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PHYSICAL REVIEW B VOLUME 5, NUMBER 7 1 APRIL 1972

Pairing Treatment of Interacting Localized Moments in Dilute Magnetic Alloys. III. Improved Treatment of Coulomb and Scattering Interactions*

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The Anderson model of a localized magnetic center is used to study a system of interacting localized moments in a dilute magnetic alloy. The operator equation-of-motion method is used to calculate both the localized and the conduction-band quasiparticle excitation spectra in a manner which carefully treats both the Coulomb and the scattering interactions. Hole-electron pairing is used to facilitate the accurate evaluation of the effective interaction between centers. This effective interaction causes the localized quasiparticle excitation energies to spread and shift by an amount proportional to $n_0^{1/2}$ (n_0 being the density of centers). The conduction-band quasiparticle excitation energies are spread and shifted by an amount proportional to n_0. There are no gaps in the conduction-band spectrum. The Born series for the conduction-band scattering amplitude is summed analytically. It is shown that spurious gaps are an artifact of any finite order of Born approximation. Self-consistency is achieved both in calculating thermal averages (especially local magnetic moments) and in satisfying the Friedel sum rule.

I. INTRODUCTION

In this paper the study of an *interacting* system of localized moments in a dilute magnetic alloy will be continued, with each localized center containing a magnetic moment being represented by the model of Anderson.[1] The paper shall examine the quasiparticle excitation spectrum associated both with the localized centers and with the conduction band of the host metal when n_0, the density of centers, is small but *finite*. In order to properly account for the interaction between centers, particularly in the *paramagnetic* phase of the system, it is important to introduce the idea of *pairing*. Specifically, one pairs an electron in some single-particle orbital, spin up, with a hole in some single-particle orbital, spin down. For the case where the two spatial orbitals are the same, this amounts to leaving unspecified the orientation of the spin of the electron occupying the orbital.

The quasiparticle excitation spectrum shall be determined by means of the operator equation-of-motion method.[2] While doing so, special care will be taken to achieve *self-consistency* in two senses of the word. First of all, the various thermal averages will be determined self-consistently. This assures that the net magnetic moment on any center is evaluated self-consistently with regard to both magnitude and direction. Second, the parameters of the Anderson model will be chosen such that there is consistency with the Friedel sum rule,[3] corresponding to the fact that the electric field associated with any excess charge on a localized center must be screened out by the surrounding conduction electrons. In the absence of a local moment, the usual form of the Friedel sum rule applies to the Ander-

son model, as has been shown by Langreth.[4] This author shall assume that this is also true in the presence of a local moment. The satisfying of the Friedel sum rule will be carried out in a fashion analogous to that recently developed for treating the extraorbital model of a dilute metallic alloy.[5]

In the original treatment of interacting localized moments by this author,[6] use was made of a generalized effective field. Specifically, this means that the commutator $[c_{l\sigma}, H]$ was *linearized* with respect to the complete set of one-electron destruction operators $c_{l\sigma}$ (H being the Hamiltonian of the system). In a second paper,[7] this procedure was generalized in order to treat the intracenter Coulomb repulsion accurately. Here the commutator $[c_{l\sigma}, H]$ was treated exactly, but the double commutator $[[c_{l\sigma}, H], H]$ was linearized with respect to $c_{l\sigma}$ and $[c_{l\sigma}, H]$. For simplicity, only the single-center problem was considered, although the calculation could have been readily extended to the many-center problem. If this had been done, the results for the localized centers (*but not for the conduction band*) would have been identical with those to be calculated in the present paper.

In this paper, the third of the series, the analysis is extended so that both $[c_{l\sigma}, H]$ and $[[c_{l\sigma}, H], H]$ are treated exactly, but the triple commutator $[[[c_{l\sigma}, H], H], H]$ is linearized in a fashion discussed in detail in Sec. II. As is apparent from the work of Kim[8] and Theumann,[9] this method of truncating the equations of motion is sufficient to allow for the appearance of Kondo-like effects[10] associated with the scattering interaction. The calculation of the conduction-band quasiparticle excitation spectrum, with Kondo effects included, involves the solution of what is, in effect, an integral equation for the conduction-band scattering amplitude. Using a technique developed for the extraorbital model of a disordered alloy,[5] the Born series for this scattering amplitude is summed analytically in the limit of low density of localized centers. The resultant conduction-band quasiparticle excitation spectrum has *no energy gaps*. In contrast, any finite order of Born approximation will lead to gaps in the conduction band in the vicinity of the localized quasiparticle excitation energies. A case in point is the results of I, where the first Born approximation was employed. This situation is an example of the fact that perturbation expansions in the scattering interaction[11] need not necessarily be convergent.

Several attempts[8,9,12,13] have been made to study the Anderson model of a single center by means of the Green's-function equation-of-motion method.[14] None of these attempts have properly satisfied self-consistency. Not only was the Friedel sum rule ignored, but, more seriously, it was assumed *a priori* that the center had equal occupancy by electrons of both directions of spin, which is equivalent to assuming a *vanishing local moment* as far as self-consistency is concerned. Once such an assumption is made, it is inappropriate to attempt, as did Theumann,[9] to infer an effective exchange constant. In contrast to recent suggestions,[11,15] the fact that Theumann's exchange constant differs from the value calculated for the Anderson model by perturbation theory[16] does not necessarily imply inaccuracies in truncating the equations of motion, but rather the absence of a local moment. It should be added that attempts such as those of Mamada and Shibata[11] to attack the problem with perturbation theory also forego self-consistency in the sense that the unperturbed state is, in general, characterized by a different value of local moment from that of the perturbed state.

II. EQUATION OF MOTION

The Hamiltonian of our system is

$$H = H_0 + H_1 , \tag{2.1}$$

$$H_0 = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \epsilon_0 \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + U_0 \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} , \tag{2.2}$$

$$H_1 = \sum_{k,i,\sigma} (V_{ki} c_{k\sigma}^\dagger c_{i\sigma} + V_{-ki} c_{i\sigma}^\dagger c_{k\sigma}) . \tag{2.3}$$

The one-electron energies ϵ_k (for the conduction band) and ϵ_0 (for the localized centers) are measured relative to the Fermi level. The total Hamiltonian represents a system of conduction-band electrons interacting with electrons in localized s orbitals on impurity centers, the index i designating centers. The positive Coulomb energy U_0 is associated with any center containing two opposite-spin electrons. We shall take

$$V_{ki}^* = V_{-ki} , \tag{2.4}$$

so that H_1 is Hermitian. We will later need the fact that

$$V_{ki} = V_k e^{-i\vec{k}\cdot\vec{R}_i} , \tag{2.5}$$

where $\vec{R}_i$ is the position of the ith center and V_k is the matrix element for a center located at the origin. If we had only one center in the whole crystal, H would be the Hamiltonian for the Anderson model of a localized magnetic center.[1] The electron creation and destruction operators obey the usual anticommutation relations.

We wish to look for an operator $\mathcal{O}$ such that

$$[\mathcal{O}, H] = \hbar\omega \mathcal{O} . \tag{2.6}$$

If Eq. (2.6) is exactly satisfied, $\hbar\omega$ is necessarily *real*. If $\hbar\omega$ is *positive*, $\mathcal{O}$ is a quasiparticle *destruction* operator associated with an excited state of the system containing one quasiparticle of energy $\hbar\omega$. If $\hbar\omega$ is *negative*, $\mathcal{O}$ is a quasiparticle

creation operator associated with an excited state of the system containing one quasiparticle of energy $|\hbar\omega|$. If Eq. (2.6) is only approximately satisfied, then $\hbar\omega$ may be *complex*. In this case, the signature of the real part of $\hbar\omega$ determines whether $\mathcal{O}$ is a quasiparticle creation or destruction operator. In any case, $\hbar\omega$ must be in either the second or the fourth quadrant of the complex ω plane to ensure that the quasiparticle excitations are *causal* (i.e., decay with increasing time). The lifetime of such an excitation is given by

$$\tau = (2|\omega_2|)^{-1}, \tag{2.7}$$

where $-i\omega_2$ is the imaginary part of ω. Values of ω in the first or third quadrant indicate instabilities.

We introduce the notation

$$N_{l\sigma} \equiv c^\dagger_{l\sigma} c_{l\sigma} \tag{2.8}$$

for the particle-number operator, in terms of which we can write

$$H_0 = \sum_{k,\sigma} \epsilon_k N_{k\sigma} + \epsilon_0 \sum_{i,\sigma} N_{i\sigma} + U_0 \sum_i N_{i\uparrow} N_{i\downarrow} . \tag{2.9}$$

We define the operators

$$\begin{aligned} \varphi_{1i\sigma} &\equiv c_{i\sigma} , \\ \varphi_{2i\sigma} &\equiv N_{i,-\sigma} c_{i\sigma} , \\ \varphi_{1ik\sigma} &\equiv N_{i,-\sigma} c_{k\sigma} - c^\dagger_{i,-\sigma} c_{i\sigma} c_{k,-\sigma} , \\ \varphi_{2ik\sigma} &\equiv c^\dagger_{k,-\sigma} c_{i,-\sigma} c_{i\sigma} . \end{aligned} \tag{2.10}$$

Calculating the commutators of H with respect to $c_{k\sigma}$ and the various φ's we get

$$[c_{k\sigma}, H] = \epsilon_k c_{k\sigma} + \sum_i V_{ki} \varphi_{1i\sigma} , \tag{2.11}$$

$$[\varphi_{1i\sigma}, H] = \epsilon_0 \varphi_{1i\sigma} + U_0 \varphi_{2i\sigma} + \sum_k V_{-ki} c_{k\sigma} , \tag{2.12}$$

$$[\varphi_{2i\sigma}, H] = (\epsilon_0 + U_0)\varphi_{2i\sigma} + \sum_k (V_{-ki}\varphi_{1ik\sigma} - V_{ki}\varphi_{2ik\sigma}) , \tag{2.13}$$

$$[\varphi_{1ik\sigma}, H_0] = \epsilon_k \varphi_{1ik\sigma} , \tag{2.14}$$

$$[\varphi_{2ik\sigma}, H_0] = (2\epsilon_0 + U_0 - \epsilon_k)\varphi_{2ik\sigma} , \tag{2.15}$$

$$[\varphi_{1ik\sigma}, H_1] = \sum_j V_{kj} c^\dagger_{i,-\sigma}(c_{i,-\sigma} c_{j\sigma} - c_{i\sigma} c_{j,-\sigma}) + \sum_{k'} V_{-k'i} c^\dagger_{i,-\sigma}(c_{k',-\sigma} c_{k\sigma} - c_{k'\sigma} c_{k,-\sigma}) - \sum_{k'} V_{k'i} c^\dagger_{k',-\sigma}(c_{k,-\sigma} c_{i\sigma} - c_{k'\sigma} c_{i,-\sigma}) , \tag{2.16}$$

$$[\varphi_{2ik\sigma}, H_1] = -\sum_j V_{-kj} c^\dagger_{j,-\sigma} c_{i,-\sigma} c_{i\sigma} + \sum_{k'} V_{-k'i} c^\dagger_{k,-\sigma}(c_{k',-\sigma} c_{i\sigma} - c_{k'\sigma} c_{i,-\sigma}) . \tag{2.17}$$

The basic approximation of this paper is now introduced. The right-hand sides of Eqs. (2.16) and (2.17) are *linearized* with respect to all possible $c_{j\sigma}$ or $c_{k'\sigma}$ operators. In other words, the operator coefficient multiplying any $c_{j\sigma}$ or $c_{k'\sigma}$ is replaced by the corresponding thermal average. It can be checked that every such thermal average has a portion independent of n_0, the density of localized centers in the crystal. In addition, the thermal average multiplying $c_{i\sigma}$ has a portion linear in n_0. We make the approximation of dropping this latter portion, valid in the dilute limit. As a consequence, thermal averages of the type

$$\langle c^\dagger_{i\sigma} c_{i'\sigma} \rangle , \quad \langle c^\dagger_{i,-\sigma} c_{i'\sigma} \rangle \text{ for } i \neq i' ,$$

$$\langle c^\dagger_{k\sigma} c_{k'\sigma} \rangle , \quad \langle c^\dagger_{k,-\sigma} c_{k'\sigma} \rangle \text{ for } \vec{k} \neq \vec{k}'$$

are ignored. We retain thermal averages of the form

$$n_{l\sigma} \equiv \langle N_{l\sigma} \rangle , \tag{2.18}$$

$$b_l \equiv \langle c^\dagger_{l\uparrow} c_{l\downarrow} \rangle , \tag{2.19}$$

$$n_{ik\sigma} \equiv \langle c^\dagger_{i\sigma} c_{k\sigma} \rangle , \tag{2.20}$$

$$b_{ik\sigma} \equiv \langle c^\dagger_{i,-\sigma} c_{k\sigma} \rangle . \tag{2.21}$$

The actual calculation of these thermal averages will be carried out in the appendices. As is shown in Appendix C, $n_{ik\sigma}$ and $b_{ik\sigma}$ are proportional to V_{ki}. Since V_{ki} is inversely proportional to the square root of the volume of the crystal, $n_{ik\sigma}$ and $b_{ik\sigma}$ vanish in the infinite-volume limit. Nevertheless, these averages make contributions to sums over k space which are finite in the infinite-volume limit, and thus must be retained. Equations (2.16) and (2.17) are replaced by

$$[\varphi_{1ik\sigma}, H_1] = \sum_j V_{kj}[n_{i,-\sigma} c_{j\sigma} - (b_i \delta_{\sigma\uparrow} + b_i^* \delta_{\sigma\downarrow}) c_{j,-\sigma}] + V_{ki}\{(n_{i,-\sigma} - n_{k,-\sigma}) c_{i\sigma} - [(b_i - b_k)\delta_{\sigma\uparrow} + (b_i^* - b_k^*)\delta_{\sigma\downarrow}] c_{i,-\sigma}\} + \sum_{k'} V_{-k'i}(n_{ik,-\sigma} c_{k'\sigma} - b_{ik\sigma} c_{k',-\sigma}) , \tag{2.22}$$

$$[\varphi_{2ik\sigma}, H_1] = -V_{-ki}\{(n_{i,-\sigma} - n_{k,-\sigma}) c_{i\sigma} - [(b_i - b_k)\delta_{\sigma\uparrow} + (b_i^* - b_k^*)\delta_{\sigma\downarrow}] c_{i,-\sigma}\} + \sum_{k'} V_{-k'i}(n^*_{ik,-\sigma} c_{k'\sigma} - b^*_{ik,-\sigma} c_{k',-\sigma}) . \tag{2.23}$$

Here we have made use of the fact, proved in Appendix C, that

$$n_{i,-k,\sigma} = n^*_{ik\sigma} , \tag{2.24}$$

$$b_{i,-k,\sigma} = b^*_{i,k,-\sigma} . \tag{2.25}$$

The assumption of finite b_l and $b_{ik\sigma}$ introduces the possibility of *pairing*. Here it is *hole-electron* pair-

ing, as in the excitonic insulator,[17] rather than *electron-electron* pairing, as in the superconductor. Unlike the excitonic insulator, however, here a finite b_l indicates only that an electron is occupying the orbital l with its spin pointing neither straight up nor straight down.

Let us, for the moment, consider some arbitrary set of operators $\psi_{p\sigma}$. We introduce the vector operators

$$\Psi_p \equiv \begin{pmatrix} \psi_{p\uparrow} \\ \psi_{p\downarrow} \end{pmatrix}, \quad \Psi_p^\dagger \equiv (\psi_{p\uparrow}^\dagger, \psi_{p\downarrow}^\dagger) . \tag{2.26}$$

We define the 2×2 matrix

$$\langle [\Psi_p ; \Psi_q^\dagger]_+ \rangle \equiv \begin{pmatrix} \langle [\psi_{p\uparrow}, \psi_{q\uparrow}^\dagger]_+ \rangle & \langle [\psi_{p\uparrow}, \psi_{q\downarrow}^\dagger]_+ \rangle \\ \langle [\psi_{p\downarrow}, \psi_{q\uparrow}^\dagger]_+ \rangle & \langle [\psi_{p\downarrow}, \psi_{q\downarrow}^\dagger]_+ \rangle \end{pmatrix} . \tag{2.27}$$

We have need of the general matrix notation

$$M \equiv \begin{pmatrix} m_{\uparrow\uparrow} & m_{\uparrow\downarrow} \\ m_{\downarrow\uparrow} & m_{\downarrow\downarrow} \end{pmatrix}, \quad M^\dagger \equiv \begin{pmatrix} m_{\uparrow\uparrow}^\dagger & m_{\downarrow\uparrow}^\dagger \\ m_{\uparrow\downarrow}^\dagger & m_{\downarrow\downarrow}^\dagger \end{pmatrix} . \tag{2.28}$$

An arbitrary M can be expanded in terms of the four matrices

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad i\tau_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$
$$\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \tau_4 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{2.29}$$

Equations (2.27) and (2.28) imply that

$$\langle [\Psi_p ; \Psi_q^\dagger]_+ \rangle = \langle [\Psi_q ; \Psi_p^\dagger]_+ \rangle^\dagger . \tag{2.30}$$

We define the vector operators

$$\Psi_{1i} \equiv \begin{pmatrix} \varphi_{1i\uparrow} \\ \varphi_{1i\downarrow} \end{pmatrix}, \quad \Phi_{2i} \equiv \begin{pmatrix} \varphi_{2i\uparrow} \\ \varphi_{2i\downarrow} \end{pmatrix},$$
$$\Phi_{1ik} \equiv \begin{pmatrix} \varphi_{1ik\uparrow} \\ \varphi_{1ik\downarrow} \end{pmatrix}, \quad \Phi_{2ik} \equiv \begin{pmatrix} \varphi_{2ik\uparrow} \\ \varphi_{2ik\downarrow} \end{pmatrix} \tag{2.31}$$

and

$$\Psi_{2i} \equiv \Phi_{2i} - \mathfrak{U}_i \Psi_{1i} ,$$
$$\Psi_{1ik} \equiv \Phi_{1ik} - \mathfrak{U}_i \Psi_k - \mathfrak{V}_{ik} \Psi_{1i} , \tag{2.32}$$
$$\Psi_{2ik} \equiv \Phi_{2ik} - \mathfrak{V}_{ik}^\dagger \Psi_{1i} ,$$

where

$$\mathfrak{U}_i \equiv \langle [\Phi_{2i} ; \Psi_{1i}^\dagger]_+ \rangle ,$$
$$\mathfrak{V}_{ik} \equiv \langle [\Phi_{1ik} ; \Psi_{1i}^\dagger]_+ \rangle , \tag{2.33}$$

and

$$\Psi_k \equiv \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} . \tag{2.34}$$

Thus we have

$$\mathfrak{U}_i = \mathfrak{U}_i^\dagger = \langle [\Phi_{2i} ; \Phi_{2i}^\dagger]_+ \rangle$$
$$= \tfrac{1}{2}(n_{i\downarrow} + n_{i\uparrow})\tau_4 + \tfrac{1}{2}(n_{i\downarrow} - n_{i\uparrow})\tau_3$$
$$- \tfrac{1}{2}(b_i + b_i^*)\tau_1 - \tfrac{1}{2}(b_i - b_i^*) i\tau_2 . \tag{2.35}$$

Similarly, we have

$$\langle [\Phi_{1ik} ; \Psi_{k'}^\dagger]_+ \rangle = \delta_{kk'} \mathfrak{U}_i ,$$
$$\langle [\Phi_{1ik} ; \Psi_{1j}^\dagger]_+ \rangle = \delta_{ij} \mathfrak{V}_{ik} , \tag{2.36}$$
$$\langle [\Phi_{2ik} ; \Psi_{1j}^\dagger]_+ \rangle = \delta_{ij} \mathfrak{V}_{ik}^\dagger .$$

Here we have used the fact that

$$\mathfrak{V}_{ik} = \begin{pmatrix} n_{ik\downarrow} & -b_{ik\uparrow} \\ -b_{ik\downarrow} & n_{ik\uparrow} \end{pmatrix} . \tag{2.37}$$

In analogy with $\mathfrak{U}_i$, it is convenient to define

$$\mathfrak{U}_k \equiv \begin{pmatrix} n_{k\downarrow} & -b_k \\ -b_k^* & n_{k\uparrow} \end{pmatrix} . \tag{2.38}$$

We see that

$$\langle [\Psi_p ; \Psi_q^\dagger]_+ \rangle = 0 \quad \text{if } p \neq q , \tag{2.39}$$

so that we have, in effect, a set of *independent* vector operators. In addition, Ψ_k and Ψ_{1i} are *normalized*, i.e.,

$$\langle [\Psi_k ; \Psi_k^\dagger]_+ \rangle = \langle [\Psi_{1i} ; \Psi_{1i}^\dagger]_+ \rangle = \tau_4 . \tag{2.40}$$

The other vectors are not normalized; for example,

$$\langle [\Psi_{2i} ; \Psi_{2i}^\dagger]_+ \rangle = \mathfrak{U}_i (\tau_4 - \mathfrak{U}_i) . \tag{2.41}$$

The normalization matrices for Ψ_{1ik} and Ψ_{2ik} are rather complicated; fortunately, they are not needed for the following developments.

Equations (2.11)–(2.15), (2.22), and (2.23) can be rewritten as

$$[\Psi_{1i}, H] = (\epsilon_0 \tau_4 + U_0 \mathfrak{U}_i)\Psi_{1i} + U_0 \Psi_{2i} + \textstyle\sum_k V_{-ki} \Psi_k , \tag{2.42}$$

$$[\Psi_{2i}, H] = [U_0 \mathfrak{U}_i (\tau_4 - \mathfrak{U}_i) + \textstyle\sum_k (V_{ki}^* \mathfrak{V}_{ik} - V_{ki} \mathfrak{V}_{ik}^\dagger)]\Psi_{1i}$$
$$+ [\epsilon_0 \tau_4 + U_0 (\tau_4 - \mathfrak{U}_i)]\Psi_{2i} + \textstyle\sum_k [V_{ki}^* \Psi_{1ik} - V_{ki} \Psi_{2ik}] , \tag{2.43}$$

$$[\Psi_{1ik}, H] = \epsilon_k \Psi_{1ik} - U_0 \mathfrak{V}_{ik} \Psi_{2i}$$
$$+ \{V_{ki}(\mathfrak{U}_i - \mathfrak{U}_k) + \mathfrak{V}_{ik}[(\epsilon_k - \epsilon_0)\tau_4 - U_0 \mathfrak{U}_i]\}\Psi_{1i} , \tag{2.44}$$

$$[\Psi_{2ik}, H] = (2\epsilon_0 + U_0 - \epsilon_k)\Psi_{2ik} - U_0 \mathfrak{V}_{ik}^\dagger \Psi_{2i}$$
$$- \{V_{ki}^*(\mathfrak{U}_i - \mathfrak{U}_k) + \mathfrak{V}_{ik}^\dagger[(\epsilon_k - \epsilon_0)\tau_4 - U_0(\tau_4 - \mathfrak{U}_i)]\}\Psi_{1i} . \tag{2.45}$$

This replacement of Φ's by Ψ's in the commutators has lead to considerable cancellation of terms.

We see that the commutator of H with any Ψ_p can be written as a linear combination of the various Ψ_p. Thus we assume that the operator $\mathcal{O}$ of Eq. (2.6) can be written in the form

$$\mathcal{O} = \textstyle\sum_p A_p^\dagger \Psi_p , \tag{2.46}$$

where

$$A_p \equiv \begin{pmatrix} a_{p'} \\ a_{p,} \end{pmatrix} \tag{2.47}$$

is a vector coefficient. Here we are using the notation

$$(p) = (\vec{k}) + (1i) + (2i) + (1i\vec{k}) + (2i\vec{k}) \ . \tag{2.48}$$

If we substitute Eq. (2.46) into (2.6), take the anticommutator with respect to $\Psi^\dagger_{p'}$, thermally average, and divide by the normalization matrix $\langle[\Psi_{p'}\,;\,\Psi^\dagger_{p'}]_+\rangle$, we get the set of equations

$$\textstyle\sum_p A^\dagger_p[K(p,p') - \hbar\omega\delta_{pp'}\tau_4] = 0 \ , \tag{2.49}$$

where we are defining

$$K(p,p') \equiv \langle[[\Psi_p, H];\ \Psi^\dagger_{p'}]_+\rangle\,\langle[\Psi_{p'}\,;\,\Psi^\dagger_{p'}]_+\rangle^{-1} \ . \tag{2.50}$$

Note that because of Eq. (2.39) every term of $\langle[[\Psi_p, H];\ \Psi^\dagger_{p'}]_+\rangle$ is automatically proportional to $\langle[\Psi_{p'}\,;\,\Psi^\dagger_{p'}]_+\rangle$. Thus it is not necessary to know the latter in order to evaluate $K(p,p')$. In turn, setting p' equal to $\vec{k}$, $1i$, $2i$, $1i\vec{k}$, and $2i\vec{k}$, we can write Eq. (2.49) as

$$A^\dagger_k(\epsilon_k - \hbar\omega) + \textstyle\sum_i V_{-ki}A^\dagger_{1i} = 0 \ , \tag{2.51}$$

$$\begin{aligned} A^\dagger_{1i}[(\epsilon_0 - \hbar\omega)\tau_4 + U_0\mathfrak{U}_i] + \textstyle\sum_k A^\dagger_k V_{ki} + A^\dagger_{2i}\,[U_0\mathfrak{U}_i(\tau_4 - \mathfrak{U}_i) + \sum_k (V^*_{ki}\mathfrak{V}_{ik} - V_{ki}\mathfrak{V}^\dagger_{ik})] \\ + \textstyle\sum_k A^\dagger_{1ik}\{V_{ki}(\mathfrak{U}_i - \mathfrak{U}_k) + \mathfrak{V}_{ik}[(\epsilon_k - \epsilon_0)\tau_4 - U_0\mathfrak{U}_i]\} \\ - \textstyle\sum_k A^\dagger_{2ik}\{V^*_{ki}(\mathfrak{U}_i - \mathfrak{U}_k) + \mathfrak{V}^\dagger_{ik}\,[(\epsilon_k - \epsilon_0)\tau_4 - U_0(\tau_4 - \mathfrak{U}_i)]\} = 0 \ , \end{aligned} \tag{2.52}$$

$$A^\dagger_{2i}[(\epsilon_0 + U_0 - \hbar\omega)\tau_4 - U_0\mathfrak{U}_i] + A^\dagger_{1i}U_0 - U_0\textstyle\sum_k (A^\dagger_{1ik}\mathfrak{V}_{ik} + A^\dagger_{2ik}\,\mathfrak{V}^\dagger_{ik}) = 0 \ , \tag{2.53}$$

$$A^\dagger_{1ik}(\epsilon_k - \hbar\omega) + A^\dagger_{2i}V^*_{ki} = 0 \ , \tag{2.54}$$

$$A^\dagger_{2ik}(2\epsilon_0 + U_0 - \epsilon_k - \hbar\omega) - A^\dagger_{2i}V_{ki} = 0 \ . \tag{2.55}$$

These last two equations immediately give

$$A^\dagger_{1ik} = -\,A^\dagger_{2i}V^*_{ki}(\epsilon_k - \hbar\omega)^{-1} \ , \tag{2.56}$$

$$A^\dagger_{2ik} = +\,A^\dagger_{2i}V_{ki}(2\epsilon_0 + U_0 - \epsilon_k - \hbar\omega)^{-1} \ . \tag{2.57}$$

It is shown in Appendix D that

$$\begin{aligned} \textstyle\sum_k [V^*_{ki}\mathfrak{V}_{ik}(\epsilon_k - \hbar\omega)^{-1} + V_{ki}\mathfrak{V}^\dagger_{ik}(\epsilon_k + \hbar\omega - 2\epsilon_0 - U_0)^{-1}] \\ = (\kappa - 1)U_0^{-1}[(\epsilon_0 + U_0)\tau_4 - U_0\mathfrak{U}_i] \ , \end{aligned} \tag{2.58}$$

$$\begin{aligned} \textstyle\sum_k |V_k|^2(\mathfrak{U}_i - \mathfrak{U}_k)[(\epsilon_k - \hbar\omega)^{-1} - (\epsilon_k + \hbar\omega - 2\epsilon_0 - U_0)^{-1}] \\ = (\lambda - 1)U_0^{-1}\epsilon_0(\epsilon_0 + U_0)\tau_4 \ . \end{aligned} \tag{2.59}$$

The proportionality factors $(\kappa - 1)$ and $(\lambda - 1)$ are *real* functions of ω. The functions κ and λ differ appreciably from unity only if the temperature T is comparable to or smaller than the Kondo temperature T_K, and even then only if $\hbar\omega$ lies in the immediate vicinity of zero or $(2\epsilon_0 + U_0)$. (By immediate vicinity we mean that the energy difference is comparable to or smaller than $k_B T_K$.) With the aid of Eqs. (2.56)–(2.59), Eqs. (2.52) and (2.53) become, respectively,

$$A^\dagger_{1i}Q_i + \textstyle\sum_k A^\dagger_k V_{ki} = 0 \ , \tag{2.60}$$

$$A^\dagger_{2i} = -\,A^\dagger_{1i}\kappa^{-1}U_0[(\epsilon_0 + U_0 - \hbar\Omega)\tau_4 - U_0\mathfrak{U}_i]^{-1} \ , \tag{2.61}$$

where we are defining

$$\Omega \equiv \kappa^{-1}\omega \ , \tag{2.62}$$

$$L = \kappa^{-1}[(\hbar\omega)^2 - (2\epsilon_0 + U_0)\hbar\omega + \lambda\epsilon_0(\epsilon_0 + U_0)] \ , \tag{2.63}$$

$$Q_i \equiv L[(\epsilon_0 + U_0 - \hbar\Omega)\tau_4 - U_0\mathfrak{U}_i]^{-1} \ . \tag{2.64}$$

Here we have made use of the identity

$$\begin{aligned} [(\epsilon_0 - \hbar\Omega)\tau_4 + U_0\mathfrak{U}_i][(\epsilon_0 + U_0 - \hbar\Omega)\tau_4 - U_0\mathfrak{U}_i] \\ - U_0^2\mathfrak{U}_i(\tau_4 - \mathfrak{U}_i) \equiv (\epsilon_0 - \hbar\Omega)(\epsilon_0 + U_0 - \hbar\Omega)\tau_4 \ . \end{aligned} \tag{2.65}$$

Equations (2.51) and (2.60) represent a system of coupled equations for the unknown $A^\dagger_{1i}$'s and $A^\dagger_k$'s. We can immediately eliminate the $A^\dagger_k$'s in favor of the $A^\dagger_{1i}$'s, or vice versa. Eliminating $A^\dagger_k$ from Eq. (2.60), we get

$$\begin{aligned} A^\dagger_{1i}(Q_i - W\tau_4) - \sum_{j\neq i} A^\dagger_{1j} \sum_k |V_k|^2 e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)}(\epsilon_k - \hbar\omega)^{-1} \\ = 0 \ , \end{aligned} \tag{2.66}$$

where

$$W \equiv \textstyle\sum_k |V_k|^2(\epsilon_k - \hbar\omega)^{-1} = (2\pi)^{-3}\int d^3k\,|V_k|^2(\epsilon_k - \hbar\omega)^{-1} \ . \tag{2.67}$$

Eliminating $A^\dagger_{1i}$ from Eq. (2.51), we get

$$\begin{aligned} A^\dagger_k[(\epsilon_k - \hbar\omega)\tau_4 - |V_k|^2\textstyle\sum_i Q_i^{-1}] \\ - \sum_{k'\neq k} A^\dagger_{k'}V^*_k V_{k'} \sum_i e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_i}Q_i^{-1} = 0 \ . \end{aligned} \tag{2.68}$$

The self-energy W is defined for ω lying in either the second or the fourth quadrant of the complex ω plane. In the first or the third quadrant, W is defined by analytic continuation across the *real axis*.[18] Since we are primarily interested in ω near the real axis, we use the Plemelj relation

$$\lim_{\eta\to 0^+}(x \pm i\eta)^{-1} = \mathcal{P}\left(\frac{1}{x}\right) \mp i\pi\delta(x) \tag{2.69}$$

in evaluating W. Writing

$$\omega = \omega_1 - i\omega_2 , \tag{2.70}$$

$$W = W_1 - iW_2 , \tag{2.71}$$

we get

$$W_1 = (2\pi)^{-3}\,\mathcal{P}\int d^3k \,|V_k|^2 (\epsilon_k - \hbar\omega_1)^{-1} , \tag{2.72}$$

$$W_2 = -\tfrac{1}{2}(2\pi)^{-2}(\mathrm{sgn}\omega_1)\int d^3k\,|V_k|^2\,\delta(\epsilon_k - \hbar\omega_1)$$
$$= -(2\pi)^{-1}(\mathrm{sgn}\omega_1)\left[k^2\left(\frac{d\epsilon_k}{dk}\right)^{-1}|V_k|^2\right]_{\epsilon_k=\hbar\omega_1} . \tag{2.73}$$

We shall later make use of the common approximation of ignoring the dependence of W on the *magnitude* of ω_1 (e.g., by setting $\omega_1 = 0$ inside the integrands for W_1 and W_2). See Appendix D.

III. LOCALIZED QUASIPARTICLES

We look for solutions to Eq. (2.66). We assume that one particular vector coefficient, say $A^\dagger_{1i}$, is much larger than all the other $A^\dagger_{1j}$ $(j \neq i)$. This approximation is certainly valid for sufficiently small density of impurity centers. Thus, for $A^\dagger_{1i}$ we have Eq. (2.66), while for $A^\dagger_{1j}$ $(j \neq i)$ we have

$$A^\dagger_{1j}(Q_j - W\tau_4)$$
$$= \sum_{p\neq j} A^\dagger_{1p}\sum_{k'}|V_{k'}|^2 e^{i\vec{k}'\cdot(\vec{R}_p - \vec{R}_j)}(\epsilon_{k'} - \hbar\omega)^{-1}$$
$$\cong A^\dagger_{1i}\sum_{k'}|V_{k'}|^2 e^{-i\vec{k}'\cdot(\vec{R}_j - \vec{R}_i)}(\epsilon_{k'} - \hbar\omega)^{-1} . \tag{3.1}$$

Substituting (3.1) into (2.66), we get

$$A^\dagger_{1i}(G_i - P_i) = 0 , \tag{3.2}$$

where we are defining

$$G_i \equiv Q_i - W\tau_4 , \tag{3.3}$$

$$P_i \equiv (2\pi)^{-6}\int\int d^3k\, d^3k' \,|V_k|^2\,|V_{k'}|^2(\epsilon_k - \hbar\omega)^{-1}$$
$$\times(\epsilon_{k'} - \hbar\omega)^{-1}\sum_{j\neq i} G_j^{-1} e^{i(\vec{k}-\vec{k}')\cdot(\vec{R}_j - \vec{R}_i)} . \tag{3.4}$$

Settting up the notation

$$p_i \equiv \epsilon_0 + U_0 - \tfrac{1}{2}U_0(n_{i\uparrow} + n_{i\downarrow}) , \tag{3.5}$$

$$q_i \equiv \tfrac{1}{2}U_0(n_{i\uparrow} - n_{i\downarrow}) , \tag{3.6}$$

$$\Delta_i \equiv U_0 b_i , \tag{3.7}$$

$$w_i \equiv (q_i^2 + |\Delta_i|^2)^{1/2} , \tag{3.8}$$

we have

$$(\epsilon_0 + U_0 - \hbar\Omega)\tau_4 - U_0\mathfrak{u}_i$$
$$= \begin{pmatrix} p_i - \hbar\Omega - q_i & \Delta_i \\ \Delta_i^* & p_i - \hbar\Omega + q_i \end{pmatrix} , \tag{3.9}$$

$$[(\epsilon_0 + U_0 - \hbar\Omega)\tau_4 - U_0\mathfrak{u}_i]^{-1}$$
$$= [(p_i - \hbar\Omega)^2 - w_i^2]^{-1}[(p_i - \hbar\Omega)\tau_4 + q_i\tau_3 - \tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1$$
$$- \tfrac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2] . \tag{3.10}$$

Defining

$$a_i \equiv L^{-1}[(p_i - \hbar\Omega)^2 - w_i^2] , \tag{3.11}$$

we have

$$G_i = a_i^{-1}\begin{pmatrix} p_i - a_iW - \hbar\Omega + q_i & -\Delta_i \\ -\Delta_i^* & p_i - a_iW - \hbar\Omega - q_i \end{pmatrix} , \tag{3.12}$$

so that

$$G_i^{-1} = a_i[(p_i - a_iW - \hbar\Omega)^2 - w_i^2]^{-1}$$
$$\times[(\epsilon_0 + U_0 - a_iW - \hbar\Omega)\tau_4 - U_0\mathfrak{u}_i] . \tag{3.13}$$

We now anticipate the following results of the calculation. It turns out that p_i and w_i are always independent of the index i. (Thus a_i is also.) In one of the two kinds of solutions, q_i and Δ_i are also independent of i; in the other kind of solution, q_i and Δ_i vary in an essentially random fashion from site to site, subject to the constraint that w_i be site independent. The former is the ordered solution; the latter is the disordered solution. We define

$$I_i \equiv (2\pi)^{-6}\int\int d^3k\, d^3k' \,|V_k|^2\,|V_{k'}|^2(\epsilon_k - \hbar\omega)^{-1}$$
$$\times(\epsilon_{k'} - \hbar\omega)^{-1}\sum_{j\neq i} e^{i(\vec{k}-\vec{k}')\cdot(\vec{R}_j - \vec{R}_i)} , \tag{3.14}$$

$$D_i \equiv a_i[(p_i - a_iW - \hbar\Omega)^2 - w_i^2]^{-1}(p_i - a_iW - \hbar\Omega)\tau_4 . \tag{3.15}$$

I_i differs from P_i by the absence of G_j^{-1}. D_i is that portion of G_i^{-1} proportional to τ_4. For the ordered solution, we can replace G_j^{-1} by G_i^{-1} in P_i, so that

$$P_i = G_i^{-1}I_i . \tag{3.16}$$

For the disordered solution, the portions of G_j^{-1} proportional to τ_1, τ_2, and τ_3 make negligible contributions to the sum over j in P_i, this being due to the random nature of q_i and Δ_i. The portion of G_j^{-1} proportional to τ_4 is equal to D_i, so that

$$P_i = D_i I_i . \tag{3.17}$$

We may now rewrite Eq. (3.2) as

$$A^\dagger_{1i}G'_i = 0 , \tag{3.18}$$

where we are defining

$$G'_i \equiv -\tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 - \tfrac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2 + q_i\tau_3$$
$$+ \alpha_i(p_i - a_iW - \hbar\Omega)\tau_4 , \tag{3.19}$$

$$\alpha_i \equiv \frac{(p_i - a_iW - \hbar\Omega)^2 - w_i^2 - a_i^2 I_i}{(p_i - a_iW - \hbar\Omega)^2 - w_i^2 + Qa_i^2 I_i} , \tag{3.20}$$

$$Q \equiv +1 , \quad \text{ordered state}$$
$$\equiv 0 , \quad \text{disordered state} . \tag{3.21}$$

In order to evaluate I_i, we approximate the sum over $j \neq i$ by the equivalent integral

$$\sum_{j\neq i} e^{i(\vec{k}-\vec{k}')\cdot(\vec{R}_j - \vec{R}_i)} = n_0\int d^3R\, e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} . \tag{3.22}$$

We are assuming a crystal of unit volume and a

density of centers n_0. Note that, having made this approximation, $I_i = I$ is independent of the index i. It can be shown[6] that

$$I = \tfrac{1}{2} n_0 (2\pi)^{-6} \int d^3k \,|V_k|^4 (\hbar^2 k^2/2m)^{-1} (\epsilon_k - \hbar\omega)^{-1} , \tag{3.23}$$

where m is the effective mass of the conduction electrons, which we shall assume is positive. Writing

$$I = I_1 - iI_2 , \tag{3.24}$$

we have

$$I_1 = \tfrac{1}{2} n_0 (2\pi)^{-6} \mathcal{P} \int d^3k \,|V_k|^4 (\hbar^2 k^2/2m)^{-1} (\epsilon_k - \hbar\omega_1)^{-1} ,$$

$$I_2 = -\tfrac{1}{4} n_0 (2\pi)^{-5} (\mathrm{sgn}\omega_1) \int d^3k \,|V_k|^4 (\hbar^2 k^2/2m)^{-1} \times \delta(\epsilon_k - \hbar\omega_1) . \tag{3.25}$$

As with W, it is usually a good approximation to ignore the ω dependence of I by setting $\omega_1 = 0$ inside the integrands of Eq. (3.25).

We return to Eq. (3.18). Corresponding to this matrix equation, there is the secular equation

$$\begin{vmatrix} \alpha_i(p_i - a_i W - \hbar\Omega) + q_i & -\Delta_i \\ -\Delta_i^* & \alpha_i(p_i - a_i W - \hbar\Omega) - q_i \end{vmatrix} = 0 , \tag{3.26}$$

which gives

$$\alpha_i(p_i - a_i W - \hbar\Omega) \pm w_i = 0 . \tag{3.27}$$

Substituting this back into (3.20), we get an equation cubic in α_i^{-1}:

$$\alpha_i^{-3} - \alpha_i^{-2} - [1 + (a_i/w_i)^2 I]\,\alpha_i^{-1} + [1 - Q(a_i/w_i)^2 I] = 0 . \tag{3.28}$$

Solving for the roots in the usual fashion, expanding in powers of the small quantity I, and keeping only the leading terms, we get

$$\alpha_i^{-1} = -1 \tag{3.29}$$

and

$$\alpha_i^{-1} = +1 \mp (a_i/w_i)\,[\tfrac{1}{2}(1+Q)I]^{1/2} . \tag{3.30}$$

The root given by (3.29) is unacceptable in that it does not reduce to $+1$ in the limit as n_0 and I vanish; the two roots given by (3.30) are acceptable in this regard. We must, however, have the sign appearing in (3.30) be opposite to that appearing in (3.27). This is necessary in order that the term involving I make a contribution to $\hbar\Omega$ lying in the same quadrant of the complex plane as does the term involving W. This can be seen by substituting (3.30) into (3.27) and getting

$$\hbar\Omega = p_i - a_i W \pm \alpha_i^{-1} w_i = p_i \pm w_i - a_i \{W + [\tfrac{1}{2}(1+Q)I]^{1/2}\} . \tag{3.31}$$

Making the assumption that the conduction-band effective mass is positive, we see that W and I lie in the same quadrant of the complex ω plane. We take the square root of I that lies in the same quadrant as I. It should be emphasized that Eq. (3.31), having been obtained by expanding in powers of (I/w_i^2), is not correct when $w_i = 0$. Under such conditions, $\hbar\Omega$ must be independent of Q, so that the appropriate solution to Eq. (3.27) is $\alpha_i = 0$, or $\hbar\Omega = p_i - a_i(W + I^{1/2})$. Thus we see that Eq. (3.31) gives the correct answer when $w_i = 0$ if we set $Q = 1$ in the equation.

Defining

$$\mu = \pm 1 , \tag{3.32}$$

$$W' \equiv W + [\tfrac{1}{2}(1+Q)I]^{1/2} , \tag{3.33}$$

so that (3.31) becomes

$$\hbar\Omega = p_i + \mu w_i - a_i W' . \tag{3.34}$$

With the aid of (3.11), we have

$$(p_i - \hbar\Omega + \mu w_i) = L^{-1}[(p_i - \hbar\Omega)^2 - w_i^2] W' \tag{3.35}$$

or

$$L = (p_i - \hbar\Omega - \mu w_i) W' . \tag{3.36}$$

Substituting (2.73) into (3.36) gives us a quadratic equation for $\hbar\Omega$. Solving for $\hbar\omega = \kappa\hbar\Omega$, we get

$$\hbar\omega = \hbar\omega_{\mu\nu} \equiv \epsilon_0 + \tfrac{1}{2}(U_0 - W') + \nu\{\tfrac{1}{4}(U_0 + W')^2 - W'[\tfrac{1}{2}U_0(n_{i\uparrow} + n_{i\downarrow}) + \mu w_i] + (1-\lambda)\,\epsilon_0(\epsilon_0 + U_0) - (1-\kappa)W'[\epsilon_0 + U_0 - \tfrac{1}{2}U_0(n_{i\uparrow} + n_{i\downarrow}) - \mu w_i]\}^{1/2} , \tag{3.37}$$

where

$$\nu = \pm 1 . \tag{3.38}$$

It is understood that the choice of sign for ν is independent of that for μ. In principle, Eq. (3.37) is only an implicit equation for $\hbar\omega$, since κ and λ are functions of $\hbar\omega$. As already mentioned, unless $\hbar\omega$ lies in the immediate vicinity of zero or $2\epsilon_0 + U_0$, κ and λ may be replaced by unity. Since such a contingency very rarely occurs for $\hbar\omega_{\mu\nu}$, we shall make the approximation $\kappa = \lambda = 1$, $\Omega = \omega$, in treating the localized quasiparticles. Thus

$$\hbar\omega_{\mu\nu} = \epsilon_0 + \tfrac{1}{2}(U_0 - W') + \nu\{\tfrac{1}{4}(U_0 + W')^2 - W'[\tfrac{1}{2}U_0(n_{i\uparrow} + n_{i\downarrow}) + \mu w_i]\}^{1/2} . \tag{3.39}$$

From this point on, the self-consistent determination of $\hbar\omega_{\mu\nu}$ follows just as in the treatment of the one-center problem as given in II. It is only necessary to replace W by W'. The determination of the thermal averages $n_{i\sigma}$ and b_i is carried out in Appendix A. Equations (A42)–(A44) express $n_{i\sigma}$ and b_i in terms of the weighted statistical factor g_μ, defined by Eq. (A45).

IV. CONDUCTION-BAND QUASIPARTICLES

We look for solutions to Eq. (2.68). It is *tentatively* assumed that one particular vector coeffi-

cient, say $A_k^\dagger$, is much larger than all other $A_{k'}^\dagger$. Unlike the corresponding assumption in Sec. III, it is by no means obvious that this assumption is true here, even in the limit as n_0, the density of centers, vanishes. We are, in effect, invoking the Born approximation. For $A_k^\dagger$, we have Eq. (2.68), which we write as

$$A_k^\dagger G_k = \sum_{k' \neq k} A_{k'}^\dagger V_k^* V_{k'} \sum_i e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_i} Q_i^{-1} , \tag{4.1}$$

where

$$G_k \equiv (\epsilon_k - \hbar\omega)\tau_4 - |V_k|^2 \textstyle\sum_i Q_i^{-1} . \tag{4.2}$$

For $A_{k'}^\dagger (\vec{k}' \neq \vec{k})$, we have

$$A_{k'}^\dagger G_{k'} = A_{k'}^\dagger V_{k'}^* V_k \sum_j e^{-i(\vec{k}-\vec{k}')\cdot\vec{R}_j} Q_j^{-1} + \sum_{k'' \neq k, k'} A_{k''}^\dagger V_{k''}^* V_{k''} \sum_j e^{-i(\vec{k}''-\vec{k}')\cdot\vec{R}_j} Q_j^{-1} . \tag{4.3}$$

We assume

$$A_{k''}^\dagger \cong A_k^\dagger V_{k''}^* V_k \textstyle\sum_p e^{-i(\vec{k}-\vec{k}'')\cdot\vec{R}_p} Q_p^{-1} G_{k''}^{-1} . \tag{4.4}$$

Substituting (4.4) into (4.3) we get

$$A_{k'}^\dagger = A_k^\dagger V_{k'}^* V_k \left(\sum_j e^{i(\vec{k}'-\vec{k})\cdot\vec{R}_j} Q_j^{-1} + \sum_{k''} |V_{k''}|^2 \sum_{j,p} e^{i(\vec{k}'\cdot\vec{R}_j - \vec{k}\cdot\vec{R}_p)} e^{-i\vec{k}''\cdot(\vec{R}_j-\vec{R}_p)} Q_p^{-1} G_{k''}^{-1} Q_j^{-1} \right) G_{k'}^{-1} . \tag{4.5}$$

Substituting (4.5) into (4.1), we get

$$A_k^\dagger \Big(G_k - |V_k|^2 \sum_{k'} |V_{k'}|^2 \sum_{i,j} e^{i(\vec{k}'-\vec{k})\cdot(\vec{R}_j-\vec{R}_i)} Q_j^{-1} G_{k'}^{-1} Q_i^{-1} - |V_k|^2 \sum_{k',k''} |V_{k'}|^2 |V_{k''}|^2 \times \sum_{i,j,p} e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_p)} e^{i\vec{k}''\cdot(\vec{R}_j-\vec{R}_i)} e^{i\vec{k}'\cdot(\vec{R}_p-\vec{R}_j)} Q_p^{-1} G_{k'}^{-1} Q_j^{-1} G_{k''}^{-1} Q_i^{-1} \Big) = 0 . \tag{4.6}$$

Equation (4.6) represents the *second* Born approximation. Due to destructive interference, the double sum over i and j reduces to a single sum ($i=j$); the triple sum over i, j, and p reduces to a double sum ($i=p$). In the sums over $\vec{k}$ and $\vec{k}'$, we can approximate G_k^{-1} and $G_{k'}^{-1}$ by their values in the limit $n_0 = 0$. Thus (4.6) becomes

$$A_k^\dagger \Big[G_k - |V_k|^2 \sum_i Q_i^{-2} \sum_{k'} |V_{k'}|^2 (\epsilon_{k'} - \hbar\omega)^{-1} - |V_k|^2 \sum_{i,j} Q_i^{-1} Q_j^{-1} Q_i^{-1} \sum_{k',k''} |V_{k'}|^2 |V_{k''}|^2 (\epsilon_{k'} - \hbar\omega)^{-1} (\epsilon_{k''} - \hbar\omega)^{-1} \times e^{-i(\vec{k}'-\vec{k}'')\cdot(\vec{R}_i-\vec{R}_j)} \Big] = 0 . \tag{4.7}$$

In the double sum over i and j, we separate out the terms $i=j$, whereupon we can write (making use of the definitions of I and W)

$$A_k^\dagger \Big[G_k - |V_k|^2 W \Big(\sum_i Q_i^{-2} + W \sum_i Q_i^{-3} \Big) - |V_k|^2 n_0^{-1} I \sum_i Q_i^{-2} \sum_{j \neq i} Q_j^{-1} \Big] = 0 . \tag{4.8}$$

Note that the terms involving W are *linear* in n_0, whereas the terms involving I are *quadratic* in n_0. Thus, in the dilute limit we can drop the latter terms, getting

$$A_k^\dagger \{ G_k - |V_k|^2 \textstyle\sum_i Q_i^{-1} [(WQ_i^{-1}) + (WQ_i^{-1})^2] \} = 0 . \tag{4.9}$$

It can be seen that if we perform the iteration process for $A_k^\dagger$ an indefinite number of times (rather than twice, as done above), then in the low-concentration limit Eq. (4.9) is replaced by

$$A_k^\dagger \Big(G_k - |V_k|^2 \sum_i Q_i^{-1} \sum_{n=1}^{\infty} (WQ_i^{-1})^n \Big) = 0 . \tag{4.10}$$

Keeping only the first n terms in the n series represents the nth *Born approximation*. Fortunately, we can sum this Born series by inspection. Making use of Eq. (3.3), we get

$$A_k^\dagger G_k' = 0 , \tag{4.11}$$

where we are defining

$$G_k' \equiv G_k - |V_k|^2 W \textstyle\sum_i Q_i^{-1} G_i^{-1} . \tag{4.12}$$

Making use of the definitions of G_k and G_i, this can be written

$$G_k' = (\epsilon_k - \hbar\omega)\tau_4 - |V_k|^2 \textstyle\sum_i G_i^{-1} . \tag{4.13}$$

In terms of $a_i = a$ [Eq. (3.11)], we have

$$G_i^{-1} = a[(p - aW - \hbar\Omega)^2 - w^2]^{-1} [(p - aW - \hbar\Omega)\tau_4 + \tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 + \tfrac{1}{2}(\Delta_i - \Delta_i^*) i\tau_2 - q_i\tau_3] . \tag{4.14}$$

Thus

$$\textstyle\sum_i G_i^{-1} = n_0 a[(p - aW - \hbar\Omega)^2 - w^2]^{-1} \{ (p - aW - \hbar\Omega)\tau_4 + Q[\tfrac{1}{2}(\Delta + \Delta^*)\tau_1 + \tfrac{1}{2}(\Delta - \Delta^*) i\tau_2 - q\tau_3] \} , \tag{4.15}$$

so that

$$G_k' = \left((\epsilon_k - \hbar\omega) - \frac{n_0 a |V_k|^2 (p - aW - \hbar\Omega)}{(p - aW - \hbar\Omega)^2 - w^2} \right) \tau_4$$

$$-\frac{n_0 a|V_k|^2 Q}{(p-aW-\hbar\Omega)^2-w^2}[\tfrac{1}{2}(\Delta+\Delta^*)\tau_1+\tfrac{1}{2}(\Delta-\Delta^*)i\tau_2-q\tau_3]. \tag{4.16}$$

Corresponding to Eq. (4.11), we have the secular equation

$$\det G_k' = 0\ , \tag{4.17}$$

which gives

$$\hbar\omega = \hbar\omega_{k\mu} \equiv \epsilon_k - n_0 a|V_k|^2\left(\frac{(p-aW-\hbar\Omega)-\mu Q w}{(p-aW-\hbar\Omega)^2-w^2}\right)\ , \tag{4.18}$$

where

$$\mu = \pm 1\ . \tag{4.19}$$

The two possible roots correspond to the two possible choices of spin orientation of the conduction-band quasiparticle excitations. Note that the two roots are degenerate for either the paramagnetic ($Q=0$) phase or nonmagnetic ($w=0$) phase.

The right-hand side of Eq. (4.18) will diverge if and only if

$$\hbar\Omega = p - aW + \mu w\ . \tag{4.20}$$

Aside from containing W rather than W', Eq. (4.20) is the same as Eq. (3.34), the roots to which give the localized quasiparticle excitation energies $\hbar\omega_{i\mu\nu}$. In the dilute limit, however, the imaginary part of $\kappa^{-1}\hbar\omega_{k\mu}$ is not large enough to satisfy (4.20). This indicates that there are *no gaps* in the conduction-band spectrum, and thus *no possibility* of a second branch to the spectrum (one corresponding, for example, to conduction electrons localizing themselves in the vicinity of the impurity centers). This should be contrasted with the results we would have obtained had we stopped with *any finite order of Born approximation*. Consider, for example, the second Born approximation which gives Eq. (4.9). The corresponding secular equation leads to a self-energy for $\hbar\omega_{k\mu}$ which diverges whenever the quantity L vanishes (in turn occurring for real $\hbar\omega$). It is readily apparent that the same behavior occurs for the nth Born approximation (n finite). The conduction-band energy gaps calculated in I were an artifact of the use of the first Born approximation. We see that the summing of the series appearing in Eq. (4.10) is a crucial step in the present calculation.

Having disposed of the possibility of gaps in the dilute limit, we may, with no loss of accuracy, replace $\omega = \kappa\Omega$ by $\hbar^{-1}\epsilon_k$ everywhere on the right-hand side of (4.18) which may be written

$$\hbar\omega_{k\mu} = \epsilon_k + n_0 a|V_k|^2 \textstyle\sum_\nu \frac{1}{2}(1+\mu\nu Q)(\kappa^{-1}\epsilon_k + aW - p - \nu w)^{-1}, \tag{4.21}$$

where we are defining

$$\nu = \pm 1\ . \tag{4.22}$$

The self-energy W appearing in (4.21) is to be evaluated at $\hbar\omega_1 = \epsilon_k$ while

$$a = L^{-1}(p - \kappa^{-1}\epsilon_k + \omega)(p - \kappa^{-1}\epsilon_k - w)\ , \tag{4.23}$$

$$\kappa L = \epsilon_k^2 - (2\epsilon_0 + U_0)\epsilon_k + \lambda\epsilon_0(\epsilon_0 + U_0)\ , \tag{4.24}$$

Defining

$$W_{3\nu} \equiv a^{-1}(p - \kappa^{-1}\epsilon_k + \nu w) = L(p - \kappa^{-1}\epsilon_k - \nu w)^{-1}$$
$$= \frac{\epsilon_k^2 - (2\epsilon_0 + U_0)\epsilon_k + \lambda\epsilon_0(\epsilon_0 + U_0)}{\kappa[\epsilon_0 + U_0(1 - g_{-\nu})] - \epsilon_k}\ , \tag{4.25}$$

we can write (4.21) as

$$\hbar\omega_{k\mu} = \epsilon_k + n_0|V_k|^2 \textstyle\sum_\nu \frac{1}{2}(1+\mu\nu Q)(W - W_{3\nu})^{-1}\ . \tag{4.26}$$

Making use of the fact that W is the only complex quantity in (4.26), and defining the angle

$$\delta_{\nu k} \equiv \arctan[W_2(W_1 - W_{3\nu})^{-1}]\ , \tag{4.27}$$

we have

$$\hbar\omega_{k\mu} = \epsilon_k + n_0|V_k|^2 \textstyle\sum_\nu \frac{1}{2}(1+\mu\nu Q)[(W_1 - W_{3\nu})^2 + W_2^2]^{-1/2} e^{i\delta_{\nu k}}\ . \tag{4.28}$$

The cross section for scattering of a quasiparticle of wave vector $\vec{k}$ by a localized center is

$$\sigma_k = (n_0 v_k \tau_k)^{-1}\ , \tag{4.29}$$

where τ_k is given by Eq. (2.9). We may approximate the quasiparticle velocity v_k by its value in the dilute limit, namely,

$$v_k = \hbar^{-1}\frac{d\epsilon_k}{dk}\ . \tag{4.30}$$

Combining Eqs. (2.9), (2.84), and (4.27)–(4.30), we get

$$\sigma_k = (4\pi/k^2)\textstyle\sum_\nu \frac{1}{2}(1+\mu\nu Q)\sin^2\delta_{\nu k}\ . \tag{4.31}$$

But, in general, we must have

$$\sigma_k = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_{lk}\ , \tag{4.32}$$

where δ_{lk} is the phase shift of the lth partial wave associated with the quasiparticle of wave vector $\vec{k}$. Thus

$$\textstyle\sum_\nu \frac{1}{2}(1+\mu\nu Q)\sin^2\delta_{\nu k} = \sum_{l=0}^{\infty}(2l+1)\sin^2\delta_{lk}\ . \tag{4.33}$$

As discussed in the Introduction, we invoke the Friedel sum rule[3]

$$Z = \frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)\delta_l\ . \tag{4.34}$$

Here δ_l is δ_{lk} evaluated on the Fermi surface, and Z is the excess number of conduction electrons introduced into the system by each center. As it stands, Eq. (4.34) is not appropriate to a ferromagnetic system. Thus we restrict ourselves to

the nonmagnetic ($w=0$) or paramagnetic ($Q=0$) phase in combining (4.33) and (4.34). If we make the approximation that only s-wave scattering is important (i.e., $\delta_{lk}=0$ for $l>0$), then (4.34) combined with (4.33) becomes

$$\tfrac{1}{2}\sum_\nu \sin^2\delta_\nu = \sin^2(\tfrac{1}{2}\pi Z)\ , \tag{4.35}$$

where δ_ν is $\delta_{\nu k}$ evaluated on the Fermi surface. It is a reasonable approximation to restrict ourselves to $T=0$ in satisfying (4.35), whereupon δ_ν is obtained by substituting into (4.27) the value of $W_{3\nu}$ given by

$$W_{3\nu}=\frac{\epsilon_0(\epsilon_0+U_0)}{\epsilon_0+U_0(1-g_{-\nu})}\ . \tag{4.36}$$

Here we are making use of the fact that

$$\lim_{\omega\to 0,T\to 0}\left(\frac{\lambda}{\kappa}\right)=1\ . \tag{4.37}$$

APPENDIX A

For the purposes of calculating $n_{i\sigma}$ and b_i, we can approximate the quasiparticle operator $\mathcal{O}_i$ by

$$\mathcal{O}_i \cong A_{1i}^\dagger \Psi_{1i} + A_{2i}^\dagger \Psi_{2i}\ . \tag{A1}$$

In other words, we restrict the sum of Eq. (2.46) to terms involving a single center. We hasten to add, however, that the $A_{1i}^\dagger$ and $A_{2i}^\dagger$ in Eq. (A1) are those already calculated in Eqs. (2.61) and (3.18) by taking into account the interaction between centers. For the time being, we drop the center index i. We need to invert Eq. (A1) in order to get Ψ_1 as a function of the four possible $\mathcal{O}$'s (corresponding to the four roots for $\hbar\omega$). Knowing Ψ_1, we can calculate n_σ and b.

First of all, we need to determine the vector coefficients $A_1^\dagger$ and $A_2^\dagger$. Writing

$$\begin{aligned} A_{1\mu}^\dagger &= (a_{1\uparrow\mu}^*,\ a_{1\downarrow\mu}^*)\ , \\ A_{2\mu}^\dagger &= (a_{2\uparrow\mu}^*,\ a_{2\downarrow\mu}^*)\ , \end{aligned} \tag{A2}$$

μ being the quantity of Eq. (3.32), we can express Eq. (3.18) as

$$(a_{1\uparrow\mu}^*,\ a_{1\downarrow\mu}^*)\begin{pmatrix} \mu w-q & \Delta \\ \Delta^* & \mu\omega+q\end{pmatrix}=0\ . \tag{A3}$$

Solving this, we get

$$\begin{aligned} A_{1+}^\dagger &= C_+^{-1}(w+q,\ -\Delta)\ , \\ A_{1-}^\dagger &= C_-^{-1}(+\Delta^*,\ w+q)\ , \end{aligned} \tag{A4}$$

where the C_μ are as yet unknown normalization factors. Equations (2.61) and (3.10), when combined with (A4), yield (setting $\kappa=1$)

$$A_{2\mu}^\dagger = -U_0(p-\hbar\omega-\mu w)^{-1}A_{1\mu}^\dagger\ . \tag{A5}$$

In order to find the normalization factors, we use

$$\langle[\mathcal{O}_\mu,\mathcal{O}_\mu^\dagger]_+\rangle=1\ , \tag{A6}$$

a consequence of $\mathcal{O}_\mu$ being a *fermion* quasiparticle operator. Substituting (A1) into (A6), while making use of Eqs. (2.39)–(2.41), we get

$$A_{1\mu}^\dagger A_{1\mu}+A_{2\mu}^\dagger \mathfrak{U}(\tau_4-\mathfrak{U})A_{2\mu}=1\ . \tag{A7}$$

Equation (2.65) can be written

$$\begin{aligned} U_0^2\mathfrak{U}(\tau_4-\mathfrak{U}) &= -(\epsilon_0-\hbar\omega)(\epsilon_0+U_0-\hbar\omega)\tau_4 \\ &\quad -[(\epsilon_0+U_0-\hbar\omega)\tau_4-U_0\mathfrak{U}]^2+2(\epsilon_0+\tfrac{1}{2}U_0-\hbar\omega) \\ &\quad \times[(\epsilon_0+U_0-\hbar\omega)\tau_4-U_0\mathfrak{U}]\ . \end{aligned} \tag{A8}$$

Thus

$$\begin{aligned} &U_0^2 A_{2\mu}^\dagger \mathfrak{U}(\tau_4-\mathfrak{U})A_{2\mu} \\ &= U_0^2[-(\epsilon_0-\hbar\omega)(\epsilon_0+U_0-\hbar\omega)(p-\hbar\omega-\mu w)^{-2}-1 \\ &\quad +2(\epsilon_0+\tfrac{1}{2}U_0-\hbar\omega)(p-\hbar\omega-\mu w)^{-1}]A_{1\mu}^\dagger A_{1\mu}\ , \end{aligned} \tag{A9}$$

and (A7) becomes

$$\begin{aligned} &[-(\epsilon_0-\hbar\omega)(\epsilon_0+U_0-\hbar\omega)+2(\epsilon_0+\tfrac{1}{2}U_0-\hbar\omega) \\ &\quad \times(p-\hbar\omega-\mu w)](p-\hbar\omega-\mu w)^{-2}A_{1\mu}^\dagger A_{1\mu}=1\ . \end{aligned} \tag{A10}$$

From (A4), we have

$$A_{1\mu}^\dagger A_{1\mu}=|C_\mu|^{-2}2w(w+q)\ . \tag{A11}$$

Thus

$$\begin{aligned} |C_\mu|^2 &= 2w(w+q)(p-\hbar\omega-\mu w)^{-2} \\ &\quad \times 2[(\epsilon_0+\tfrac{1}{2}U_0-\hbar\omega)(p-\hbar\omega-\mu w) \\ &\quad -(\epsilon_0-\hbar\omega)(\epsilon_0+U_0-\hbar\omega)]\ . \end{aligned} \tag{A12}$$

We now introduce the notation $A_{1\mu\nu}^\dagger$, $A_{2\mu\nu}^\dagger$, $\mathcal{O}_{\mu\nu}$, expressing the fact that these quantities depend on both μ and ν. We define

$$\tilde{\mathcal{O}}\equiv\begin{pmatrix}\mathcal{O}_{++}\\ \mathcal{O}_{-+}\\ \mathcal{O}_{+-}\\ \mathcal{O}_{--}\end{pmatrix}\ , \tag{A13}$$

$$\tilde{U}^{-1}\equiv\begin{pmatrix} A_{1++}^\dagger & A_{2++}^\dagger \\ A_{1-+}^\dagger & A_{2-+}^\dagger \\ A_{1+-}^\dagger & A_{2+-}^\dagger \\ A_{1--}^\dagger & A_{2--}^\dagger\end{pmatrix}\ , \tag{A14}$$

$$\tilde{\Psi}\equiv\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}\ . \tag{A15}$$

$\tilde{\mathcal{O}}$ and $\tilde{\Psi}$ are fourth-order column vectors, while $\tilde{U}^{-1}$ is a 4×4 matrix. Equation (A1) can be written

$$\tilde{\mathcal{O}}=\tilde{U}^{-1}\tilde{\Psi}\ , \tag{A16}$$

so that

$$\tilde{\Psi}=\tilde{U}\,\tilde{\mathcal{O}}\ , \tag{A17}$$

where $\tilde{U}$ is the inverse of $\tilde{U}^{-1}$. We define the 2×2 diagonal matrices

$$\tilde{A}_\nu \equiv \begin{pmatrix} a_{+,\nu} & 0 \\ 0 & a_{-,\nu} \end{pmatrix} , \tag{A18}$$

$$\tilde{B}_\nu \equiv \begin{pmatrix} b_{+,\nu} & 0 \\ 0 & b_{-,\nu} \end{pmatrix} , \tag{A19}$$

where

$$a_{\mu\nu} \equiv (p - \hbar\omega_{\mu\nu} - \mu w)\, b_{\mu\nu} , \tag{A20}$$

$$b_{\mu\nu} \equiv [2(\epsilon_0 + \tfrac{1}{2}U_0 - \hbar\omega_{\mu\nu})(p - \hbar\omega_{\mu\nu} - \mu w) - (\epsilon_0 - \hbar\omega_{\mu\nu})(\epsilon_0 + U_0 - \hbar\omega_{\mu\nu})]^{-1/2} . \tag{A21}$$

Here we have written $\hbar\omega_{\mu\nu}$ to indicate that $\hbar\omega$ depends explicitly on μ and ν. [Do not confuse $a_{\mu\nu}$ and $b_{\mu\nu}$ with the a_i of Eq. (3.11) and the b_l of Eq. (2.19).] We also define the 2×2 matrix

$$\mathcal{W}^{-1} \equiv [2w(w+q)]^{-1/2} \begin{pmatrix} w+q & -\Delta \\ +\Delta^* & w+q \end{pmatrix} . \tag{A22}$$

Note that the inverse of this matrix is

$$\mathcal{W} = [2w(w+q)]^{-1/2} \begin{pmatrix} w+q & +\Delta \\ -\Delta^* & w+q \end{pmatrix} . \tag{A23}$$

We define the 4×4 matrix, written in 2×2 block form, as

$$\tilde{M}^{-1} \equiv \begin{pmatrix} \tilde{A}_+ & \tilde{B}_+ \\ \tilde{A}_- & \tilde{B}_- \end{pmatrix} . \tag{A24}$$

Note that the inverse of this matrix is

$$\tilde{M} = \begin{pmatrix} \tilde{B}_- & -\tilde{B}_+ \\ -\tilde{A}_- & \tilde{A}_+ \end{pmatrix} \tilde{D} , \tag{A25}$$

where

$$\tilde{D} \equiv (\tilde{A}_+ \tilde{B}_- - \tilde{B}_+ \tilde{A}_-)^{-1} . \tag{A26}$$

Equation (A25) should be understood to mean that the upper left-hand block of $\tilde{M}$ is $\tilde{B}_-\tilde{D}$, the upper right-hand block is $-\tilde{B}_+\tilde{D}$, etc. Defining

$$d_\mu \equiv (a_{\mu,+} b_{\mu,-} - a_{\mu,-} b_{\mu,+})^{-1} , \tag{A27}$$

we have

$$\tilde{D} = \begin{pmatrix} d_+ & 0 \\ 0 & d_- \end{pmatrix} . \tag{A28}$$

The point of all these definitions is that we can write

$$\tilde{U}^{-1} = \tilde{M}^{-1} \mathcal{W}^{-1} , \tag{A29}$$

so that

$$\tilde{U} = \mathcal{W} \tilde{M} . \tag{A30}$$

The portion of Eq. (A17) of interest here can be written

$$\Psi_1 = \begin{pmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ U_{21} & U_{22} & U_{23} & U_{24} \end{pmatrix} \tilde{\mathcal{O}} \tag{A31}$$

or

$$\begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ U_{21} & U_{22} & U_{23} & U_{24} \end{pmatrix} \begin{pmatrix} \mathcal{O}_{++} \\ \mathcal{O}_{-+} \\ \mathcal{O}_{+-} \\ \mathcal{O}_{--} \end{pmatrix} . \tag{A32}$$

We have

$$\begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \mathcal{W} \tilde{B}_- \tilde{D} = [2w(w+q)]^{-1/2} \begin{pmatrix} w+q & +\Delta \\ -\Delta^* & w+q \end{pmatrix} \begin{pmatrix} b_{+-} d_+ & 0 \\ 0 & b_{--} d_- \end{pmatrix} , \tag{A33}$$

$$\begin{pmatrix} U_{13} & U_{14} \\ U_{23} & U_{24} \end{pmatrix} = -\mathcal{W} \tilde{B}_+ \tilde{D} = -[2w(w+q)]^{-1/2} \begin{pmatrix} w+q & +\Delta \\ -\Delta^* & w+q \end{pmatrix} \begin{pmatrix} b_{++} d_+ & 0 \\ 0 & b_{-+} d_- \end{pmatrix} . \tag{A34}$$

Substituting (A32) into the equations

$$\langle [c_\sigma, c_\sigma^\dagger]_+ \rangle = 1 , \tag{A35}$$

while making use of

$$\langle [\mathcal{O}_{\mu\nu} \mathcal{O}^\dagger_{\mu'\nu'}]_+ \rangle = \delta_{\mu\mu'} \delta_{\nu\nu'} , \tag{A36}$$

we get the results

$$(|U_{11}|^2 + |U_{12}|^2 + |U_{13}|^2 + |U_{14}|^2) = (|U_{21}|^2 + |U_{22}|^2 + |U_{23}|^2 + |U_{24}|^2) = 1 . \tag{A37}$$

Inserting (A33) and (A34) into (A37), we find

$$|d_\mu|^{-2} = \textstyle\sum_\nu |b_{\mu\nu}|^2 . \tag{A38}$$

We define the statistical factor

$$f \equiv \pi^{-1} |\omega_2| \int d\omega' [(\omega' - \omega_1)^2 + \omega_2^2]^{-1} \times (e^{\beta\hbar\omega'} + 1)^{-1} \tag{A39}$$

associated with the excitation

$$\omega \equiv \omega_1 - i\omega_2 \tag{A40}$$

(ω_1 and ω_2 being real). It can be shown that

$$\langle \mathcal{O}^\dagger_{\mu\nu} \mathcal{O}_{\mu'\nu'} \rangle = f_{\mu\nu} \delta_{\mu\mu'} \delta_{\nu\nu'} , \tag{A41}$$

where $f_{\mu\nu}$ is the statistical factor associated with $\omega_{\mu\nu}$. Substituting (A32) into the definitions of $n_{i\sigma}$ and b_i, while making use of (A33), (A34), and (A38), we get

$$(n_{i\uparrow} + n_{i\downarrow}) = (g_- + g_+) , \tag{A42}$$

$$(n_{i\uparrow} - n_{i\downarrow}) = (q_i/w)(g_- - g_+) , \tag{A43}$$

$$b_i = (\Delta_i/2w)(g_- - g_+) , \tag{A44}$$

where we are defining the *weighted* statistical factor

$$g_\mu \equiv (\textstyle\sum_\nu |b_{\mu\nu}|^{-2})^{-1} (\sum_\nu |b_{\mu\nu}|^{-2} f_{\mu\nu}) . \quad \text{(A45)}$$

Note that both $f_{\mu\nu}$ and g_μ are real, and lie between zero and one. Equations (A42)–(A45) were used (but not derived) in II. The matrix $\mathfrak{u}_i$ of Eq. (2.38) can be written as

$$\mathfrak{u}_i = (2w)^{-1} \textstyle\sum_\mu g_\mu \{ w\tau_4 + \mu [q_i \tau_3 - \frac{1}{2} (\Delta_i + \Delta_i^*) \tau_1 - \frac{1}{2} (\Delta_i - \Delta_i^*) i\tau_2] \} . \quad \text{(A46)}$$

APPENDIX B

For purposes of calculating $n_{k\sigma}$ and b_k, we can approximate the quasiparticle operator $\mathcal{O}_k$ by

$$\mathcal{O}_k \cong A_k^\dagger \Psi_k . \quad \text{(B1)}$$

In other words, we restrict the sum of Eq. (2.46) to the term involving a single Bloch wave. We hasten to add, however, that the $A_k^\dagger$ in Eq. (B1) is that calculated in Eq. (4.11) by taking into account the interaction between Bloch waves. It is necessary to invert Eq. (B1) in order to get Ψ_k as a function of the two possible $\mathcal{O}_k$'s (corresponding to the two roots for $\hbar\omega_k$). Knowing Ψ_k, we can calculate $n_{k\sigma}$ and b_k. For the time being, we restrict ourselves to the case $Q=1$ [where Q is given by Eq. (3.21)], whereupon q_i and Δ_i are independent of the site index i.

Writing

$$A_{k\mu}^\dagger = (a_{k\uparrow\mu}^*, a_{k\downarrow\mu}^*) , \quad \text{(B2)}$$

μ being the quantity of Eq. (4.19), we can express Eq. (4.11) as

$$(a_{k\uparrow\mu}^*, a_{k\downarrow\mu}^*) \begin{pmatrix} \mu w - q & \Delta \\ \Delta^* & \mu w + q \end{pmatrix} = 0 . \quad \text{(B3)}$$

Solving for $A_{k\mu}^\dagger$, we find

$$\begin{aligned} A_{k+}^\dagger &= [2w(w+q)]^{-1/2} (w+q, -\Delta) , \\ A_{k-}^\dagger &= [2w(w+q)]^{-1/2} (+\Delta^*, w+q) . \end{aligned} \quad \text{(B4)}$$

Here we have chosen the normalization such that

$$A_{k\mu}^\dagger A_{k\mu} = 1 , \quad \text{(B5)}$$

thereby ensuring that $\mathcal{O}_\mu$ satisfies Eq. (A6).

Writing

$$\tilde{\mathcal{O}}_k \equiv \begin{pmatrix} \mathcal{O}_{k+} \\ \mathcal{O}_{k-} \end{pmatrix} , \quad \text{(B6)}$$

we can reexpress Eq. (B1) as

$$\tilde{\mathcal{O}}_k = \mathcal{W}^{-1} \Psi_k , \quad \text{(B7)}$$

so that

$$\Psi_k = \mathcal{W} \tilde{\mathcal{O}}_k , \quad \text{(B8)}$$

W being the 2×2 matrix of Appendix A. We substitute (B8) into the definitions of $n_{k\sigma}$ and b_k, while making use of

$$\langle \mathcal{O}_{k\mu}^\dagger \mathcal{O}_{k\mu'} \rangle = f_{k\mu} \delta_{\mu\mu'} , \quad \text{(B9)}$$

$f_{k\mu}$ being the statistical factor [Eq. (A39)] associated with $\omega_{k\mu}$. We obtain

$$(n_{k\downarrow} + n_{k\uparrow}) = (f_{k-} + f_{k+}) , \quad \text{(B10)}$$

$$(n_{k\downarrow} - n_{k\uparrow}) = (q/w)(f_{k-} - f_{k+}) , \quad \text{(B11)}$$

$$b_k = (\Delta/2w)(f_{k-} f_{k+}) . \quad \text{(B12)}$$

Although these results were derived for the case $Q=1$, they are actually true for the case $Q=0$ as well, where $(n_{k\downarrow} - n_{k\uparrow})$ and b_k vanish. For the latter case, $\hbar\omega_{k+} = \hbar\omega_{k-}$ and $\mathcal{O}_{k\mu}$ is an *arbitrary* linear combination of $c_{k\uparrow}$ and $c_{k\downarrow}$. The use of Eq. (B4) for $Q=0$ corresponds to taking $\mathcal{O}_{k\mu}$ to be a quasiparticle operator associated with a spin parallel (or antiparallel) to the net spin associated with a localized center having $q_i = q$, $\Delta_i = \Delta$. The thermal averages $n_{k\sigma}$ and b_k are necessarily independent of what linear combination of $c_{k\uparrow}$ and $c_{k\downarrow}$ is used in constructing $\mathcal{O}_{k\mu}$.

The matrix $\mathfrak{u}_k$ of Eq. (2.38) can be written as

$$\mathfrak{u}_k = (2w)^{-1} \textstyle\sum_\mu f_{k\mu} \{ w\tau_4 + \mu [q\tau_3 - \frac{1}{2} (\Delta + \Delta^*) \tau_1 - \frac{1}{2} (\Delta - \Delta^*) i\tau_2] \} . \quad \text{(B13)}$$

APPENDIX C

For purposes of calculating $n_{ik\sigma}$ and $b_{ik\sigma}$, and thus the elements of the matrix $\mathfrak{v}_{ik}$, we need to approximate the quasiparticle operators $\mathcal{O}_i$ and $\mathcal{O}_k$ more accurately than was done in Appendixes A and B. It is convenient to concentrate on some particular $\vec{k}$ and i. This allows us to use the same matrix $\mathcal{W}$, in connection with $\mathcal{O}_k$, for both cases $Q=0$ and and $Q=1$, just as was done in Appendix B.

First we consider $\mathcal{O}_i$. Rather than Eq. (A1), we write

$$\mathcal{O}_i \cong A_{1i}^\dagger \Psi_{1i} + A_{2i}^\dagger \Psi_{2i} + A_k^\dagger \Psi_k . \quad \text{(C1)}$$

But here

$$\begin{aligned} A_k^\dagger &= -(\epsilon_k - \hbar\omega_i)^{-1} \textstyle\sum_j A_{1j}^\dagger V_{kj}^* \\ &\cong -(\epsilon_k - \hbar\omega_i)^{-1} A_{1i}^\dagger V_{ki}^* , \end{aligned} \quad \text{(C2)}$$

since $A_{1j}^\dagger \gg A_{1i}^\dagger$ for $j \neq i$. Thus

$$\mathcal{O}_i \cong A_{1i}^\dagger \Psi_{1i} + A_{2i}^\dagger \Psi_{2i} - (\epsilon_k - \hbar\omega_i)^{-1} A_{1i}^\dagger V_{ki}^* \Psi_k . \quad \text{(C3)}$$

We define the 4×4 matrix, written in 2×2 block form, as

$$\tilde{Z} \equiv \begin{pmatrix} \tilde{Z}_+ & 0 \\ 0 & \tilde{Z}_- \end{pmatrix} , \quad \text{(C4)}$$

where

$$\tilde{Z}_\nu \equiv \begin{pmatrix} z_{+\nu} & 0 \\ 0 & z_{-\nu} \end{pmatrix} , \quad \text{(C5)}$$

$$z_{\mu\nu} \equiv (\epsilon_k - \hbar\omega_{i\mu\nu})^{-1} . \quad \text{(C6)}$$

In matrix form, Eq. (C3) can be written

$$\tilde{\mathcal{O}}_i = \tilde{U}^{-1}\tilde{\Psi}_i - \tilde{Z}\,(\tilde{U}^{-1})_{\text{left}}\,V_{ki}^{*}\Psi_k\,, \tag{C7}$$

where $(\tilde{U}^{-1})_{\text{left}}$ is a 4×2 matrix consisting of the left half of the 4×4 matrix $\tilde{U}^{-1}$ of Appendix A. We also designate by $\tilde{U}_{\text{top}}$ the 2×4 matrix consisting of the top half of the $\tilde{U}$ matrix. Premultiplying (C7) by $\tilde{U}_{\text{top}}$, we get

$$\tilde{U}_{\text{top}}\tilde{\mathcal{O}}_i = \Psi_{1i} - \tilde{U}_{\text{top}}\tilde{Z}\,(\tilde{U}^{-1})_{\text{left}}\,V_{ki}^{*}\Psi_k\,. \tag{C8}$$

With the aid of Eqs. (A29), (A30), and (B8), this becomes

$$\Psi_{1i} = \tilde{U}_{\text{top}}\tilde{\mathcal{O}}_i + V_{ki}^{*}\tilde{\mathcal{W}}\tilde{\mathcal{K}}_k\tilde{\mathcal{O}}_k\,, \tag{C9}$$

where we are defining the 2×2 matrix

$$\tilde{\mathcal{K}}_k \equiv \tilde{M}_{\text{top}}\tilde{Z}(\tilde{M}^{-1})_{\text{left}}\,. \tag{C10}$$

From the definition of $\tilde{M}$ in Appendix A, we get

$$\tilde{\mathcal{K}}_k = \tilde{D}(\tilde{B}_-\tilde{A}_+\tilde{Z}_+ - \tilde{B}_+\tilde{A}_-\tilde{Z}_-)\,. \tag{C11}$$

Writing

$$\tilde{\mathcal{K}}_k = \begin{pmatrix} \mathcal{K}_{k+} & 0 \\ 0 & \mathcal{K}_{k-} \end{pmatrix}, \tag{C12}$$

we have

$$\mathcal{K}_{k\mu} = d_\mu\,(b_\mu - a_{\mu+}z_{\mu+} - b_{\mu+}a_{\mu-}z_{\mu-})$$

$$= \frac{(a_{\mu+}/b_{\mu+})\,z_{\mu+} - (a_{\mu-}/b_{\mu-})\,z_{\mu-}}{(a_{\mu+}/b_{\mu+}) - (a_{\mu-}/b_{\mu-})}\,. \tag{C13}$$

Equations (A20) and (C6) allow this to be rewritten as

$$\mathcal{K}_{k\mu} = (\hbar\omega_{i\mu-} - \hbar\omega_{i\mu+})^{-1}$$

$$\times\left[\left(\frac{p-\mu w-\hbar\omega_{i\mu+}}{\epsilon_k-\hbar\omega_{i\mu+}}\right) - \left(\frac{p-\mu w-\hbar\omega_{i\mu-}}{\epsilon_k-\hbar\omega_{i\mu-}}\right)\right]. \tag{C14}$$

It is convenient to make the decomposition

$$\tilde{\mathcal{K}}_k = \mathcal{K}_{k3}\tau_3 + \mathcal{K}_{k4}\tau_4\,, \tag{C15}$$

where

$$\mathcal{K}_{k3} \equiv \tfrac{1}{2}\,(\mathcal{K}_{k+} - \mathcal{K}_{k-})\,,$$
$$\mathcal{K}_{k4} \equiv \tfrac{1}{2}\,(\mathcal{K}_{k+} + \mathcal{K}_{k-})\,. \tag{C16}$$

Thus Eq. (C9) becomes

$$\Psi_{1i} = \tilde{U}_{\text{top}}\tilde{\mathcal{O}}_i + V_{ki}^{*}(\mathcal{K}_{k4}\,\mathcal{W} + \mathcal{K}_{k3}\,\mathcal{W}\tau_3)\,\tilde{\mathcal{O}}_k\,. \tag{C17}$$

This result differs from Eq. (A31) by the presence of the term containing $\tilde{\mathcal{O}}_k$.

Next we consider $\mathcal{O}_k$. Rather than Eq. (B1), we write

$$\mathcal{O}_k \cong A_k^{\dagger}\Psi_k + A_{1i}^{\dagger}\Psi_{1i}\,. \tag{C18}$$

But now

$$A_{1i}^{\dagger} = -L^{-1}\textstyle\sum_{k'} A_{k'}^{\dagger}\,V_{k'i}\,[(\epsilon_0 + U_0 - \hbar\Omega_k)\,\tau_4 - U_0\,\mathfrak{U}_i\,]$$

$$\cong -L^{-1}A_k^{\dagger}\,V_{ki}\,[(\epsilon_0 + U_0 - \hbar\Omega_k)\,\tau_4 - U_0\mathfrak{U}_i\,]\,, \tag{C19}$$

since $A_{k'}^{\dagger} \ll A_k^{\dagger}$ for $\vec{k}' \neq \vec{k}$. In a manner analogous to the proof of Eq. (A5), we can show that the above expression can be rewritten as

$$A_{1i\mu}^{\dagger} = -L^{-1}(p - \mu w - \kappa^{-1}\hbar\omega_{k\mu})\,V_{ki}A_k^{\dagger}\,. \tag{C20}$$

In matrix form, Eq. (C18) becomes

$$\tilde{\mathcal{O}}_k = \mathcal{W}^{-1}\Psi_k - \tilde{g}_k\mathcal{W}^{-1}V_{ki}\Psi_{1i}\,, \tag{C21}$$

where we are defining the 2×2 matrix as

$$\tilde{g}_k \equiv \begin{pmatrix} g_{k+} & 0 \\ 0 & g_{k-} \end{pmatrix}, \tag{C22}$$

$$g_{k\mu} \equiv L^{-1}(p - \mu w - \kappa^{-1}\hbar\omega_{k\mu})\,. \tag{C23}$$

Here

$$L = \kappa^{-1}\,[(\hbar\omega_{k\mu})^2 - (2\epsilon_0 + U_0)\,\hbar\omega_{k\mu} + \lambda\epsilon_0(\epsilon_0 + U_0)]$$

$$= \kappa^{-1}\,[(\epsilon_0 - \hbar\omega_{k\mu})\,(\epsilon_0 + U_0 - \hbar\omega_{k\mu}) + (\lambda - 1)\,\epsilon_0(\epsilon_0 + U_0)]\,. \tag{C24}$$

Premultiplying Eq. (C21) by $\mathcal{W}$, and making use of Eq. (A31), we get

$$\Psi_k = \mathcal{W}\tilde{\mathcal{O}}_k + V_{ki}\mathcal{W}\tilde{g}_k\mathcal{W}^{-1}U_{\text{top}}\tilde{\mathcal{O}}_i\,. \tag{C25}$$

Just as with $\mathcal{K}_k$, it is convenient to make the decomposition

$$\tilde{g}_k = g_{k3}\tau_3 + g_{k4}\tau_4\,, \tag{C26}$$

$$g_{k3} \equiv \tfrac{1}{2}\,(g_{k+} - g_{k-})\,,$$
$$g_{k4} \equiv \tfrac{1}{2}\,(g_{k+} + g_{k-})\,. \tag{C27}$$

Thus Eq. (C25) becomes

$$\Psi_k = \mathcal{W}\tilde{\mathcal{O}}_k + V_{ki}\,(g_{k4}\,\tilde{U}_{\text{top}} + g_{k3}\,\tilde{U}'_{\text{top}})\,\tilde{\mathcal{O}}_i\,, \tag{C28}$$

where we are defining the 4×4 matrix

$$\tilde{U}' \equiv \mathcal{W}\tau_3\tilde{M}\,. \tag{C29}$$

This result differs from Eq. (B8) by the presence of the term involving $\tilde{\mathcal{O}}_i$.

With the aid of Eqs. (C17) and C28), we can now determine $n_{ik\sigma}$ and $b_{ik\sigma}$. The results are most conveniently expressed in the form

$$(n_{ik\uparrow} + n_{ik\uparrow}) = V_{ki}\textstyle\sum_\mu\,(g_{k\mu}\,g_\mu + \mathcal{K}_{k\mu}f_{k\mu})\,, \tag{C30}$$

$$(n_{ik\uparrow} - n_{ik\uparrow}) = V_{ki}(q_i/w)\textstyle\sum_\mu\,\mu\,(g_{k\mu}\,g_\mu + \mathcal{K}_{k\mu}\,f_{k\mu})\,, \tag{C31}$$

$$b_{ik\uparrow} = V_{ki}(\Delta_i/2w)\textstyle\sum_\mu\,\mu\,(g_{k\mu}\,g_\mu + \mathcal{K}_{k\mu}\,f_{k\mu})\,, \tag{C32}$$

$$b_{ik\downarrow} = V_{ki}(\Delta_i^{*}/2w)\textstyle\sum_\mu\,\mu\,(g_{k\mu}\,g_\mu + \mathcal{K}_{k\mu}\,f_{k\mu})\,, \tag{C33}$$

where g_μ and $f_{k\mu}$ are the statistical factors defined in Appendixes A and B, respectively. In order to evaluate $g_{k\mu}$ and $\mathcal{K}_{k\mu}$, we introduce the approximations

$$\hbar\omega_{i\mu\nu} \cong \epsilon_\nu \equiv \epsilon_0 + \tfrac{1}{2}\,(1+\nu)\,U_0\,, \tag{C34}$$

$$\hbar\omega_{k\mu} \cong \epsilon_k \tag{C35}$$

into Eqs. (C14) and (C23), respectively, obtaining

$$\mathcal{K}_{k\mu} = -U_0^{-1} \sum_\nu \nu(p - \mu w - \epsilon_\nu)(\epsilon_k - \epsilon_\nu)^{-1}$$

$$= -(p - \mu w - \epsilon_k)(\epsilon_0 - \epsilon_k)^{-1}(\epsilon_0 + U_0 - \epsilon_k)^{-1} , \tag{C36}$$

and

$$\mathcal{G}_{k\mu} = [(\epsilon_0 - \epsilon_k)(\epsilon_0 + U_0 - \epsilon_k) + (\lambda - 1)\epsilon_0(\epsilon_0 + U_0)]^{-1} \times [\kappa(p - \mu w) - \epsilon_k] . \tag{C37}$$

[In (C37), λ and κ are to be evaluated at $\hbar\omega = \epsilon_k$.] These approximate expressions for $\hbar\omega_{i\mu\nu}$ and $\hbar\omega_{k\mu}$ are correct in the limit $V_{ki} \to 0$. Thus (C36) and (C37), inserted into (C30)–(C33), will result in values of $n_{ik\sigma}$ and $b_{ik\sigma}$ accurate to terms linear in V_{ki}, which is sufficient for our purposes. Making use of Eq. (2.4) and the fact that ϵ_k has inversion symmetry in k space, we immediately obtain Eqs. (2.24) and (2.25). The matrix $\mathcal{U}_{ik}$ of Eq. (2.37) can be expressed as

$$V_{ki}^* \mathcal{U}_{ki} = (2w)^{-1} |V_k|^2 \sum_\mu (\mathcal{G}_{k\mu} g_\mu + \mathcal{K}_{k\mu} f_{k\mu}) \times \{w\tau_4 + \mu[q_i\tau_3 - \tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 - \tfrac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2]\} . \tag{C38}$$

APPENDIX D

For purposes of calculating the sums of Eq. (2.58), we can approximate κ and λ by unity in $\mathcal{G}_{k\mu}$ [Eq. (C37)], as it appears in $V_{ki}^* \mathcal{U}_{ki}$ [Eq. (C38)]. This approximation gives

$$\mathcal{G}_{k\mu} = -\mathcal{K}_{k\mu} = U_0^{-1} \sum_\nu \nu(p - \mu w - \epsilon_\nu)(\epsilon_k - \epsilon_\nu)^{-1} , \tag{D1}$$

so that (C38) becomes

$$V_{ki}^* \mathcal{U}_{ki} = (4wU_0)^{-1} |V_k|^2 \sum_{\mu,\nu} \nu(p - \mu w - \epsilon_\nu)(\epsilon_k - \epsilon_\nu)^{-1} \times \{w\tau_4 + \mu[q_i\tau_3 - \tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 - \tfrac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2]\} \times [(1 - 2f_{k\mu}) - (1 - 2g_\mu)] . \tag{D2}$$

First we consider the matrix sum

$$S_i \equiv \sum_k V_{ki}^* \mathcal{U}_{ki}(\epsilon_k - \hbar\omega)^{-1} . \tag{D3}$$

Substituting (D2) into (D3), we note that the contribution to S_i coming from terms proportional to $(1 - 2g_\mu)$ can always be expressed as a linear combination of the self-energy differences $[W(\hbar\omega) - W(\epsilon_\nu)]$. Invoking the approximation that $W(\hbar\omega)$ is independent of the magnitude of ω_1, then these differences will vanish. (We shall ignore the possibility of any residual imaginary portions in the combination of differences of the W's.) Invoking (C35) in the evaluation of $(1 - 2f_{k\mu})$, i.e.,

$$(1 - 2f_{k\mu}) = \tanh(\tfrac{1}{2}\beta\epsilon_k) , \tag{D4}$$

we see that S_i can be written as

$$S_i = (2U_0)^{-1} \times \sum_\nu [(p - \epsilon_\nu)\tau_4 - q_i\tau_3 + \tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 + \tfrac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2] \times \sum_k |V_k|^2 (\epsilon_k - \epsilon_\nu)^{-1}(\epsilon_k - \hbar\omega)^{-1} \tanh(\tfrac{1}{2}\beta\epsilon_k) . \tag{D5}$$

Approximating the factor $(\epsilon_k - \epsilon_\nu)^{-1}$ by its value at $\epsilon_k = 0$, we get

$$S_i = [p\tau_4 - q_i\tau_3 + \tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 + \tfrac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2] \times [2\epsilon_0(\epsilon_0 + U_0)]^{-1} \sum_k |V_k|^2 (\epsilon_k - \hbar\omega)^{-1} \tanh(\tfrac{1}{2}\beta\epsilon_k) . \tag{D6}$$

Comparing this with Eq. (3.9), we see that

$$S_i = U_0^{-1} P(\hbar\omega)[(\epsilon_0 + U_0)\tau_4 - U_0\mathfrak{U}_i] , \tag{D7}$$

where

$$P(\hbar\omega) \equiv [2\epsilon_0(\epsilon_0 + U_0)]^{-1} U_0 \sum_k |V_k|^2 (\epsilon_k - \hbar\omega)^{-1} \tanh(\tfrac{1}{2}\beta\epsilon_k) . \tag{D8}$$

In a similar fashion, if we consider the sum

$$S_i' \equiv \sum_k V_{ki} \mathcal{U}_{ki}^\dagger (\epsilon_k - \hbar\omega')^{-1} , \tag{D9}$$

where

$$\hbar\omega' \equiv 2\epsilon_0 + U_0 - \hbar\omega , \tag{D10}$$

then we find

$$S_i' = U_0^{-1} P(\hbar\omega')[(\epsilon_0 + U_0)\tau_4 - U_0\mathfrak{U}_i] . \tag{D11}$$

Substituting (D7) and (D11) into Eq. (2.58), we see that

$$\kappa = 1 + P(\hbar\omega) + P(\hbar\omega') . \tag{D12}$$

We next consider the sums of Eq. (2.59). In particular, we define

$$\bar{S}_i \equiv \sum_k |V_k|^2 (\mathfrak{U}_i - \mathfrak{U}_k)[(\epsilon_k - \hbar\omega)^{-1} - (\epsilon_k - \hbar\omega')^{-1}] . \tag{D13}$$

Using Eqs. (A46) and (B13), we have

$$\bar{S}_i = (4w)^{-1} \sum_k |V_k|^2 [(\epsilon_k - \hbar\omega)^{-1} - (\epsilon_k - \hbar\omega')^{-1}] \times \sum_\mu [(1 - 2f_{k\mu}) - (1 - 2g_\mu)]\{\omega\tau_4 + \mu[q_i\tau_3 - \tfrac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 - \tfrac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2]\} . \tag{D14}$$

As with the previous sums, the contributions to $\bar{S}_i$ coming from terms proportional to $(1 - 2g_\mu)$ can be expressed as linear combinations of the self-energy differences $[W(\hbar\omega) - W(\hbar\omega')]$, which will be neglected. Approximating $(1 - 2f_{k\mu})$ by (D4), we get

$$\bar{S}_i = \tfrac{1}{2}\sum_k |V_k|^2 [(\epsilon_k - \hbar\omega)^{-1} - (\epsilon_k - \hbar\omega')^{-1}] \tanh(\tfrac{1}{2}\beta\epsilon_k)\tau_4 . \tag{D15}$$

Substituting (D8) and (D15) into Eq. (2.59), we see that

$$\lambda = 1 + P(\hbar\omega) - P(\hbar\omega') . \tag{D16}$$

In the k sum defining $P(\hbar\omega)$, we assume that $|V_k|^2$ is an *even* function of ϵ_k. Since $\tanh(\frac{1}{2}\beta\epsilon_k)$ is *odd* in ϵ_k, we can replace $(\epsilon_k - \hbar\omega)^{-1}$ in the summand by its *odd* portion, namely, $\epsilon_k[\epsilon_k^2 - (\hbar\omega)^2]^{-1}$. Thus we have

$$P(\hbar\omega) = [2\epsilon_0(\epsilon_0 + U_0)]^{-1} U_0 \sum_k |V_k|^2 \times \epsilon_k[\epsilon_k^2 - (\hbar\omega)^2]^{-1} \tanh(\tfrac{1}{2}\beta\epsilon_k) \ . \quad \text{(D17)}$$

Let us invoke Eq. (2.69) in evaluating (D17). We see that the imaginary parts of the summand cancel, and

$$P(\hbar\omega) = P(\hbar\omega_1) = (2\pi)^{-3}[2\epsilon_0(\epsilon_0 + U_0)]^{-1} U_0 \times \mathcal{P} \int d^3k \, |V_k|^2 [\epsilon_k^2 - (\hbar\omega_1)^2]^{-1} \epsilon_k \tanh(\tfrac{1}{2}\beta\epsilon_k) \ . \quad \text{(D18)}$$

For simplicity, we now make the usual assumptions:

$$(2\pi)^{-3} \int d^3k = \rho \int_{-D}^{+D} d\epsilon_k \ , \quad \text{(D19)}$$

$$|V_k|^2 = V^2 \ , \quad \text{(D20)}$$

so that

$$P(\hbar\omega_1) = -\tfrac{1}{2}\Gamma \int_{-D}^{+D} [\epsilon^2 - (\hbar\omega_1)^2]^{-1} \epsilon \tanh(\tfrac{1}{2}\beta\epsilon) \, d\epsilon \ , \quad \text{(D21)}$$

where we are defining

$$\Gamma \equiv -\rho V^2 U_0 / \epsilon_0(\epsilon_0 + U_0) \ .$$

As has been shown by Theumann,[9] (D21) can be written approximately as

$$P(\hbar\omega_1) = \Gamma \ln\left(\frac{[(\pi k_B T)^2 + (\hbar\omega_1)^2]^{1/2}}{D + |\hbar\omega_1|}\right) \ . \quad \text{(D22)}$$

For $|\hbar\omega_1| \ll D$, we have

$$1 + P(\hbar\omega_1) = \Gamma \ln\{T_K^{-1}[T^2 + (\hbar\omega_1/\pi k_B)^2]^{1/2}\} \ , \quad \text{(D23)}$$

where

$$T_K = \pi^{-1} D e^{-1/\Gamma} \quad \text{(D24)}$$

is the Kondo temperature.

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*Work supported in part by the U. S. Office of Naval Research.

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