of lower-energy modes caused by the advent of surface states. The alloy spectrum [Fig. 1(c)] shows interesting peaks near $60J_0$, which is the range in which local s modes are predicted to arise when an $S=\frac{7}{2}$ impurity is placed in $S=\frac{5}{2}$ host (with a doubling of J). In fact, the exact prediction for an isolated impurity[7] is $57J_0$.

The specific heat and magnetization can be calculated readily using the prescriptions given by previous authors.[9,10] Dramatic specific-heat changes, for example, would not be expected[16] in the alloy treated numerically above, since $\epsilon(=J'/J-1)$ had the value $\frac{1}{2}$ or -1; the low-lying resonance modes which enhance the specific heat greatly are present for $0<|\epsilon|<0.2$, the latter inequality being approximate. Combining the condition for low-lying resonances with the ability to calculate detailed magnetic spectra of alloys allows one to design materials with substantially altered specific heats and theoretically predict that property.

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Localized Correlations in Narrow Conduction Bands. I

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We have studied the effects of an exchange-enhanced substitutional impurity on a host metal by double-time Green's functions. We have used a simplification of the Wolff model to describe this system, i.e., a one-band model in which Coulomb interactions in the host lattice are neglected, and the impurity is represented by $Un_\sigma n_{\bar{\sigma}}+V(n_\sigma+n_{\bar{\sigma}})$, where n_σ is the electron occupation number for spin σ at the impurity site. A decoupling scheme is used in which operators on the exchange-enhanced site are never separated from each other in the process of decoupling. This leads to a singular integral equation for the localized Green's function of the exchange-enhanced site, in terms of which all the one-electron properties of the system are expressible. The integral equation, assuming essentially a Lorentzian density of states for the host lattice, is exactly solvable in the U-infinite, V-finite limit, as well as for the special case of electron-hole symmetry, $U+2V=0$. Numerical results for the U-infinite, V-zero limit for zero temperature are obtained for n_0, the number of electrons on the impurity site, and for the one-electron t matrix as a function of energy. n_0 has a value of 0.4, which may be compared with the values $n_0=0$ predicted by the Hartree-Fock theory and $n_0=\frac{2}{3}$ obtained by using a determinantal wave function from which the doubly occupied state is projected out. The t matrix is found to exhibit a characteristic Kondo-like resonance at zero energy, and indicates a resistivity which falls rapidly with increasing temperature, as well as a specific-heat anomaly.

I. INTRODUCTION

THE purpose of this paper is to establish the basis for a new approach to the problem of a magnetic impurity in a narrow energy band.

Until a few years ago, it was generally believed that the localized Coulomb interaction associated with magnetic impurities in metals and heavily doped semiconductors could be understood within the context of Hartree-Fock theory.[1,2] The inadequacy of this point of view became clear with the now famous work of Kondo[3] on the logarithmic divergence in the host conduction-electron t matrix. In the model studied by Kondo, the s-d Hamiltonian, strong localized correlations enter indirectly through the assumption that a local spin exists in the electron gas. In order to study the strong Coulomb interactions present on certain impurities a model which explicitly exhibits these interactions is obviously needed. The extraorbital model of a magnetic impurity due to Anderson meets this requirement, and considerable effort has been expended[4] during the past few years in studying correlations in this system. It appears clear that for certain situations, namely, for transition-metal impurities in transition metals and particularly for heavily doped semiconductors,[5] a one-band model such as was studied within

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the Hartree-Fock approximation by Wolff[2] is more appropriate. Because of our interest in the above-mentioned systems, we have adopted a modification of the Wolff model to study. The model consists of a narrow conduction band in which Coulomb and potential scattering is effective at only one Wannier site, the impurity site. The model resembles the one studied by Hubbard,[6] with the crucial difference that in our case only one site has the Coulomb interaction.

Central to obtaining an adequate understanding of the behavior of this model is a careful treatment of electron correlations at the impurity site. To this end we have found the equation-of-motion technique well suited. In decoupling the equations of motions, we have been guided by the requirement of never violating equal-time electron correlations at the impurity site. Equations of motion for the electron Green's functions consistent with this requirement have been obtained and solved for in certain limiting cases.

An alternative approach to localized correlations within the one-band model has been taken by Suhl and co-workers.[7,8] They employ diagrammatic techniques and configuration averaging to obtain localization. Their approach, which attempts to properly renormalize the low-frequency singularity in the susceptibility present within the Hartree-Fock approximation, is very different from ours and we have found it difficult at present to draw any parallels between their work and ours.

This paper represents the first in a series in which we hope to extend our treatment to finite magnetic fields, generalize our model to include the possibility that the impurity site has a different coupling to its neighbors from that of the remaining sites, and do a better job of treating unequal-time correlations at the impurity site. Considerable progress has already been made on the first two objectives and we hope to publish this shortly.

As this paper is a rather long one, we include below a summary of the material contained in the succeeding sections. In Sec. II, the model is described in detail and certain exact results for the Green's function are derived. In Sec. III, the approximation scheme is introduced and an integral equation for the impurity site Green's function is obtained. In Sec. IV, a particular density of states for the host lattice is chosen and the integral equation solved for two special cases (a) infinite Coulomb potential and (b) Coulomb and scattering potential chosen in such a way that electron-hole symmetry exists. Finally in Sec. VI, the solution to the integral equation for case (a) is put in a form suitable for numerical calculations. The average impurity site occupation number and the energy dependence of the imaginary part of the t matrix are calculated.

II. MODEL HAMILTONIAN AND GREEN'S-FUNCTION METHOD

The Hamiltonian for the model is

$$H=\sum_{ij\sigma} T_{ij}c_{i\sigma}{}^{\dagger}c_{j\sigma}+V\sum_{\sigma} n_{0,\sigma}+\tfrac{1}{2}U\sum_{\sigma} n_{0\sigma}n_{0\bar{\sigma}} -h\sum_{i,\sigma}\sigma n_{i,\sigma}\,, \quad (2.1)$$

where $c_{i\sigma}{}^{\dagger}$ creates an electron of spin σ at lattice site i and $n_{0,\sigma}$ is the number of electrons of spin σ at the impurity site. The difference in one-electron potential between host and impurity sites is measured by V. A Coulomb repulsion U is operative only between electrons of opposite spin located at the impurity site (the Pauli principle forbids two electrons of the same spin being at the same site). A uniform external magnetic field is described by the last term in (2.1). The kinetic energy may be written as

$$\sum_{ij\sigma} T_{ij}c_{i\sigma}{}^{\dagger}c_{j\sigma}=\sum_{\mathbf{q}\sigma}\epsilon_{\mathbf{q}}c_{\mathbf{q}\sigma}{}^{\dagger}c_{\mathbf{q}\sigma}\,,$$
$$\epsilon_{\mathbf{q}}=(1/N)\sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}T_{ij}\,, \quad (2.2)$$

where $\epsilon_{\mathbf{q}}$ is the band energy of the host and

$$c_{\mathbf{q}\sigma}{}^{\dagger}(c_{\mathbf{q}\sigma}{}^{\dagger}=N^{-1/2}\sum_i c_{i,\sigma}{}^{\dagger}e^{i\mathbf{q}\cdot\mathbf{R}_i})$$

creates an electron of spin σ and momentum $\mathbf{q}$. Throughout this paper, momenta will be designated by $\mathbf{q}$ or $\mathbf{q}'$, lattice site indices by i, j, k, or l.

Our analysis is based on the equation of motion of the retarded (+) and advanced (−) Green's functions defined by[9]

$$\langle\langle A(t),B(t')\rangle\rangle^{(\pm)}=\mp i\theta[\pm(t-t')]\langle[A(t),B(t')]\rangle\,, \quad (2.3)$$

where $A(t)$, $B(t)$ are operators in the Heisenberg representation and

$$\theta(x)=1\,,\quad x>0 \quad (2.4a)$$

$$\theta(x)=0\,,\quad x<0\,. \quad (2.4b)$$

Differentiation of (2.3) with respect to t yields

$$i(d/dt)\langle\langle A(t),B(t')\rangle\rangle^{(\pm)}=\delta(t-t')\langle[A(t),B(t)]\rangle +\langle\langle[[A(t),H],B(t')]\rangle\rangle^{(\pm)}\,, \quad (2.5)$$

where use has been made of the relations

$$(d/dt)\theta(t-t')=\delta(t-t') \quad (2.6)$$

and

$$i(d/dt)A=[A,H]\,. \quad (2.7)$$

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Differentiation of (2.3) with respect to t' gives

$$i(d/dt')\langle\langle A(t),B(t')\rangle\rangle^{(\pm)}=-\delta(t-t')\langle[A(t),B(t)]\rangle+\langle\langle[A(t),[B(t'),H]]\rangle\rangle^{(\pm)}. \quad (2.8)$$

The Green's functions defined by (2.3) are functions of $t-t'$ only, and one can define the Fourier transform

$$\langle\langle A,B\rangle\rangle_E{}^{(\pm)}=\frac{1}{2\pi}\int_{-\infty}^{\infty}\langle\langle A(t),B(0)\rangle\rangle^{(\pm)}e^{iEt}dt. \quad (2.9)$$

In the case of the retarded $(+)$ Green's function, the integral (2.9) converges for $\mathrm{Im}E>0$, and in the case of the advanced Green's function $(-)$ it converges for $\mathrm{Im}E<0$. The function

$$\langle\langle A,B\rangle\rangle_E=\langle\langle A,B\rangle\rangle_E{}^{(+)},\quad \mathrm{Im}E>0 \quad (2.10a)$$

$$=\langle\langle A,B\rangle\rangle_E{}^{(-)},\quad \mathrm{Im}E<0 \quad (2.10b)$$

is analytic except on the real axis. The equations of motion of $\langle\langle A,B\rangle\rangle_E$ follow from (2.5) and (2.8), respectively.

$$E\langle\langle A,B\rangle\rangle_E=\langle[A,B]\rangle/2\pi+\langle\langle[A,H],B\rangle\rangle_E, \quad (2.11a)$$

$$E\langle\langle A,B\rangle\rangle_E=\langle[A,B]\rangle/2\pi-\langle\langle A,[B,H]\rangle\rangle_E. \quad (2.11b)$$

The equation usually used is (2.11a). The equation of motion for the desired quantity $\langle\langle A,B\rangle\rangle$ is given by (2.11a) and (2.11b). In order to find $\langle\langle A,B\rangle\rangle$, it is necessary to know the higher-order Green's function $\langle\langle[A,H],B\rangle\rangle_E$ whose equation of motion is determined by (2.11a) and (2.11b) and involves $\langle\langle[[A,H],H],B\rangle\rangle_E$. At some stage, a higher-order Green's function is approximated by lower-order Green's functions and the system of equations of motion becomes a set of simultaneous equations which may be solved for the lower-order Green's functions. If $\langle\langle A;B\rangle\rangle_E$ is known then $\langle B(t')A(t)\rangle$, the expectation value of $B(t')A(t)$, is given by

$$\langle B(t')A(t)\rangle=i\int_{-\infty}^{\infty}[\langle\langle A;B\rangle\rangle_{E+i\delta}-\langle\langle A;B\rangle\rangle_{E-i\delta}]\times\frac{e^{-iE(t-t')}}{e^{\beta(E-\mu)}+1}dE, \quad (2.12)$$

where here and later in the paper the quantity δ is taken to mean the limit $\delta\rightarrow+0$. As a consequence, all the one-electron properties of the system can be calculated once

$$G_{ij}{}^{\sigma}(E)\equiv\langle\langle c_{i\sigma};c_{j\sigma}{}^{\dagger}\rangle\rangle_E \quad (2.13)$$

is known.

Using Eqs. (2.1) and (2.11a) yields the equation of motion for $G_{l,m}{}^{\sigma}$

$$(E+h\sigma)G_{l,m}{}^{\sigma}=(\delta_{l,m}/2\pi)+\sum_j T_{lj}G_{jm}{}^{\sigma}+\delta_{l,0}(VG_{0,m}{}^{\sigma}+U\Gamma_{000,m}{}^{\sigma}), \quad (2.14)$$

where $\Gamma_{000,m}{}^{\sigma}$ is a higher-order Green's function given by

$$\Gamma_{000,m}{}^{\sigma}=\langle\langle n_{0\bar{\sigma}}c_{0\sigma};c_{m\sigma}{}^{\dagger}\rangle\rangle. \quad (2.15)$$

The Fourier transform of $G_{l,m}{}^{\sigma}$ is given by

$$G_{\mathbf{q},\mathbf{q}'}{}^{\sigma}(E)=(1/N)\sum_{l,m}e^{i\mathbf{q}\cdot\mathbf{R}_l}G_{l,m}{}^{\sigma}(E)e^{-i\mathbf{q}'\cdot\mathbf{R}_m}, \quad (2.16)$$

and obeys the equation of motion

$$(E+h\sigma-\epsilon_{\mathbf{q}})G_{\mathbf{q},\mathbf{q}'}{}^{\sigma}=\delta_{\mathbf{q},\mathbf{q}'}/2\pi+VG_{0,\mathbf{q}'}{}^{\sigma}/N^{1/2}+U\Gamma_{000,\mathbf{q}'}{}^{\sigma}/N^{1/2}, \quad (2.17)$$

where we have used (2.2), (2.14), (2.16), and

$$G_{0\mathbf{q}'}{}^{\sigma}=(1/N)^{1/2}\sum_m G_{0,m}e^{-i\mathbf{q}'\cdot\mathbf{R}_m}, \quad (2.18a)$$

$$\Gamma_{000,\mathbf{q}'}{}^{\sigma}=(1/N)^{1/2}\sum_m \Gamma_{000,m}{}^{\sigma}e^{-i\mathbf{q}'\cdot\mathbf{R}_m}. \quad (2.18b)$$

Throughout this paper, the subscript 0 appearing, for example, in $G_{0,\mathbf{q}'}{}^{\sigma}$ means the lattice site 0 (the impurity site) and not $q=0$. Note that

$$G_{0,\mathbf{q}'}{}^{\sigma}=(1/N^{1/2})\sum_{\mathbf{q}}G_{\mathbf{q},\mathbf{q}'}{}^{\sigma}.$$

It is helpful to define some quantities which will be used in the remainder of the paper:

$$F_{\mathbf{q}}{}^{\sigma}=1/(E+h\sigma-\epsilon_{\mathbf{q}}), \quad (2.19a)$$

$$F^{\sigma}=(1/N)\sum_{\mathbf{q}}F_{\mathbf{q}}{}^{\sigma}, \quad (2.19b)$$

$$B^{\sigma}=(1/N)\sum_{\mathbf{q}}\epsilon_{\mathbf{q}}F_{\mathbf{q}}{}^{\sigma}=-1+(E+h\sigma)F^{\sigma}. \quad (2.19c)$$

We now relate $G_{\mathbf{q},\mathbf{q}'}{}^{\sigma}$ to $G_{00}{}^{\sigma}$. Multiplying both sides of (2.17) by $(1/N^{1/2})F_{\mathbf{q}}{}^{\sigma}$ and summing on $\mathbf{q}$ yields

$$U\Gamma_{000,\mathbf{q}'}{}^{\sigma}=\frac{G_{0\mathbf{q}'}{}^{\sigma}(1-F^{\sigma}V)-F_{\mathbf{q}'}{}^{\sigma}/2\pi N^{1/2}}{F^{\sigma}}. \quad (2.20)$$

This relation is used to eliminate $U\Gamma_{000,\mathbf{q}'}{}^{\sigma}$ from (2.17) to obtain

$$G_{\mathbf{q}\mathbf{q}'}{}^{\sigma}=F_{\mathbf{q}}{}^{\sigma}[(\delta_{\mathbf{q}\mathbf{q}'}/2\pi)+(G_{0\mathbf{q}'}{}^{\sigma}/F^{\sigma}N^{1/2})-(F_{\mathbf{q}'}{}^{\sigma}/2\pi F^{\sigma})]. \quad (2.21)$$

Multiplying both sides of (2.17) by $F_{\mathbf{q}}{}^{\sigma}/N^{1/2}$ and summing on q' yields

$$G_{\mathbf{q},0}{}^{\sigma}=(F_{\mathbf{q}}{}^{\sigma}/N^{1/2})[1/2\pi+VG_{0,0}{}^{\sigma}+U\Gamma_{000,0}{}^{\sigma}]. \quad (2.22)$$

With the aid of the two equations of motion (2.11a) and (2.11b) it can be shown (Appendix A) that

$$G_{\mathbf{q},\mathbf{q}'}{}^{\sigma}=G_{\mathbf{q}',\mathbf{q}}{}^{\sigma}. \quad (2.23)$$

Equation (2.23) implies $G_{0\mathbf{q}'}{}^{\sigma}=G_{\mathbf{q}'0}{}^{\sigma}$, thus (2.21) and (2.22) give the important result

$$G_{\mathbf{q},\mathbf{q}'}{}^{\sigma}=(\delta_{\mathbf{q}\mathbf{q}'}/2\pi)F_{\mathbf{q}}{}^{\sigma}+(1/N)F_{\mathbf{q}}{}^{\sigma}T^{\sigma}F_{\mathbf{q}'}{}^{\sigma}, \quad (2.24)$$

where the t matrix is a function of energy, but not momentum

$$T^\sigma = (VG_{00}{}^\sigma + U\Gamma_{000,0}{}^\sigma)/F^\sigma. \tag{2.25}$$

The relationship between $G_{00}{}^\sigma$ and $\Gamma_{000,0}{}^\sigma$ is obtained by summing (2.22) over q,

$$G_{00}{}^\sigma = (1/2\pi + U\Gamma_{000,0}{}^\sigma)F^\sigma/(1-F^\sigma V). \tag{2.26}$$

T^σ then takes the relatively simple form

$$T^\sigma = (G_{00}{}^\sigma/F^\sigma - 1/2\pi)(1/F^\sigma). \tag{2.27}$$

Hence we have succeeded in relating $G_{\mathbf{q}\mathbf{q}'}{}^\sigma$ to $G_{00}{}^\sigma$. For simplicity, in the remainder of the paper we set $N=1$.

III. APPROXIMATE SOLUTION OF EQUATIONS OF MOTION

In order to determine $\Gamma_{000,0}{}^\sigma$, we use (2.1) and (2.11a) to write the equation of motion

$$(E+h\sigma-U-V)\Gamma_{000,0}{}^\sigma = (1/2\pi)\langle n_{0\bar\sigma}\rangle + \sum_j T_{0j}[\Gamma_{00j,0}{}^\sigma + \Gamma_{0j0,0}{}^\sigma - \Gamma_{j00,0}{}^\sigma], \tag{3.1}$$

where

$$\Gamma_{ijk,l}{}^\sigma = \langle\langle c_{i\bar\sigma}{}^\dagger c_{j\bar\sigma} c_{k\sigma};\, c_{l\sigma}{}^\dagger\rangle\rangle_E. \tag{3.2}$$

Again making use of (2.1) and (2.11a), we write the equations of motion for $\Gamma_{00j,0}{}^\sigma$, $\Gamma_{0j0,0}{}^\sigma$, and $\Gamma_{j00,0}{}^\sigma$ which appear on the right-hand side of (3.1):

$$(E+h\sigma)\Gamma_{00j,0}{}^\sigma = \sum_k T_{jk}\Gamma_{00k,0}{}^\sigma + \sum_k T_{0k}(\Gamma_{0kj,0}{}^\sigma - \Gamma_{k0j,0}{}^\sigma), \quad j\neq 0 \tag{3.3}$$

$$(E+h\sigma)\Gamma_{0j0,0}{}^\sigma = \langle c_{0\bar\sigma}{}^\dagger c_{j\bar\sigma}\rangle/2\pi + \sum_k T_{0k}(\Gamma_{0jk,0}{}^\sigma - \Gamma_{kj0,0}{}^\sigma) + \sum_k T_{jk}\Gamma_{0k0,0}{}^\sigma, \quad j\neq 0 \tag{3.4}$$

$$(E+h\sigma-U-2V)\Gamma_{j00,0}{}^\sigma = \langle c_{j\bar\sigma}{}^\dagger c_{0\bar\sigma}\rangle/2\pi + \sum_k T_{0k}[\Gamma_{j0k,0}{}^\sigma + \Gamma_{jk0,0}{}^\sigma] - \sum_k T_{jk}\Gamma_{k00,0}{}^\sigma, \quad j\neq 0. \tag{3.5}$$

We are free to choose the zero of energy at

$$T_{i,i} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} = 0, \tag{3.6}$$

Approximations are now introduced in such a way as to treat correlations on the impurity site (where there is a Coulomb interaction) as accurately as is feasible. We treat Green's function $\Gamma_{ijk,0}{}^\sigma$ exactly when two or more of the indices i, j, k refer to the impurity site. If only one of the indices refers to the impurity site we make a Hartree-Fock-type approximation

$$\Gamma_{ijk,0}{}^\sigma \simeq \langle c_{i\bar\sigma}{}^\dagger c_{j\bar\sigma}\rangle G_{k,0}{}^\sigma, \quad \text{at most one of } i,\, j,\, k \text{ equals } 0. \tag{3.7}$$

This approximational scheme is based on the notion that it is the correlations between electrons at the impurity site which are of prime importance in this problem. Making use of (3.7), Eqs. (3.3)–(3.5) are approximated by (3.8)–(3.10), respectively:

$$(E+h\sigma)\Gamma_{00j,0}{}^\sigma = \sum_k T_{jk}\Gamma_{00k,0}{}^\sigma, \quad j\neq 0 \tag{3.8}$$

where we have used the relation $\langle c_{0\bar\sigma}{}^\dagger c_{k\bar\sigma}\rangle = \langle c_{k\bar\sigma}{}^\dagger c_{0\bar\sigma}\rangle$ which follows from (2.23) and (2.12),

$$(E+h\sigma)\Gamma_{0j0,0}{}^\sigma = \langle c_{0\bar\sigma}{}^\dagger c_{j\bar\sigma}\rangle[1/2\pi + \sum_k T_{0k}G_{k0}{}^\sigma] - G_{00}{}^\sigma \sum_k T_{0k}\langle c_{k\bar\sigma}{}^\dagger c_{j\bar\sigma}\rangle + \sum_k T_{jk}\Gamma_{0k0,0}{}^\sigma, \quad j\neq 0 \tag{3.9}$$

$$(E+h\sigma-U-2V)\Gamma_{j00,0}{}^\sigma = \langle c_{j\bar\sigma}{}^\dagger c_{0\bar\sigma}\rangle[1/2\pi + \sum_k T_{0k}G_{k,0}{}^\sigma] + G_{00}{}^\sigma \sum_k T_{0k}\langle c_{j\bar\sigma}{}^\dagger c_{k\bar\sigma}\rangle - \sum_k T_{jk}\Gamma_{k00,0}{}^\sigma, \quad j\neq 0. \tag{3.10}$$

The quantities

$$\sum_j T_{0j}\Gamma_{00j,0}{}^\sigma,$$

etc., which appear in (3.1) may be obtained from (3.8)–(3.10) which all have the general form

$$a\Gamma_j = b_j \pm \sum_k T_{jk}\Gamma_k, \quad j\neq 0 \tag{3.11}$$

where Γ_j stands for $\Gamma_{00j,0}{}^\sigma$, $\Gamma_{0j0,0}{}^\sigma$, or $\Gamma_{j00,0}{}^\sigma$. It is shown in Appendix B that (3.11) implies

$$\sum_j T_{0j}\Gamma_j = \pm\{-b_0 + (1/J) \times [\pm K\Gamma_0 + \sum_{\mathbf{q}} b_{\mathbf{q}}(a\mp\epsilon_{\mathbf{q}})^{-1}]\}, \tag{3.12}$$

where

$$J = \sum_{\mathbf{q}} (a\mp\epsilon_{\mathbf{q}})^{-1}, \quad K = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}}(a\mp\epsilon_{\mathbf{q}})^{-1}, \tag{3.13}$$

and it is understood that

$$b_{\mathbf{q}} = \sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i} b_i.$$

With the aid of (3.12), we find from (3.8)

$$\sum_j T_{0j}\Gamma_{00j,0}{}^\sigma = B^\sigma\Gamma_{000,0}{}^\sigma/F^\sigma, \tag{3.14a}$$

where F^σ, B^σ as well as $F_{\mathbf{q}}{}^\sigma$ are defined in (2.19).

The approximation (3.14a) for $\sum_j T_{0j}\Gamma_{00j,0}{}^{\sigma}$ has a flaw. In the limit that U is very large, $\Gamma_{000,0}{}^{\sigma}$ goes to zero as U^{-1}; this is clear from (3.1) and reflects the fact that the probability of finding two electrons on the impurity site must be very small if the repulsion between them is very large. There is no reason based on equal-time correlations why $\Gamma_{00j,0}{}^{\sigma}$ should be small in the large U limit. An alternative to (3.14a) consistent with our decoupling rules is obtained by applying the Hartree-Fock approximation (3.7) to $\Gamma_{00j,0}{}^{\sigma}$ to obtain

$$\sum_j T_{0j}\Gamma_{00j0}{}^{\sigma}=\langle n_{0\bar{\sigma}}\rangle\sum_j T_{0j}G_{j,0}{}^{\sigma}. \qquad (3.14\text{b})$$

Actual computations show that the final result for $G_{00}{}^{\sigma}$ is relatively insensitive to which approximation is used with (3.14b) leading to about 10% increase in the electron occupation number at the impurity. It is interesting to note that while (3.14b) does not vanish as $U\to\infty$, it does fail to satisfy the dynamic sum rule

$$\int_{-\infty}^{\infty}\mathrm{Im}\langle\langle c_{0\bar{\sigma}}{}^{\dagger}c_{0\bar{\sigma}}c_{j\sigma};\,c_{0\sigma}{}^{\dagger}\rangle\rangle_{\omega+i\delta}f(\omega)d\omega=0\,,\quad \text{as } U\to\infty\,, \qquad (3.15)$$

which clearly is satisfied by approximation (3.14a). This sum rule follows trivially from the fact that

$$\langle c_{0\sigma}{}^{\dagger}c_{0\bar{\sigma}}{}^{\dagger}c_{0\bar{\sigma}}c_{j\bar{\sigma}}\rangle=0\,,\quad \text{as } U\to\infty\,.$$

In the light of the above and the desire to treat all the correlations at the same stage in the decoupling we continue with (3.14a).

From (3.9) and (3.12), we find

$$\begin{aligned}\sum_j T_{0j}\Gamma_{0j0,0}{}^{\sigma}=&-\{\langle n_{0\bar{\sigma}}\rangle[1/2\pi+\sum_k T_{0k}G_{k,0}{}^{\sigma}]\\&-G_{00}{}^{\sigma}\sum_k T_{0k}\langle c_{k\bar{\sigma}}{}^{\dagger}c_{0\bar{\sigma}}\rangle\}\\&+(F^{\sigma})^{-1}\sum_{\mathbf{q}}F_{\mathbf{q}}{}^{\sigma}\{\langle c_{0\bar{\sigma}}{}^{\dagger}c_{\mathbf{q}\bar{\sigma}}\rangle[1/2\pi+\sum_k T_{0k}G_{k0}{}^{\sigma}]\\&-G_{00}{}^{\sigma}\sum_k T_{0k}\langle c_{k\bar{\sigma}}{}^{\dagger}c_{\mathbf{q}\bar{\sigma}}\rangle\}+B^{\sigma}\Gamma_{000,0}{}^{\sigma}/F^{\sigma}. \qquad (3.16)\end{aligned}$$

From (3.10) and (3.12), we find

$$\begin{aligned}\sum_j T_{0j}\Gamma_{j00,0}{}^{\sigma}=&\{\langle n_{0\bar{\sigma}}\rangle[1/2\pi+\sum_k T_{0k}G_{k,0}{}^{\sigma}]\\&+G_{00}{}^{\sigma}\sum_k T_{0k}\langle c_{0\bar{\sigma}}{}^{\dagger}c_{k\bar{\sigma}}\rangle\}\\&-(A^{\sigma})^{-1}\sum_{\mathbf{q}}A_{\mathbf{q}}{}^{\sigma}\{\langle c_{\mathbf{q}\bar{\sigma}}{}^{\dagger}c_{0\bar{\sigma}}\rangle[1/2\pi+\sum_k T_{0k}G_{k0}{}^{\sigma}]\\&+G_{00}{}^{\sigma}\sum_k T_{0k}\langle c_{q\bar{\sigma}}{}^{\dagger}c_{k\bar{\sigma}}\rangle\}+C^{\sigma}\Gamma_{000,0}{}^{\sigma}/A^{\sigma}, \qquad (3.17)\end{aligned}$$

where

$$A_{\mathbf{q}}{}^{\sigma}=(E+h\sigma-U-2V+\epsilon_{\mathbf{q}})^{-1},\quad A^{\sigma}=\sum_{\mathbf{q}}A_{\mathbf{q}}{}^{\sigma},\quad C^{\sigma}=\sum_{\mathbf{q}}\epsilon_{\mathbf{q}}A_{\mathbf{q}}{}^{\sigma}. \qquad (3.18)$$

Using (3.15)–(3.17) in (3.1) yields

$$\begin{aligned}&[E+h\sigma-U-V-2(B^{\sigma}/F^{\sigma})+(C^{\sigma}/A^{\sigma})]\Gamma_{000,0}{}^{\sigma}\\&=-(1/2\pi)\langle n_{0\bar{\sigma}}\rangle-2\langle n_{0\bar{\sigma}}\rangle\sum_k T_{0k}G_{k0}{}^{\sigma}+(F^{\sigma})^{-1}\sum_{\mathbf{q}}F_{\mathbf{q}}{}^{\sigma}\\&\quad\times\{\langle c_{0\bar{\sigma}}{}^{\dagger}c_{\mathbf{q}\bar{\sigma}}\rangle[(1/2\pi)+\sum_k T_{0k}G_{k0}{}^{\sigma}]\\&\quad-G_{00}{}^{\sigma}\sum_k T_{0k}\langle c_{k\bar{\sigma}}{}^{\dagger}c_{\mathbf{q}\bar{\sigma}}\rangle\}\\&\quad+(A^{\sigma})^{-1}\sum_k A_{\mathbf{q}}{}^{\sigma}\{\langle c_{\mathbf{q}\bar{\sigma}}{}^{\dagger}c_{0\bar{\sigma}}\rangle[(1/2\pi)+\sum_k T_{0k}G_{k0}{}^{\sigma}]\\&\quad+G_{00}{}^{\sigma}\sum_k T_{0k}\langle c_{\mathbf{q}\bar{\sigma}}{}^{\dagger}c_{k\bar{\sigma}}\rangle\}. \qquad (3.19)\end{aligned}$$

Noting that

$$\sum_k T_{0k}G_{k0}{}^{\sigma}=B^{\sigma}G_{00}{}^{\sigma}/F^{\sigma} \qquad (3.20)$$

and writing $\Gamma_{000,0}{}^{\sigma}$ in (3.9) in terms of $G_{00}{}^{\sigma}$ via (2.26) gives

$$\begin{aligned}2\pi G_{00}{}^{\sigma}=&\bigg\{[L^{\sigma}(1-F^{\sigma}V)/(UF^{\sigma})]+2\langle n_{0\bar{\sigma}}\rangle\\&\times\frac{B^{\sigma}}{F^{\sigma}}-\frac{\beta^{\sigma}\beta^{\sigma}}{(F^{\sigma})^2}+\frac{\gamma^{\sigma}}{F^{\sigma}}-\frac{\beta'^{\sigma}B^{\sigma}}{F^{\sigma}A^{\sigma}}-\frac{\gamma'^{\sigma}}{A^{\sigma}}\bigg\}^{-1}\\&\times\bigg\{-\langle n_{0\bar{\sigma}}\rangle+\frac{\beta^{\sigma}}{F^{\sigma}}+\frac{\beta'^{\sigma}}{A^{\sigma}}+\frac{L^{\sigma}}{U}\bigg\}\,, \qquad (3.21)\end{aligned}$$

where

$$L^{\sigma}=E+h\sigma-U-V-2(B^{\sigma}/F^{\sigma})+(C^{\sigma}/A^{\sigma})\,, \qquad (3.22)$$

$$\beta^{\sigma}=\sum_{\mathbf{q}}\langle c_{0\bar{\sigma}}{}^{\dagger}c_{\mathbf{q}\bar{\sigma}}\rangle F_{\mathbf{q}}{}^{\sigma}\,, \qquad (3.23)$$

$$\beta'^{\sigma}=\sum_{\mathbf{q}}\langle c_{\mathbf{q}\bar{\sigma}}{}^{\dagger}c_{0\bar{\sigma}}\rangle A_{\mathbf{q}}{}^{\sigma}\,, \qquad (3.24)$$

$$\gamma^{\sigma}=\sum_{\mathbf{q}}F_{\mathbf{q}}{}^{\sigma}\sum_k T_{0k}\langle c_{k\bar{\sigma}}{}^{\dagger}c_{q\bar{\sigma}}\rangle\,, \qquad (3.25)$$

$$\gamma'^{\sigma}=\sum_{\mathbf{q}}A_{\mathbf{q}}\sum_k T_{0k}\langle c_{q\bar{\sigma}}{}^{\dagger}c_{k\bar{\sigma}}\rangle\,. \qquad (3.26)$$

The expectation value appearing in say (3.23) may be related to an integral over energy of $G_{0,\mathbf{q}}{}^{\sigma}(E)$ by (2.12), $G_{0,\mathbf{q}}{}^{\sigma}(E)$ is then written in terms of $G_{0,0}{}^{\sigma}(E)$ by use of (2.24)–(2.26). Hence, Eq. (3.21) represents an integral equation for the quantity $G_{00}{}^{\sigma}(E)$.

We next rewrite (3.21) in such a way as to exhibit explicitly the fact that it is an integral equation. Define an operator $O_{E'}$

$$O_{E'}\{A(E')\}=i\int_{-\infty}^{\infty}dE'\,f(E')\times[A(E'+i\delta)-A(E'-i\delta)]. \qquad (3.27)$$

It follows that[10]

$$\beta^\sigma(E)=\sum_{\mathbf{q}}\langle c_{0\bar\sigma}{}^\dagger c_{\mathbf{q}\bar\sigma}\rangle F_{\mathbf{q}}{}^\sigma(E)=\sum_{\mathbf{q}}F_{\mathbf{q}}{}^\sigma(E)O_{E'}\{G_{\mathbf{q},0}{}^{\bar\sigma}(E')\}$$

$$=\sum_{\mathbf{q}}F_{\mathbf{q}}{}^\sigma(E)O_{E'}\{F_{\mathbf{q}}{}^{\bar\sigma}(E')G_{00}{}^{\bar\sigma}(E')/F^{\bar\sigma}(E')\}$$

$$=O_{E'}\{\sum_{\mathbf{q}}F_{\mathbf{q}}{}^\sigma(E)F_{\mathbf{q}}{}^{\bar\sigma}(E')G_{00}{}^{\bar\sigma}(E')/F^{\bar\sigma}(E')\}$$

$$=O_{E'}\left\{\frac{[F^{\bar\sigma}(E')-F^\sigma(E)]}{E-E'+2h\sigma}\frac{G_{00}{}^{\bar\sigma}(E')}{F^{\bar\sigma}(E')}\right\}, \tag{3.28}$$

$$\beta'^\sigma(E)=\sum_{\mathbf{q}}\frac{-1}{-[E+h\sigma-U-2V]-\epsilon_{\mathbf{q}}}\langle c_{0\bar\sigma}{}^\dagger c_{\mathbf{q}\bar\sigma}\rangle$$

$$=-\beta^\sigma(-[E+2h\sigma-U-2V]), \tag{3.29}$$

$$\gamma^\sigma(E)=\sum_{\mathbf{q}}F_{\mathbf{q}}{}^\sigma\sum_j T_{0j}\langle c_{j\bar\sigma}{}^\dagger c_{\mathbf{q}\bar\sigma}\rangle$$

$$=\sum_{\mathbf{q}\mathbf{q}'}F_{\mathbf{q}}{}^\sigma\epsilon_{\mathbf{q}'}O_{E'}\{G_{\mathbf{q},\mathbf{q}'}{}^{\bar\sigma}(E')\}$$

$$=O_{E'}\left\{\sum_{\mathbf{q}\mathbf{q}'}F_{\mathbf{q}}{}^\sigma(E)\epsilon_{\mathbf{q}'}\times\left(\frac{\delta_{\mathbf{q}\mathbf{q}'}F_{\mathbf{q}}{}^{\bar\sigma}(E')}{2\pi}-\frac{F_{\mathbf{q}}{}^{\bar\sigma}(E')F_{\mathbf{q}'}{}^{\bar\sigma}(E')}{2\pi F^{\bar\sigma}(E')}+\frac{F_{\mathbf{q}}{}^{\bar\sigma}(E')F_{\mathbf{q}'}{}^{\bar\sigma}(E')}{(F^{\bar\sigma}(E'))^2}G_{00}{}^{\bar\sigma}(E')\right)\right\}$$

$$=\frac{1}{2\pi}O_{E'}\left\{\frac{B^{\bar\sigma}(E')-B^\sigma(E)}{E-E'+2h\sigma}\right\}-\frac{1}{2\pi}O_{E'}\left\{\frac{F^{\bar\sigma}(E')-F^\sigma(E)}{E-E'+2h\sigma}\frac{B^{\bar\sigma}(E')}{F^{\bar\sigma}(E')}\right\}+O_{E'}\left\{\frac{[F^{\bar\sigma}(E')-F^\sigma(E)]}{E-E'+2h\sigma}\times\frac{B^{\bar\sigma}(E')}{[F^{\bar\sigma}(E')]^2}G^{\bar\sigma}(E')\right\}, \tag{3.30}$$

$$\gamma'^\sigma(E)=-\gamma^\sigma(-[E+2h-U-2V]). \tag{3.31}$$

An examination of (3.28)–(3.31) reveals that (3.21) represents a singular nonlinear set of simultaneous integral equations for the four quantities $G_{00}{}^\sigma(E+i\delta)$, $G_{00}{}^{\bar\sigma}(E\pm i\delta)$.

IV. FINAL FORM OF INTEGRAL EQUATION

To proceed further, we must choose a particular form for the density of states $\eta(E)$ of the host lattice. If one hopes to obtain an analytic solution to the integral equation $\eta(E)$ should be analytic in the complex plane with the exception of a few isolated poles. In addition, as a practical matter, it must be chosen to effect a maximum simplification of (3.21). A Lorentzian density of states

$$\eta(E)\equiv(D/\pi)(E^2+D^2)^{-1} \tag{4.1}$$

is, as other workers have found, ideally suited for this. It has, however, one very serious drawback—the one-electron band energy is infinite for this density of states. For problems which have electron-hole symmetry, such as for the s-d Hamiltonian and the present model when $U+2V=0$, this drawback never manifests itself. When electron-hole symmetry is lacking, as it generally is for the model studied here, logarithmic divergences are introduced because of the slowness with which the $\eta(E)$ goes to zero for large energies. There are two ways one can attempt to circumvent this problem. One is simply to use a density of states which falls off much more rapidly; these, however, lead to integral equations which have so far proved intractable to analytic methods. The second is to introduce a cutoff into the integrals which reflects the fact that all physical density of states do go to zero above a certain energy. It is this second course we adopt in this paper.

To maintain a certain consistancy, we shall cutoff all integrals at $\pm nD$ whether they are divergent or not. The value of n will be left unspecified at present so that the sensitivity of our solution to the size of the cutoff can be studied.

Specializing now to the Lorentzian density of states we find

$$F^\sigma(E=\omega+i\tau)=(\omega+h\sigma+iD\operatorname{sgn}\tau)^{-1}, \tag{4.2}$$

$$B^\sigma(E=\omega+i\tau)=-iD\operatorname{sgn}\tau/(\omega+h\sigma+iD\operatorname{sgn}\tau). \tag{4.3}$$

It is shown in Appendix C that (3.28) and (3.30) take the form

$$\beta^\sigma(\omega+i\delta)=F^\sigma(\omega+i\delta)[\langle n_{0\bar\sigma}\rangle+2D\varphi_1{}^\sigma(\omega+i\delta)], \tag{4.4}$$

$$\gamma^\sigma(\omega+i\delta)=F^\sigma(\omega+i\delta)[\alpha^\sigma+(D/\pi)Y^\sigma(\omega+i\delta)+2iD^2\varphi_1{}^\sigma(\omega+i\delta)], \tag{4.5}$$

where

$$Y^\sigma(\omega+i\delta)=\int_{-nD}^{nD}\frac{f(\omega')d\omega'}{\omega-\omega'+2h\sigma+i\delta}, \tag{4.6}$$

$$\varphi_1{}^\sigma(\omega+i\delta)=\int_{-nD}^{nD}\frac{f(\omega')G_{00}{}^{\bar\sigma}(\omega'+i\delta)^*d\omega'}{\omega-\omega'+2h\sigma+i\delta}, \tag{4.7}$$

$$\alpha^\sigma=D\int_{-nD}^{nD}f(\omega')[G_{00}{}^{\bar\sigma}(\omega'+i\delta)+G_{00}{}^{\bar\sigma}(\omega'+i\delta)^*]d\omega'. \tag{4.8}$$

We also note that

$$B^\sigma/F^\sigma=-iD\operatorname{sgn}\tau \tag{4.9}$$

and

$$C^\sigma/A^\sigma=iD\operatorname{sgn}\tau. \tag{4.10}$$

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

Finally, from (3.29) and (4.4), we find

$$\beta'^\sigma(\omega+i\delta)=F^\sigma(\omega-U-2V+i\delta)\times[\langle n_{0\bar\sigma}\rangle-2D\varphi_2{}^\sigma(\omega+i\delta)], \quad (4.11)$$

where

$$\varphi_2{}^\sigma(\omega+i\delta)=\int_{-nD}^{nD}\frac{f(\omega')G_{00}{}^{\bar\sigma}(\omega'+i\delta)d\omega'}{\omega-U-2V+\omega'+i\delta}. \quad (4.12)$$

From (3.31) and (4.5), we find

$$\gamma'^\sigma(\omega+i\delta)=F^\sigma(\omega-U-2V+i\delta)[\alpha^\sigma-(D/\pi)Z^\sigma(\omega+i\delta)+2iD^2\varphi_2{}^\sigma(\omega+i\delta)], \quad (4.13)$$

where

$$Z(\omega+i\delta)=\int_{-nD}^{nD}\frac{f(\omega')d\omega'}{\omega-U-2V+\omega'+i\delta}. \quad (4.14)$$

We now use (4.4)–(4.14) to rewrite the integral equation (3.21) as

$$G_{00}{}^\sigma(\omega+i\delta)=\frac{a^\sigma(\omega)+(D/\pi)[\varphi_1{}^\sigma(\omega+i\delta)-\varphi_2{}^\sigma(\omega+i\delta)]}{b^\sigma(\omega)+(D/\pi)[Y^\sigma(\omega+i\delta)+Z(\omega+i\delta)]+4iD^2[\varphi_1{}^\sigma(\omega+i\delta)-\varphi_2{}^\sigma(\omega+i\delta)]}, \quad (4.15)$$

where

$$2\pi a^\sigma(\omega)=\langle n_{0\sigma}\rangle+(\omega+h\sigma-U-V+3iD)U^{-1}, \quad (4.16)$$

$$b^\sigma(\omega)=(\omega+h\sigma-U-V+3iD)\times(\omega+h\sigma-V+iD)U^{-1}. \quad (4.17)$$

Introducing the function

$$\psi^\sigma(\omega+i\delta)=4\pi iDG_{00}{}^\sigma(\omega+i\delta)-1, \quad (4.18)$$

Eq. (4.15) is transformed into

$$\psi_\sigma(\omega+i\delta)=4\pi iD\frac{a(\omega)-b(\omega)-(D/\pi)[Y^\sigma(\omega+i\delta)+Z(\omega+i\delta)]}{b(\omega)-(D/\pi)[\varphi_3{}^\sigma(\omega+i\delta)+\varphi_4{}^\sigma(\omega+i\delta)]}, \quad (4.19)$$

where

$$\varphi_3{}^\sigma(\omega+i\delta)=\int_{-nD}^{nD}\frac{f(\omega')\psi^{\bar\sigma}(\omega'+i\delta)^*d\omega'}{\omega-\omega'+2h\sigma+i\delta}, \quad (4.20)$$

$$\varphi_4{}^\sigma(\omega+i\delta)=\int_{-nD}^{nD}\frac{f(\omega')\psi^{\bar\sigma}(\omega'+i\delta)d\omega'}{\omega-U-2V+\omega'+i\delta}. \quad (4.21)$$

If approximation (3.14b) had been used rather than (3.14a) the integral equation (4.19) would have the same form (4.19) but with $a(\omega)$ and $b(\omega)$ changed to

$$2\pi a(\omega)\rightarrow\langle n_{0\bar\sigma}\rangle+(\omega+h\sigma-U-V+2iD)U^{-1}, \quad (4.22)$$

$$b(\omega)\rightarrow iD\langle n_{0\bar\sigma}\rangle+(\omega+h\sigma-U-V+2iD)\times(\omega+h\sigma-V+iD)U^{-1}. \quad (4.23)$$

This is our final form for the integral equation, actually (4.19) represents four simultaneous integral equations; taking the complex conjugate of (4.19) and or making the change $\sigma\rightarrow-\sigma$ gives three more integral equations.

V. SOLUTION OF INTEGRAL EQUATIONS FOR TWO SPECIAL CASES

In the first part of this section, we solve the integral equations (4.19) under the assumptions (a) D/U, $V/U\ll1$ and (b) $h=0$ (the finite field case, $h\neq0$, can be solved by a straightforward generalization of the method presented here). Later in the second, we examine the case $V+\frac{1}{2}U=0$.

The integral equations (4.19) for $\psi(\omega+i\delta)$ and $\psi^*(\omega+i\delta)$ take the form

$$\psi_R(\omega)=[d(\omega)+Y_+(\omega)]/[g(\omega)+\varphi_A{}^+(\omega)], \quad (5.1)$$

$$\psi_A(\omega)=[\tilde d(\omega)+Y_-(\omega)]/[\tilde g(\omega)+\varphi_R{}^-(\omega)], \quad (5.2)$$

where

$$\psi_R(\omega)=\psi(\omega+i\delta),\quad \psi_A(\omega)=\psi^*(\omega+i\delta), \quad (5.3)$$

$$Y_\pm(\omega)=\frac{1}{\pi}\int_{-nD}^{nD}\frac{f(\omega')d\omega'}{\omega-\omega'\pm i\delta}, \quad (5.4)$$

$$\varphi_A{}^\pm(\omega)=\frac{1}{\pi}\int_{-nD}^{nD}\frac{d\omega'f(\omega')\psi_A(\omega')}{\omega-\omega'\pm i\delta},\quad \varphi_R{}^\pm(\omega)=\frac{1}{\pi}\int_{-nD}^{nD}\frac{d\omega'f(\omega')\psi_R(\omega')}{\omega-\omega'\pm i\delta}, \quad (5.5)$$

$$d(\omega)=[(V-\omega)/D]+i(1-\langle n_0\rangle),\quad \tilde d(\omega)=[(V-\omega)/D]-i(1-\langle n_0\rangle), \quad (5.6)$$

where $\langle n_0\rangle$ is the average number of electrons at the impurity site and

$$g(\omega)=[(\omega-V)/D]+i,\quad \tilde g(\omega)=[(\omega-V)/D]-i. \quad (5.7)$$

The integral equations (5.1) and (5.2) are similar to those solved by Bloomfield and Hamann[11] for the *s-d* model Kondo problem. We adapt their method of solution to (5.1) and (5.2), and sketch the procedure below. For more details the reader is referred to their paper. Define

$$\pi_A{}^\pm=g+\varphi_A{}^\pm,\quad \pi_R{}^\pm=\tilde g+\varphi_R{}^\pm. \quad (5.8)$$

One finds from (5.1), (5.2), (5.5), and (5.8)

$$\pi_A{}^+-\pi_A{}^-=[Y^+-Y^-][\tilde d+Y_-]/\pi_R{}^-, \quad (5.9)$$

$$\pi_R{}^+-\pi_R{}^-=[Y^+-Y^-][d+Y_+]/\pi_A{}^+. \quad (5.10)$$

[11] P. E. Bloomfield and D. R. Hamann, Phys. Rev. **164**, 856 (1967).

Multiply both sides of (5.9) by π_R^- and both sides of (5.10) by π_A^+ and add the two resulting equations to obtain

$$\pi_A^+\pi_R^+ - (d+\tilde{d})Y^+ - Y^{+2} = \pi_A^-\pi_R^- - (d+\tilde{d})Y^- - Y^{-2}. \quad (5.11)$$

Since all of the functions appearing in (5.11) are either analytic or sectionally holomorphic (analytic in upper and lower half-planes but discontinuous across the real axis from $-nD$ to nD), we conclude that $j(z) = \pi_A(z)\pi_R(z) - [d(z)+\tilde{d}(z)]Y(z) - Y(z)^2$ is either analytic or sectionally holomorphic. Because $j(z)$ is continuous across the real axis by (5.11) it must be analytic. It can be determined by the behavior of $\pi_A\pi_R - (d+d)Y - Y^2$ at infinity.

From (5.4) and (4.6),

$$\lim_{z\to\infty} [d(z)+\tilde{d}(z)]Y(z) = -\frac{2}{\pi D}\int_{-nD}^{nD} f(E')dE', \quad (5.12)$$

$$\lim_{z\to\infty} Y(z)^2 = 0. \quad (5.13)$$

From (5.5), (5.7), and (5.8),

$$\lim_{z\to\infty} \pi_A(z) = \frac{z}{D} + \left(i - \frac{V}{D}\right) + \frac{1}{\pi z}\int_{-nD}^{nD} f(E')\psi_A(E')dE', \quad (5.14)$$

$$\lim_{z\to\infty} \pi_R(z) = \frac{z}{D} - \left(i + \frac{V}{D}\right) + \frac{1}{\pi z}\int_{-nD}^{nD} f(E')\psi_R(E')dE'. \quad (5.15)$$

The above two equations give

$$\lim_{z\to\infty} \pi_A(z)\pi_R(z) = \left(\frac{1}{D}\right)^2(z-V)^2 + 1 + \frac{1}{\pi D}\int_{-nD}^{nD} f(E')[\psi_A(E')+\psi_R(E')]dE'. \quad (5.16)$$

The integral in (5.16) is simply

$$2\langle n_0\rangle - (2/\pi D)\int_{-nD}^{nD} f(E')dE'$$

as is evident from the definition of ψ in terms of G_{00}^{-nD}. We have, finally,

$$\lim_{z\to\infty} \pi_A\pi_R - (d+\tilde{d})Y - Y^2 = (1/D)^2(z-V)^2 + 1 + 2\langle n_0\rangle. \quad (5.17)$$

[12] J. Zittartz and E. Müller-Hartmann, Z. Physik **212**, 380 (1968).

Thus, we find

$$j(z) = (1/D^2)(z-V)^2 + 1 + 2\langle n_0\rangle \quad (5.18)$$

and

$$\pi_A(z)\pi_R(z) = j(z) + (d(z)+\tilde{d}(z))Y(z) + Y^2(z). \quad (5.19)$$

Returning to (5.9) and (5.10), multiply both sides of (5.9) by π_R^- and both sides of (5.10) by π_R^+ and subtract (5.10) from (5.9) to obtain

$$\pi_A^+\pi_R^- = \tfrac{1}{2}[\pi_A^-\pi_R^- + \pi_A^+\pi_R^+ + (Y^+-Y^-)(\tilde{d}-d) - (Y^+-Y^-)^2]. \quad (5.20)$$

Using (5.19) and recalling $\pi(\omega\pm i\delta) = \pi^\pm(\omega)$, we find

$$\pi_A^+\pi_R^- = j + Y^+\tilde{d} + Y^-d + Y^+Y^-. \quad (5.21)$$

Taking the limit $z \to \omega + i\delta$ in (5.19) and dividing (5.19) by (5.21), we find

$$(\pi_R^+/\pi_R^-) = [j + (d+\tilde{d})Y^+ + Y^{+2}]/[j + Y^+\tilde{d} + Y^-d + Y^+Y^-] \equiv H(\omega), \quad (5.22)$$

from which

$$\pi_R(z) = P(z)\exp\left[-\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{d\omega'}{z-\omega'}\ln H(\omega')\right]. \quad (5.23)$$

The polynomial $P(z)$ is determined by (a) infinities of $\ln H(\omega')$ for $-nD \le \omega' \le nD$ and (b) asymptotic behavior of π_A. In Appendix D, we show $\ln H(\omega')$ has no infinities on the interval $-nD \le \omega' \le nD$, thus $P(z)$ is determined by (2) only. We know the asymptotic behavior of π_R from (5.15), also

$$\lim_{z\to\infty}\exp\left[-\frac{1}{2\pi i}\int\frac{d\omega'}{z-\omega'}\ln H(\omega')\right] \to 1 + \frac{i}{2\pi z}\int_{-nD}^{nD} d\omega' \ln H(\omega'), \quad (5.24)$$

thus

$$P(z) = P_0 + P_1 z, \quad (5.25)$$

where

$$P_0 = -i\left[1 + (1/2\pi D)\times\int_{-nD}^{nD} d\omega' \ln H(\omega')\right] - (V/D), \quad (5.26)$$

$$P_1 = 1/D. \quad (5.27)$$

Finally, from (5.2), (5.8), (5.23), and (5.25),

$$\psi_A(\omega) = [\tilde{d}(\omega) + Y^-(\omega)][P_0 + P_1\omega]^{-1} \times \exp\left(\frac{1}{2\pi i}\int_{-nD}^{nD} d\omega' \frac{\ln H(\omega')}{\omega - \omega' - i\delta}\right), \quad (5.28)$$

which constitutes a formal solution of the simultaneous integral equations (5.1) and (5.2). The quantity $\langle n_0\rangle$ which appears in $H(\omega')$ must be calculated self-consistently. We also note that

$$\pi_A(z)=(P_0^*+P_1^*z)\exp\left(\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{d\omega'}{z-\omega'}\ln H^*(\omega')\right), \quad (5.29)$$

$$\psi_R(\omega)=[d(\omega)+Y^+(\omega)][P_0^*+P_1^*\omega]^{-1}\times\exp\left(-\frac{1}{2\pi i}\int_{-nD}^{nD}d\omega'\frac{\ln H^*(\omega')}{\omega-\omega'+i\delta}\right). \quad (5.30)$$

We now examine the case $2V+U=0$ with a half-filed band and $h=0$. In this case, the Hamiltonian (2.1) has electron-hole symmetry and solutions of (2.1) should exhibit this symmetry, in particular, one expects $\langle n_{0\sigma}\rangle=\langle n_{0\bar\sigma}\rangle$. This is evident even within the Hartree-Fock approximation; the Coulomb and potential scattering cancel for this case, since

$$V\sum n_{0\sigma}+U\sum_\sigma \langle n_{0\bar\sigma}\rangle n_{0\sigma}=0.$$

The integral equation (4.19) exhibits "reasonances" at $\omega=0$ and $\omega=U+2V$, since $Y(\omega+i\delta)$ is singular at $\omega=0$ (for zero temperature) and $Z(\omega+i\delta)$ is singular at $\omega=U+2V$.

If $U+2V=0$, these "resonances" are both at $\omega=0$ and cancel. The integral equation (4.15) for $G_{00}{}^{\sigma}(\omega+i\delta)$ is

$$G_{00}{}^{\sigma}(\omega+i\delta)=\left(A(\omega)+(D/\pi)\int_{-nD}^{nD}\frac{[f(\omega')-\frac{1}{2}][G_{00}{}^{\sigma}(\omega'+i\delta)^*+G_{00}{}^{\bar\sigma}(-\omega'+i\delta)]d\omega'}{\omega-\omega'+i\delta}\right)\Bigg/\left(B(\omega)+4iD^2\int_{-nD}^{nD}\frac{[f(\omega')-1/2][G_{00}{}^{\sigma}(\omega'+i\delta)^*+G_{00}{}^{\bar\sigma}(-\omega'+i\delta)]d\omega'}{\omega-\omega'+i\delta}\right), \quad (5.31)$$

$$A(\omega)=(1/4\pi)(2\langle n_{0\bar\sigma}\rangle-1)-(1/4\pi)(\omega+3iD)V^{-1}, \quad (5.32)$$

$$B(\omega)=\tfrac{1}{2}V^{-1}[V^2-(\omega+iD)(\omega+3iD)]. \quad (5.33)$$

Equation (5.31) is obtained from (4.15) by noting

$$f(-\omega)=1-f(\omega)\quad\text{and}\quad\int_{-nD}^{nD}\frac{G(\omega'+i\delta)d\omega'}{\omega+\omega'+i\delta}=0.$$

If $\langle n_{0\bar\sigma}\rangle=\frac{1}{2}$ as expected then $A(\omega)^*=-A(-\omega)$, also $B(\omega)^*=B(-\omega)$, thus,

$$G_{00}{}^{\sigma}(\omega+i\delta)=A(\omega)/B(\omega) \quad (5.34)$$

satisfies (5.31) as $G_{00}{}^{\bar\sigma}(\omega+i\delta)^*=-G_{00}{}^{\bar\sigma}(-\omega+i\delta)$. It is easily shown that for this solution

$$\langle n_{0\sigma}\rangle=O_{\omega'}\{A(\omega')/B(\omega')\}=\tfrac{1}{2}, \quad (5.35)$$

as assumed.

VI. NUMERICAL RESULTS AND DISCUSSION

In this section, the average impurity site occupation $\langle n_0\rangle$ and the energy dependence of the imaginary part of the t matrix are evaluated at zero temperature for the special case $U=\infty$, $h=0$ considered in Sec. V. The scattering potential V is also taken to be zero. In order to calculate $\langle n_0\rangle$, we express it in terms of the first and second moments of $H(\omega)$:

$$\langle n_0\rangle=2\langle n_{0\sigma}\rangle=2O_{\omega'}\{G_{00}{}^{\sigma}(\omega')\}=2(4\pi D)^{-1}\int_{-nD}^{nD}f(\omega')\times\{\psi_R(\omega')+\psi_A(\omega')+2\}d\omega', \quad (6.1)$$

where use has been made of (4.18), (5.1), and (5.2). From the definition (5.5) of $\varphi_R(\omega)$, we obtain

$$\lim_{\omega\to\infty}\varphi_R(\omega)=(\pi\omega)^{-1}\int_{-nD}^{nD}f(\omega')\psi_R(\omega')d\omega'. \quad (6.2)$$

Noting that $\psi_A(\omega)=\psi_R(\omega)^*$, Eq. (6.1) for $\langle n_0\rangle$ becomes

$$\lim_{\omega\to\infty}\langle n_0\rangle=D^{-1}\,\mathrm{Re}\{\omega\varphi_R(\omega)\}+n/\pi. \quad (6.3)$$

Equations (5.8), (5.23), (5.25) give

$$\varphi_R(\omega)=\pi_R(\omega)-\tilde g(\omega)=D^{-1}[\omega-iD-(1/2\pi)iM_0]\times\exp\left(-\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{d\omega'\ln H(\omega')}{\omega-\omega'}\right)-D^{-1}[\omega-iD], \quad (6.4)$$

where

$$M_m=\int_{-nD}^{nD}d\omega\,\omega^m\ln H(\omega). \quad (6.5)$$

The exponential term appearing in (6.4) may be expanded for large ω

$$\exp\left(-\frac{1}{2\pi i}\int_{-nD}^{nD}d\omega'\frac{\ln H(\omega')}{\omega-\omega'}\right)=1+\frac{iM_0}{2\pi\omega}+\frac{1}{\omega^2}\times\left[\frac{iM_1}{2\pi}-\frac{1}{8\pi^2}M_0^2\right]+O\left(\frac{1}{\omega^3}\right). \quad (6.6)$$

Combining (6.4) and (6.6) yields

$$\omega\varphi_A(\omega)=(M_0/2\pi)+(iM_1/2\pi D)+(M_0{}^2/8\pi^2 D)+O(1/\omega)\,. \quad (6.7)$$

Use of (6.7) in (6.3) gives a self-consistent equation for $\langle n_0\rangle$, since the moments M_0 and M_1 depend on $\langle n_0\rangle$ via the dependence of $H(\omega)$ on $\langle n_0\rangle$. The equation was solved numerically using standard interval halving techniques and the moments evaluated by Gaussian quadrature techniques. Absolute accuracy of 10^{-4} is obtained. The resultant value of $\langle n_0\rangle$ depends to some extent on the choice of the cutoff nD. For $n=3$, 6, and 10 the value of $\langle n_0\rangle$, the total number of electrons on the impurity site, is 0.40, 0.42, 0.42, respectively. The value for $\langle n_0\rangle$ gives some indication of the adequacy of our approximations in treating correlations. The Hartree-Fock approximation yields $\langle n_0\rangle=0$. The correlated function $(1-n_{0\downarrow}n_{0\uparrow})|0\rangle$, where $|0\rangle$ is the unperturbed Fermi sea, yields a larger value of $\langle n_0\rangle$, 0.66.

In comparing this value with that obtained from the decoupling scheme, it should be kept in mind that there are two factors tending to reduce the latter which are not general features of the decoupling scheme. The first factor is our truncation of the spectral range of all integrals to $(-nD, nD)$, and the second is the presence of a logarithmic infinity as $n\to\infty$ in the denominator of Eq. (4.15) which defines $G_{00}(\omega+i\delta)$. Both factors result from our use of a Lorentzian density of states, and the use of a more realistic density of states would eliminate them. We estimate that our value of n_0 might be increased by 25% for a realistic band structure,[13] but this would still be less than the $\langle n_0\rangle$ obtained from the correlated wave function $(1-n_{0\downarrow}n_{0\uparrow})|0\rangle$. It is hoped that the inclusion of unequal-time correlations will increase the size of $\langle n_0\rangle$.

We turn now to a calculation of $T(\omega)$. In order to evaluate $\operatorname{Im}T(\omega)$, it is necessary to put Eq. (5.28) for $\psi_A(\omega)$ into a form that is more suitable for computation. The quantity

$$K(z)=j+(d+\tilde{d})Y+Y^2=2\langle n_0\rangle+1+[(z/D)-Y]^2, \quad (6.8)$$

appearing in (5.19) has real and imaginary parts

$$\operatorname{Re}K=2\langle n_0\rangle+1+\{\operatorname{Re}[(z/D)-Y]\}^2-\{\operatorname{Im}[(z/D)-Y]\}^2, \quad (6.9\text{a})$$

$$\operatorname{Im}K=2\{\operatorname{Re}[(z/D)-Y]\}\{\operatorname{Im}[(z/D)-Y]\}\,. \quad (6.9\text{b})$$

For reasons which will be apparent shortly, it is necessary to know if $K(z)$ has any zeros in the complex plane. From (6.9), we see that this is possible if

$$\operatorname{Re}[(z/D)-Y]=0$$

and

$$\{\operatorname{Im}[(z/D)-Y]\}^2=2\langle n_0\rangle+1\,. \quad (6.10)$$

Clearly, if $z=z_0$ satisfies (6.10), then $z_0{}^*$ also does. It will be assumed that $K(z)$ has two zeros, z_0 and $z_0{}^*$, this assumption has been checked by numerical calculation for values of $\langle n_0\rangle$ in the range of interest. The dimensionless quantity

$$\Gamma(z)=K(z)D^2/|z-z_0|^2 \quad (6.11)$$

has no zeros, thus $\ln\Gamma(z)$ is not singular (except for the cut of Y, $-nD<\omega<nD$) and may be written as

$$\ln\Gamma(z)=-\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{d\omega'}{z-\omega'}\ln\frac{\Gamma^+(\omega')}{\Gamma^-(\omega')}\,. \quad (6.12)$$

From the definition of $H(\omega)$, Eq. (5.22), we see

$$\operatorname{Im}\{\ln K^+\}=\operatorname{Im}\{\ln H(\omega)\}\,. \quad (6.13)$$

Also,

$$\Gamma^+(\omega)/\Gamma^-(\omega)=K^+(\omega)/K^-(\omega)\,, \quad (6.14)$$

$$\operatorname{Re}\{\ln K^+(\omega)\}=\operatorname{Re}\{\ln K^-(\omega)\}\,, \quad (6.15\text{a})$$

$$\operatorname{Im}\{\ln K^+(\omega)\}=-\operatorname{Im}\{\ln K^-(\omega)\}\,. \quad (6.15\text{b})$$

Equations (6.13)–(6.15) lead to the relation

$$\ln\{(\Gamma^+(\omega)/\Gamma^-(\omega)\}=2i\operatorname{Im}\{\ln H(\omega)\}\,. \quad (6.16)$$

With the help of (6.12)

$$\begin{aligned}\exp[\tfrac{1}{2}\ln\Gamma(\omega-i\delta)]&=\exp\left(-\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{d\omega'}{\omega-\omega'-i\delta}\operatorname{Im}\{\ln H(\omega')\}\right)\\&=\exp\left(-\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{d\omega'}{\omega-\omega'-i\delta}\times[\ln H(\omega')-\ln|H(\omega')|]\right)\end{aligned} \quad (6.17)$$

and from the definition of $\Gamma(\omega-i\delta)$

$$\exp[\tfrac{1}{2}\ln\Gamma(\omega-i\delta)]=[K(\omega-i\delta)D^2/|\omega-z_0|^2]^{1/2}. \quad (6.18)$$

These results allow the expression (5.28) for $\psi_A(\omega)$ to be put in the form

$$\psi_A(\omega)=[\tilde{d}+Y^-][P_0+P_1\omega]^{-1}|\omega-z_0|[(|H|/D^2K^-)]^{1/2}\times\exp\left(\frac{1}{2\pi i}P\int_{-nD}^{nD}\frac{d\omega'\ln|H(\omega')|}{\omega-\omega'}\right), \quad (6.19)$$

which is suitable for numerical computations. The constant z_0 can be expressed in terms of moments of $H(\omega)$. Use of (6.16) in (6.12) yields

$$\ln\Gamma(\omega)=-\frac{1}{\pi}\int_{-nD}^{nD}\frac{d\omega'}{\omega-\omega'}\operatorname{Im}\{\ln H(\omega')\} \quad (6.20)$$

[13] We have arrived at this estimate by taking the value of $\langle n_0\rangle$ for $n=1$, where only half the spectral weight of the Lorentzian has been exhausted, but where the logarithmic singularity is not yet too large, and doubling it.

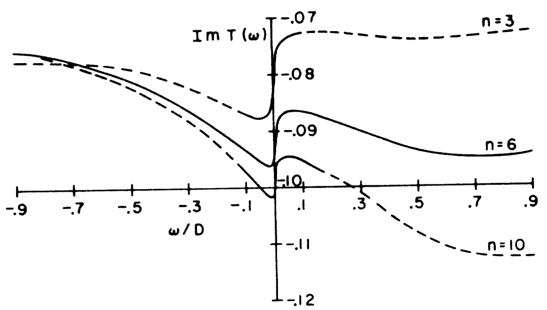

FIG. 1. Imaginary part of the t matrix versus energy for an energy range $-0.9D<\omega<0.9D$ in units of the bandwitdh D. [For infinite potential scattering $\mathrm{Im}T(\omega=0)=-\frac{1}{2}\pi$.] The three curves correspond to the three different values of the cutoff $\pm nD$ as discussed in the second paragraph of Sec. IV. The temperature dependence of the one-electron properties depends primarily on the shape of $\mathrm{Im}T(\omega)$.

from which

$$\lim_{\omega\to\infty}\ln\Gamma(\omega)=-(\pi\omega)^{-1}[\mathrm{Im}\{M_0\}+\omega^{-1}\,\mathrm{Im}\{M_1\}]. \quad (6.21)$$

From the definition of $\Gamma(\omega)$, Eq. (6.11), we find

$$\lim_{\omega\to\infty}\ln\Gamma(\omega)=2\omega^{-1}\,\mathrm{Re}\{z_0\}+\omega^{-2}[2(\mathrm{Re}\{z_0\})^2-|z_0|^2+D^2(1+2\langle n_0\rangle-2n/\pi)]. \quad (6.22)$$

Direct comparison of (6.21) and (6.22) yields

$$\mathrm{Re}\{z_0\}=-(1/2\pi)\,\mathrm{Im}\{M_0\}, \quad (6.23)$$

$$(\mathrm{Im}\{z_0\})^2=D^2[1+2\langle n_0\rangle-(2n/\pi)]+(\mathrm{Im}\{M_0\}/2\pi)^2+(\mathrm{Im}\{M_1\}/\pi). \quad (6.24)$$

Expressing $\langle n_0\rangle$ in terms of moments by use of (6.7) in (6.3) and using that relationship in (6.24) gives

$$(\mathrm{Im}\{z_0\})^2=[D+(1/2\pi)\,\mathrm{Re}\{M_0\}]^2. \quad (6.25)$$

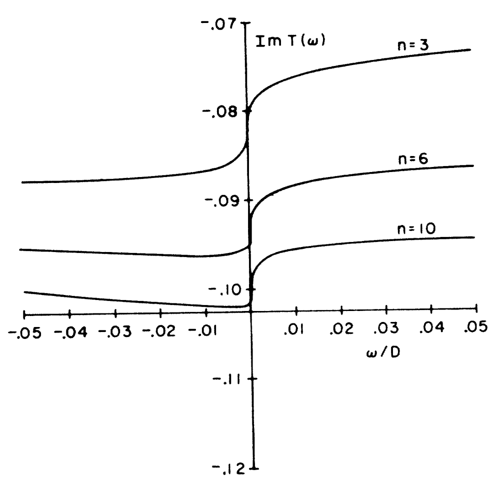

FIG. 2. Imaginary part of the t matrix versus energy for an energy range $-0.05D<\omega<0.05D$. The curves are the same ones shown in Fig. 1 but are plotted over an energy range more appropriate to thermal energies.

Finally,

$$z_0^{\pm}=\pm i[D+(1/2\pi)\,\mathrm{Re}\{M_0\}]-(1/2\pi)\,\mathrm{Im}\{M_0\}, \quad (6.26)$$

where $z_0^{\pm}$ denotes z_0 or z_0^*. Comparing (5.26) and (6.26) yields

$$\omega-z_0^{+}=D(P_0+P_1\omega). \quad (6.27)$$

This can be used in (6.19). The relationship (6.26) is checked by direct calculation of $z_0^{\pm}$, i.e., by finding the roots of $K(z)$ through a numerical root finding procedure and comparing the roots found with those calculated from the relation (6.26). The results are in very good agreement, thereby serving as a check to our numerical procedures.

At zero temperature, $H(\omega)=1$ for $\omega>0$, so the integral in (6.19) is from $-nD$ to 0. The integral is written as

$$\int_{-nD}^{0}\frac{d\omega'\ln|H(\omega')|}{\omega-\omega'}=\int_{-nD}^{0}\frac{d\omega'(\ln|H(\omega')|-\ln|H(\omega)|)}{\omega-\omega'}+H(\omega)\int_{-nD}^{0}\frac{d\omega'}{\omega-\omega'}. \quad (6.28)$$

The interval $(-nD, 0)$ is divided into as many as six subintervals so that the integrand changes by at most a factor of 30 within any subinterval. The integral over each subinterval is evaluated by Gaussian quadrature techniques. The case $\omega=0$ is treated by writing

$$\int_{-nD}^{0}\frac{d\omega'\ln|H(\omega')|}{\omega'}=\int_{-nD}^{-10^{-4}D}\frac{d\omega'\ln|H(\omega')|}{\omega'}+\int_{-10^{-4}D}^{0}\frac{d\omega'\ln|H(\omega')|}{\omega'}. \quad (6.29)$$

The first integral from $-nD$ to $-10^{-4}D$ is evaluated by the numerical procedure described above and the integral from $-10^{-4}D$ to 0 is evaluated analytically after $H(\omega)$ is approximated by

$$H(\omega)=\frac{2\langle n_0\rangle+[g(\omega)]^2-2ig(\omega)}{4\langle n_0\rangle+[g(\omega)]^2}, \quad (6.30)$$

where

$$g(\omega)=(1/\pi)\ln|(nD+\omega)/\omega|. \quad (6.31)$$

The values for ψ_A $(\omega=\pm10^{-6}D)$ and $\omega_A(0)$ as determined by (6.28) and (6.29), respectively, are in good agreement and differ by less than 1%, with $\psi_A(0)$ lying between $\psi_A(+10^{-6}D)$ and $\psi_A(-10^{-6}D)$, further serving as a check for our numerical calculations.

The imaginary part of the $T(\omega)$ matrix as a function of energy is shown in Figs. 1 and 2. (Figures 1 and 2 differ in the energy scale.) In each figure, the different curves correspond to different values of the limits of the integral in (6.19), the values $nD=3D$, $6D$, and $10D$ are used. The shapes of the curves are quite similar particularly in the region of small energy (Fig. 2). It is the shape of $\mathrm{Im}T(\omega)$ in the low-energy region which determines the temperature dependence of the one-particle properties of the system through the relationship $\tau(\omega)^{-1}=-2\,\mathrm{Im}T(\omega)$, where $\tau(\omega)$ is the relaxation time of the conduction electrons in the presence of the impurity. The uncertainty as to the exact form of $\mathrm{Im}T(\omega)$ as evidenced in Figs. 1 and 2 was sufficiently great to dissuade us from carrying out detailed calculations of such quantities as the resistivity and specific heat. The sensitivity of the solution to the cutoff stems from the fact that the nature of the scattering center must be calculated self-consistently and this depends on $D_{\mathbf{q},\mathbf{q}'}(\omega)$ over a broad frequency range. It is clear, however, from the figures that ρ and c_v will show anomalous behavior at low temperatures. In particular, it is clear from $\tau^{-1}\propto\mathrm{Im}T$ that the resistivity will decrease with increasing temperature much faster than for nonresonant scattering.

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APPENDIX A

We prove (2.23), $G_{\mathbf{q}\mathbf{q}'}{}^{\sigma}=G_{\mathbf{q}'\mathbf{q}}{}^{\sigma}$. First choose $A=c_{m,\sigma}$ in (2.11a) and $B=c_{m,\sigma}{}^{\dagger}$ in (2.11b), H is given by (2.1), and upon carrying out the indicated commutations we find

$$(E+h\sigma)\langle\langle c_{m\sigma},B\rangle\rangle =(2\pi)^{-1}\langle[c_{m\sigma},B]\rangle+\sum_j T_{mj}\langle\langle c_{j\sigma},B\rangle\rangle +\delta_{m,0}(V\langle\langle c_{0\sigma},B\rangle\rangle+U\langle\langle n_{0\bar\sigma}c_{0\sigma},B\rangle\rangle)\,,\quad\text{(A1)}$$

$$(E+h\sigma)\langle\langle A,c_{m\sigma}{}^{\dagger}\rangle\rangle =(2\pi)^{-1}\langle[A,c_{m\sigma}{}^{\dagger}]\rangle+\sum_j T_{mj}\langle\langle A,c_{j\sigma}{}^{\dagger}\rangle\rangle +\delta_{m0}(V\langle\langle A,c_{0\sigma}{}^{\dagger}\rangle\rangle+U\langle\langle A,n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle)\,.\quad\text{(A2)}$$

Let $B=c_{l\sigma}{}^{\dagger}$ in (A1), $A=c_{l\sigma}$ in (A2) to obtain

$$(E+h\sigma)G_{m,l}{}^{\sigma} =(2\pi)^{-1}\delta_{m,l}+\sum_j T_{mj}\,G_{jl}{}^{\sigma}+\delta_{m,0}(V\langle\langle c_{0\sigma},c_{l\sigma}{}^{\dagger}\rangle\rangle +U\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{l\sigma}{}^{\dagger}\rangle\rangle)\,,\quad\text{(A3)}$$

$$(E+h\sigma)G_{l,m}{}^{\sigma} =(2\pi)^{-1}\delta_{l,m}+\sum_j T_{mj}\,G_{lj}{}^{\sigma}+\delta_{m,0}(V\langle\langle c_{l\sigma}{}^{\dagger},c_{0\sigma}\rangle\rangle +U\langle\langle c_{l\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle)\,.\quad\text{(A4)}$$

Fourier transforming (A3) and (A4) gives

$$G_{\mathbf{q}\mathbf{q}'}{}^{\sigma}=F_{\mathbf{q}}{}^{\sigma}[(2\pi)^{-1}\delta_{\mathbf{q}\mathbf{q}'}+VG_{0\mathbf{q}'}{}^{\sigma} +U\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{\mathbf{q}'\sigma}{}^{\dagger}\rangle\rangle]\,,\quad\text{(A5)}$$

$$G_{\mathbf{q}'\mathbf{q}}{}^{\sigma}=F_{\mathbf{q}}[(2\pi)^{-1}\delta_{\mathbf{q}\mathbf{q}'}+VG_{\mathbf{q}',0}{}^{\sigma} +U\langle\langle c_{\mathbf{q}'\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle]\,.\quad\text{(A6)}$$

Next let $B=n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}$ in (A1) $A=n_{0\bar\sigma}c_{0\sigma}$ in (A2), then

$$(E+h\sigma)\langle\langle c_{m\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle =\delta_{m,0}(2\pi)^{-1}\langle n_{0\bar\sigma}\rangle+\sum_j T_{mj}\langle\langle c_{j\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle +\delta_{m,0}(V\langle\langle c_{0\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle+U\langle\langle n_{0\bar\sigma}c_{0\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle)\,,\quad\text{(A7)}$$

$$(E+h\sigma)\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{m\sigma}\rangle\rangle =\delta_{m,0}(2\pi)^{-1}\langle n_{0\bar\sigma}\rangle+\sum_j T_{mj}\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{j\sigma}{}^{\dagger}\rangle\rangle +\delta_{m,0}(V\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{0\sigma}{}^{\dagger}\rangle\rangle+U\langle\langle n_{0\bar\sigma}c_{0\sigma},n_0c_{0\bar\sigma\sigma}{}^{\dagger}\rangle\rangle)\,.\quad\text{(A8)}$$

Fourier transforming (A7) and (A8) one obtains

$$\langle\langle c_{\mathbf{q}\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle=F_{\mathbf{q}}{}^{\sigma}[(2\pi)^{-1}\langle n_{0\bar\sigma}\rangle+V\langle\langle c_{0\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle +U\langle\langle n_{0\bar\sigma}c_{0\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle]\,,\quad\text{(A9)}$$

$$\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{\mathbf{q}\sigma}{}^{\dagger}\rangle\rangle=F_{\mathbf{q}}{}^{\sigma}[(2\pi)^{-1}\langle n_{0\bar\sigma}\rangle+V\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{0\sigma}{}^{\dagger}\rangle\rangle +U\langle\langle n_{0\bar\sigma}c_{0\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle]\,.\quad\text{(A10)}$$

Summing (A9) and (A10) over q and solving for $\langle\langle c_{\mathbf{q}\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle$ and $\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{\mathbf{q}\sigma}{}^{\dagger}\rangle\rangle$, respectively, gives the result

$$\langle\langle c_{0\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle=\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{0\sigma}{}^{\dagger}\rangle\rangle\,.\quad\text{(A11)}$$

Equations (A9) and (A10) now yield $\langle\langle c_{\mathbf{q}\sigma},n_{0\bar\sigma}c_{0\sigma}{}^{\dagger}\rangle\rangle =\langle\langle n_{0\bar\sigma}c_{0\sigma},c_{\mathbf{q}\sigma}{}^{\dagger}\rangle\rangle$ and comparison of (A5) with (A6) gives $G_{\mathbf{q}\mathbf{q}'}{}^{\sigma}=G_{\mathbf{q}'\mathbf{q}}{}^{\sigma}$.

APPENDIX B

We prove that if (3.11) holds, then (3.12) follows. First write (3.11) as

$$a\Gamma_j=b_j\pm\sum_k T_{jk}\Gamma_k=b_j\pm T_{j0}\Gamma_0\pm\sum_{k\neq0} T_{jk}\Gamma_k\,,\quad j\neq0.\quad\text{(B1)}$$

Define the restricted Fourier transformer of Γ by

$$\hat\Gamma_{\mathbf{q}}=\sum_{j\neq0} e^{i\mathbf{q}\cdot\mathbf{R}_j}\Gamma_j.\quad\text{(B2)}$$

Multiply both sides of (B1) by $e^{i\mathbf{q}\cdot\mathbf{R}_j}$ and sum over j excluding $j=0$,

$$a\hat\Gamma_{\mathbf{q}}=b_{\mathbf{q}}-b_0\pm\epsilon_{\mathbf{q}}\Gamma_0\pm\epsilon_{\mathbf{q}}\hat\Gamma_{\mathbf{q}}\mp\sum_{\mathbf{q}'}\epsilon_{\mathbf{q}'}\hat\Gamma_{\mathbf{q}'}.\quad\text{(B3)}$$

We wish to solve for

$$\sum_j T_{0j}\Gamma_j=\sum_{\mathbf{q}}\epsilon_{\mathbf{q}}\Gamma_{\mathbf{q}}=\sum_{\mathbf{q}}\epsilon_{\mathbf{q}}\hat\Gamma_{\mathbf{q}}.\quad\text{(B4)}$$

Noting that from (B2)

$$\sum_{\mathbf{q}} \hat{\Gamma}_{\mathbf{q}} = 0, \tag{B5}$$

solving (B3) for $\hat{\Gamma}_{\mathbf{q}}$, and summing over q gives

$$0 = \sum_{\mathbf{q}} \frac{b_{\mathbf{q}}}{a \mp \epsilon_{\mathbf{q}}} - b_0 \sum_{\mathbf{q}} \frac{1}{a \mp \epsilon_{\mathbf{q}}} \pm \sum_{\mathbf{q}} \frac{\epsilon_{\mathbf{q}}}{a \mp \epsilon_{\mathbf{q}}} \Gamma_0 \mp \sum_{\mathbf{q}} \frac{1}{a \mp \epsilon_{\mathbf{q}}} \sum_{\mathbf{q}'} \epsilon_{\mathbf{q}'} \Gamma_{\mathbf{q}'} . \tag{B6}$$

Use of (B4) in (B6) gives (3.12).

APPENDIX C

Equations (4.4) and (4.5) are derived here. From (3.26) and (3.27), we obtain

$$\beta^{\sigma}(\omega+i\delta) = i\int_{-\infty}^{\infty} d\omega' F(\omega') \left[\frac{F^{\bar{\sigma}}(\omega'+i\delta) - F^{\sigma}(\omega+i\delta)}{\omega-\omega'+2h\sigma} \frac{G_{00}{}^{\bar{\sigma}}(\omega'+i\delta)}{F^{\bar{\sigma}}(\omega'+i\delta)} - \frac{F^{\sigma}(\omega'-i\delta) - F^{\sigma}(\omega+i\delta)}{\omega-\omega'+2h\sigma+i\delta} \frac{G_{00}{}^{\bar{\sigma}}(\omega'-i\delta)}{F^{\bar{\sigma}}(\omega'-i\delta)} \right]. \tag{C1}$$

The unperturbed Green's function F^{σ} is given by (4.2) from which

$$\frac{F^{\bar{\sigma}}(\omega'+i\delta) - F^{\sigma}(\omega+i\delta)}{\omega-\omega'+2h\sigma} \frac{1}{F^{\bar{\sigma}}(\omega'+i\delta)} = \frac{1}{\omega+h\sigma+iD} \tag{C2}$$

$$\frac{F^{\bar{\sigma}}(\omega'-i\delta) - F^{\sigma}(\omega+i\delta)}{\omega-\omega'+2h\sigma+i\delta} \frac{1}{F^{\bar{\sigma}}(\omega'-i\delta)} = \frac{1}{\omega+h\sigma+iD}\left[1 + \frac{2iD}{\omega-\omega'+2h\sigma+i\delta}\right]. \tag{C3}$$

Substituting (C2) and (C3) in (C1) gives

$$\beta^{\sigma}(\omega+i\delta) = \frac{1}{\omega+h\sigma+iD}\left[\langle n_{0\bar{\sigma}}\rangle + 2D\int_{-\infty}^{\infty} d\omega'\, f(\omega')(G_{00}{}^{\bar{\sigma}}(\omega'-i\delta) \; (\omega-\omega'+2h\sigma+i\delta))\right]. \tag{C4}$$

In order to find γ, we see from (3.29) that we require

$$O_{\omega'}\left(\frac{F^{\bar{\sigma}}(\omega') - F^{\sigma}(\omega)}{\omega-\omega'+2h\sigma} \frac{\beta^{\bar{\sigma}}(\omega')G_{00}{}^{\bar{\sigma}}(\omega')}{[F^{\bar{\sigma}}(\omega')]^2} \right) = i\int_{-\infty}^{\infty} d\omega'\, f(\omega') \left(\frac{F^{\bar{\sigma}}(\omega'+i\delta) - F^{\sigma}(\omega+i\delta)}{\omega-\omega'+2h\sigma} \frac{\beta^{\bar{\sigma}}(\omega'+i\delta)}{F^{\bar{\sigma}}(\omega'+i\delta)} \frac{G_{00}{}^{\bar{\sigma}}(\omega'+i\delta)}{F^{\bar{\sigma}}(\omega'+i\delta)} - \frac{F^{\bar{\sigma}}(\omega'-i\delta) - F^{\sigma}(\omega+i\delta)}{\omega-\omega'+2h\sigma+i\delta} \frac{\beta^{\bar{\sigma}}(\omega'-i\delta)}{F^{\bar{\sigma}}(\omega'-i\delta)} \frac{G_{00}{}^{\bar{\sigma}}(\omega'-i\delta)}{F^{\bar{\sigma}}(\omega'-i\delta)} \right)$$

[making use of (4.2) and (4.3)]

$$= i\int_{-\infty}^{\infty} d\omega'\, f(\omega') \left[\frac{-iDG_{00}{}^{\bar{\sigma}}(\omega'+i\delta)}{\omega+h\sigma+iD} + \frac{-iD}{\omega+h\sigma+iD}\left(1 + \frac{2iD}{\omega-\omega'+2h\sigma+i\delta}\right) \times G_{00}{}^{\bar{\sigma}}(\omega'-i\delta) \right]. \tag{C4}$$

Also required is

$$\frac{1}{2\pi} O_{\omega'} \left\{ \frac{B^{\bar{\sigma}}(\omega') - B^{\sigma}(\omega)}{\omega-\omega'+2h\sigma} \right\} - \frac{1}{2\pi} O_{\omega'} \left\{ \left(\frac{F^{\bar{\sigma}}(\omega') - F^{\sigma}(\omega)}{\omega-\omega'+2h\sigma} \right) \frac{B^{\bar{\sigma}}(\omega')}{F^{\bar{\sigma}}(\omega')} \right\}$$

$$= \frac{1}{2\pi} O_{\omega'} \left\{ \frac{1}{\omega-\omega'+2h\sigma} \left[(\omega'-h\sigma)F^{\bar{\sigma}}(\omega') - (\omega+h\sigma)F^{\sigma}(\omega) - (F^{\bar{\sigma}}(\omega') - F^{\sigma}(\omega)) \left(\frac{1}{F^{\bar{\sigma}}(\omega')} - \omega' + h\sigma \right) \right] \right\}$$

$$= \frac{1}{2\pi} O_{\omega'} \left\{ \frac{F^{\bar{\sigma}}(\omega') - F^{\sigma}(\omega)}{\omega-\omega'+2h\sigma} \frac{1}{F^{\bar{\sigma}}(\omega')} \right\} = \frac{(D\ \pi)}{\omega+h\sigma+iD} \int_{-\infty}^{\infty} \frac{f(\omega')}{\omega-\omega'+2h\sigma+i\delta} d\omega' \tag{C5}$$

[where we used $\beta^\sigma(\omega)=-1+(\omega+h\sigma)F^\sigma(\omega)$]. Combining (C4) and (C5) gives

$$\gamma^\sigma(\omega+i\delta)=\frac{(D/\pi)}{\omega+h\sigma+iD}\left[\int_{-\infty}^{\infty}\frac{d\omega' f(\omega')}{\omega-\omega'+2h\sigma+i\delta}+2iD^2\int_{-\infty}^{\infty}d\omega' f(\omega')\frac{G_{00}^{\bar\sigma}(\omega'-i\delta)}{\omega-\omega'+2h\sigma+i\delta}\right.$$
$$\left.+D\int_{-\infty}^{\infty}d\omega' f(\omega')[G_{00}^{\bar\sigma}(\omega'+i\delta)+G_{00}^{\bar\sigma}(\omega'-i\delta)]\right]. \quad \text{(C6)}$$

Again using (4.2) and (4.3), we obtain

$$\alpha^\sigma(\omega+i\delta)\equiv O_{\omega'}\left\{\frac{B^{\bar\sigma}(\omega')G^{\bar\sigma}(\omega')}{F^{\bar\sigma}(\omega')}\right\}=D\int_{-\infty}^{\infty}d\omega' f(\omega')[G_{00}^{\bar\sigma}(\omega'+i\delta)+G_{00}^{\bar\sigma}(\omega'-i\delta)]. \quad \text{(C7)}$$

With the result (C7) it is clear that (C6) is equivalent to (4.5).

The density of states (4.1) allows for a great simplica- tion in the integral equation (3.20) as evidenced by (4.19). Unfortunately, the density of states (4.1) goes to zero rather slowly as $E\rightarrow\pm\infty$ the direct result of this is that the real part of the integral

$$Y^\sigma(\omega+i\delta)=\int_{-\infty}^{\infty}\frac{f(\omega')d\omega'}{\omega-\omega'+2h\sigma+i\delta} \quad \text{(C8)}$$

is infinite. This behavior is unphysical and a cutoff at $\pm nD$ is introduced

$$Y^\sigma(\omega+i\delta)\simeq\int_{-nD}^{nD}\frac{f(\omega')d\omega'}{\omega-\omega'+2h\sigma+i\delta}. \quad \text{(C9)}$$

This introduces a singularity (at zero temperature) into the real part of $Y^\sigma(\omega\pm i\delta)$ at $\omega=\pm nD-2h\sigma$ which is also unphysical. Fortunately, we are only interested in energies close to the Fermi energy and we expect that a judicious choice on n will lead to meaningful results. It is found that our numerical results are fairly insensitive to the choice of n for $n=3$, 6, and 10.

APPENDIX D

We show that the function $H(\omega)$ of (5.22) has no zeros or singularities for $-nD\leq\omega\leq nD$. Define

$$d=d_R+id_I, \quad \tilde{d}=d_R-id_I, \quad Y^{\pm}=Y_R\pm iY_I, \quad \text{(D1)}$$

where d_R, d_I, Y_R, and Y_I are real and j is real by (5.18), then

$$H(\omega)=\frac{j+2d_RY_R+Y_R^2-Y_I^2+2iY_I(d_R+Y_R)}{j+2(d_RY_R+d_IY_I)+Y_R^2+Y_I^2}, \quad \text{(D2)}$$

where

$$d_R=(V-\omega)/D, \quad d_I=1-\langle n_0\rangle, \quad j=(\omega-V)^2D^{-2}+1+2\langle n_0\rangle. \quad \text{(D3)}$$

Use of (D3) in (D2) gives

$$H(\omega)=\frac{2\langle n_0\rangle+(1-f^2)+[(V-\omega)D^{-1}+Y_R]^2-2if[(V-\omega)D^{-1}+Y_R]}{2\langle n_0\rangle(1+f)+[(V-\omega)D^{-1}+Y_R]^2+(1-f)^2}, \quad \text{(D4)}$$

where we have used $Y_I=-f$, $f=$ Fermi function.

From (D4) we see that $H(\omega)$ has no zeros or poles on the real axis.