

extrinsic material can be done using relatively thick samples whereas those on intrinsic material require very thin samples. Furthermore, there is no photon frequency in the intrinsic case which can be related to a carrier concentration.

Interference fringes in a plane parallel slab of InSb have been observed to shift in an external magnetic field due to the changes in the free carrier contribution to the index of refraction.<sup>13</sup> The fringe effects are best observed using circular and linear polarization in the longitudinal and transverse orientations, respectively. At fixed wavelength, this shift in fringes with field could produce oscillations in the transmission as the orders of interference passed the wavelength of observation. However, the oscillations would be periodic in  $H$ . For the particular samples used, the fringes would be about  $1 \text{ cm}^{-1}$  apart, appreciably less than the spectral resolution of  $10 \text{ cm}^{-1}$  used. Therefore, the shift of interference fringes is not likely the cause of the observed phenomenon.

A few comments may be worthwhile concerning the relationship of the oscillatory optical absorption phenomena discussed in this paper and other oscillatory effects such as the de Haas-van Alphen effect and the Shubnikov-de Haas effect. The latter two effects de-

<sup>13</sup> E. D. Palik, Appl. Optics (to be published).

pend critically on the existence of a sharp Fermi surface. If the carriers become nondegenerate, oscillations characteristic of these effects disappear. In the optical absorption effects, on the other hand, the basic requirement for oscillations is that the optical radiation excite carriers to final states at an energy coincident with the edge of a well-defined magnetic level. The existence of a sharp Fermi surface is not essential, but does make possible an identification such as Eq. (2) which then leads to the useful Eq. (6). If the relaxation time of the carriers is too short, however, the edges of the magnetic levels will be poorly defined and the oscillations will be smeared out.

*Note added in proof.* Free carrier oscillations have been observed in 1-mm-thick  $n$ -type InAs containing about  $5 \times 10^{16}$  carriers / $\text{cm}^3$  at liquid nitrogen temperature. An effective mass ratio of 0.028 was obtained in good agreement with the effective mass obtained from cyclotron resonance measurements in the same magnetic field range 100–150 kG.

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## Exchange Narrowing of $d$ Bands in Antiferromagnets\*

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The theory of exchange narrowing of  $d$  bands presented in a previous paper for the ferromagnet is extended to the case of the antiferromagnet. It is shown that the dynamic spin wave-electron interaction gives rise to a narrowing factor  $e^{-\zeta}$ .  $\zeta$  depends upon the state of excitation of the spin system and increases with the number of antiferromagnetic magnons and hence with temperature. It is suggested that this effect may contribute to the high resistivity of a large number of antiferromagnetic compounds.

### I. INTRODUCTION

IN a previous paper<sup>1</sup> (hereafter referred to as I) it was shown that in the tight-binding approximation a  $d$  electron moving through a ferromagnetic crystal with a Bloch-type wave function would be coupled to the spin-wave system. A semiphenomenological theory describing the interaction of the  $d$  electron with the spin waves was formulated. The intra-atomic exchange arising in the Hartree-Fock equations was treated as an electron-magnon coupling operator. The coupled Hamil-

tonian was then separated into effective perturbed electron and spin-wave Hamiltonians. The average effect of the spin waves on electron was shown to result in a dynamic interaction which gave rise to a localization of the electron and a narrowing of the  $d$  band. The electronic bandwidth was found to depend parametrically upon the state of excitation of the spin system, and decreased with temperature (analogous to the polaron effect).

In this paper we consider the problem of an itinerant  $d$  electron in an antiferromagnet and show that a similar band narrowing can result. Our principal interest is in the effect of the spin waves on the electronic wave function and bandwidth and we shall not concern

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<sup>1</sup> T. Wolfram and J. Callaway, Phys. Rev. **127**, 1605 (1962).

ourselves with the actual exchange mechanism by which the crystal has attained an antiferromagnetic configuration. The calculations are quite similar to those presented in I, and will not be presented in such great detail here.

## II. THE SEMIPHENOMENOLOGICAL ONE-ELECTRON HAMILTONIAN

In dealing with the antiferromagnet it is convenient to assume that the spin configuration can be decomposed into two sublattices, and therefore, we restrict ourselves to the simple and body-centered cubic structures which can be divided into sublattice 1 and 2 in such a way that all the nearest neighbors of an atom on sublattice 1 are on sublattice 2 and vice versa. We adopt the convention that  $\mathbf{R}_i$  refers to the sublattice with spin "up" and  $\mathbf{R}_j$  to the spin "down" sublattice.

The Hamiltonian for a single electron coupled to a system of antiferromagnetically aligned spins can be taken from I, Eq. (7), to be (neglecting spin-orbit effects)

$$H = (\mathbf{p} - e\mathbf{A}/c)^2/2m + \sum_i U_1(\mathbf{r} - \mathbf{R}_i) + \sum_j U_2(\mathbf{r} - \mathbf{R}_j) - \sum_i G_1(\mathbf{r} - \mathbf{R}_i)\mathbf{S}_e \cdot \mathbf{S}_i - \sum_j G_2(\mathbf{r} - \mathbf{R}_j)\mathbf{S}_e \cdot \mathbf{S}_j + H_{s.w.} \quad (1)$$

The first term is the kinetic-energy operator appropriate in the presence of a magnetic field.  $\mathbf{A}$  is the vector potential. The second and third terms are the effective electrostatic potentials due to the other electrons and may be different for the two sublattices, 1 and 2. The fourth and fifth terms describe the effective exchange coupling of the itinerant electron with the atomic electrons.  $\mathbf{S}_e$  is the itinerant electron-spin operator,  $\mathbf{S}_i$  and  $\mathbf{S}_j$  are the net atomic-spin operators, and  $G_1$  and  $G_2$  are effective exchange potentials. The last term is the unperturbed spin-wave Hamiltonian,

$$H_{s.w.} = 2J \sum_{n\theta i} \mathbf{S}_i \cdot \mathbf{S}_j - g\beta H_1 \sum_i S_{iz} - g\beta H_2 \sum_j S_{jz},$$

$$H_1 = H + H_A,$$

$$H_2 = H - H_A, \quad (2)$$

where  $H$  is the external magnetic field and  $H_A$  is the effective anisotropic internal magnetic field.<sup>2</sup>  $S_{iz}$  and  $S_{jz}$  are the  $z$  components of the atomic spin operators,  $g$  is the spectroscopic splitting factor, and  $\beta$  is the Bohr magneton. The addition of  $H_{s.w.}$  to the one-electron Hamiltonian can be justified by arguments similar to those given in the case of the ferromagnet.

We wish to make a tight-binding calculation of the electron energy bands. The Bloch functions will be constructed from the localized wave functions obtained

<sup>2</sup> See, for example, J. Van Kranendonk and J. H. Van Vleck, Rev. Mod. Phys. **30**, 1 (1958).

by adding an excess electron to an orbital on a lattice site  $\mathbf{R}_k$ . The tight-binding wave function for the electron localized in the neighborhood of the lattice site  $\mathbf{R}_i$  with spin up will be an eigenstate of the Hamiltonian  $H^0(\mathbf{R}_i)$ ,

$$H^0(\mathbf{R}_i) = (\mathbf{p} - e\mathbf{A}/c)^2/2m + U_1(\mathbf{r} - \mathbf{R}_i) - G_1(\mathbf{r} - \mathbf{R}_i)\mathbf{S}_e \cdot \mathbf{S}_i + H_{s.w.} \quad (3)$$

## III. THE ANTIFERROMAGNETIC SPIN-WAVE REPRESENTATION

The unperturbed spin-wave Hamiltonian,  $H_{s.w.}$ , can be written in terms of the antiferromagnetic spin-wave annihilation and creation operators by successive canonical transformations. First, we transform to spin deviation operators defined by

$$S_{iz} = S - a_i^* a_i,$$

$$S_i^+ = (2S)^{1/2} a_i,$$

$$S_i^- = (2S)^{1/2} a_i^*, \quad (4)$$

and

$$S_{jz} = a_j^* a_j - S,$$

$$S_j^+ = (2S)^{1/2} a_j^*,$$

$$S_j^- = (2S)^{1/2} a_j,$$

where

$$S^\pm = S_x \pm iS_y. \quad (6)$$

Next we Fourier transform the spin deviation operators in terms of the reciprocal lattice vectors of the Brillouin zone defined by the sublattice,<sup>2</sup>

$$a_i = (2/N)^{1/2} \sum_k \exp(-i\mathbf{k} \cdot \mathbf{R}_i) a_{1k},$$

$$a_j = (2/N)^{1/2} \sum_k \exp(i\mathbf{k} \cdot \mathbf{R}_j) a_{2k}. \quad (7)$$

The final transformation,

$$a_{1k} = C_{1k} A_k + C_{2k} B_k^*,$$

$$a_{2k} = C_{1k} B_k + C_{2k} A_k^*, \quad (8)$$

defines the spin-wave annihilation and creation operators  $A_k$  and  $A_k^*$ , and  $B_k$  and  $B_k^*$  for the two antiferromagnetic spin-wave modes. The transformation coefficients are given by<sup>2</sup>

$$C_{1k} = \rho_k (\rho_k^2 - \gamma_k^2)^{-1/2},$$

$$C_{2k} = -\gamma_k (\rho_k^2 - \gamma_k^2)^{-1/2}, \quad (9)$$

where

$$\rho_k = (1 + H_A/H_E) + [(1 + H_A/H_E)^2 - \gamma_k^2]^{1/2},$$

$$\gamma_k = (1/z) \sum_{\Delta} \exp(i\mathbf{k} \cdot \Delta),$$

$$H_E = 2JSz/g\beta. \quad (10)$$

The sum over  $\Delta$  is a sum over the  $z$  vectors that join an atom on one sublattice with its nearest neighbors on the other sublattice. In terms of the annihilation and creation operators defined by Eq. (8),  $H_{s.w.}$  assumes the standard form

$$H_{s.w.} = E_S + \sum_k \{ A_k^* A_k \hbar\omega_{1k} + B_k^* B_k \hbar\omega_{2k} \}, \quad (11)$$

where the two antiferromagnetic spin-wave frequencies are given by

$$\begin{aligned}\hbar\omega_{1\mathbf{k}} &= g\beta[(H_E+H_A)^2-\gamma_{\mathbf{k}}^2 H_E^2]^{1/2}+g\beta H, \\ \hbar\omega_{2\mathbf{k}} &= g\beta[(H_E+H_A)^2-\gamma_{\mathbf{k}}^2 H_E^2]^{1/2}-g\beta H,\end{aligned}\quad (12)$$

and

$$E_S = \sum_{\mathbf{k}} \frac{1}{2}(\hbar\omega_{1\mathbf{k}} + \hbar\omega_{2\mathbf{k}}) - JS^2 zN - H_A g\beta N. \quad (13)$$

The coupling term of Eq. (3),  $GS_e \cdot \mathbf{S}_i$ , similarly can be expressed in terms of the annihilation and creation operators of Eq. (8), with the result

$$\begin{aligned}-G_1(\mathbf{r}-\mathbf{R}_i)\mathbf{S}_e \cdot \mathbf{S}_i &= -G_1(\mathbf{r}-\mathbf{R}_i)\{(S-\eta/N)S_e^z \\ &+ (S/N)^{1/2}[S_e^+ \sum_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{R}_i)(C_{1\mathbf{k}}A_{\mathbf{k}}^* + C_{2\mathbf{k}}B_{\mathbf{k}}) \\ &+ S_e^- \sum_{\mathbf{k}} \exp(-i\mathbf{k} \cdot \mathbf{R}_i)(C_{1\mathbf{k}}A_{\mathbf{k}} + C_{2\mathbf{k}}B_{\mathbf{k}}^*)]\},\end{aligned}\quad (14)$$

where we have replaced  $a_i^*a_i$  by the total number of spin deviations in the system,  $\eta$ , divided by total number of lattice sites,  $N$ .

The Hamiltonian of Eq. (3) can now be written as

$$H^0(\mathbf{R}_i) = H_{el} + H_{int} + H_{s.w.}, \quad (15)$$

where

$$\begin{aligned}H_{el} &= (\mathbf{p} - e\mathbf{A}/c)^2/2m + U_1(\mathbf{r}-\mathbf{R}_i) \\ &- G_1(\mathbf{r}-\mathbf{R}_i)(S-\eta/N)S_e^z,\end{aligned}\quad (16)$$

and

$$\begin{aligned}H_{int} &= (S/N)^{1/2}[S_e^+ \sum_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{R}_i)(C_{1\mathbf{k}}A_{\mathbf{k}}^* + C_{2\mathbf{k}}B_{\mathbf{k}}) \\ &+ S_e^- \sum_{\mathbf{k}} \exp(-i\mathbf{k} \cdot \mathbf{R}_i)(C_{1\mathbf{k}}A_{\mathbf{k}} + C_{2\mathbf{k}}B_{\mathbf{k}}^*)].\end{aligned}\quad (17)$$

#### IV. THE PERTURBED SPIN WAVES

As a trial solution to (15), we take the product function

$$\Psi = \Phi X = \begin{pmatrix} \phi_1(\mathbf{r}-\mathbf{R}_i) \\ \phi_2(\mathbf{r}-\mathbf{R}_i) \end{pmatrix} X, \quad (18)$$

where  $\Phi$  is a two-component spin orbital and is a function which depends only "itinerant" electron coordinates, and  $X$  is a spin-wave state which depends only on the spin-wave dynamical variables. (Both, of course, depend upon the lattice site.) Proceeding as in the ferromagnetic case we obtain the variational self-consistent equations for the perturbed and spin-wave functions:

$$[H_{el} + \langle X | H_{int} | X \rangle] \Phi = \mathcal{E}^0 \Phi, \quad (19)$$

$$\left[ H_{s.w.} + \int \Phi^* H_{int} \Phi d\tau \right] X = \lambda X, \quad (20)$$

where the parameters  $\mathcal{E}^0$  and  $\lambda$  are Lagrange multipliers arising from the constraint that the function  $\Phi$  and  $X$  be normalized. Equation (19) is the effective Schrödinger equation for the itinerant electron perturbed by the spin waves, and similarly Eq. (20) is the equation for the spin waves perturbed by the itinerant electron. The term  $\langle X | H_{int} | X \rangle$ , as we shall see, is negative and may be interpreted as an additional attractive potential which results from the dynamic interaction of the

electron with the spin waves. (Note that the static exchange is contained in  $H_{el}$ .)

The coupling term in Eq. (20) can be reduced to a spin-wave operator by integrating over the electron coordinates. Thus, we obtain

$$\begin{aligned}\langle \Phi | H_{int} | \Phi \rangle &= (S/N)^{1/2} \sum_{\mathbf{k}} [J_{12} \exp(i\mathbf{k} \cdot \mathbf{R}_i)(C_{1\mathbf{k}}A_{\mathbf{k}}^* + C_{2\mathbf{k}}B_{\mathbf{k}}) \\ &+ J_{12}^* \exp(-i\mathbf{k} \cdot \mathbf{R}_i)(C_{1\mathbf{k}}A_{\mathbf{k}} + C_{2\mathbf{k}}B_{\mathbf{k}}^*)],\end{aligned}\quad (21)$$

where

$$J_{12} = \int \phi_1^* G_1(\mathbf{r}-\mathbf{R}_i) \phi_2 d^3r. \quad (22)$$

The Hamiltonian for the perturbed spin waves,  $H_{s.w.}'$ , is

$$\begin{aligned}H_{s.w.}' &= \sum_{\mathbf{k}} [A_{\mathbf{k}}^* A_{\mathbf{k}} + \Gamma_{1\mathbf{k}}(\mathbf{R}_i) A_{\mathbf{k}}^* + \Gamma_{1\mathbf{k}}^*(\mathbf{R}_i) A_{\mathbf{k}}] \hbar\omega_{1\mathbf{k}} \\ &+ \sum_{\mathbf{k}} [B_{\mathbf{k}}^* B_{\mathbf{k}} + \Gamma_{2\mathbf{k}}(\mathbf{R}_i) B_{\mathbf{k}}^* \\ &+ \Gamma_{2\mathbf{k}}^*(\mathbf{R}_i) B_{\mathbf{k}}] \hbar\omega_{2\mathbf{k}},\end{aligned}\quad (23)$$

where

$$\begin{aligned}\Gamma_{1\mathbf{k}}(\mathbf{R}_i) &= -J_{12}(S/N)^{1/2}(C_{1\mathbf{k}}/\hbar\omega_{1\mathbf{k}}) \exp(i\mathbf{k} \cdot \mathbf{R}_i), \\ \Gamma_{2\mathbf{k}}(\mathbf{R}_i) &= -J_{12}^*(S/N)^{1/2}(C_{2\mathbf{k}}/\hbar\omega_{2\mathbf{k}}) \exp(i\mathbf{k} \cdot \mathbf{R}_i).\end{aligned}\quad (24)$$

At low temperatures, the operators  $A_{\mathbf{k}}$ ,  $A_{\mathbf{k}}^*$ ,  $B_{\mathbf{k}}$ , and  $B_{\mathbf{k}}^*$  approximate annihilation and creation operators for two noninteracting Bose systems. If we approximate the commutators by

$$\begin{aligned}[A_{\mathbf{k}}, A_{\mathbf{k}'}^*] &\approx \delta_{\mathbf{k}\mathbf{k}'}, \\ [B_{\mathbf{k}}, B_{\mathbf{k}'}^*] &\approx \delta_{\mathbf{k}\mathbf{k}'},\end{aligned}\quad (25)$$

then the unperturbed spin-wave states  $\chi^0(n_{1\mathbf{k}})$  and  $\chi^0(n_{2\mathbf{k}})$  obey the rules

$$\begin{aligned}A_{\mathbf{k}}^* A_{\mathbf{k}} \chi^0(n_{1\mathbf{k}}) &= n_{1\mathbf{k}} \chi^0(n_{1\mathbf{k}}), \\ A_{\mathbf{k}}^* \chi^0(n_{1\mathbf{k}}) &= (n_{1\mathbf{k}}+1)^{1/2} \chi^0(n_{1\mathbf{k}}+1), \\ A_{\mathbf{k}} \chi^0(n_{1\mathbf{k}}) &= (n_{1\mathbf{k}})^{1/2} \chi^0(n_{1\mathbf{k}}-1),\end{aligned}\quad (26)$$

$$\begin{aligned}B_{\mathbf{k}}^* B_{\mathbf{k}} \chi^0(n_{2\mathbf{k}}) &= n_{2\mathbf{k}} \chi^0(n_{2\mathbf{k}}), \\ B_{\mathbf{k}}^* \chi^0(n_{2\mathbf{k}}) &= (n_{2\mathbf{k}}+1)^{1/2} \chi^0(n_{2\mathbf{k}}+1), \\ B_{\mathbf{k}} \chi^0(n_{2\mathbf{k}}) &= (n_{2\mathbf{k}})^{1/2} \chi^0(n_{2\mathbf{k}}-1).\end{aligned}\quad (27)$$

The antiferromagnetic spin-wave state for the electron at  $R_i$  is

$$X(\mathbf{R}_i) = \prod_{\mathbf{k}} \chi(n_{1\mathbf{k}}, \mathbf{R}_i) \chi(n_{2\mathbf{k}}, \mathbf{R}_i). \quad (28)$$

We may then expand the eigenstates of  $H_{s.w.}'$  in terms of the unperturbed states  $\chi^0(n_{1\mathbf{k}})$  and  $\chi^0(n_{2\mathbf{k}})$ . We obtain using second-order perturbation

$$\begin{aligned}\chi(n_{1\mathbf{k}}, \mathbf{R}_i) &= [1 - \frac{1}{2}(2n_{1\mathbf{k}}+1)|\Gamma_{1\mathbf{k}}|^2] \chi^0(n_{1\mathbf{k}}) \\ &+ (n_{1\mathbf{k}})^{1/2} \Gamma_{1\mathbf{k}}^*(\mathbf{R}_i) \chi^0(n_{1\mathbf{k}}-1) \\ &- (n_{1\mathbf{k}}+1)^{1/2} \Gamma_{1\mathbf{k}}(\mathbf{R}_i) \chi^0(n_{1\mathbf{k}}+1) + O(1/N),\end{aligned}\quad (29)$$

and

$$\begin{aligned}\chi(n_{2\mathbf{k}}, \mathbf{R}_i) &= [1 - \frac{1}{2}(2n_{2\mathbf{k}}+1)|\Gamma_{2\mathbf{k}}|^2] \chi^0(n_{2\mathbf{k}}) \\ &+ (n_{2\mathbf{k}})^{1/2} \Gamma_{2\mathbf{k}}^*(\mathbf{R}_i) \chi^0(n_{2\mathbf{k}}-1) \\ &- (n_{2\mathbf{k}}+1)^{1/2} \Gamma_{2\mathbf{k}}(\mathbf{R}_i) \chi^0(n_{2\mathbf{k}}+1) + O(1/N).\end{aligned}\quad (30)$$

### V. THE PERTURBED ONE-ELECTRON HAMILTONIAN

In Sec. IV we found the perturbed spin-wave states  $\chi(n_{1k}, \mathbf{R}_i)$  and  $\chi(n_{2k}, \mathbf{R}_i)$  as solutions to the effective spin-wave Hamiltonian. We are now able to evaluate the perturbation term,  $\langle X | H_{\text{int}} | X \rangle$ , occurring in the electronic Hamiltonian.

This is easily accomplished using Eqs. (26)–(30). The effective perturbed electron Hamiltonian for the itinerant electron localized at  $\mathbf{R}_i$  is then

$$\begin{aligned} H_{e1}'(\mathbf{R}_i) &= (\mathbf{p} - e\mathbf{A}/c)^2/2m + U_1(\mathbf{r} - \mathbf{R}_i) \\ &\quad - G_1(\mathbf{r} - \mathbf{R}_i)(S - n/N)S_e^z \\ &\quad - G_1(\mathbf{r} - \mathbf{R}_i) \left[ \left( \frac{S}{N} \right) \sum_{\mathbf{k}} (J_{12}^* S_e^+ + J_{12} S_e^-) \right. \\ &\quad \left. \times \left( \frac{C_{1k}^2}{\hbar\omega_{1k}} + \frac{C_{2k}^2}{\hbar\omega_{2k}} \right) \right]. \quad (31) \end{aligned}$$

The first term involving  $G_1(\mathbf{r} - \mathbf{R}_i)$  is the usual static exchange potential with a correction for the average number of spin deviations present on the  $i$ th lattice site. The last term is a dynamic spin-wave interaction. This Hamiltonian should be compared with the corresponding ferromagnetic one-electron Hamiltonian given by Eq. (33) of I. It will be seen that the spin-wave perturbation is quite similar. However, it should be noted that the spin-wave frequency is proportional to  $k^2$  in the ferromagnet and as  $k$  in the antiferromagnetic case for small propagation vectors.

We may repeat the same calculation for the itinerant electron localized on a site with spin “down” centered at  $\mathbf{R}_j$ . The tight binding functions will be solutions to the local Hamiltonian,  $H^0(\mathbf{R}_j)$ ,

$$\begin{aligned} H^0(\mathbf{R}_j) &= (\mathbf{p} - e\mathbf{A}/c)^2/2m + U_2(\mathbf{r} - \mathbf{R}_j) \\ &\quad - G_2(\mathbf{r} - \mathbf{R}_j) \mathbf{S}_e \cdot \mathbf{S}_j + H_{s.w.} \quad (32) \end{aligned}$$

Again assuming a product solution

$$\tilde{\Psi} = \tilde{\Phi}(\mathbf{R}_j) \tilde{X}(\mathbf{R}_j) = \begin{pmatrix} \tilde{\phi}_1(\mathbf{r} - \mathbf{R}_j) \\ \tilde{\phi}_2(\mathbf{r} - \mathbf{R}_j) \end{pmatrix} \tilde{X}(\mathbf{R}_j), \quad (33)$$

we find that

$$\tilde{X}(\mathbf{R}_j) = \prod_{\mathbf{k}} \chi(n_{1k}, \mathbf{R}_j) \chi(n_{2k}, \mathbf{R}_j), \quad (34)$$

where

$$\begin{aligned} \chi(n_{1k}, \mathbf{R}_j) &= [1 - \frac{1}{2}(2n_{1k} + 1) |\tilde{\Gamma}_{1k}|^2] \chi^0(n_{1k}) \\ &\quad + (n_{1k})^{1/2} \tilde{\Gamma}_{1k}(\mathbf{R}_j) \chi^0(n_{1k} + 1) \\ &\quad - (n_{1k} + 1)^{1/2} \tilde{\Gamma}_{1k}(\mathbf{R}_j) \chi^0(n_{1k} + 1) + O(1/N), \quad (35) \end{aligned}$$

and

$$\begin{aligned} \chi(n_{2k}, \mathbf{R}_j) &= [1 - \frac{1}{2}(2n_{2k} + 1) |\tilde{\Gamma}_{2k}|^2] \chi^0(n_{2k}) \\ &\quad + (n_{2k})^{1/2} \tilde{\Gamma}_{2k}^*(\mathbf{R}_j) \chi^0(n_{2k} - 1) \\ &\quad - (n_{2k} + 1)^{1/2} \tilde{\Gamma}_{2k}(\mathbf{R}_j) \chi^0(n_{2k} + 1) + O(1/N), \quad (36) \end{aligned}$$

with

$$\begin{aligned} \tilde{\Gamma}_{1k} &= -\tilde{J}_{12}(S/N)^{1/2} \exp(i\mathbf{k} \cdot \mathbf{R}_j) C_{2k}/\hbar\omega_{1k}, \\ \tilde{\Gamma}_{2k} &= -\tilde{J}_{12}^*(S/N)^{1/2} \exp(i\mathbf{k} \cdot \mathbf{R}_j) C_{1k}/\hbar\omega_{2k}, \quad (37) \end{aligned}$$

$$\tilde{J}_{12} = \int \tilde{\phi}_1^* G_2(\mathbf{r} - \mathbf{R}_j) \tilde{\phi}_2 d^3r.$$

The corresponding effective one-electron Hamiltonian is

$$\begin{aligned} H_{e1}' &= (\mathbf{p} - e\mathbf{A}/c)^2/2m + U_2(\mathbf{r} - \mathbf{R}_j) \\ &\quad - G_2(\mathbf{r} - \mathbf{R}_j)(n/N - S)S_e^z \\ &\quad - G_2(\mathbf{r} - \mathbf{R}_j) \left[ (\tilde{J}_{12}^* S_e^+ + \tilde{J}_{12} S_e^-) \right. \\ &\quad \left. \times \sum_{\mathbf{k}} \left( \frac{C_{1k}^2}{\hbar\omega_{2k}} + \frac{C_{2k}^2}{\hbar\omega_{1k}} \right) \right]. \quad (38) \end{aligned}$$

### VI. BAND NARROWING IN THE ANTIFERROMAGNET

From the discussion of the ferromagnet it is clear that the electronic band narrowing factor arises from the transformation function for neighboring spin-wave states:

$$e^{-\tau} = \langle X(\mathbf{R}_i) | X(\mathbf{R}_j = \mathbf{R}_i + \Delta) \rangle, \quad (39)$$

where  $\Delta$  is a nearest-neighbor vector. Equation (39) may be written as

$$\begin{aligned} e^{-\tau} &= \prod_{\mathbf{k}} \langle \chi(n_{1k}, \mathbf{R}_i = 0) | \chi(n_{1k}, \mathbf{R}_j = \Delta) \rangle \\ &\quad \times \langle \chi(n_{2k}, \mathbf{R}_i = 0) | \chi(n_{2k}, \mathbf{R}_j = \Delta) \rangle. \quad (40) \end{aligned}$$

The first factor is easily evaluated

$$\begin{aligned} \prod_{\mathbf{k}} \langle \chi(n_{1k}, 0) | \chi(n_{1k}, \Delta) \rangle &= \prod_{\mathbf{k}} \{ [1 - \frac{1}{2}(2n_{1k} + 1) |\Gamma_{1k}(0)|^2] \\ &\quad \times [1 - \frac{1}{2}(2n_{1k} + 1) |\tilde{\Gamma}_{1k}(\Delta)|^2] + n_{1k} \Gamma_{1k}(0) \tilde{\Gamma}_{1k}^*(\Delta) \\ &\quad + (n_{1k} + 1) \Gamma_{1k}^*(0) \tilde{\Gamma}_{1k}(\Delta) + O(N^{-3/2}) \}. \quad (41) \end{aligned}$$

We may rewrite this as an exponential:

$$\begin{aligned} \prod_{\mathbf{k}} \langle \chi(n_{1k}, 0) | \chi(n_{1k}, \Delta) \rangle &= \exp \{ -\sum_{\mathbf{k}} \frac{1}{2} (2n_{1k} + 1) [ |\Gamma_{1k}(0)|^2 + |\tilde{\Gamma}_{1k}(\Delta)|^2 ] \\ &\quad - n_{1k} \Gamma_{1k}(0) \tilde{\Gamma}_{1k}^*(\Delta) \\ &\quad - (n_{1k} + 1) \Gamma_{1k}^*(0) \tilde{\Gamma}_{1k}(\Delta) + O(N^{-2}) \}. \quad (42) \end{aligned}$$

In the absence of an external magnetic field, the two antiferromagnetic normal modes become degenerate with  $\omega_{1k} = \omega_{2k}$  so that  $n_{1k} = n_{2k}$ . In this case, the two spin-wave modes for a given  $k$  vector are identical except that the spin vectors are reversed. Neglecting the anisotropy field<sup>3</sup>  $H_A$  the electron eigenstates  $\Phi(R_i)$  and  $\Phi(R_j)$  differ only by the direction of quantization

<sup>3</sup>The assumption of an anisotropic field  $H_A$  is necessary to insure the stability of the antiferromagnetic configuration. It may, however, be neglected in comparison with the exchange field  $H_E$ . Typical values are  $H_A = 10^2$  Oe and  $H_E = 10^6$  Oe, so that  $H_A$  is  $10^{-4}$  smaller than  $H_E$ .

and perhaps a phase factor  $\gamma$

$$\tilde{\Phi}(\mathbf{R}_j) = \begin{pmatrix} \tilde{\phi}_1(\mathbf{r}-\mathbf{R}_j) \\ \tilde{\phi}_2(\mathbf{r}-\mathbf{R}_j) \end{pmatrix} = \begin{pmatrix} \phi_2(\mathbf{r}-\mathbf{R}_j) \\ \phi_1(\mathbf{r}-\mathbf{R}_j) \end{pmatrix} e^{i\gamma}, \quad (43)$$

where  $\phi_1$  and  $\phi_2$  are the components of the spinor for an electron at a spin-up site. Thus, we have in this case  $\tilde{J}_{12} = J_{12}^*$ , so that,

$$\begin{aligned} & \prod_{\mathbf{k}} \langle \chi(n_{1\mathbf{k}}, 0) | \chi(n_{1\mathbf{k}}, \mathbf{\Delta}) \rangle \\ &= \exp \left\{ -|J_{12}|^2 \left( \frac{2n_{1\mathbf{k}}+1}{2} \right) \left( \frac{S}{N} \right) \right. \\ & \quad \left. \times \sum_{\mathbf{k}} \frac{C_{1\mathbf{k}}^2 + C_{2\mathbf{k}}^2 - 2C_{1\mathbf{k}}C_{2\mathbf{k}} \cos(\mathbf{k} \cdot \mathbf{\Delta})}{(\hbar\omega_{1\mathbf{k}})^2} \right\}. \quad (44) \end{aligned}$$

An identical contribution is obtained from the second factor in Eq. (40) and, therefore, the band-narrowing exponent is

$$\begin{aligned} \zeta(n_{\mathbf{k}}) &= (2n_{\mathbf{k}}+1) \left( \frac{S}{N} \right) |J_{12}|^2 \\ & \quad \times \sum_{\mathbf{k}} \frac{C_{1\mathbf{k}}^2 + C_{2\mathbf{k}}^2 - 2C_{1\mathbf{k}}C_{2\mathbf{k}} \cos(\mathbf{k} \cdot \mathbf{\Delta})}{(\hbar\omega_{\mathbf{k}})^2}, \quad (45) \end{aligned}$$

where  $n_{1\mathbf{k}} = n_{2\mathbf{k}} = n_{\mathbf{k}}$  and  $\omega_{1\mathbf{k}} = \omega_{2\mathbf{k}} = \omega_{\mathbf{k}}$ .

In order to estimate the magnitude of  $\zeta$  we consider a body-centered cubic crystal with lattice constant  $a$ . At low temperatures we may set  $n_{\mathbf{k}}$  equal to zero. This must give an underestimate of  $\zeta$  because there are always spin deviations present in an antiferromagnet. Anderson<sup>4</sup> has calculated that at any given site there is a 7% probability of one or more spin deviations and a 93% probability of no spin deviations. The sum over the sublattice Brillouin zone may be approximated by an integral so that

$$\zeta(0) = \frac{S|J_{12}|^2}{\Omega} \int_{\Omega} \frac{C_{1\mathbf{k}}^2 + C_{2\mathbf{k}}^2 - 2C_{1\mathbf{k}}C_{2\mathbf{k}} \cos(\mathbf{k} \cdot \mathbf{\Delta})}{(\hbar\omega_{\mathbf{k}})^2} d^3k, \quad (46)$$

where  $\Omega$  is the volume of the zone. In evaluating the constants  $C_{1\mathbf{k}}$  and  $C_{2\mathbf{k}}$  and  $\omega_{\mathbf{k}}$ , we set the external magnetic field,  $H$ , and anisotropy field,  $H_A$ , equal to zero. We then obtain

$$\zeta(0) = \frac{|J_{12}/J|^2}{1024S} \left\{ \frac{1}{\Omega} \int_{\Omega} \frac{d^3k}{(1 - \cos^2 k_x \cos^2 k_y \cos^2 k_z)^{1/2}} \right\}, \quad (47)$$

where  $k_x$ ,  $k_y$ , and  $k_z$  are the Cartesian components of  $\mathbf{k}$  and  $J$  is the spin-wave exchange parameter. The quantity in parentheses was evaluated numerically and found to be 1.12. The Néel temperature of many

antiferromagnets is small and the ratio  $J_{12}/J$  may be as large as 50. For  $S=2$  we obtain a value of 1.4 for  $\zeta(0)$ .

## VII. DISCUSSION AND CONCLUSION

A large number of antiferromagnetic binary compounds are insulators. In particular, many of the transition element oxides and sulfides such as MnO, FeO, NiO, MnS and others are insulators. Simple band theoretical arguments would predict that these compounds should be conductors since their  $d$  bands are unfilled. Slater<sup>5</sup> has suggested that the nonconducting nature of these compounds with unfilled  $d$  bands is due to antiferromagnetic exchange effects. According to the Hartree-Fock approximation the exchange potential is attractive for electrons with parallel spins and repulsive for electrons with antiparallel spins. The periodicity of the exchange potential is, therefore, twice that of the ordinary potential. A band gap will consequently develop in the interior of the Brillouin zone. If the full Brillouin zone contains  $N$  states,  $N/2$  of these will lie below the gap. Then, for example, an antiferromagnet with one electron per atom can be an insulator at absolute zero if the gap is sufficiently large. In this theory the energy gap depends upon the existence of antiferromagnetic ordering. Mott<sup>6</sup> has pointed out several difficulties with Slater's theory. In particular, Mott has argued that according to this model the crystal should become conducting above the Néel temperature since the energy gap vanishes with the loss of magnetic order. On the other hand, since short-range order may persist above the Néel temperature, it is not clear that the energy gap need vanish.

Slater's theory can be improved by considering in addition to the exchange energy gap, the effect of the dynamic spin wave-electron interaction. If the electron-magnon interaction is large, then the dynamic effect of the spin waves can cause the electron band width to decrease with increasing temperature. Thus, as the temperature increases the energy gap decreases, but simultaneously the electron effective mass increases. The increase in effective mass may be sufficient to compensate for the diminishing of energy gap so that the resistivity remains large.

The theory of exchange narrowing presented in this paper is, of course, very crude and we cannot suppose that it is directly applicable to the antiferromagnetic compounds that we have been discussing. Similar effects due to the formation of polarons may be equally important. Nevertheless, it seems plausible that dynamic exchange effects may contribute significantly to the resistivity at temperatures below the Néel temperature. Since spin deviations are always present in an antiferromagnet, the dynamic interaction will be nonvanishing even at absolute zero.

<sup>4</sup> P. W. Anderson, Phys. Rev. **86**, 694 (1952).

<sup>5</sup> J. C. Slater, Phys. Rev. **82**, 538 (1951).

<sup>6</sup> N. F. Mott, Suppl. Nuovo Cimento **8**, 312 (1958).