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Localized Correlations in Narrow Conduction Bands. II

Joel A. Appelbaum
Bell Telephone Laboratories, Murray Hill, New Jersey 07974

and

David R. Penn*
Brown University, Providence, Rhode Island 02912
(Received 13 July 1070)

The problem of a magnetic impurity in a narrow conduction band is studied using double-time Green's functions. We have used a Wolff model in which a repulsive Coulomb interaction of strength U is limited to the impurity site. The coupling of the impurity site to its neighbors because of the kinetic energy is reduced by a scale factor relative to the coupling of host atoms to their neighbors. The difference in the one-electron potential between host and impurity sites is also taken into account. We have solved the decoupled Green's-function equations in the infinite-U limit in the presence of a finite magnetic field. From this solution, a conserving calculation of the zero-field magnetic susceptibility χ is performed and numerical results obtained. We find that for a sufficiently weak coupling between the impurity atom and its neighbors, a Curie-law behavior of χ can be obtained over the four decades of temperature studied. Evidence of Kondo saturation of χ is found for more strongly coupled impurities. The susceptibility shows no evidence of singular behavior at zero temperature.

I. INTRODUCTION

Recently the authors undertook a study of the problem of a magnetic impurity in a narrow energy band.[1-3] An equation-of-motion technique was used in which particular care was taken in the treatment of electron correlations at the impurity site. A similar decoupling scheme has also been used in the study of the Anderson model.[4]

The model studied by the authors was a modification of the Wolff[5] model; it was assumed that the sole effect of the magnetic impurity was the introduction of a strong repulsive interaction between electrons of opposite spin on the impurity site. The coupling of the impurity to its neighbors via the hopping term in the kinetic energy was assumed to be the same as that for any other atom and its neighbors. The one-electron potential of the impurity was assumed to be the same as that of a host atom. Our purpose is to study this model, relaxing the above-mentioned restrictions (equal coupling and equal one-electron potentials), in the presence of a magnetic field. We show that the procedures used by Appelbaum and Penn in Ref. 2 (to be referred to as I) carry over to this more general case. The equation for the localized Green's functions at the impurity site is then virtually identical to that for the extra orbital in the Anderson model.[4,6]

The singular integral equation obtained from the equation-of-motion scheme can be solved in the infinite-U limit, where U measures the strength of the Coulomb repulsion on the impurity site. The static zero-field magnetic susceptibility of the impurity is found by a direct calculation in the zero-field limit of $(n_{0-}-n_{0+})/H$, where $n_{0\pm}$ is the occupation number of the impurity site for spin up (down) and H is the magnetic field.

The outline of this paper is as follows. In Sec. II we apply an equation-of-motion technique to obtain a self-consistant equation for the impurity Green's function. The equation is solved formally in Sec. III. In Sec. IV this solution is used to reduce the calculation of the magnetic susceptibility to quadratures. The magnetic susceptibility is evaluated numerically and the results presented in Sec. V. A comparison of this work with other calculations of the magnetic susceptibility is contained in Sec. VI.

II. EQUATION OF MOTION

The Hamiltonian we study is

$$\mathcal{H}=\sum_{ij\sigma}T_{ij}d^\dagger_{i\sigma}d_{j\sigma}+\frac{U}{2}\sum_\sigma n_{0\sigma}n_{0\bar\sigma}+V\sum_\sigma n_{0\sigma}+\Delta\sum_{i\sigma}\sigma n_{i\sigma}\ , \tag{2.1}$$

where $d^\dagger_{i\sigma}$ creates an electron with spin $\frac{1}{2}\sigma=\pm\frac{1}{2}$ at site i, U is the strength of the Coulomb repulsion at site $i=0$, V is the shift in the zero of energy at the impurity site, and Δ is the magnetic energy of the electrons due to the external field; the g value of the electron at all sites is assumed equal.

The hopping integral T_{ij} is taken to have the form

$$T_{ij}=T(i-j)+T'_{0j}\delta_{i,0}+T'_{i0}\delta_{j,0}\ , \tag{2.2}$$

where

$$T'_{i0}=T'_{0i}\equiv\gamma T(i)\ , \tag{2.3}$$

and we make the choice $T(0)=0$. In other words, we assume the coupling of the impurity site to its neighbors is the same as for host sites, except for a scale factor. The factor $1+\gamma$ is expected to be significantly less than unity because T_{ij} is proportional to the overlap of wave functions located at sites i and j. This overlap occurs in the exponentially decreasing tails of the wave functions and the impurity-atom wave function is more contracted than that of a host atom.

We introduce the retarded double-time Green's function[7]

$$\langle\langle A,B\rangle\rangle_\omega=-\frac{i}{2\pi}\int_0^\infty\langle A(t)B(0)-B(0)A(t)\rangle e^{i\omega t}dt\ . \tag{2.4}$$

The equation of motion for the one-electron Green's function is

$$(\omega-\sigma\Delta)D^\sigma_{ij}=\frac{\delta_{ij}}{2\pi}+\sum_k T_{ik}D^\sigma_{kj}+U\delta_{i0}\langle\langle n_{0\bar\sigma}d_{0\sigma};\ d^\dagger_{j\sigma}\rangle\rangle+V\delta_{i0}D^\sigma_{0j}\ , \tag{2.5}$$

where

$$D^\sigma_{ij}=\langle\langle d_{i\sigma};\ d^\dagger_{j\sigma}\rangle\rangle_\omega\ . \tag{2.6}$$

Introducing

$$a_{\vec k\sigma}\equiv(1/N^{1/2})\textstyle\sum_i e^{-i\vec k\cdot\vec r_i}d_{i\sigma}\ , \tag{2.7}$$

one finds that (2.5) can be rewritten as

$$(\omega-\sigma\Delta-\epsilon_{\vec k})G^\sigma_{\vec k\vec k'}=\frac{1}{2\pi}\delta_{\vec k\vec k'}+\frac{\gamma}{N}\sum_{\vec q}\epsilon_{\vec q}G^\sigma_{\vec q\vec k'}+(\gamma\epsilon_{\vec k}+V)\times\frac{1}{N}\sum_{\vec q}G^\sigma_{\vec q\vec k'}+\frac{1}{N^{1/2}}U\langle\langle n_{0\bar\sigma}d_{0\sigma};a^\dagger_{\vec k'\sigma}\rangle\rangle\ , \tag{2.8}$$

where

$$G^\sigma_{\vec k\vec k'}\equiv\langle a_{\vec k\sigma};\ a^\dagger_{\vec k'\sigma}\rangle\ , \tag{2.9}$$

$$\epsilon_{\vec q}=(1/N^{1/2})\textstyle\sum_i e^{i\vec q\cdot(\vec r_i-\vec r_j)}T(i-j)\ . \tag{2.10}$$

Introducing

$$G^\sigma_{\vec k'}=\textstyle\sum_{\vec k}G^\sigma_{\vec k\vec k'};\quad E^\sigma_{\vec k'}=\sum_{\vec k}\epsilon_{\vec k}G^\sigma_{\vec k,\vec k'}\ , \tag{2.11}$$

one obtains from (2.8) the equations

$$[1-\gamma F^1(\omega-\sigma\Delta)-VF(\omega-\sigma\Delta)]G^\sigma_{\vec k'}(\omega)-\gamma F(\omega-\sigma\Delta)E^\sigma_{\vec k'}=\frac{1}{2\pi}\frac{1}{\omega-\sigma\Delta-\epsilon_{\vec k'}}+UN^{1/2}F(\omega-\sigma\Delta)\langle\langle n_{0\bar\sigma}d_{0\sigma};a^\dagger_{\vec k'\sigma}\rangle\rangle, \tag{2.12}$$

$$[\gamma F^2(\omega-\sigma\Delta)+VF^1(\omega-\sigma\Delta)]G^\sigma_{\vec k'}(\omega)+[\gamma F^1(\omega-\sigma\Delta)-1]E^\sigma_{\vec k'}=-\frac{1}{2\pi}\frac{\epsilon_{\vec k'}}{\omega-\epsilon_{\vec k'}-\sigma\Delta}-UN^{1/2}F^1\times(\omega-\sigma\Delta)\langle\langle n_{0\bar\sigma}d_{0\sigma};\ a^\dagger_{\vec k'\sigma}\rangle\rangle\ , \tag{2.13}$$

where

$$F^n(\omega) = (1/N)\sum_{\vec{k}} \epsilon_{\vec{k}}^n/(\omega - \epsilon_{\vec{k}}) , \qquad (2.14)$$

$$F(\omega) \equiv F^0(\omega);\; F^1(\omega) = \omega F(\omega) - 1;\; F^2(\omega) = \omega F^1(\omega) , \qquad (2.15)$$

assuming the band is symmetric about the zero of energy. The zero of energy coincides here with the Fermi energy, the case of half-filled conduction band is being considered. By summing over $\vec{k}'$ in (2.12) and (2.13), one finds after some algebra that

$$\langle\langle d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = \frac{1}{N}\sum_{\vec{k}'} G_{\vec{k}'}^\sigma = \frac{F(\omega-\sigma\Delta)(1/2\pi + U\langle\langle n_{0\bar\sigma} d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle)}{1-(2\gamma+\gamma^2)F^1(\omega-\sigma\Delta) - VF(\omega-\sigma\Delta)} . \qquad (2.16)$$

As in I, we write an equation for the two-particle Green's function $\langle\langle n_{0\bar\sigma} d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle$:

$$(\omega - \sigma\Delta - UV)\langle\langle n_{0\bar\sigma} d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = \frac{\langle n_{0\bar\sigma}\rangle}{2\pi} + \sum_{j'} T_{0j'}\langle\langle n_{0\bar\sigma} d_{j'\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle - \sum_{j'} T_{0j'}\langle\langle d_{0\bar\sigma}^\dagger d_{0\sigma} d_{j'\bar\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle - \sum_{j'} T_{j'0}\langle\langle d_{0\bar\sigma} d_{0\sigma} d_{j'\bar\sigma}^\dagger\,;\, d_{0\sigma}^\dagger\rangle\rangle . \qquad (2.17)$$

Since we will be interested in the infinite-U case, we can ignore the last term on the right-hand side of (2.17).

The equation for $\langle\langle n_{0\bar\sigma} d_{j'\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle$ after decoupling is

$$(\omega-\sigma\Delta)\langle\langle n_{0\bar\sigma}\, d_{j'\sigma}\,; d_{0\sigma}^\dagger\rangle\rangle = \sum_k T_{j'k}\langle\langle n_{0\bar\sigma} d_{k\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle :\quad j' \neq 0, \qquad (2.18)$$

where we have used the decoupling approximation

$$\langle\langle d_{i\bar\sigma}^\dagger d_{j\bar\sigma} d_{j'\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = \langle d_{i\bar\sigma}^\dagger d_{j\bar\sigma}\rangle\langle\langle d_{j'\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle :\quad \text{at most one of } i,j,j' = 0 . \qquad (2.19)$$

See I for a complete discussion of the decoupling procedure. By Fourier analyzing (2.18) one finds

$$(\omega - \sigma\Delta - \epsilon_{\vec{q}})\Gamma_{\vec{q}}^\sigma = -(1/N)\sum_{\vec{k}'} \epsilon_{\vec{k}'}\Gamma_{\vec{k}'} + (\omega - \sigma\Delta + \gamma\epsilon_{\vec{q}})(1/N)\sum_{\vec{k}'}\Gamma_{\vec{k}'} , \qquad (2.20)$$

where

$$\Gamma_{\vec{q}}^\sigma = \langle\langle n_{0\bar\sigma} a_{\vec{q}\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle . \qquad (2.21)$$

Dividing (2.19) by $(\omega - \sigma\Delta - \epsilon_{\vec{q}})$ and summing on $\vec{q}$ one finds that

$$\sum_{\vec{k}'} \epsilon_{\vec{k}'}\Gamma_{\vec{k}'} = \frac{(1+\gamma)F^1(\omega-\sigma\Delta)}{F(\omega-\sigma\Delta)}\sum_{\vec{k}'}\Gamma_{\vec{k}'} . \qquad (2.22)$$

Since

$$\sum T_{0j'}\langle\langle n_{0\bar\sigma} d_{j'\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = (1/N^{1/2})(1+\gamma)\sum_{\vec{q}}\epsilon_{\vec{q}}\Gamma_{\vec{q}} , \qquad (2.23)$$

$$\langle\langle n_{0\bar\sigma} d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = (1/N^{1/2})\sum_{\vec{q}}\Gamma_{\vec{q}} , \qquad (2.24)$$

we obtain

$$\sum_{j'} T_{0j'}\langle\langle n_{0\bar\sigma} d_{j'\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = (1+\gamma)^2(\omega - \sigma\Delta - F^{-1}) \times \langle\langle n_{0\bar\sigma} d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle . \qquad (2.25)$$

We now need an equation for

$$\langle\langle d_{0\bar\sigma}^\dagger d_{0\sigma} d_{j'\bar\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle : j' \neq 0 .$$

After decoupling according to (2.19) it takes the form

$$(\omega-\sigma\Delta)\langle\langle d_{0\bar\sigma}^\dagger d_{0\sigma} d_{j'\bar\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = -\langle d_{0\bar\sigma}^\dagger d_{j'\bar\sigma}\rangle(1/2\pi + \sum_k T_{0k}\langle\langle d_{k\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle) + \sum_k T_{j'k}\langle\langle d_{0\bar\sigma}^\dagger d_{0\sigma} d_{k\bar\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle + \sum_i T_{i0}\langle d_{i\bar\sigma}^\dagger d_{j'\bar\sigma}\rangle\langle\langle d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle . \qquad (2.26)$$

By Fourier analyzing (2.26) one obtains

$$(\omega-\sigma\Delta-\epsilon_{\vec{k}})\Gamma_{\vec{k}}'^\sigma - (\omega-\sigma\Delta)\frac{1}{N}\sum_{\vec{q}}\Gamma_{\vec{q}}'^\sigma = -\left(\langle d_{0\bar\sigma}^\dagger a_{\vec{k}\bar\sigma}\rangle - \frac{1}{N}\sum_{\vec{q}}\langle d_{0\bar\sigma}^\dagger a_{\vec{q}\bar\sigma}\rangle\right)\left(\frac{1}{2\pi} + (1+\gamma)E\right) - \frac{1}{N}\sum_{\vec{q}}\epsilon_{\vec{q}}\Gamma_{\vec{q}}'^\sigma + \gamma\epsilon_{\vec{k}}\frac{1}{N}\sum_{\vec{q}}\Gamma_{\vec{q}}'^\sigma + \sum_i T_{i0}\left(\langle d_{i\bar\sigma}^\dagger a_{\vec{k}\bar\sigma}\rangle - \frac{1}{N}\sum_{\vec{k}}\langle d_{i\bar\sigma}^\dagger a_{\vec{k}\bar\sigma}\rangle\right) D_{00}^\sigma , \qquad (2.27)$$

where

$$D_{00}^\sigma = \langle\langle d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle , \qquad (2.28)$$

$$\Gamma_{\vec{k}}'^\sigma = \langle\langle d_{0\bar\sigma}^\dagger d_{0\sigma} a_{\vec{k}\bar\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle , \qquad (2.29)$$

and

$$E = (1/N)\sum_{\vec{k}} E_{\vec{k}}^\sigma . \qquad (2.30)$$

Using

$$\sum_{j'} T_{0j'}\langle\langle d_{0\bar\sigma}^\dagger d_{0\sigma} d_{j'\bar\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = \frac{1+\gamma}{N^{1/2}}\sum_{\vec{q}'}\epsilon_{\vec{q}'}\Gamma_{\vec{q}}'^\sigma \qquad (2.31)$$

and (2.27),

$$\sum_{j'} T_{0j'}\langle\langle d_{0\bar\sigma}^\dagger d_{0\sigma} d_{j'\bar\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle = -(1+\gamma)^2[\omega-\sigma\Delta - F^{-1}(\omega-\sigma\Delta)]\langle\langle n_{0\bar\sigma} d_{0\sigma}\,;\, d_{0\sigma}^\dagger\rangle\rangle + \frac{B^\sigma(\omega-\sigma\Delta)D_{00}^\sigma(\omega)}{F(\omega-\sigma\Delta)} - (1+\gamma)^2 A^\sigma(\omega-\sigma\Delta)\,\frac{1/2\pi + (1+\gamma)E(\omega)}{F(\omega-\sigma\Delta)} , \qquad (2.32)$$

where

$$A^{\sigma}(\omega-\sigma\Delta)=\frac{1}{N^{1/2}(1+\gamma)}\sum_{\vec{k}}\left(\langle d_{0\bar{\sigma}}^{\dagger}a_{\vec{k}\bar{\sigma}}\rangle-N^{-1}\sum_{\vec{q}}\langle d_{0\bar{\sigma}}^{\dagger}a_{\vec{q}\bar{\sigma}}\rangle\right)\Big/(\omega-\sigma\Delta-\epsilon_{\vec{k}}) , \tag{2.33}$$

$$B^{\sigma}(\omega-\sigma\Delta)=\frac{(1+\gamma)}{N^{1/2}}\sum_{i\vec{k}}T_{i0}\left(\langle d_{i\bar{\sigma}}^{\dagger}a_{\vec{k}\bar{\sigma}}\rangle-N^{-1}\sum_{\vec{k}'}\langle d_{i\bar{\sigma}}^{\dagger}a_{\vec{k}\bar{\sigma}}\rangle\right)\Big/(\omega-\sigma\Delta-\epsilon_{\vec{k}}) . \tag{2.34}$$

Combining (2.32) and (2.25) into (2.17) and (2.16) one finds for the local Green's function in the infinite-U limit,

$$D_{00}^{\sigma}(\omega+i\delta)=F(\omega-\sigma\Delta)[(1-\langle n_{0\bar{\sigma}}\rangle)/2\pi-(1+\gamma)^2A^{\sigma}(\omega-\sigma\Delta)/2\pi F(\omega-\sigma\Delta)]\,[(1+\gamma)^2-(2\gamma+\gamma^2)(\omega-\sigma\Delta)$$
$$\times F(\omega-\sigma\Delta)-B^{\sigma}(\omega-\sigma\Delta)-VF(\omega-\sigma\Delta)-(1+\gamma)^4(F^{-1}(\omega-\sigma\Delta)-\omega+\sigma\Delta)A^{\sigma}(\omega-\sigma\Delta)]^{-1} . \tag{2.35}$$

III. INTEGRAL EQUATION

Converting (2.35) into a closed explicit equation for $D_{00}^{\sigma}(\omega)$ involves expressing $A^{\sigma}(\omega)$ and $B^{\sigma}(\omega)$ in terms of integral operators acting on $D_{00}^{\sigma}(\omega)$. This is done in Appendix A for a truncated Lorentzian density of states. We find that

$$A^{\sigma}(\omega-\sigma\Delta+i\delta)=F(\omega-\sigma\Delta)2D\int_{-nD}^{nD}\frac{f(\omega'-\sigma\Delta)D_{00}^{\bar{\sigma}}(\omega'-i\delta-\sigma\Delta)d\omega'}{\omega-\sigma\Delta-\omega'+i\delta} , \tag{3.1}$$

$$B^{\sigma}(\omega-\sigma\Delta+i\delta)=\frac{(1+\gamma)^2DF(\omega-\sigma\Delta)}{\pi}\int_{-nD}^{nD}\frac{f(\omega'-\sigma\Delta)d\omega'}{\omega-\sigma\Delta-\omega'+i\delta}$$
$$+\frac{(1+\gamma)^4DF(\omega-\sigma\Delta)}{\pi}\int_{-nD}^{nD}\frac{f(\omega'-\sigma\Delta)D_{00}^{\bar{\sigma}}(\omega'-i\delta-\sigma\Delta)d\omega'}{\omega-\sigma\Delta-\omega'+i\delta} . \tag{3.2}$$

Substituting (3.1) and (3.2) into (2.35) we obtain

$$D_{00}^{+}(\omega+i\delta)=\left(\frac{(1-\langle n_{0+}\rangle)}{2\pi}-\frac{d}{\pi}\int_{-nD}^{nD}\frac{f(\omega'-\Delta)d\omega'}{\omega-\omega'-\Delta+i\delta}D_{00}^{-}(\omega'-\Delta-i\delta)\right)\Big/$$
$$\left(\omega-\Delta-V-\frac{d}{\pi}\int_{-nD}^{nD}\frac{d\omega' f(\omega'-\Delta)}{\omega-\omega'-\Delta+i\delta}-4id^2\int_{-nD}^{nD}\frac{d\omega' f(\omega'-\Delta)}{\omega-\omega'-\Delta+i\delta}D_{00}^{-}(\omega'-\Delta-i\delta)\right) , \tag{3.3}$$

where

$$d=(1+\gamma)^2D . \tag{3.4}$$

Examination of this equation and Eq. (26) of Ref. 4 reveals that our equation for the impurity-level Green's function and Theumann's for the extra-orbital Green's function in the Anderson model are identical if one makes the correspondence $d\to\pi\rho^0V_{kd}^2$ and $V\to\epsilon_d$, where ρ^0 is the density of states of the conduction band, V_{kd} the s-d mixing strength, and ϵ_d the d-electron energy level. Theumann's integral equation is derived for a constant density of states and the asssmption that $F(\omega+i\delta)$ may be replaced by $-i\pi\rho(\omega)$. It should be pointed out that while the t matrix in the Anderson model is proportional to $D_{00}(\omega)$, this is not true here, as we show in Appendix C.

The key to solving (3.3) is to notice that while there are in principle four sets of integral equations for $D^{+}(\omega\pm i\delta)$ and $D^{-}(\omega\pm i\delta)$, the equations separate so that $D^{+}(\omega+i\delta)$ couples with only $D^{-}(\omega-i\delta)$ and similarly for the other two quantities.

With the substitutions

$$\Psi^{\sigma}(\omega+i\delta)=4\pi i d D_{00}^{\sigma}(\omega+i\delta)-1 , \tag{3.5a}$$

$$\Psi^{\sigma}(\omega+i\delta)=\Psi^{\sigma}(\omega-i\delta)^{*} , \tag{3.5b}$$

the two simultaneous equations we need to solve are

$$\Psi^{+}(\omega+i\delta)=\frac{b^{-}+i(\omega-\Delta-V)/d+X_1(\omega-\Delta+i\delta)}{1-i(\omega-\Delta-V)/d+\Phi_1(\omega-\Delta+i\delta)} , \tag{3.6}$$

$$\Psi^{-}(\omega-i\delta)=\frac{b^{+}-i(\omega+\Delta-V)/d+X_2(\omega+\Delta-i\delta)}{1+i(\omega+\Delta-V)/d+\Phi_2(\omega+\Delta+i\delta)} , \tag{3.7}$$

with

$$X_1(Z)=\frac{1}{\pi i}\int_{-nD}^{nD}\frac{f(\omega'-\Delta)d\omega'}{Z-\omega'} ,$$
$$X_2(Z)=-\frac{1}{\pi i}\int_{-nD}^{nD}\frac{f(\omega'+\Delta)d\omega'}{Z-\omega'} , \tag{3.8}$$

$$\Phi_1(Z)=\frac{1}{\pi i}\int_{-nD}^{nD}\frac{f(\omega'-\Delta)\Psi^{-}(\omega'-\Delta-i\delta)d\omega'}{Z-\omega'} , \tag{3.9}$$

$$\Phi_2(Z)=-\frac{1}{\pi i}\int_{-nD}^{nD}\frac{f(\omega'+\Delta)\Psi^{+}(\omega'+\Delta+i\delta)d\omega'}{Z-\omega'} , \tag{3.10}$$

and

$$b^{\pm}=1-2\langle n_{0\pm}\rangle\ . \qquad (3.11)$$

Examining the discontinuity of $\Phi_1(Z)$ and $\Phi_2(Z)$ across the real axis one finds

$$\Phi_1(\omega+\Delta+i\delta)-\Phi_1(\omega+\Delta-i\delta)$$
$$=[X_1(\omega+\Delta+i\delta)-X_1(\omega+\Delta-i\delta)]\Psi^-(\omega-i\delta)$$
$$(-D<\omega+\Delta<D)\ , \qquad (3.12)$$

$$\Phi_2(\omega-\Delta+i\delta)-\Phi_2(\omega-\Delta-i\delta)$$
$$=[X_2(\omega-\Delta+i\delta)-X_2(\omega-\Delta-i\delta)]\Psi^+(\omega+i\delta)$$
$$(-D<\omega-\Delta<D)\ . \qquad (3.13)$$

Substituting (3.13) and (3.12) into (3.6) and (3.7), respectively, and then translating the frequency axis in (3.6) by $+\Delta$ and (3.7) by $-\Delta$ one finds

$$\frac{\Phi_1(\omega+i\delta)-\Phi_1(\omega-i\delta)}{X_1(\omega+i\delta)-X_1(\omega-i\delta)}=\frac{b^+ +(\omega-V)/id+X_2(\omega+i\delta)}{1-(\omega-V)/id+\Phi_2(\omega-i\delta)}$$
$$(-D<\omega<D)\ , \qquad (3.14)$$

$$\frac{\Phi_2(\omega+i\delta)-\Phi_2(\omega-i\delta)}{X_2(\omega+i\delta)-X_2(\omega-i\delta)}=\frac{b^- -(\omega-V)/id+X_1(\omega+i\delta)}{1+(\omega-V)/id+\Phi_1(\omega+i\delta)}$$
$$(-D<\omega<D)\ . \qquad (3.15)$$

Equations (3.14) and (3.15) can now be solved as in I. Clearing fractions in (3.14) and (3.15) and adding, one finds that

$$-X_1(Z)X_2(Z)+\Phi_1(Z)\Phi_2(Z)$$
$$-X_1(Z)[b^+-i(Z-V)/d]-X_2(Z)[b^-+i(Z-V)/d]$$
$$+\Phi_2(Z)[1-i(Z-V)/d]+\Phi_1(Z)[1+i(Z-V)/d] \qquad (3.16)$$

is continuous across the cut $(-D,D)$. Since the function is analytic above and below the cut and continuous across the cut, it must be a polynomial. Examination of the asymptotic form of (3.16) reveals that (3.16) is a constant, denoted here as A,

$$A=\lim_{Z\to\infty}\frac{Z}{id}[\Phi_2(Z)-\Phi_1(Z)]+\frac{Z}{id}[X_2(Z)-X_1(Z)]$$
$$=4i\int_{-nD}^{nD}[D_{00}^{+}(\omega'+\Delta+i\delta)f(\omega'+\Delta)$$
$$-D_{00}^{-}(\omega'-\Delta-i\delta)f(\omega'-\Delta)]d\omega'\ . \qquad (3.17)$$

Using (3.15)–(3.17) one obtains after some rather simple algebraic manipulation the boundary value problem

$$\frac{\Phi_1(\omega+i\delta)+1-i(\omega-V)/d}{\Phi_1(\omega-i\delta)+1-i(\omega-V)/d}=H'=\frac{H_N'}{H_D'}\ , \qquad (3.18)$$

$$H_N'=1+A+(\omega-V)^2/d^2+X_2(\omega-i\delta)X_1(\omega+i\delta)$$
$$+X_2(\omega-i\delta)[b^-+i(\omega-V)/d]$$
$$+X_1(\omega+i\delta)[b^+-i(\omega-V)/d]\ , \qquad (3.19)$$

$$H_D'=1+A+(\omega-V)^2/d^2+X_1(\omega-i\delta)[b^+-i(\omega-V)/d]$$
$$+X_2(\omega-i\delta)[b^-+i(\omega-V)/d]$$
$$+X_2(\omega-i\delta)X_1(\omega-i\delta)\ . \qquad (3.20)$$

The solution to (3.18) can be written down by inspection and is

$$\Phi_1(Z)+1-\frac{i(Z-V)}{d}$$
$$=\frac{C-iZ}{d}\exp\left(-\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{\ln H'(\omega')d\omega'}{Z-\omega'}\right). \qquad (3.21)$$

The constant C is determined by expanding both sides of (3.21) in a Taylor-Laurent series. One finds

$$C=1+\frac{iV}{d}-(2\pi d)^{-1}\int_{-nD}^{nD}\ln H'(\omega')d\omega'\ . \qquad (3.22)$$

Equation (3.21) constitutes a solution to (3.18); it is necessary however, to determine A and $b^{\pm}$ self-consistently by examining the asymptotic form of Φ_1 and Φ_2. To this end it is advantagous to obtain a form of Φ_2 symmetric with that of (3.21); going back to (3.15)–(3.17) we obtain an alternative to (3.18),

$$\frac{\Phi_2(\omega+i\delta)+1+i(\omega-V)/d}{\Phi_2(\omega-i\delta)+1+i(\omega-V)/d}=H\equiv\frac{H_N}{H_D}\ , \qquad (3.23)$$

$$H_N=1+A+(\omega-V)^2/d^2-i(\omega-V)[X_1(\omega+i\delta)$$
$$-X_2(\omega+i\delta)]/d+X_1(\omega+i\delta)X_2(\omega+i\delta)$$
$$+b^+X_1(\omega+i\delta)+b^-X_2(\omega+i\delta)\ , \qquad (3.24)$$

$$H_D=1+A+(\omega-V)^2/d^2-i(\omega-V)[X_1(\omega+i\delta)$$
$$-X_2(\omega-i\delta)]/d+X_1(\omega+i\delta)X_2(\omega-i\delta)$$
$$+b^+X_1(\omega+i\delta)+b^-X_2(\omega-i\delta)\ , \qquad (3.25)$$

whose solution is

$$\Phi_2(Z)+\frac{1+i(Z-V)}{d}$$
$$=\frac{C'+iZ}{d}\exp\left(-\frac{1}{2\pi i}\int_{-nD}^{nD}\frac{\ln H(\omega')\,d\omega'}{Z-\omega'}\right), \qquad (3.26)$$

with

$$C'=1-\frac{iV}{d}+(2\pi d)^{-1}\int_{-nD}^{nD}\ln H(\omega')d\omega'\ . \qquad (3.27)$$

Expanding (3.21) and (3.26) in Taylor-Laurent series and equating equal powers of Z one finds

$$\lim_{Z\to\infty}Z\Phi_1(Z)=\left(1-\frac{V}{id}\right)\frac{iM_0'}{2\pi}+\frac{M_1'}{2\pi d}-\frac{iM_0'^2}{8\pi^2 d}\ , \qquad (3.28)$$

$$\lim_{Z\to\infty} Z\Phi_2(Z) = \left(1+\frac{V}{id}\right)\frac{iM_0}{2\pi} - \frac{M_1}{2\pi d} + \frac{iM_0^2}{8\pi^2 d}, \quad (3.29)$$

with

$$M_r = \int_{-nD}^{nD} \ln H(\omega)\omega^r d\omega, \quad M_r' = \int_{-nD}^{nD} \ln H'(\omega)\omega^r d\omega . \quad (3.30)$$

Substituting (3.28) and (3.29) into (3.17) results in an implicit transcendental equation for A and $b^{\pm}$. We need two more such equations so we can determine the three unknowns A and $b^{\pm}$.

Expanding (3.9) in powers of $1/Z$ one finds

$$\lim_{Z\to\infty} Z\Phi_1(Z) = (\pi i)^{-1}\int_{-nD}^{nD} d\omega' f(\omega'-\Delta)\Psi^-(\omega'-\Delta-i\delta),$$

$$\lim_{Z\to\infty} \operatorname{Im} Z\Phi_1(Z) = 4d\int_{-nD}^{nD} d\omega f(\omega)\operatorname{Im}D_{00}^-(\omega+i\delta) - 4d\int_{-nD-\Delta}^{nD} d\omega f(\omega)\operatorname{Im}D_{00}^-(\omega-i\delta) + \frac{1}{\pi}\int_{-nD-\Delta}^{nD-\Delta} f(\omega)d\omega , \quad (3.31)$$

$$\lim_{Z\to\infty} \operatorname{Im} Z\Phi_1(Z) = -2dn_{0-} + \frac{nD}{\pi} + \Delta\left(\frac{1}{\pi} + 4d\operatorname{Im}D_{00}^-(-nD+i\delta)\right) \quad (3.32)$$

$$\cong -2dn_{0-} + \frac{nD}{\pi} + \frac{\Delta}{\pi} . \quad (3.33)$$

In going from (3.32) to (3.33) we have dropped the term $4d\operatorname{Im}D_{00}^-(-nD+i\delta)$. Now $\operatorname{Im}D_{00}^-(-nD+i\delta)$ is the density of states of the impurity level at the host-band edge. Physically that region cannot be of any importance and the density of states should go to zero there. This result is not in accord with the behavior of the integral equation (3.3), where the spurious logarithmic singularity introduced by the truncated density of states forces $\operatorname{Im}D(\omega+i\delta)$ to have unphysically large values near the band edge. The region over which this behavior occurs, however, can be shown to be of the order $(nD/\pi)e^{-nD/d}$ and consequently does not affect the calculation of such quantities as $n^{\pm}$ in the limit $nD/d \gg 1$, and clearly has no influence on such things as resistivity and specific heat. Expanding (3.10) in powers of $1/Z$ one finds similarly that

$$\lim_{Z\to\infty} Z\operatorname{Im}\Phi_2(Z) = 2dn_{0+} - \frac{nD}{\pi} + \frac{\Delta}{\pi} . \quad (3.34)$$

Equations (3.34), (3.31), and (3.17), together with (3.28)–(3.30) serve to define three transcentral equations from which n_{0+} and A can be found. The formal solution to (3.3) has been completed.

IV. MAGNETIC SUSCEPTIBILITY

Our aim in this section is to convert the formal solution we have obtained in the previous section for $D_{00}^{\pm}(\omega)$ into a calculation of the static zero-field magnetic susceptibility. In Appendix B we show that the magnetic susceptibility of the host and impurity is just the sum of the Pauli susceptibility of the host and the local susceptibility of the impurity. There is no net polarization induced in the host for a Lorentzian density of states. The quantity to be calculated is therefore

$$\chi = \lim_{\Delta\to\infty} \frac{n_{0-} - n_{0+}}{\Delta} . \quad (4.1)$$

Equation (4.1) is the usual definition of χ if we set $\mu_B = 1$; adding (3.33) and (3.34) yields

$$\lim_{Z\to\infty} Z\operatorname{Im}(\Phi_1+\Phi_2) = -2d\chi\Delta + \frac{2\Delta}{\pi} . \quad (4.2)$$

We now expand Φ_1 and Φ_2 in powers of Δ. The first step is to expand H and H' in (3.19) and (3.20) and (3.24) and (3.25) in powers of Δ. For H' one finds

$$H'(\omega) = \frac{H_D^0 + 2i\Delta[gf' - fj + b_0 j - \chi g - (\omega - V)f'/d + \frac{1}{2}a]}{H_N^{0*} + 2\Delta(\chi f - b_0 f') + 2i\Delta(b_0 j - \chi g + \frac{1}{2}a)}, \quad (4.3)$$

$$H_N^0 = 1 - f^2(\omega) + 2n_0 + [(\omega - V)/d - g(\omega)]^2 + 2if(\omega)[(\omega - V)/d - g(\omega)] , \quad (4.4)$$

$$H_D^0 = 2n_0[1 + f(\omega)] + [(\omega - V)/d - g(\omega)]^2 + [1 - f(\omega)]^2 , \quad (4.5)$$

$$a = \lim_{\Delta\to 0} \frac{dA}{d\Delta} , \quad (4.6)$$

$$g(\omega) = \frac{1}{\pi}\int_{-nD}^{nD} \frac{d\omega' f(\omega')}{\omega - \omega'}, \quad j(\omega) = \frac{1}{\pi}\int_{-nD}^{nD} \frac{d\omega' f'(\omega')}{\omega - \omega'}, \quad (4.7)$$

$$n_0 = n_{0+} + n_{0-}, \qquad b_0 = 1 - n_0 , \quad (4.8)$$

and where the superscript prime indicates derivative with respect to frequency.

$$H(\omega) = \frac{H_N^0(\omega) + 2\Delta[b_0 f' - \chi f] + 2i\Delta[b_0 j - \chi g + \frac{1}{2}a]}{H_D^0(\omega) + 2i\Delta\{f'g - jf + b_0 j - \chi g - [(\omega - V)/d]f' + \frac{1}{2}a\}} . \quad (4.9)$$

If (4.3) and (4.4) are inserted into (3.30) and $\ln H(\omega)$ and $\ln H'(\omega)$ are expanded in powers of Δ, one obtains expressions for M_r and M_r' in powers of Δ. Inserting these into (3.28) and (3.29) and then in turn into (4.2) generates a linear equation for χ and a, whose coefficients are complicated integrals of H_N^0, H_D^0, etc.

We need a second equation in the two unknowns

χ and a to complete our solution. This is obtained from (4.6) and (3.17). Examination of (3.17) using (3.33) and (3.34) reveals that

$$\mathrm{Re}A = 2n_0 + O(\Delta^2) , \tag{4.10}$$

so that

$$\lim_{\Delta\to 0} \frac{d\,\mathrm{Re}A}{d\Delta} = 0 .$$

Using (3.17), (3.18), and (3.29) we find

$$\mathrm{Im}A = \frac{1}{d}\left(\frac{\mathrm{Re}(M_1+M_1')}{2\pi d} + \frac{\mathrm{Im}(M_0-M_0')}{2\pi} - \frac{V\,\mathrm{Re}(M_0+M_0')}{2\pi d} + \frac{1}{4\pi^2 d}\left(\mathrm{Re}M_0\,\mathrm{Im}M_0 + \mathrm{Re}M_0'\,\mathrm{Im}M_0\right)\right) . \tag{4.11}$$

Examining (4.11) it is easily shown that it is of order Δ, so that

$$a = \lim \mathrm{Im}(A)/\Delta \quad \text{as } \Delta \to 0 . \tag{4.12}$$

Equations (4.11) and (4.12) furnish us with our second linear equation in χ and a. The solution to (4.2) and (4.12) is straightforward, though tedious. We find for χ,

$$\chi = (a_{12}B - a_{22}C)(a_{11}a_{22} - a_{12}a_{21})^{-1} ,$$
$$C = f_1^{(0)}\alpha + f_4^{(0)}\beta + f_4^{(1)}\gamma + 1/\pi d , \tag{4.13}$$

$$B = \gamma f_1^{(1)} - \alpha f_4^{(0)} + \beta f_1^{(0)} ,$$
$$a_{11} = -1 + f_2^{(0)}\alpha + f_5^{(0)}\beta + f_5^{(1)}\gamma ,$$
$$a_{12} = \alpha f_3^{(0)} + f_6^{(0)}\beta + f_6^{(1)}\gamma ,$$
$$a_{21} = \gamma f_2^{(1)} - \alpha f_5^{(0)} + \beta f_5^{(0)} , \tag{4.14}$$
$$a_{22} = -\tfrac{1}{2} + \gamma f_3^{(1)} - \alpha f_6^{(0)} + \beta f_3^{(0)} ,$$

where

$$\alpha = -1/\pi d - (1/2\pi^2 d^2)\int_{-nD}^{nD} d\omega \ln|H_N/H_D| ,$$
$$\beta = (1/2\pi^2 d^2)\int_{-nD}^{nD} d\omega \arg H_N - V/\pi d^2 , \tag{4.15}$$
$$\gamma = 1/\pi d^2 .$$

We have defined $f_r^{(m)}$ as

$$f_r^{(m)} = \int_{-nD}^{nD} \omega^m f_r(\omega)\, d\omega , \tag{4.16}$$

with

$$f_1 = (1-n_0)(f' H_N^R + j H_N^I)|H_N|^{-2} ,$$
$$f_2 = -(f H_N^R + g H_N^I)|H_N|^{-2} ,$$
$$f_3 = \tfrac{1}{2} H_N^I |H_N|^2 ,$$
$$f_4 = (1-n_0)\, j\left(\frac{H_N^R}{|H_N|^2} - \frac{1}{H_D}\right) - \frac{f' H_N^I}{|H_N|^2} + \frac{[(\omega - V)/d] f' + jf + f'g}{H_D} , \tag{4.17}$$
$$f_5 = \frac{f H_N^I}{|H_N|^2} - g\left(\frac{H_N^R}{|H_N|^2} - \frac{1}{H_D}\right) ,$$
$$f_6 = \frac{1}{2}\left(\frac{H_N^R}{|H_N|^2} - \frac{1}{H_D}\right) .$$

The problem of calculating χ has thus been reduced to quadratures.

V. NUMERICAL PROCEDURE AND RESULTS

The evaluation of χ given in (4.13) reduces to a rather long delicate numerical problem. The temperature dependence of χ, which we expect physically to be Curie-like, means that if we study χ over a temperature range of four decades, we can expect that χ may vary by four decades. A study of (4.13)–(4.17) indicates that this comes about through a cancellation among the terms making up the denominator of (4.13). The implication of this analysis is that we must be prepared to calculate the integrals entering (4.14) to five places or better if we are to expect at least 10% accuracy at the lowest temperatures. To accomplish this aim, the domain of integration of the integrals in (4.16) was broken into a large number of parts and these parts were integrated by an eight-point Gaussian-integration routine. The accuracy of this procedure was tested by using trial integrands of similar structure to $f_r(\omega)$ which could be done exactly.[8]

As our main aim was to study the susceptibility in a range where we could expect Curie behavior we chose for our parameters $V = -1$ and $d = 0.1$. Before we can evaluate χ in (4.13) we need to know n_0. This is found in the same way as described in I, where this calculation is discussed extensively. We find $n_0 = 0.94996$. n_0 is quoted to five figures because, as we shall see, χ is a very sensitive function of n_0. Thus the integrals entering n_0 were evaluated to six significant figures.

In Table I we list χ calculated at various temperatures. For $D = 1$ eV this covers a range from 1100–0.11 °K. We notice that while χ is certainly temperature dependent, it does not vary as $1/T$. The results imply a strongly magnetic impurity, but not free-spin-like.

At this point it was felt worthwhile to investigate the sensitivity of χ to n_0. While n_0 has been determined self-consistently we also know that the energy cutoff introduced in the host band structure (Appendix A) results in an approximate error of 1% in n_0. We have therefore treated n_0 as an adjustable parameter with a freedom of variation on

TABLE I. The susceptibility as a function of temperature for the case $d=0.1$ eV, $D=1$ eV, $V=-1$ eV, and $n_0=0.94996$ is determined self-consistently.

T (°K)	χ
0.11×10^4	8.1
0.11×10^3	64.5
0.11×10^2	251
0.11×10^1	465
0.11×10^0	683

TABLE III. The susceptibility as a function of temperature for the case $d=0.2725$ eV, $D=1$ eV, $V=-1$ eV and $n_0=0.8556$ is determined self-consistently.

T (°K)	χ
0.11×10^4	5.75
0.11×10^3	23.3
0.11×10^2	58.8
0.11×10^1	127
0.11×10^0	226

the order of 1%. We find a very small change in n_0 results in a susceptibility which is Curie-like. In Table II we have listed C, the Curie constant, defined at $\chi T=C(T)$, as a function of T. It has very little variation over four decades of temperature. Its rms value differs from its average value by 3%.

We have also investigated the case where $V=-1$, $d=0.2725$. We find for this case that $n_0\sim0.8556$ when determined self-consistently. Values for χ are shown in Table III. Again we find behavior similar to that found for $d=0.1$ in Table II.

In attempting to vary n_0 for this case it proved impossible to achieve Curie-law behavior over the four decades. At $T/D=10^{-4}$, saturation has occured for the example shown in Table IV. This is not entirely suprising since if we calculate the expected Kondo temperature[9] for this system we find $T_k/D\sim1.1\times10^{-5}$. It is a characteristic feature of decoupling procedures that the transition in physical properties predicted by decoupling theories occurs over a number of decades[10] around T_k. We therefore believe we are observing a saturation of the susceptibility due to the Kondo effect in this case.

It is difficult to access the proper role that n_0 serves as an adjustable parameter. It may of course be that since we have treated n_0 approximately due to our introduction of an energy cutoff it is not unreasonable to expect that the proper n_0 for χ might differ somewhat from that we have obtained "self-consistently."

Another possibility is as follows. A major feature of decoupling schemes is that they introduce in a realistic fashion width to the impurity levels due to their interaction with the band electrons. It is the finite width of the impurity levels which makes it difficult to obtain a Curie-like susceptibility, this width tending to peg the susceptibility at a value more like that of the host band than an isolated spin. We know that the strong Coulomb repulsion on the impurity site acts in such a way as to overcome this tendency and to effectively suppress this one-particle width in so far as it enters χ. What we may be observing in this calculation is that a small part of the one-particle spectral width enters into the calculation of χ due to the unavoidable error in the treatment of higher-order nonsingular terms by the decoupling procedure. By varying n_0 we are effectively compensating for this temperature-independent piece and thereby allowing the Fermi-surface singularities[11,12] to operate to generate the Curie law.

VI. COMPARISON AND DISCUSSION

There have been a large number of calculations of the magnetic susceptibility of a local moment in a host metal over the last few years, and a comparison of this calculation to all of them is clearly impractical. Our aim in this section is to place our work within the broad context of this literature and to make a detailed comparison for only a few closely related works.

The first category of calculations has been done for the s-d model. These, by force, produce a Curie law at higher temperatures, since an isolated spin is assumed *a priori* to exist and be only weakly coupled to the conduction band. The calculation due to Zittartz[13] is the most advanced in this category and uses a Kubo expression for χ. Using the Nagaoka[14] decoupling and Hamann's integral equation[15] he finds that χ goes negative at the lowest temperature. There are two sources of difficulty which

TABLE II. The Curie constant $C(T)\equiv T\chi$ as a function of temperature for the case $d=0.1$ eV, $D=1$ eV, $V=-1$ eV, and $n_0=0.949429$.

T (°K)	$C(T)$
0.11×10^4	0.82
0.11×10^3	0.83
0.11×10^2	0.77
0.11×10^1	0.69
0.11×10^0	0.74

TABLE IV. The Curie constant $C(T)\equiv T\chi$ as a function of temperature for the case $d=0.2725$ eV, $D=1$ eV, $V=-1$ eV and $n_0=0.838$.

T (°K)	$C(T)$
0.11×10^4	0.846
0.11×10^3	0.834
0.11×10^2	0.377
0.11×10^1	0.084
0.11×10^0	0.0144

could produce this result. The first is simply an inadequacy in the decoupling procedure. The second is that the decoupling scheme is not a conserving approximation[16] with respect to a calculation of χ using the Kubo formula. This second possibility is what prompted us to determine χ from a direct calculation of $\lim_{H\to 0}(n_{0-}-n_{0+})/H$. This procedure is of neccessity conserving.

More closely related to the present work are those calculations in which a local spin is not assumed to exist on the impurity. A number of these approximations[17] use time-dependent Hartree-Fock on random-phase approximation (RPA). In general, they do not yield temperature-dependent values of χ; a large enhancement of χ over that expected from a band electron can only be obtained by artificially restricting U to a very narrow range. This present calculation is aimed at remedying this situation by using an equation-of-motion technique.

An alternate attempt to remedy this difficulty is due to Suhl and co-workers and has been referred to as a renormalized RPA. This approach did succeed in producing a reasonably Curie law for high temperatures, albeit with a Curie constant only 40% of the expected one, but fails in its treatment of saturation due to the Kondo effect.[18]

The most successful calculations to date involve the use of functional integral techniques for calculating the grand partition function from which the susceptibility has been obtained.[18,19] This gives Curie-law behavior in the high-temperature regime with a Curie constant which approaches the expected one for a free spin as $U\to\infty$. The method suffers from the difficulty of being extremely complex when extended to low temperature,[20] and only a small amount of success has been obtained in calculatnig any other physical properties using this method.

Since the completion of the calculation described in this paper, a report by Mamada and Takano[21] has been brought to our attention. Their aim is also to calculate χ and they adopt the Anderson model to study. They follow the decoupling procedure used by Theumann and ourselves and consequently arrive at precisely the same integral equation (3.3) as ours.

At this point our approach diverges. Mamada and Takano[21] calculate χ from the expression

$$\chi=(g^2\mu_B^2/T)\langle S_{\mathrm{total}}^2\rangle\ , \qquad (6.1)$$

as was done by Zittartz.[13] In the process of performing this calculation they are forced to introduce new equations of motion for Green's functions which do not previously appear in the hierarchy of equations for $D_{00}(\omega)$. These equations can only be solved by introducing a decoupling procedure which goes beyond that employed for the calculation of $D_{00}(\omega)$. In particular, their extra decoupling procedure, translated into the notion and context of this paper, adds the factorization

$$\langle d_{i\sigma}^\dagger d_{j\sigma} d_{k\sigma}\,;\, d_{0\sigma}^\dagger\rangle \to =\langle d_{i\sigma}^\dagger d_{j\sigma}\rangle\langle d_{k\sigma}\,;\, d_{i\sigma}^\dagger\rangle - \langle d_{i\sigma}^\dagger d_{k\sigma}\rangle\langle d_{j\sigma}\,;\, d_{0\sigma}\rangle : \qquad (6.2)$$

at most one of $i,j,k=0$.

This means that one is separating like-spin electrons as well as electrons of opposite spin. This complicates the question of whether the χ they calculate is conserving with respect to the decoupling procedure they use for $D_{00}^{\sigma}(\omega)$. For high temperature they find a Curie law; for very low temperature they find that χ diverges as $(T_k/T)\ln(T/T_k)$. This latter result is in disagreement with the numerical studies we have done here, which show very rapid saturation of χ for $T \lesssim T_k$. It is in further disagreement with studies done by Anderson and coworkers[22,23] that show there are no low-temperature singular properties associated with a magnetic impurity in a metal.

APPENDIX A

By definition

$$A^\sigma(\omega-\sigma\Delta)=\frac{1}{N^{1/2}}\frac{1}{(1+\gamma)}\sum_{\vec{k}}\left(\langle d_{0\bar\sigma}^\dagger a_{\vec{k}\bar\sigma}\rangle-\frac{1}{N}\sum_{\vec{q}}\langle d_{0\bar\sigma}^\dagger a_{\vec{q}\bar\sigma}\rangle\right)\Big/(\omega-\sigma\Delta-\epsilon_{\vec{k}})\ . \qquad (A1)$$

Introducing the operator

$$F_{\omega'}O_{\omega'}=i\int f(\omega')(O_{\omega'+i\delta}-O_{\omega'-i\delta})d\omega'\ , \qquad (A2)$$

we have

$$\langle d_{0\bar\sigma}^\dagger a_{\vec{k}\bar\sigma}\rangle = F_{\omega'}\langle\langle a_{\vec{k}\bar\sigma}\,;\,d_{0\bar\sigma}^\dagger\rangle\rangle_{\omega'} = F_{\omega'}(1/N^{1/2})\textstyle\sum_{\vec{q}'}G_{\vec{k}\vec{q}'}^{\bar\sigma}\ . \qquad (A3)$$

Using (B4) and (B5) it is easy to show that

$$\sum_{\vec{q}'}G_{\vec{k}\vec{q}'}^{\bar\sigma}=D_{00}^{\bar\sigma}\left(-\gamma+\frac{(1+\gamma)F^{-1}(\omega+\sigma\Delta)}{\omega+\sigma\Delta+\epsilon_{\vec{k}}}\right), \qquad (A4)$$

since

$$\frac{1}{N}\sum_{\vec{q}}\langle d_{0\bar\sigma}^\dagger a_{\vec{q}\bar\sigma}\rangle=D_{00}^{\bar\sigma}\ ,$$

$$\langle d_{0\bar\sigma}^\dagger a_{\vec{k}\bar\sigma}\rangle-\frac{1}{N}\sum_{\vec{q}}\langle d_{0\bar\sigma}^\dagger a_{\vec{q}\bar\sigma}\rangle = \frac{(1+\gamma)}{N^{1/2}}F_{\omega'}\left[D_{00}^{\bar\sigma}(\omega')\left(\frac{F^{-1}(\omega'+\sigma\Delta)}{\omega'+\sigma\Delta-\epsilon_{\vec{k}}}-1\right)\right]\ . \qquad (A5)$$

Inserting (A5) into (A1) yields $A^\sigma(\omega)$ in terms of $D_{00}^{\bar\sigma}(\omega)$,

$$A^\sigma(\omega)=F(\omega)F_{\omega'}\left[D_{00}^{\bar\sigma}(\omega')\left(\frac{F^{-1}(\omega)-F^{-1}(\omega'+\sigma\Delta)}{\omega-\omega'-\sigma\Delta}\right)\right]\ . \qquad (A6)$$

We turn now to $B^\sigma(\omega-\sigma\Delta)$. By definition

$$B^\sigma(\omega-\sigma\Delta)=\frac{(1+\gamma)}{N^{1/2}}\sum_{i,\vec{k}}T_{i0}\left(\langle d_{i\bar\sigma}^\dagger a_{\vec{k}\bar\sigma}\rangle-N^{-1}\sum_{\vec{k}'}\langle d_{i\bar\sigma}^\dagger a_{\vec{k}'\bar\sigma}\rangle\right)\Big/$$

$$(\omega-\sigma\Delta-\epsilon_{\vec{k}})\ . \tag{A7}$$

By Fourier transformation

$$\sum_i T_{i0}\left(\langle d^\dagger_{i\bar\sigma}a_{\vec{k}\bar\sigma}\rangle - N^{-1}\sum_{\vec{k}'}\langle d^\dagger_{i\bar\sigma}a_{\vec{k}'\bar\sigma}\rangle\right)$$

$$=(1+\gamma)N^{-1/2}\sum_{\vec{k}'}\epsilon_{\vec{k}'}\left[\langle a^\dagger_{\vec{k}'\bar\sigma}a_{k\bar\sigma}\rangle - N^{-1}\sum_{\vec{q}}\langle a^\dagger_{\vec{k}'\bar\sigma}a_{\vec{q}\bar\sigma}\rangle\right] \tag{A8}$$

$$=(1+\gamma)N^{-1/2}F_{\omega'}\left(\sum_{\vec{k}'}\epsilon_{\vec{k}}G^{\bar\sigma}_{\vec{k}\vec{k}'} - N^{-1}\sum_{\vec{q},\vec{k}'}\epsilon_{\vec{k}'}G^{\bar\sigma}_{\vec{q}\vec{k}'}\right)\ . \tag{A9}$$

With the help of (A4) and (B4) and (B5) one finds

$$\sum_{\vec{k}'}\epsilon_{\vec{k}'}G_{\vec{k}\vec{k}'} = -\frac{1}{2\pi}+\frac{F^{-1}(\omega+\sigma\Delta)}{2\pi(\omega+\sigma\Delta-\epsilon_{\vec{k}})}$$
$$-\gamma(\gamma+1)D^{\bar\sigma}_{00}[\omega+\sigma\Delta-F(\omega+\sigma\Delta)]$$
$$+\frac{(1+\gamma)^2F^1(\omega+\sigma\Delta)[F(\omega+\sigma\Delta)]^{-2}D^{\bar\sigma}_{00}}{\omega+\sigma\Delta-\epsilon_k} \tag{A10}$$

and

$$E^{\bar\sigma}\equiv N^{-1}\sum_{\vec{k},\vec{k}'}\epsilon_{\vec{k}'}G^{\bar\sigma}_{\vec{k}\vec{k}'} = (1+\gamma)[\omega+\sigma\Delta-F(\omega+\sigma\Delta)]D^{\bar\sigma}_{00}\ . \tag{A11}$$

Substituting (A10) and (A11) into (A9) one finds

$$\sum T_{i0}\left(\langle d^\dagger_{i\bar\sigma}a_{\vec{k}\bar\sigma}\rangle - N^{-1}\sum_{\vec{k}'}\langle d_{i\bar\sigma}a'_{k\bar\sigma}\rangle\right)$$
$$=(1+\gamma)N^{-1/2}F_\omega\left(-\frac{1}{2\pi}+\frac{F^{-1}(\omega+\sigma\Delta)}{2\pi(\omega+\sigma\Delta-\epsilon_{\vec{k}})}\right.$$
$$-(1+\gamma)^2D^{\bar\sigma}_{00}[\omega+\sigma\Delta-F(\omega+\sigma\Delta)]$$
$$\left.+\frac{(1+\gamma)^2F^1(\omega+\sigma\Delta)D^{\bar\sigma}_{00}}{[F(\omega+\sigma\Delta)]^2(\omega+\sigma\Delta-\epsilon_{\vec{k}})}\right)\ . \tag{A12}$$

Substituting (A12) into (A7) yields

$$B^\sigma(\omega)=(1+\gamma)^2B^\sigma_1(\omega)+(1+\gamma)^4B^\sigma_2(\omega)\ , \tag{A13}$$

$$B^\sigma_1(\omega)=F(\omega)F_{\omega'}\left(\frac{1}{2\pi}\frac{F^{-1}(\omega'+\sigma\Delta)-F^{-1}(\omega)}{\omega'+\sigma\Delta-\omega}\right), \tag{A14}$$

$$B^\sigma_2(\omega)=F(\omega)F_{\omega'}\left[[\omega'+\sigma\Delta-F^{-1}(\omega'+\sigma\Delta)]\times D^{\bar\sigma}_{00}\left(\frac{F^{-1}(\omega)-F^{-1}(\omega'+\sigma\Delta)}{\omega-\omega'-\sigma\Delta}-1\right)\right]\ . \tag{A15}$$

We now specialize to a Lorentzian density of states. As was discussed in I, this leads to convergence problems which necessitate the introduction of a cutoff parameter. Because of the presence of the magnetic field this cutoff must be introduced with particular care. The cutoff in fact arises from terms like

$$[F^{-1}(\omega'+\sigma\Delta)-F^{-1}(\omega)]/(\omega'+\sigma\Delta-\omega)\ ,$$

which reflect the density of states of the host band. We must remove the explicit field (Δ) dependence of those terms so that our cutoff does not become field dependent. This involves making a change in variables from $\omega'+\sigma\Delta$ to ω' before the cutoff is introduced, and then introducing the cutoff. We have dwelled on this point since failure to take due care of it leads spurious contribution to the susceptibility from the band edge.[24]

For a Lorentzian density of states $\rho^0(\omega)$,

$$\rho^0(\omega)=\frac{D}{\pi}\frac{1}{\omega^2+D^2} \tag{A16}$$

and

$$F(\omega)=(\omega+iD)^{-1}. \tag{A17}$$

Substituting (A17) into (A6) and (A13)–(A15), and introducing a cutoff $\pm nD$ in the integral (after the change of variables discussed above), one finds for $A^\sigma(\omega-\sigma\Delta+i\delta)$ and $B^\sigma(\omega-\sigma\Delta+i\delta)$ the expressions given in (3.1) and (3.2).

APPENDIX B

From (2.8) one obtains directly

$$\sum_{\vec{k}}G^\sigma_{\vec{k}\vec{k}}=\frac{N}{2\pi}F(\omega-\sigma\Delta)+\frac{\gamma}{N}\sum_{\vec{q},\vec{k}}\epsilon_{\vec{q}}G^\sigma_{\vec{q}\vec{k}}(\omega-\sigma\Delta-\epsilon_{\vec{k}})^{-1}+\frac{1}{N}\sum_{\vec{k},\vec{q}}\frac{\gamma\epsilon_{\vec{k}}+V}{\omega-\sigma\Delta-\epsilon_{\vec{k}}}G_{\vec{q}\vec{k}}+\frac{U}{N^{1/2}}\sum_{\vec{q}}\Gamma^\sigma_{\vec{q}}(\omega-\sigma\Delta-\epsilon_{\vec{q}})^{-1}\ , \tag{B1}$$

$$\sum_{\vec{k}}G^\sigma_{\vec{k}\vec{k}}=\frac{N}{2\pi}F(\omega-\sigma\Delta)-\gamma D^\sigma_{00}(\omega)+\frac{1}{N}\sum_{\vec{k}}(\omega-\sigma\Delta-\epsilon_{\vec{k}})^{-1}[\gamma E^\sigma_{\vec{k}}+N^{1/2}U\Gamma^\sigma_{\vec{k}}+(\gamma(\omega-\sigma\Delta)+V)G^\sigma_{\vec{k}}]\ . \tag{B2}$$

Using (2.12) this becomes

$$\sum_{\vec{k}}G^\sigma_{\vec{k}\vec{k}}=\frac{N}{2\pi}F(\omega-\sigma\Delta)-\gamma D^\sigma_{00}(\omega)+\frac{1}{N}\sum_{\vec{k}'}\frac{(\omega-\sigma\Delta-\epsilon'_{\vec{k}})^{-1}}{F(\omega-\sigma\Delta)}\{(1+\gamma)G^\sigma_{\vec{k}'}(\omega)-[2\pi(\omega-\sigma\Delta-\epsilon_{\vec{k}})]^{-1}\}\ . \tag{B3}$$

Solving (2.12) and (2.13) for $G^\sigma_{k'}$,

$$G^\sigma_{\vec{k}'}(\omega)=[F^1(2\gamma+\gamma^2)+VF-1]^{-1}\left(-UN^{1/2}F\Gamma_{\vec{k}'}+\frac{\gamma F}{2\pi}-\frac{(1+\gamma)}{2\pi}(\omega-\epsilon_{\vec{k}}-\sigma\Delta)^{-1}\right)\ , \tag{B4}$$

and using

$$\Gamma_{\vec{q}} = \frac{\langle\langle n_{0\bar\sigma} d_{0\sigma};\ d_{0\sigma}^\dagger \rangle\rangle}{N^{1/2}} \left(\frac{-(1+\gamma)[\omega - \sigma\Delta - F^{-1}(\omega - \sigma\Delta)] + \omega - \sigma\Delta + \gamma\epsilon_{\vec{q}}}{\omega - \sigma\Delta - \epsilon_{\vec{q}}} \right) , \tag{B5}$$

one arrives at

$$\sum_{\vec{k}} G_{\vec{k}'}(\omega)(\omega - \sigma\Delta - \epsilon_{\vec{k}})^{-1} = \frac{D_{00}^\sigma(\omega)}{F(\omega - \sigma\Delta)} \{F^{-1}(\omega - \sigma\Delta) + \gamma[F(\omega - \sigma\Delta)]^2\} . \tag{B6}$$

Inserting (B6) into (B3) one finds that

$$\sum_{\vec{k}} G_{\vec{k}\vec{k}}^\sigma = \frac{NF(\omega - \sigma\Delta)}{2\pi} + \frac{1}{2\pi} \frac{d\ln F(\omega - \sigma\Delta)}{d\omega} - D_{00}^\sigma \left(2\gamma + \gamma^2 + \frac{(1+\gamma)^2}{F} \frac{d\ln F}{d\omega} \right) . \tag{B7}$$

Equation (B7) can be used to calculate N^σ, the total number of electron of spin σ in magnetic field Δ. For a Lorentzian density of states

$$F(\omega) = (\omega + iD)^{-1} , \tag{B8}$$

hence

$$\frac{d}{d\omega} \ln F(\omega) = -F(\omega) , \tag{B9}$$

$$\sum_{\vec{k}} G_{\vec{k}\vec{k}}^\sigma = \frac{N-1}{2\pi} F(\omega - \sigma\Delta) + D_{00}^\sigma(\omega) . \tag{B10}$$

Now

$$\begin{aligned} N^\sigma &= \int f(\omega)\, \mathrm{Im} \textstyle\sum_{\vec{k}} G_{\vec{k}\vec{k}}^\sigma(\omega) d\omega \\ &= (N-1) \int f(\omega) \rho^0(\omega - \Delta) d\omega + n_0^\sigma , \end{aligned} \tag{B11}$$

where $\rho^0(\omega)$ is the host density of states per atom and n_0^σ the occupation numbers for the impurity level. Aside from the Pauli susceptibility, the total excess susceptibility due to the impurity is calculated from $n_{0+} - n_{0-}$. The arguments above, which carry through exactly for the Lorentzian density of states, are approximately valid for any smoothly varying density of states if $(1+\gamma)$ is small, corresponding to a narrow impurity level.

APPENDIX C

In this Appendix we obtain an expression for the conduction electron t matrix. Starting from (2.8)

$$\begin{aligned} (\omega - \sigma\Delta - \epsilon_{\vec{k}}) G_{\vec{k},\vec{k}'}^\sigma &= \frac{\delta_{\vec{k}\vec{k}'}}{2\pi} + \frac{\gamma}{N} E_{\vec{k}'}^\sigma + (\gamma\epsilon_{\vec{k}} + V) \\ &\times \frac{1}{N} G_{\vec{k}'} + \frac{U}{N^{1/2}} \langle\langle n_{0\bar\sigma} d_{0\sigma};\ a_{\vec{k}'\sigma}^\dagger \rangle\rangle . \end{aligned} \tag{C1}$$

Using (A4), (A10), together with (B5) it is straightforward to show that

$$\begin{aligned} G_{\vec{k}\vec{k}'}^\sigma = &\frac{\delta_{\vec{k}\vec{k}'}}{2\pi(\omega - \epsilon_{\vec{k}} - \sigma\Delta)} + \frac{\gamma^2 D_{00}^\sigma}{N} \\ &- \frac{1}{N} \frac{\gamma(1+\gamma) D_{00}^\sigma F^{-1}(\omega - \sigma\Delta)}{\omega - \epsilon_{\vec{k}\sigma} - \sigma\Delta} \\ &- \frac{1}{N} \frac{\gamma(1+\gamma) D_{00}^\sigma F^{-1}(\omega - \sigma\Delta)}{\omega - \epsilon_{\vec{k}'} - \sigma\Delta} \\ &+ \frac{1}{N} \frac{[(1+\gamma)^2 D_{00}^\sigma F^{-2}(\omega - \sigma\Delta) - F^{-1}(\omega - \sigma\Delta)/2\pi]}{(\omega - \epsilon_{\vec{k}} - \sigma\Delta)(\omega - \epsilon_{\vec{k}'} - \sigma\Delta)} . \end{aligned} \tag{C2}$$

Equation (C2) is easily interpreted. The first term describes electron propagation in the host lattice, no scattering. The second term describes the impurity resonance in the total Green's function. The next two terms reflect the fact that the impurity level is a resonance in the host band, and therefore the electron may resonate between the scattering states and the impurity level. The final term just measures the scattering rate of the conduction electrons due to the impurity. Notice that if $\gamma \to -1$, decoupling of the impurity from the conduction electrons, the resonanting terms vanishes and the host electron scattering rate is just

$$-F^{-1}(\omega - \sigma\Delta)/2\pi .$$

This is just the t matrix for scattering from a vacancy in the host lattice.

In general we identify the t matrix as

$$t^\sigma(\omega) = (1+\gamma)^2 D_{00}^\sigma(\omega) F^{-2}(\omega - \sigma\Delta) - F^{-1}(\omega - \sigma\Delta)/2\pi . \tag{C3}$$

As we observed in Sec. III, the t matrix in the Anderson model, t_A, is just proportional to the extraorbital Green's function. The extraorbital Green's function and $D_{00}^\sigma(\omega)$ are identical within the decoupling scheme; consequently

$$t_A^\sigma(\omega) = 2\pi V_{\vec{k}d}^2 D_{00}^\sigma(\omega) , \tag{C4}$$

$$t_A^\sigma(\omega) = 2(1+\gamma)^2 D/\rho^0 . \tag{C5}$$

Inserting (C5) into (C3), and evaluating $F(\omega)$ near the Fermi surface, one finds (we set $\Delta = 0$)

$$t(\omega) = iD\left(\tfrac{1}{2}\, i t_A(\omega) \rho^0 - 1/2\pi\right) . \tag{C6}$$

Now we know[15,25] that as $\omega \to 0$, $t_A(\omega) \to 1/\pi i \rho^0$, the unitarity limit. This means that $t(\omega) \to 0$. As the Kondo state is formed in the d-band level the scattering in the d band tends to zero.

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Determination of the Kondo Temperature and Internal Field Distribution in Dilute *Au*Mn Alloys*

J. W. Loram, T. E. Whall, and P. J. Ford
University of Sussex, Brighton, United Kingdom
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The resistivities of several *Au*Mn alloys, containing between 0.005 and 1.5 at.% Mn, have been measured in the temperature range 0.5–40 °K. The magnitude of the spin resistivity is determined from the decrease in resistance due to ordering in internal fields. This, combined with a measurement of the coefficient of the logarithmic term in the resistance at temperatures well above the resistance maximum, allows the Kondo temperature to be determined, the value so obtained being of the order of 10^{-13} °K. The predicted resistivity at $T=0$, in the absence of interactions, is shown to be comparable with the unitarity limit for d-wave scattering. Information is also obtained concerning the magnitude and distribution of internal fields within the alloys. The distribution is found to approximate to a Gaussian, but with a dip in the region of very low fields.

I. INTRODUCTION

Previous investigations,[1,2] and the present results, demonstrate that the temperature dependence of the resistivity of dilute *Au*Mn alloys is qualitatively the same as that observed in many other dilute-magnetic-alloy systems. In very low concentration alloys, the resistivity increases logarithmically with decreasing temperature in the liquid-helium temperature range. At rather higher concentrations the logarithmic increase is terminated and a broad maximum is observed, associated with the onset of magnetic ordering, and the resistance falls as the temperature is lowered further. The main quantitative difference is the rather small magnitude of the logarithmic term, which is approximately 15 times smaller in *Au*Mn alloys[2] than in *Au*Fe alloys[3] of comparable concentration. As the spin value of Mn in Au is significantly larger than that of Fe in Au, it may be concluded that the Kondo temperature in *Au*Mn is extremely low.

In the present investigation, the resistances of *Au*Mn alloys containing between 0.005 and 1.5% Mn have been measured in the temperature range 0.5–40 °K. The decrease in resistance below the ordering temperature is combined with the magnitude of the logarithmic term at higher temperatures to provide an estimate of the Kondo temperature. The deviation of the resistance from a logarithmic temperature dependence is used to provide information on the magnitude and distribution of internal fields within the alloy.