the domain alignment field.

Cooper[2] has correctly pointed out that if the resonances reported by Bagguley and Liesegang in Tb are direct $k=0$ spin-wave excitations, the frozen-lattice model cannot be valid at their experimental frequency. Marsh and Sievers[5] studied far-infrared absorption in Tb and concluded that the frozen-lattice model better explained their data. Our high-frequency microwave data[1] provided a definitive test: They could only be explained on the basis of the frozen-lattice model. (The free-lattice model could not even qualitiatively explain the experimental results.[1,2]) To understand the difference in behavior between the low-frequency microwave results of Bagguley and Liesegang and those of the above-mentioned far-infrared and high-frequency microwave regions, Marsh has proposed a two-sublattice model.[6] Brooks[7] has also discussed the possibility of a frequency-dependent mechanism which might allow the free-lattice model to be operative at low microwave frequencies. Our earlier high-frequency results,[1] together with the low-frequency investigation presented in this paper, provide a natural and satisfying resolution of the apparent discrepancy. Thus the conjectures related to the Tb problem made by the aforementioned authors [2,6,7] are no longer necessary.

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Addendum to "Localized Correlations in Narrow Conduction Bands. I"

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The self-consistent equations derived by Appelbaum and Penn (AP) for a single strongly correlated impurity site in a narrow conduction band are solved using a rapidly converging density of states. This rectifies the convergence difficulties AP found when they used a Lorentzian density of states. We find that n_0, the total electron occupation number at the impurity site, is 0.497, compared to 0.4 found by AP. Results for the resistivity as a function of temperature are also presented.

Recently, Appelbaum and Penn[1] (AP) have treated the problem of localized correlations in a narrow conduction band by means of an equation-of-motion decoupling scheme. In the process of solving the resulting self-consistent equation for the local-correlated-site Green's function, they were forced to use a Lorentzian density of states

$$\eta(E)=(D/\pi)\,1/(E^2+D^2) \tag{1}$$

to describe the energy dispersion in the conduction band. As discussed by AP, the slow convergence of the Lorentzian density of states introduced unphysical divergences into their self-consistent equations which required the introduction of an extraneous cutoff energy to which the final results were sensitive.

It is the purpose of this paper to obtain a solution of AP's self-consistent equations using a density of states which does not suffer from these divergences, and to present numerical results for the electron occupation number at the correlated site as well as the resistivity as a function of temperature. It will be found that AP's qualitative conclusions remain valid.

It will be assumed that the reader is familiar with the contents and notation of AP. For convenience, the model Hamiltonian used by AP is written

$$H=\sum_{ij,\sigma} T_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}+\tfrac{1}{2}U\sum_{\sigma}n_{0\sigma}\,n_{0\bar{\sigma}} \ , \tag{2}$$

where $c^{\dagger}_{i\sigma}$ creates an electron of spin σ at lattice site i and $n_{0\sigma}$ is the number of electrons of spin σ at the correlated or impurity site.

The properties of the system are described by D^{σ}, the impurity Green's function, defined as

$$D^{\sigma}(\omega)=\langle\langle c_{0\sigma}\,;\,c^{\dagger}_{0\sigma}\rangle\rangle_{\omega} \tag{3}$$

in the notation of Zubarev.[2]

The general equation for $D^{\sigma}(\omega)$ is given in Eq. (3.21) of AP and accompanying defining relations and will not be repeated here. It was found that a density of states of the form

$$\eta(\omega)=\sqrt{2}\,\pi^{-1}/(\omega^4+1) \tag{4}$$

has the property of rapid convergence plus sufficient analytic simplicity so that a solution of Eq. (3.21) of AP can be effected. Using (4), Eq. (3.21) of AP becomes

$$\begin{aligned}2\pi D(\omega+i\sigma)=(\omega^2+2)[A^{+}(\omega)-2\sqrt{2}\,\phi_1^{+}(\omega)]\\ \times\{(\omega-i\sqrt{2})B^{+}(\omega)-8i[\phi_1^{+}(\omega)-\phi_1(i\sqrt{2})]\\ -(\sqrt{2}/\pi)(\omega^2+2)g_1^{+}(\omega)\}^{-1}\ ,\end{aligned} \tag{5}$$

$$\begin{aligned}\phi_1(z)&=\int\frac{f(\omega')-\frac{1}{2}}{\omega'^2+2}\,\frac{D(\omega'-i\delta)}{z-\omega'}\,d\omega'\ ,\\ \phi_2(z)&=\int\frac{f(\omega')-\frac{1}{2}}{\omega'^2+2}\,\frac{D(\omega'+i\delta)}{z-\omega'}\,d\omega'\ ,\end{aligned} \tag{6}$$

$$g(z)=\int\frac{f(\omega')-\frac{1}{2}}{\omega'^2+2}\,\frac{1}{z-\omega'}\,d\omega'\ , \tag{7}$$

and where $A^{+}(\omega)=\frac{2}{3}(1-\eta_0)-iA_0/(\omega+i\sqrt{2})\ ,$ (8)

$$\begin{aligned}B^{+}(\omega)=\omega^2+i\sqrt{2}\,\omega+iA_0/(\omega+i\sqrt{2})-\tfrac{3}{2}\\ -iB_0+2\sqrt{2}\,\phi_1(i\sqrt{2})\ ,\end{aligned} \tag{9}$$

with

$$\eta_0=i\int[f(\omega')-\tfrac{1}{2}][D(\omega'+i\delta)-D(\omega'-i\delta)]\,d\omega'\ , \tag{10}$$

$$A_0=\int\frac{[f(\omega')-\frac{1}{2}]}{\omega'+i\sqrt{2}}[D(\omega'+i\delta)-D(\omega'-i\delta)]\,d\omega'\ , \tag{11}$$

$$B_0=\int\frac{f(\omega')-\frac{1}{2}}{\omega'+i\sqrt{2}}\left(\frac{D(\omega'+i\delta)}{\omega'+i\sqrt{2}}-\frac{D(\omega'-i\delta)}{\omega'-i\sqrt{2}}\right)d\omega'\ . \tag{12}$$

In the above, the superscript (±) means

$$x^{\pm}(\omega)=x(\omega\pm i\delta),\qquad \delta\to 0\ . \tag{13}$$

Equation (5) along with its complex-conjugate equation constitutes a coupled set of nonlinear integral equations which can be transformed into a Riemann-Hilbert boundary value problem in a way similar to that applied to Eqs. (5.1) and (5.2) of AP. It is a reasonably straightforward task to establish that the Riemann-Hilbert problem can be formulated in terms of the functions

$$\begin{aligned}\pi_1(z)=(z-i\sqrt{2})B^{+}(z)+8i\phi_1(i\sqrt{2})\\ -(\sqrt{2}/\pi)(z^2+2)g(z)-8i\phi_1(z)\ ,\end{aligned} \tag{14}$$

$$\begin{aligned}\pi_2(z)=(z+i\sqrt{2})B^{+*}(z)-8i\phi_2(-i\sqrt{2})\\ -(\sqrt{2}/\pi)(z^2+2)g(z)+8i\phi_2(z)\ .\end{aligned} \tag{15}$$

Using (14) and (15), one finds that Eq. (5) and its complex conjugate take the form

$$\begin{aligned}\left[\left(\pi_1^{+}+\frac{\sqrt{2}}{\pi}(\omega^2+2)g^{+}\right)-\left(\pi_1^{-}+\frac{\sqrt{2}}{\pi}(\omega^2+2)g^{-}\right)\right]\pi_2^{-}\\ =-8i(g^{+}-g^{-})\,[(\omega^2+2)/2\pi]\\ \times[\theta^{-}-(\omega^2+2)g^{-}/2\pi i-\pi_2^{-}/2\sqrt{2}\,i]\end{aligned} \tag{16}$$

and

$$\begin{aligned}\left[\left(\pi_2^{+}+\frac{\sqrt{2}}{\pi}(\omega^2+2)g^{+}-\left(\pi_2^{-}+\frac{\sqrt{2}}{\pi}(\omega^2+2)g^{-}\right)\right]\pi_1^{+}\\ =8i(g^{+}-g^{-})[(\omega^2+2)/2\pi]\,[\theta^{+}+(\omega^2+2)g^{+}/2\pi i\\ +\pi_1^{+}/2\sqrt{2}\,i]\ ,\end{aligned} \tag{17}$$

with

$$\begin{aligned}\theta^{+}=A^{+}-(1/2\sqrt{2}\,i)\,[(\omega-i\sqrt{2})B^{+}+8i\phi_1(i\sqrt{2})]\ ,\\ \theta^{-}=(\theta^{+})^{*}\ .\end{aligned} \tag{18}$$

Using (14)–(17), one can establish that

$$\begin{aligned}\pi_1(z)\pi_2(z)-(4i/\pi)g(z)(z^2+2)[\theta^{+}(z)-\theta^{-}(z)]\\ -(2/\pi^2)(z^2+2)^2g^2(z)=p(z)\ ,\end{aligned} \tag{19}$$

where $p(z)$ is a sixth-order polynomial given by

$$p(z)=[z^3+(B_{00}+2)z+p_0]^2+8n_0+\tfrac{9}{2}\ , \tag{20}$$

with $p_0=4\,\mathrm{Im}D_1-16\phi_1(i\sqrt{2})\ ,$ (21)

$$B_{00}=-\tfrac{3}{2}-2\,\mathrm{Im}D_0+4\sqrt{2}\,\mathrm{Re}\phi_1(i\sqrt{2})\ , \tag{22}$$

and $$D_n=\int d\omega'\,\omega'^n\,\frac{G(\omega'-i\delta)[f(\omega')-\frac{1}{2}]}{\omega'^2+2}\ . \tag{23}$$

Combining (19) with (16) and (17) results in

$$\ln\pi_2^+-\ln\pi_1^-=\ln H(\omega)\ , \tag{24}$$

$$H(\omega)=\frac{p(z)+(4i/\pi)(\omega^2+2)g^-(\theta^+-\theta^-)+(2/\pi^2)(\omega^2+2)^2g^{+2}}{p(z)+(4i/\pi)(\omega^2+2)(g^-\theta^+-g^+\theta^-)+(2/\pi^2)(\omega^2+2)^2g^+g^-}\ . \tag{25}$$

The solution to the boundary-value problem in (24) is easily established to be

$$\pi_2(z)=\frac{z^4+b_3z^3+b_2z^2+b_1z+b_0}{z-i\sqrt{2}}\times\exp\left(-\frac{1}{2\pi i}\int\frac{\ln H(\omega)\,d\omega}{z-\omega}\right)\ , \tag{26}$$

where b_n are complex constants. An examination of $H(\omega)$ establishes that its index is zero,[3] so that (26) constitutes the unique solution to (24).

The conversion of (26) into usable form involves the determination of the b_n as well as η_0, A_0, and B_0. By expanding both sides of (26) in power of $1/\omega$ to order $1/\omega^3$ and equating coefficients, one obtains a set of three simultaneous nonlinear transcendental equations from which all the unknown parameters are obtainable.

These equations have been solved by standard numerical techniques. We find that the total electron occupation number for both spins at the impurity site $n_0=0.494$. This result is in excellent agreement with our previous estimate in AP that a more realistic band structure would increase our original estimate for n_0, which was 0.4, by 25%.

We have calculated the resistivity by standard techniques,[4] and this is plotted versus temperature in Fig. 1. The resistivity changes by one percent between $T_0=0$ and $T_1=10^{-3}D$. If D is taken as 1 eV, $T_1\sim10\,^\circ\mathrm{K}$. This is a small change on the scale we are usually used to thinking of in connection with the magnetic impurity problem.[5] It is, however, a very large change compared to what we would expect from the usual T/D corrections associated with ordinary impurities. This behavior can be understood by recognizing that the coupling of the impurity to the band is comparable to the bandwidth. We are therefore in the strong-coupling regime, the result of which is that the

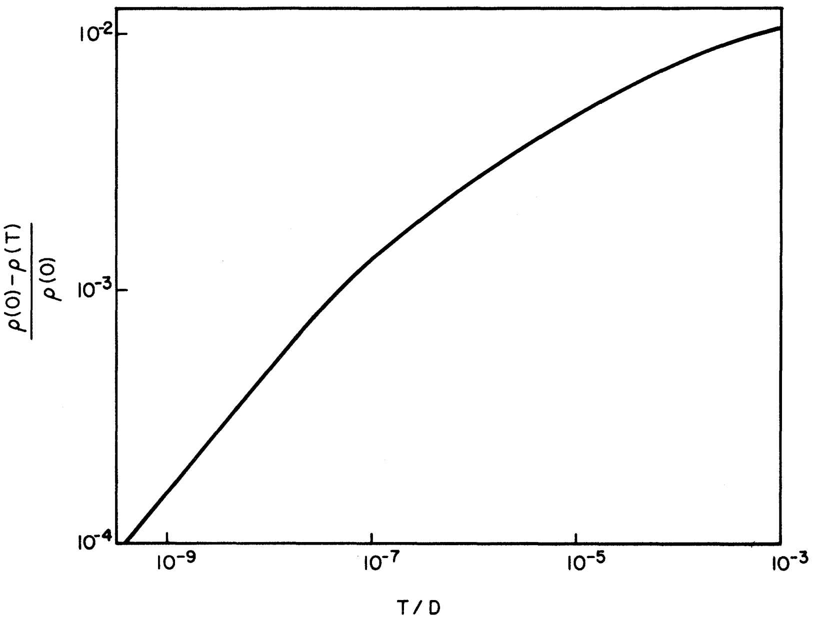

FIG. 1. Resistivity due to the substitutional impurity is plotted versus temperature, measured in units of bandwidth.

Kondo effect is drastically reduced.

Very recently, Theumann[6] has published a study of the Anderson model which employed an essentially identical decoupling scheme to that used by AP for the Wolff model. Theumann treated the case where v was infinite and the Anderson mixing term V was small compared to the deep impurity level E_D. She first specialized to the case of a very deep impurity level. In this case, she found behavior quite similar to that found by Bloomfield and Hamann[7] for the s-d model, if the results for the resistivity were expressed in terms of T/T_K, where T_K, the Kondo temperature, was $T_K = De^{-E_D/\rho V^2}/\pi$, where D was the bandwidth, ρ was the density of conduction electrons, and V was the mixing term.

Our result essentially complements Theumann's by considering the strong-coupling Wolff-model case. It also contains the difficulty briefly discussed by Theumann, that not all the Kondo-like "leading logarithmic terms" are contained in the decoupling scheme.

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Magnon-Coupled Nuclear Spin-Phonon Interaction[*]

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The magnon-coupled nuclear spin-phonon interaction first proposed by Silverstein is discussed on the basis of a classical model. In addition to being conceptually quite simple, the model points out several interesting new features of this coupling mechanism.

The magnon-coupled nuclear spin-phonon interaction first proposed by Silverstein[1] has been observed in at least one antiferromagnet[2] and probably in several others.[3-5] The purpose of this paper is to discuss this coupling mechanism from a point of view different from that of Silverstein.

Following Silverstein[1] we consider a uniaxial two-sublattice antiferromagnet in which the nuclear spin system is coupled to the electronic spins via an isotropic hyperfine interaction. (A good example is the Mn^{55} nuclear spin system in MnF_2.) The Hamiltonian of such a system consists of the following terms:

$$\mathcal{H} = \mathcal{H}_{\mathrm{P}} + \mathcal{H}_{\mathrm{MP}} + \mathcal{H}_{\mathrm{ex}} + \mathcal{H}_{\mathrm{A}} + \mathcal{H}_{\mathrm{ZM}} + \mathcal{H}_{\mathrm{hyp}} + \mathcal{H}_{\mathrm{ZN}} \quad . \qquad (1)$$

The individual terms correspond to the phonon, the magnon-phonon, the exchange, the magnetic anisotropy, the electronic Zeeman, the hyperfine, and the nuclear Zeeman contributions to the total Hamiltonian. Silverstein's solution to the problem involved expressing each term of Eq. (1) in terms of phonon and spin-wave operators, performing an average over the intermediate electronic spin system, and thus deriving an effective nuclear spin-phonon interaction, which is then used to calculate an ultrasonic absorption coefficient. This two-step process is described as follows: An acoustic phonon interacts with the electronic spin system (via $\mathcal{H}_{\mathrm{MP}}$) creating a virtual magnon; the magnon is then coupled to the nuclear spin system and produces a nuclear spin transition via the hyperfine interaction $\mathcal{H}_{\mathrm{hyp}}$. The calculation is clearly restricted to low temperatures ($T \ll T_N =$ Néel temperature) and, because of the average over the electronic spin states, any time correlation existing between the electronic and nuclear spins is lost.

An alternative approach to the problem is to calculate the elementary excitation spectrum of the complete system represented by the Hamiltonian of Eq. (1). Since the average over the electronic spin states is then unnecessary, time cor-