi)+3i\Delta/U]D^{-1}(A+)\\&-[f(\omega')+(\omega'+\epsilon_F)/U-(\omega-\epsilon_k+i\epsilon)/U-(1-\xi)-3i\Delta/U]D^{-1}(A-)\},\end{aligned}\tag{B9}$$

where $D(A\pm)$ is the exact denominator of $G_d(\omega)$ [Eq. (3.8) is just the second-order approximation; the required expression will be obtained in the succeeding paper], and where

$$A\pm=\frac{V^2}{\pi U\xi(1-3)}\sum_{k'}(f_{k'}-\tfrac{1}{2})\{[\pm(\omega-\epsilon_k+i\epsilon)+\omega'\pm i\Gamma(\pm(\omega-\epsilon_k)+\omega'-\epsilon_{k'})-\epsilon_{k'}]^{-1}$$
$$+[\epsilon_{k'}\pm(\omega-\epsilon_k+i\epsilon)+\omega'-U(1-2\xi)\pm i\Gamma(\pm(\omega+\epsilon_k)+\omega')-U(1-2\xi)]^{-1}\}. \quad \text{(B10)}$$

We note that $\Gamma(\omega-\epsilon_k+i\epsilon)$ satisfies the identity

$$\Gamma(\omega-\epsilon_k+i\epsilon)=-\tilde{\Gamma}(-\omega+\epsilon_k-i\epsilon), \quad \text{(B11)}$$

where $\tilde{\Gamma}$ is the charge conjugate of Γ (i.e., $-\theta\rightleftarrows 1-\theta$; $\xi\rightleftarrows 1-\xi$; see Appendix A). From Eq. (B4) we see that the intrinsic width of the d electron resonance line $\Gamma(T)+\pi(JP)^2T\to O(T_c)$ for $T\to 0$.

Since $D(A\pm)\to O(U)$ for $T\gg T_c$, we see that $\Gamma\to 0$ for $T\gg T_c$ (though Γ is finite at all T) and thus in this paper where we are considering $T\gg T_c$ we may neglect Γ with respect to T[Γ is at best $0(T_c)$ for $T\to 0$].

Consider now the self-energy corrections to the $\ln|U(1-2\xi)/W|$ part of $A^\sigma(\omega)$ [Fig. 3(g)] given by the four diagrams of Fig. 10. These terms yield the expression

$$-\sum_{k\to k_2}V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(D_{2d+U-k}{}^{\sigma})^2D_{k_1+d-k}{}^{g\sigma}(f_k{}^{-\sigma}\,\delta_{k,k_2})G_d{}^{\sigma(0)}$$
$$-\sum_{k\to k_2}V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(D_{2d+U-k}{}^{\sigma})^2D_{k_1+d-k}{}^{(2-g)\sigma}(f_k{}^{-\sigma}\,\delta_{k,k_2})G_d{}^{\sigma(0)}$$
$$-\sum_{k\to k_3}V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(f_k{}^{-\sigma}\,\delta_{k,k_3})(f_{k_1}{}^{\sigma}\,\delta_{k_1,k_2})(D_{2d+U-k}{}^{\sigma})^2(-D_{k_1+d-k}{}^{g\sigma}+D_{k_1+d-k+U})G_d{}^{\sigma(0)}$$
$$-\sum_{k\to k_3}V^4(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})(f_{k_1}{}^{\sigma}\,\delta_{k_1,k_2})(-D_{k_1-k+d}{}^{(2-g)\sigma}+D_{k_1-k+d+U}{}^{(2-g)\sigma})(f_k{}^{-\sigma}\,\delta_{k,k_3})(D_{2d+U-k}{}^{\sigma})^2G_d{}^{\sigma(0)}. \quad \text{(B12)}$$

These terms do not cancel for $\omega\approx\epsilon_k$ and hence, even for the case $\xi=\frac{1}{2}$, the terms involving $\sum_k D_{2d+U-k}{}^{\sigma}f_k{}^{-\sigma}$ yield expression of order $\ln(W/\Delta)$ rather than $\ln(W/T)$.

APPENDIX C: SELF-ENERGY CORRECTIONS TO $2i\Delta(D_k{}^\sigma)^2$ TERM

The self-energy corrections to the $2i\Delta(D_k{}^\sigma)^2$ term are of two types: those that modify the coefficient ($2i\Delta$) and those that modify the denominators $D_k{}^\sigma$. To first order in Δ, only the latter appear. The corrections to the first $D_k{}^\sigma$ are represented by Figs. 11(a)–11(d), with an equivalent set of diagrams (not shown) modifying the second $D_k{}^\sigma$. The contribution from Fig.

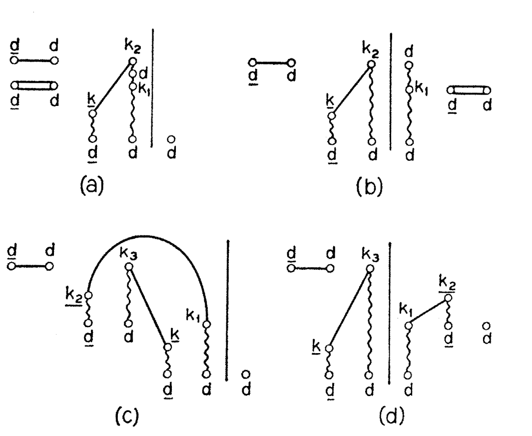

FIG. 10. Second-order self-energy corrections to $D^\sigma{}_{2d+U-k}$.

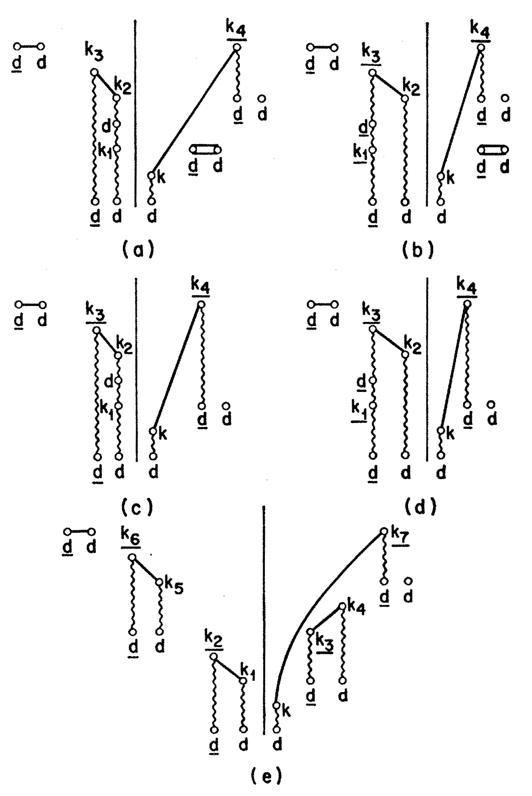

FIG. 11. Second-order self-energy corrections to $2i\Delta(D_k{}^\sigma)^2$.

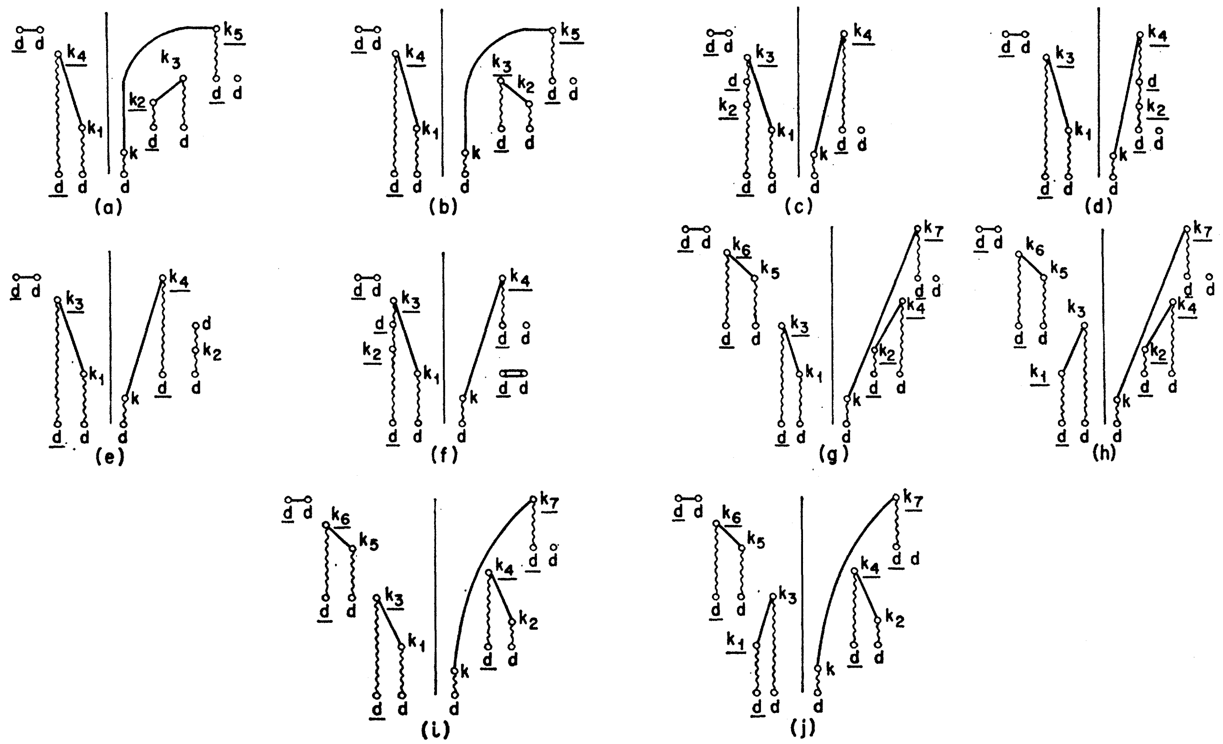

FIG. 12. Fourth-order self-energy corrections to $2i\Delta(D_k^\sigma)^2$.

11(a)–11(d) may be written

$$-\sum_{k\to k_2} V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^3 D_{k+k_1-d}^{g\sigma}(D_{k+k_2-d-U}^{g\sigma}-D_{k+k_2-d}^{g\sigma})f_k^\sigma f_{k_2}^{-\sigma}G_d^\sigma$$
$$-\sum_{k\to k_2} V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^3 D_{k-k_1+d}^{(2-g)\sigma}(D_{k+k_2-d-U}^{g\sigma}-D_{k+k_2-d}^{g\sigma})f_k^\sigma f_{k_2}^{-\sigma}G_d^\sigma$$
$$-\sum_{k\to k_2} V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^3 (D_{k+k_1-d-U}^{g\sigma}-D_{k+k_1-d}^{g\sigma})(D_{k+k_2-d-U}^{g\sigma})f_k^\sigma f_{k_2}^{-\sigma}G_d^\sigma$$
$$-\sum_{k\to k_2} V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^3 (D_{k-k_1+d+U}^{g\sigma}-D_{k-k_1+d}^{g\sigma})(D_{k+k_2-d-U}^{g\sigma})f_k^\sigma f_{k_2}^{-\sigma}G_d^\sigma. \quad \text{(C1)}$$

The last two terms give no contribution; from the first two we obtain

$$D_k^\sigma \to D_{k-2i\Delta}^\sigma. \quad \text{(C2)}$$

From Fig. 11(e) we see that the product $2i\Delta(D_{k-2i\Delta}^\sigma)^2$ is the first term in a series:

$$2i\Delta(D_{k-2i\Delta}^\sigma)^2[1+(2i\Delta D_{k-2i\Delta}^\sigma)^2+\cdots]=\frac{2i\Delta}{(\omega-\epsilon_{k_\sigma}+2i\Delta)^2}\,\frac{1}{1+4\Delta^2/(\omega-\epsilon_{k_\sigma}+2i\Delta)^2}$$
$$=\frac{2i\Delta}{(\omega-\epsilon_{k_\sigma}'+2i\Delta)^2+4\Delta^2}$$
$$=\tfrac{1}{2}[(\omega-\epsilon_{k\sigma})^{-1}-(\omega-\epsilon_{k_\sigma}+4i\Delta)^{-1}]. \quad \text{(C3)}$$

The second-order (in Δ) corrections to the denominators D_k^σ are represented in Fig. 12(g)–12(j). These self-energy terms may be written (for $H=0$) as

$$2i\frac{\Delta^2}{U}\bar{\gamma}=-V^4\sum_{k_1,k_2}\{(D_{k_1+k-d-U}-D_{k_1+k-d})[D_{k_1+k-k_2}(D_{k-k_2+d+U}-D_{k-k_2+d})+D_{k+k_1+k_2-2d-U}$$
$$\times(D_{k+k_2-d-U}-D_{k+k_2-d})]+(D_{k-k_1+d+U}-D_{k-k_1+d})[D_{k-k_1-k_2+2d+U}(D_{k-k_2+d+U}-D_{k-k_2-d})+D_{k-k_1+k_2}$$
$$\times D_{k+k_2-d-U}-D_{k+k_2-d})]\}f_{k_1}f_{k_2}, \quad \text{(C4)}$$

where we have written

$$D_k^\sigma \to D_{k-2i\Delta-2i(\Delta^2/U)\bar{\gamma}}^\sigma. \tag{C5}$$

The second-order correction to the $(2i\Delta)$ term is represented in Figs. 12(a)–12(f) (there exists a similar set where k_1 is replaced by $\bar{k}_1$, etc.; not shown). These terms yield

$$\begin{aligned}2i\gamma\frac{\Delta^2}{U}=-V^4\sum_{k_1,k_2}\{&(D_{k_1+k-d-U}-D_{k_1+k-d})^2(D_{k+k_1-k_2}+D_{k+k_1+k_2-2d-U})f_{k_2}-(D_{k+k_1-d-U}-D_{k_1+k-d})\\&\times[D_{k+k_1-d-U}(2D_{k+k_1-k_2}+D_{k+k_1+k_2-2d-U})+(D_{k+k_1-d}D_{k+k_1-k_2})]+(D_{k-k_1+d+U}-D_{k-k_1+d})^2\\&\times(D_{k-k_1-k_2+2d+U}+D_{k+k_2-k_1})f_{k_2}-(D_{k-k_1+d+U}-D_{k-k_1+d})\\&\times[D_{k-k_1+d+U}(2D_{k-k_1+k_2}+D_{k-k_1-k_2+2d+U})+D_{k-k_1+d}D_{k+k_2-k_1}]\}f_{k_1},\end{aligned} \tag{C6}$$

where we have written

$$2i\Delta\to 2i\Delta+(2i\Delta^2/U)\gamma. \tag{C7}$$

Thus, to second order in Δ we find

$$\begin{aligned}2i\Delta(D_k^\sigma)\to 2i\Delta+2i\frac{\Delta^2}{U}\gamma&\left\{\frac{1}{[\omega-\epsilon_k+2i\Delta+2i\bar{\gamma}(\Delta^2/U)]^2}\,\frac{1}{1-[2i\Delta+2i\gamma(\Delta^2/U)]^2/[\omega-\epsilon_k+2i\Delta+2i\bar{\gamma}(\Delta^2/U)]^2}\right.\\&\left.=\frac{1}{2}\left[\frac{1}{\omega-\epsilon_k}-\frac{1}{\omega-\epsilon_k+4i\Delta+4i(\Delta^2/U)\gamma}\right]\right\},\end{aligned} \tag{C8}$$

where we have made use of the fact that $\gamma=\bar{\gamma}$, neglecting terms of order $(\Delta/U)^2T$, as may be seen by comparing expressions (C4) and (C6) for $\bar{\gamma}-\gamma$ with expression (B3) for the second-order (in Δ) self-energy correction to $D_k^{(2g-1)\sigma}$. Again we see that the perturbation terms vanish for $T\to 0$; whereas there exists a nonanalytic temperature and energy-dependent self-energy $i\Gamma$:

$$2i\Delta(D_k^\sigma)^2\to\frac{1}{2}\left[\frac{1}{\omega-\epsilon_{k_\sigma}+i\Gamma(\omega-\epsilon_k+i\epsilon)}-\frac{1}{\omega-\epsilon_{k_\sigma}+4i\Delta+(4i\Delta^2/U)\gamma+\cdots}\right]. \tag{C9}$$

APPENDIX D: SELF-ENERGY CORRECTIONS TO $(\Delta/U)^2\ln^2(W/T)$ TERMS

The self-energy corrections to the $(\Delta/U)^2\ln^2(W/T)$ terms are of two types; the corrections to the $D_k^{(2g-1)\sigma}$ term (which has been considered in Appendix B) and the self-energy correction to D_k^σ. These latter corrections are represented, to first order in Δ, by Figs. 13(a)–13(e). The contribution from Figs. 13(a)–13(d) may be written

$$\begin{aligned}&-\sum_{k\to k_4}V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^2D_{k_1+k-d}^{g\sigma}(D_{k+k_2-d-U}^{g\sigma}-D_{k+k_2-d}^{g\sigma})D_{k_2}^{(2g-1)\sigma}f_{k_2}^{-\sigma}\,\delta_{k_2,k_4}f_k^\sigma\,\delta_{k,k_3}G_d^{\sigma(0)}\\&-\sum_{k\to k_4}V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^2D_{k-k_1+d}^{(2-g)\sigma}(D_{k+k_2-d-U}^{g\sigma}-D_{k+k_2-d}^{g\sigma})D_{k_2}^\sigma f_k^\sigma\,\delta_{k,k_3}f_{k_2}^{-\sigma}\,\delta_{k_2,k_4}G_d^{\sigma(0)}\\&-\sum_{k\to k_4}V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^2(D_{k+k_1-d-U}^{g\sigma}-D_{k+k_1-d}^{g\sigma})D_{k+k_2-d-U}^{g\sigma}D_{k_2}^{(2g-1)\sigma}f_k^\sigma\,\delta_{k,k_3}f_{k_2}^{-\sigma}\,\delta_{k_2,k_4}G_d^{\sigma(0)}\\&-\sum_{k\to k_4}V^6(D_{d+U}^{g\sigma}-D_d^{g\sigma})(D_k^\sigma)^2(D_{k+d+U-k_1}^{(2-g)\sigma}-D_{k+d+k_1}^{(2-g)\sigma})D_{k+k_2-d-U}^{g\sigma}D_{k_2}^{(2g-1)\sigma}f_k^\sigma\,\delta_{k,k_3}f_{k_2}^{-\sigma}\,\delta_{k_2,k_4}G_d^{\sigma(0)}.\end{aligned} \tag{D1}$$

From these terms we see that

$$D_k^\sigma\to D_{k-2i\Delta}^\sigma, \tag{D2}$$

whereas from Fig. 13(e) (plus $k_1\to\bar{k}_1$, $k_3\to\bar{k}_3$, etc.) we see that $D_{k-2i\Delta}^\sigma$ is the first term in the series

$$\begin{aligned}D_{k-2i\Delta}^\sigma&(1+(2i\Delta D_{k-2i\Delta}^\sigma)^2+\cdots)\\&=\frac{1}{(\omega-\epsilon_{k_\sigma}+2i\Delta)}\,\frac{1}{1-(2i\Delta)^2/(\omega-\epsilon_{k_\sigma}+2i\Delta)^2}\\&=\tfrac{1}{2}[(\omega-\epsilon_{k_\sigma})^{-1}+(\omega-\epsilon_{k_\sigma}+4i\Delta)^{-1}].\end{aligned} \tag{D3}$$

It is easy to see that upon inclusion of the exact propagators we have, as in Appendix C,

$$D_{k-2i\Delta}^\sigma\to\tfrac{1}{2}[D_{k-i\Gamma}^\sigma+D_{k-4i\Delta-4i(\Delta^2/U)\gamma+\cdots}^\sigma]. \tag{D4}$$

APPENDIX E: VANISHING OF THE $f_{kk_1}(k\neq k_1)$ TERM OF $A^\sigma(\omega)$ FOR ξU, $(1-\xi)U\ll W$

There is an additional term which would appear to be of order $i(\Delta/U)[(\Delta/U)\ln(W/T)]$. This term corresponds to Fig. 3(b) [which gave rise to $A^\sigma(\omega)$ when the factor $f_k^{-\sigma}\,\delta_{k,k_1}$ is replaced by $f_{kk_1}^{-\sigma}$ for $k\neq k_1$], where, using Eq. (2.9),

$$f_{kk_1}{}^{-\sigma}=\frac{V^2}{\pi}\int_{-\infty}^{\infty} f(\omega')\ \mathrm{Im}\left[\frac{G_d{}^{-\sigma}(\omega')}{(\omega'-\epsilon_{k-\sigma})(\omega'-\epsilon_{k_1-\sigma})}\right]d\omega'. \tag{E1}$$

Thus this contribution from Fig. 3(b) is given by

$$-\sum_{k,k_1} i\frac{V^4}{2\pi}(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})D_k{}^{(2g-1)\sigma}[D_{d+U+k-k_1}{}^{g\sigma}(n^{-\sigma})+D_{d+k-k_1}{}^{g\sigma}(1-n^{-\sigma})]$$

$$\times\int_{-\infty}^{\infty} d\omega' f(\omega')\left\{\frac{G_d{}^{-\sigma}(\omega'+i\delta)}{(\omega'-\epsilon_{k-\sigma}+i\delta)(\omega'-\epsilon_{k_1-\sigma}+i\delta)}-\frac{G_d{}^{-\sigma}(\omega'-i\delta)}{(\omega'-\epsilon_{k-\sigma}-i\delta)(\omega'-\epsilon_{k_1-\sigma}-i\delta)}\right\}. \tag{E2}$$

Let us consider the summation over k_1 first. We note that

$$\sum_{k_1}\frac{1}{(\omega'-\epsilon_{k_1-\sigma}-i\delta)(\omega-\epsilon_{d-U}+\epsilon_{k_1}+g\sigma H-\epsilon_k+i\epsilon)}=0,$$

so only the first term in integrand contributes, and by closing the contour in the upper ϵ_{k_1} plane we find

$$-\sum_k\frac{V^4}{\pi}(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})\int_{-\infty}^{\infty}d\omega'\left[\frac{n^{-\sigma}}{\omega-\epsilon_{d-U}-\epsilon_k+\omega'+g\sigma H+i\epsilon+i\delta}+\frac{(1-n^{-\sigma})}{\omega-\epsilon_d-\epsilon_k+\omega'+g\sigma H+i\epsilon+i\delta}\right]$$

$$\times\left[\frac{f(\omega')G_d{}^{-\sigma}(\omega'+i\delta)}{(\omega'-\epsilon_{k-\sigma}+i\delta)}\right][\omega-\epsilon_k+(2g-1)\sigma H+i\epsilon]^{-1}. \tag{E3}$$

However, we now note that all ϵ_k denominators have positive imaginary parts, and hence upon performing the sum over k we see that this term gives no contribution. If we had considered a Lorentzian density of states function $\rho(\epsilon_k)=\rho W^2/(\epsilon_k-\epsilon_F)^2+W^2$, the above procedure may be carried out, leading to the result [to order $(\Delta/U)^2$]

$$-\frac{i\Delta^2}{\pi}(D_{d+U}{}^{g\sigma}-D_d{}^{g\sigma})G_d{}^{\sigma(0)}(iW)\int_{-\infty}^{\infty}d\omega' f(\omega')\frac{G_d{}^{-\sigma}(\omega')^*}{\omega-\omega'+i\epsilon}, \tag{E4}$$

where

$$G_d{}^{\sigma(0)}(iW)=-\left[\frac{n^{-\sigma}}{iW+\xi U}+\frac{1-n^{-\sigma}}{iW-(1-\xi)U}\right]. \tag{E5}$$

Thus this particular $i(\Delta/U)^2\ln(W/T)$ term [which would in general lead to a nonlinear integral equation for $G_d{}^\sigma(\omega)$ in contrast to the linear equation obtained in the succeeding paper] may be dropped in the limit ξU, $(1-\xi)U\ll W$. It is of interest to note that had we written the truncation approximation, Eq. (3.6), as

$$G_{(k_1k)d}{}^{\sigma}=(f_k{}^{-\sigma}\delta_{k,k_1}+f_{kk_1}{}^{-\sigma})G_d{}^{\sigma}(\omega), \tag{E6}$$

we would in effect be including expression (E4) with $W=0$, whereas the equation which would give the exact perturbation result, Eq. (E4), with $W\gg\xi U$, $(1-\xi)U$, is

$$G_{(k_1k)d}{}^{\sigma}=f_k{}^{-\sigma}\delta_{k,k_1}G_d{}^{\sigma}(\omega)+f_{kk_1}{}^{-\sigma}G_d{}^{\sigma}(\omega-\epsilon_k+\epsilon_{k_1}). \tag{E7}$$

Equation (E4) is not quite correct, however, in that while we allowed for the energy difference $\epsilon_k-\epsilon_{k_1}$ in the argument of $G_d{}^\sigma(\omega)$, we set $\langle n^{-\sigma}C_{k_1-\sigma}{}^\dagger C_{k-\sigma}\rangle=n^{-\sigma}\langle C_{k_1-\sigma}{}^\dagger C_{k-\sigma}\rangle$. We shall see in Appendix H that this is a valid approximation to the order required for $k=k_1$; for $k\neq k_1$, however, the above analysis holds only for the explicit terms $\langle C_{k_1\pm\sigma}{}^\dagger C_{k\pm\sigma}\rangle$ and $\langle n^{-\sigma}C_{k_1\sigma}{}^\dagger C_{k\sigma}\rangle$; the term $\langle n^{-\sigma}C_{k_1-\sigma}{}^\dagger C_{k-\sigma}\rangle$ $(k\neq k_1)$ does yield a contribution

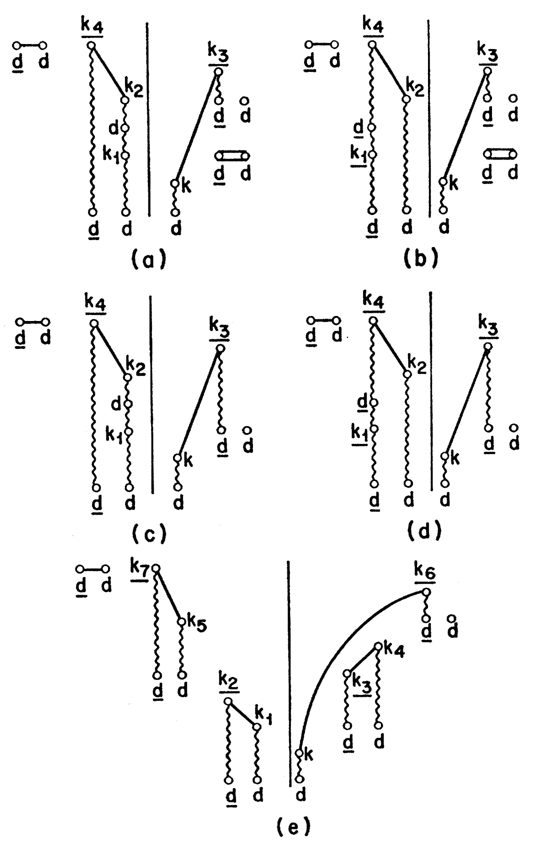

FIG. 13. Second-order self-energy corrections to $D_k{}^\sigma$.

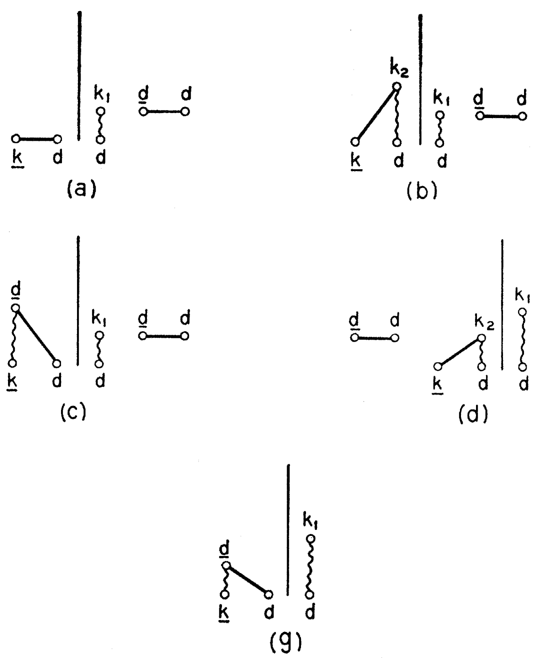

FIG. 14. Representation of $\langle C^{\dagger}_{k-\sigma} d_{-\sigma} d_{\sigma} \mid C^{\dagger}_{k_1\sigma}\rangle$.

of order Δ/U (because this contribution comes from the region $\epsilon_k \approx \epsilon_d$, rather than ϵ_F, we nevertheless obtain a linear integral equation). However, for $H=0$, this contribution is cancelled by an additional fourth-order term, and thus plays no role; even for $H\neq 0$ this additional term goes to zero as $U\to\infty$ (with ϵ_d finite) and thus plays no essential role.

APPENDIX F: EVALUATION OF $\langle d_{-\sigma}{}^{\dagger} C_{k-\sigma} d_{\sigma}{}^{\dagger} C_{k_1\sigma}\rangle$

The thermal average $\langle d_{-\sigma}{}^{\dagger} C_{k-\sigma} d_{\sigma}{}^{\dagger} C_{k_1\sigma}\rangle$ may be obtained from the equation

$$\langle d_{-\sigma}{}^{\dagger} C_{k-\sigma} d_{\sigma}{}^{\dagger} C_{k_1\sigma}\rangle = \langle C_{k_1\sigma}{}^{\dagger} d_{\sigma} C_{k-\sigma}{}^{\dagger} d_{-\sigma}\rangle^{*}, \tag{F1}$$

where

$$\langle C_{k_1\sigma}{}^{\dagger} d_{\sigma} C_{k-\sigma}{}^{\dagger} d_{-\sigma}\rangle = \pi^{-1}\int_{-\infty}^{\infty} d\omega\, f(\omega)\ \mathrm{Im}\langle C_{k-\sigma}{}^{\dagger} d_{-\sigma} d_{\sigma} \mid C_{k_1\sigma}{}^{\dagger}\rangle_{\omega}. \tag{F2}$$

If we define $F_{kk_1}{}^{\sigma}(\omega)$ by

$$\langle C_{k-\sigma}{}^{\dagger} d_{-\sigma} d_{\sigma} \mid C_{k_1\sigma}{}^{\dagger}\rangle_{\omega} \equiv F_{kk_1}{}^{\sigma}(\omega), \tag{F3}$$

we see that $F^{\sigma}(\omega)$ is a quantity very similar to $G_d{}^{\sigma}(\omega)$ and may be computed to any order of Δ/U by means of the diagrammatic representation presented in Sec. III. The lowest-order diagrams are shown in Fig. 14.

Diagrams (c) and (e) of Fig. 14 do not contribute for the same reason f_{kk_1} for $k_1\neq k$ does not contribute to $A^{\sigma}(\omega)$ (see Appendix E). The remaining diagrams yield

$$\begin{aligned} F_{kk_1}{}^{\sigma} = D_{2d+U-k}{}^{\sigma}\{ &-V\langle \hat{n}_{kd}{}^{-\sigma}\hat{n}^{\sigma}\rangle (D_{k_1+d+U-k}{}^{(2-g)\sigma} - D_{k_1+d-k}{}^{(2-g)\sigma}) - V n_{kd}{}^{-\sigma} D_{k_1+d-k}{}^{(2-g)\sigma} \\ &- V^2 f_k{}^{-\sigma} D_{k_1}{}^{\sigma}(n^{\sigma} D_{k_1+d+U-k}{}^{(2-g)\sigma} + (1-n^{\sigma}) D_{k_1+d-k}{}^{(2-g)\sigma}) + V^2 f_k{}^{-\sigma} D_{k_1}{}^{\sigma} G_d{}^{\sigma}\}. \end{aligned} \tag{F4}$$

The quantity $\langle \hat{n}_{kd}{}^{-\sigma}\hat{n}^{\sigma}\rangle$ must be evaluated. We may write

$$\langle n_{kd}{}^{-\sigma}\hat{n}^{\sigma}\rangle = \pi^{-1}\int_{-\infty}^{\infty} f(\omega)\ \mathrm{Im} G_{(dd)k}{}^{-\sigma}(\omega). \tag{F5}$$

It is clear that to the order required

$$G_{(dd)k}{}^{-\sigma}(\omega) = \tfrac{1}{2} V G_{+d}{}^{-\sigma}(\omega)[D_k{}^{-\sigma} + D_{k-4i\Delta}{}^{-\sigma}], \tag{F6}$$

where we have allowed for renormalization effects. The denominator $D_{k_1}{}^{\sigma}$ is likewise to be renormalized as shown in Eq. (D4) (we neglect Γ for $T\gg T_c$). If we integrate over ω in Eq. (F2) we obtain, to lowest order in Δ/U (neglecting the σH terms in the denominators),

$$\begin{aligned} \langle d_{-\sigma}{}^{\dagger} C_{k-\sigma} d_{\sigma}{}^{\dagger} C_{k_1\sigma}\rangle = {} & V n_{kd}{}^{-\sigma}\left[\frac{f_{2d+U-k} - f_{k_1+d-k}}{\epsilon_d + U - \epsilon_{k_1}}\right] + \left\{\frac{V^2}{\pi}\int_{-\infty}^{\infty} d\omega' f(\omega')\ \mathrm{Im}\left\{\frac{G_{+d}{}^{-\sigma}(\omega')}{\omega' - \epsilon_{k-\sigma}}\right\}\right. \\ & \times\left\{\frac{f_{2d+U-k} - f_{k_1+d+U-k}}{\epsilon_d - \epsilon_{k_1}} - \frac{f_{2d+U-k} - f_{k_1+d-k}}{\epsilon_d + U - \epsilon_{k_1}}\right\} + (V^2 f_k{}^{-\sigma})(1-n^{-\sigma})\left[\frac{f_{2d+U-k}}{(\epsilon_{d+U} - \epsilon_{k_1})(2\epsilon_{d+U} - \epsilon_k - \epsilon_{k_1})}\right. \\ & \left. + \frac{f_{k_1+d-k}}{(\epsilon_{k_1} - \epsilon_d - U)(\epsilon_d - \epsilon_k)} + \frac{f_{k_1}}{(\epsilon_{k_1} - 2\epsilon_d - U + \epsilon_k)(\epsilon_k - \epsilon_d)}\right] + V^2 n^{-\sigma}(f_k{}^{-\sigma})\left[\frac{f_{2d+U-k}}{(\epsilon_d - \epsilon_k)(2\epsilon_{d+U} - \epsilon_k - \epsilon_{k_1})}\right. \\ & \left. + \frac{f_{d+U}}{(\epsilon_k - \epsilon_d)(\epsilon_d + U - \epsilon_{k_1})} + \frac{f_{k_1}}{(\epsilon_{k_1} + \epsilon_k - 2\epsilon_d - U)(\epsilon_{k_1} - \epsilon_d - U)}\right] + V^2 f_k{}^{-\sigma}(1-n^{\sigma})\left[\frac{f_{2d+U-k}}{(\epsilon_{d+U} - \epsilon_{k_1})(2\epsilon_d + U - \epsilon_k - \epsilon_{k_1})}\right. \\ & \left. + \frac{f_d}{(\epsilon_k - \epsilon_d - U)(\epsilon_d - \epsilon_{k_1})} + \frac{f_{k_1}}{(\epsilon_{k_1} - \epsilon_d)(\epsilon_{k_1} + \epsilon_k - 2\epsilon_d - U)}\right] + V^2 f_k{}^{-\sigma} n^{\sigma}\left[\frac{f_{2d+U-k}}{(\epsilon_d - \epsilon_{k_1})(2\epsilon_d + U - \epsilon_k - \epsilon_{k_1})}\right. \\ & \left.\left. + \frac{f_{k_1}}{(\epsilon_{k_1} - \epsilon_d)(\epsilon_d + U - \epsilon_k)} + \frac{f_{k_1}}{(\epsilon_{d+U} - \epsilon_{k_1})(2\epsilon_d + U - \epsilon_k - \epsilon_{k_1})}\right]\right\}. \end{aligned} \tag{F7}$$

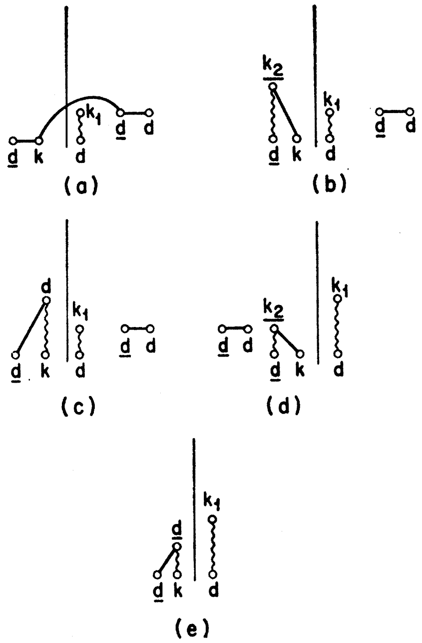

FIG. 15. Representation of $\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}d_{\sigma} \mid C^{\dagger}{}_{k1\sigma}\rangle$.

APPENDIX G: EVALUATION OF $\langle C_{k_1-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle$

The thermal average $\langle C_{k_1-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle$ may be obtained from the equation

$$\langle C_{k_1-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle=\pi^{-1}\int_{-\infty}^{\infty}d\omega\, f(\omega)\ \mathrm{Im}G_{kk_1}{}^{-\sigma}(\omega), \quad \text{(G1)}$$

where

$$G_{kk_1}{}^{\sigma}(\omega)=\langle d_{-\sigma}{}^{\dagger}C_{k-\sigma}d_{\sigma} \mid C_{k_1\sigma}{}^{\dagger}\rangle. \quad \text{(G2)}$$

The graphical representation of the lowest-order terms of $G_{kk_1}{}^{\sigma}(\omega)$ is given in Fig. 15. Again we note that diagrams (c) and (e) give no contribution upon summing over k and k_1 for the reasons presented in Appendix E. The remaining terms yield

$$\begin{aligned}G_{kk_1}{}^{\sigma}=D_k{}^{(2g-1)\sigma}\{&-V\langle n_{dk}{}^{-\sigma}\hat{n}^{\sigma}\rangle(D_{k+k_1-d-U}{}^{g\sigma}-D_{k+k_1-d}{}^{g\sigma})\\&-Vn_{dk}{}^{-\sigma}D_{k+k_1-d}{}^{g\sigma}-V^2D_{k_1}{}^{\sigma}f_k{}^{-\sigma}G_d{}^{\sigma}+V^2D_{k_1}{}^{\sigma}f_k{}^{-\sigma}\\&\times[n^{\sigma}D_{k+k_1-d-U}{}^{g\sigma}+(1-n^{\sigma})D_{k+k_1-d}{}^{g\sigma}]\},\end{aligned} \quad \text{(G3)}$$

where the denominator $D_{k_1}{}^{\sigma}$ is to be renormalized as in Eq. (D4).

Upon performing the integration over ω called for in Eq. (G1), making use of Eqs. (F5) and (F6), we obtain

$$\begin{aligned}\langle C_{k_1-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle=&\,Vn_{dk}{}^{\sigma}\left(\frac{f_k-f_{k+k_1-d}}{\epsilon_d-\epsilon_{k_1}}\right)+\left\{\frac{V^2}{\pi}\int_{-\infty}^{\infty}d\omega'\, f(\omega')\ \mathrm{Im}\left\{\frac{G_{+d}{}^{\sigma}(\omega')}{\omega'-\epsilon_{k\sigma}}\right\}\left[\frac{f_k-f_{k+k_1-d-U}}{\epsilon_d+U-\epsilon_{k_1}}-\frac{f_k-f_{k+k_1-d}}{\epsilon_d-\epsilon_{k_1}}\right]\right.\\&-V^2f_k{}^{\sigma}n^{-\sigma}\left[\frac{f_k}{(\epsilon_d+U-\epsilon_{k_1})(\epsilon_k-\epsilon_{k_1})}+\frac{f_{k_1}}{(\epsilon_{k_1}-\epsilon_k)(\epsilon_d+U-\epsilon_k)}\ \frac{f_{k+k_1-d-U}}{(\epsilon_d+U-\epsilon_{k_1})(\epsilon_d+U-\epsilon_k)}\right]\\&-V^2f_k{}^{\sigma}(1-n^{-}\ )\left[\frac{f_k}{(\epsilon_d-\epsilon_{k_1})(\epsilon_k-\epsilon_{k_1})}+\frac{f_{k_1}}{(\epsilon_{k_1}-\epsilon_k)(\epsilon_d-\epsilon_k)}\ \frac{f_{k+k_1-d}}{(\epsilon_d-\epsilon_{k_1})(\epsilon_d-\epsilon_k)}\right]\\&-V^2f_k{}^{\sigma}n^{-\sigma}\left[\frac{f_k}{(\epsilon_k-\epsilon_{k_1})(\epsilon_k-\epsilon_d-U)}+\frac{f_{k_1}}{(\epsilon_{k_1}-\epsilon_k)(\epsilon_{k_1}-\epsilon_d-U)}\right]\\&\left.-V^2f_k{}^{\sigma}(1-n^{-\sigma})\left[\frac{f_k}{(\epsilon_k-\epsilon_{k_1})(\epsilon_k-\epsilon_d)}+\frac{f_{k_1}}{(\epsilon_{k_1}-\epsilon_k)(\epsilon_{k_1}-\epsilon_d)}+\frac{1}{(\epsilon_k-\epsilon_d)(\epsilon_{k_1}-\epsilon_d)}\right]\right\}.\end{aligned} \quad \text{(G4)}$$

APPENDIX H: EVALUATION OF $\langle \hat{n}^{-\sigma}C_{k_1-\sigma}{}^{\dagger}C_{k-\sigma}\rangle$

In this appendix we examine the thermal average $\langle \hat{n}^{-\sigma}C_{k_1-\sigma}{}^{\dagger}C_{k-\sigma}\rangle$. We shall see that to order Δ/U this average is given by

$$n^{-\sigma}f_k{}^{-\sigma}\,\delta_{k,k_1}+(1-\delta_{k,k_1})\,\langle \hat{n}^{-\sigma}C_{k_1-\sigma}{}^{\dagger}C_{k-\sigma}\rangle^{(2)}, \quad \text{(H1)}$$

where for $H=0$ we may write

$$\langle \hat{n}^{-\sigma}C_{k_1-\sigma}{}^{\dagger}C_{k-\sigma}\rangle^{(2)}=\langle C_{k_1-\sigma}{}^{\dagger}d_{-\sigma}d_{\sigma}{}^{\dagger}C_{k\sigma}\rangle^{(2)}, \quad \text{(H2)}$$

if we consequently sum over k and k_1.

Let us first consider the case $k=k_1$. The thermal average $\langle d_{-\sigma}{}^{\dagger}d_{-\sigma}C_{k-\sigma}{}^{\dagger}C_{k-\sigma}\rangle^{(2)}$ may be obtained from the equation

$$\langle d_{-\sigma}{}^{\dagger}d_{-\sigma}C_{k-\sigma}{}^{\dagger}C_{k-\sigma}\rangle=\pi^{-1}\int_{-\infty}^{\infty}f(\omega)\ \mathrm{Im}S_k{}^{\sigma(2)}(\omega)\,d\omega, \quad \text{(H3)}$$

where

$$S_k{}^{\sigma}(\omega)=\langle \hat{n}^{-\sigma}C_{k-\sigma} \mid C_{k-\sigma}{}^{\dagger}\rangle. \quad \text{(H4)}$$

The graphical representation of $S_k{}^{\sigma(2)}$ is given in Fig. 16(o) and 16(a)–16(f). These diagrams contribute the expression, in the order shown,

$$\begin{aligned}S_k{}^{\sigma(2)}=&\,D_k{}^{-\sigma}n^{-\sigma(2)}+D_k{}^{-\sigma}\sum_{k_1}\{-V(D_{k+k_1-d-U}{}^{(g-2)\sigma}-D_{k+k_1-d}{}^{(g-2)\sigma})\langle \hat{n}^{\sigma}\hat{n}_{dk_1}{}^{-\sigma}\rangle-VD_{k+k_1-d}{}^{(g-2)\sigma}n_{dk_1}{}^{-\sigma}\\&+V(D_{k-k_1+d+U}{}^{-g\sigma}-D_{k-k_1+d}{}^{-g\sigma})\langle \hat{n}^{\sigma}n_{k_1d}{}^{-\sigma}\rangle+VD_{k-k_1+d}{}^{-g\sigma}n_{k_1d}{}^{-\sigma}\}+V^2(D_k{}^{-\sigma})\\&\times\sum_{k_1}\{f_{k_1}{}^{-\sigma}n^{\sigma}(D_{k+k_1-d-U}{}^{(g-2)\sigma}-D_{k+k_1-d}{}^{(g-2)\sigma})+D_{k+k_1-d}\,f_{k_1}{}^{-\sigma}+f_{k_1}{}^{-\sigma}n^{\sigma}(D_{k-k_1+d+U}{}^{-g\sigma}-D_{k-k_1+d}{}^{-g\sigma})\\&+D_{k-k_1+d}{}^{-g\sigma}f_{k_1}{}^{-\sigma}-n^{-\sigma}(D_{k+k_1-d}{}^{(g-2)\sigma}+D_{k-k_1+d}{}^{-g\sigma})\}.\end{aligned} \quad \text{(H5)}$$

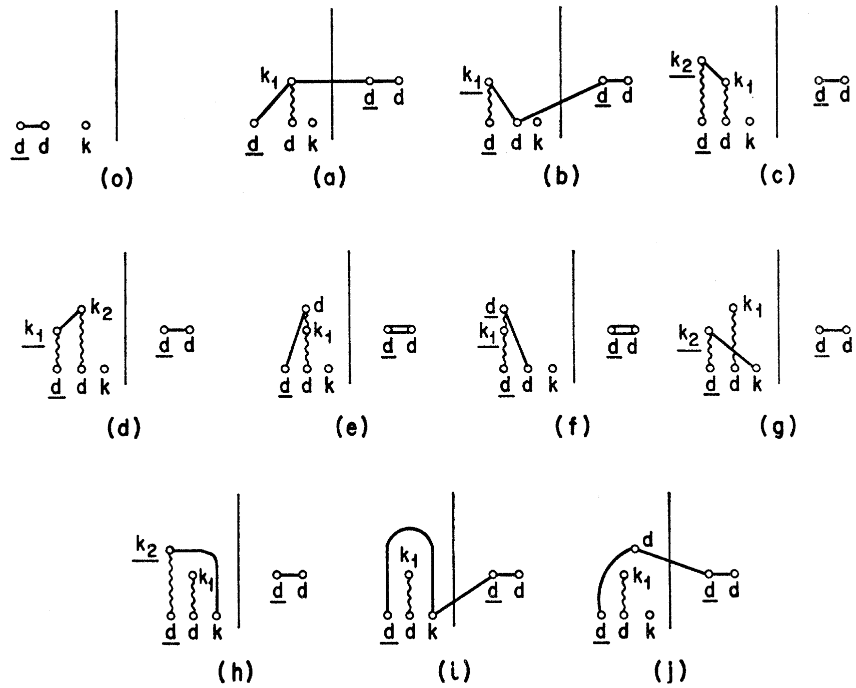

FIG. 16. Representation of $\langle n^{-\sigma}C^{\dagger}_{k-\sigma}\,|\,C_{k1-\sigma}\rangle$.

To lowest order

$$\langle n_{kd}^{-\sigma}\hat{n}^{\sigma}\rangle=\langle n_{dk}^{-\sigma}\hat{n}^{\sigma}\rangle=\frac{V}{\pi}\int_{-\infty}^{\infty}d\omega\, f(\omega)\ \mathrm{Im}\left\{\frac{G_{+d}^{-\sigma}(\omega)}{\omega-\epsilon_{k\sigma}}\right\}$$

$$=Vn^{\sigma}f_k^{-\sigma}/(\epsilon_k-\epsilon_d-U), \tag{H6}$$

so that we may write (H5), upon summing over k_1 and integrating over ω,

$$\langle d_{-\sigma}{}^{\dagger}d_{-\sigma}C_{k-\sigma}{}^{\dagger}C_{k-\sigma}\rangle=n^{-\sigma(2)}f_k^{-\sigma}+\frac{2i\Delta}{\pi}\,(n^{\sigma}+n^{-\sigma}-1)^{(0)}\ \mathrm{Re}\int_{-\infty}^{\infty}\frac{f(\omega)\,d\omega}{(\omega-\epsilon_{k-\sigma})^2}, \tag{H7}$$

where we have neglected a term proportional to $i\Delta f_k{}'\ln|(1-\xi)/\xi|$, etc. We note that $(n^{\sigma}+n^{-\sigma}-1)^{(0)}=0$, so that to order Δ/U, $\langle n^{-\sigma}C_{k-\sigma}{}^{\dagger}C_{k-\sigma}\rangle=n^{-\sigma}f_k^{-\sigma}$. We chose to keep all terms of order Δ/U explicit, rather than include the contributions of Figs. 16(e) and 16(f) as part of the renormalization of the denominator $D_k^{-\sigma}$ in Fig. 16(o) [the product $(D_k^{-\sigma})^2$ would likewise be renormalized as in Eq. (C9)] so as to show that the term $n^{-\sigma}f_k^{-\sigma}$ is the correct one, at least to order Δ/U, rather than

$$\tfrac{1}{2}n^{-\sigma}\int_{-\infty}^{\infty}d\omega\, f(\omega)\ \mathrm{Im}(D_k^{-\sigma}+D_{k-4i\Delta}{}^{-\sigma}). \tag{H8}$$

The graphical representation of $\langle n^{-\sigma}C_{k_1-\sigma}{}^{\dagger}C_{k-\sigma}\rangle$ is presented in Fig. 16(g)–16(j). We note that diagram (j) does not contribute, upon summing over k and k_1, as discussed in Appendix E. In addition, for $H=0$ diagrams 16(g)–16(i) are equivalent to diagrams (d), (b), and (a) of Fig. 15, respectively, so that we obtain Eq. (H2). As a result for $H=0$, the contribution from the last two terms of Eq. (4.11) [the contribution of Fig. 7(g) and 7(h)], is cancelled by the second-order contribution of Figs. 3(b) and 3(g), corresponding to the term $\langle\hat{n}^{-\sigma}C_{k_1-\sigma}{}^{\dagger}C_{k-\sigma}\rangle$.