

Theory of the magnetic polaron

B. Sriram Shastry and D. C. Mattis

Physics Department, University of Utah, Salt Lake City, Utah 84112

(Received 25 March 1981)

We construct exact Green's functions for a single electron in a ferromagnetic semiconductor, including both spin-conserving and spin-flip processes at $T=0$. We contrast two cases: ferromagnetic and antiferromagnetic coupling of the electron's spin to the lattice. In the former case, a small- k electron will have its spin totally polarized in the predominant direction, whereas in the latter, deviation from saturation polarization is to be expected. Crucial differences between bound- and scattering-state contributions to the electron's spectral weight are highlighted.

I. INTRODUCTION

The properties of the rare-earth chalcogenides EuO and EuS have been the subject of several recent studies, both experimental¹⁻⁹ and theoretical.¹⁰⁻¹⁷ These materials are ferromagnetic semiconductors. Conceptually, they are simpler than itinerant ferromagnetic Fe, Ni in that a clear distinction can be made between localized moments and itinerant conduction particles.

In the present work, we present a detailed analysis of the one electron Green's function zero temperature. Similar techniques could be used to extend the theory to low temperatures, in the sense of an asymptotic expansion in powers of T , but we shall not pursue this here.

We quickly dispose of the Green's function of a spin-up electron, which is trivial. The spin-down and off-diagonal (spin-flip) Green's functions are non-trivial, but exactly calculable at $T=0$. They are the principal objects of our study and may be viewed as the magnetic analogs of polarons; the basic process involving repeated emission and reabsorption of magnons with consequent recoil of the electron. For the case of *ferromagnetic coupling* of the electron's spin to the lattice, we find that the electron and the magnon effectively *repel*. After a characteristic time γ_k^{-1} , the electron, which initially has its spin down inevitably finds itself with spin up and a magnon is radiated out.

In the converse case of *antiferromagnetic coupling* to the lattice, the electron and magnon effectively *attract* and a bound, *polaron-like* state ensues. In the weak-coupling limit the electron is perfectly antiparallel to the predominant polarization. The greater the coupling constant of the electron spin to the lattice, the denser becomes the magnon cloud and the less is the degree of polarization of the electron spin in the antiparallel direction.

Evidently then, the qualitative and quantitative features of the electron dynamics depends sensitively

on whether the coupling is ferromagnetic or antiferromagnetic; yet most theories have ignored this substantial difference, arriving at conclusions that are qualitatively unsatisfactory. There are many experiments, especially on photoemitted electrons from these materials,⁴⁻⁹ and an unambiguous theoretical context is desirable and motivates the present investigation.

The paper is organized as follows: in Sec. II we set up the secular equation and obtain the eigenvalue condition. We point out the essential difference between bound and scattering states in terms of the amplitudes. In Sec. III we work out the electron Green's functions exactly. In Sec. IV we introduce a simple band structure which enables us to calculate various quantities analytically. The numerical results are given in Sec. V and in Sec. VI we discuss our results.

II. WAVE FUNCTION

In this section we construct the low-lying eigenstates of the s - d -like Hamiltonian for a magnetic semiconductor. $H = H_0 + H_1$, where

$$H_0 = \sum_k \epsilon_k a_{k\sigma}^\dagger a_{k\sigma} - \frac{1}{2} \sum_{ij} J_{ij} (\vec{S}_i \cdot \vec{S}_j - s^2) \quad (1)$$

$$H_1 = -\frac{J}{2\sqrt{N}} \sum_q \sigma_q^z S_q^z - \frac{\gamma J}{2\sqrt{N}} \sum_q (\sigma_q^+ S_q^- + \sigma_q^- S_q^+) \quad (2)$$

In the above equations, ϵ_k is the single-particle (band) energy

$$\sigma_q^+ = \sum_k a_{k\uparrow}^\dagger a_{k+q\downarrow}, \quad S_q^\alpha = \frac{1}{\sqrt{N}} \sum_i e^{-i\vec{q}\cdot\vec{R}_i} S_i^\alpha,$$

$$\sigma_q^z = \sum_{k,\sigma} z_\sigma a_{k\sigma}^\dagger a_{k+q\sigma}, \quad z_\uparrow = +1, \quad z_\downarrow = -1.$$

The S_i^α are the spin operators for the localized spins and σ 's the same for the conduction electrons. The anisotropy parameter γ can be varied from zero to unity and changes the coupling between the Ising ("Hartree") and the Heisenberg limits.

The Hamiltonian commutes with S_{tot}^z and hence we construct the low-lying eigenstates as linear superpositions of eigenstates of S_{tot}^z . In the zero particle sector the ground state of the model is readily seen to be

$$|0\rangle = |\text{vac}\rangle |\Phi\rangle, \quad (3)$$

where $|\Phi\rangle$ is the ferromagnetic state. On adding one conduction electron to the system, we may examine the $S_{\text{tot}}^z = Ns \pm 1/2$ subspaces separately.

The $S_{\text{tot}}^z = Ns + 1/2$ subspace is trivial since it is easy to verify that an exact eigenstate of H is provided by the state $|k \uparrow; 0\rangle$, where we use the notation:

$$|k \sigma; q\rangle \equiv a_{k\sigma}^\dagger |\text{vac}\rangle \frac{S_q^-}{\sqrt{2s}} |\Phi\rangle. \quad (4)$$

The transverse part of Eq. (2) annihilates $|k \uparrow; 0\rangle$ and hence

$$H|k \uparrow; 0\rangle = (\epsilon_k - Js/2)|k \uparrow; 0\rangle. \quad (5)$$

This is a stable state for $J > 0$. But for antiferromagnetic coupling ($J < 0$) it is a highly excited state.

We now turn to the $S_{\text{tot}}^z = Ns - 1/2$ subspace. Here the appropriate basis is $|k \downarrow; 0\rangle$ and $|k - q \uparrow; q\rangle$ corresponding to a down-spin electron and an up-spin plus a magnon, respectively. By direct application of H , we find

$$H|k \downarrow; 0\rangle = (\epsilon_k + Js/2)|k \downarrow; 0\rangle - \gamma J (s/2N)^{1/2} \sum_q |k - q \uparrow; q\rangle, \quad (6)$$

$$H|k - q \uparrow; q\rangle = (\epsilon_{k-q} - Js/2 + \omega_q)|k - q \uparrow; q\rangle + J/2N \sum_p |k - p \uparrow; p\rangle - \gamma J (s/2N)^{1/2} |k \downarrow; 0\rangle, \quad (7)$$

where ω_q is a magnon energy

$$\omega_q = s[J(0) - J(q)]. \quad (8)$$

We construct a linear combination

$$|\Psi_k\rangle = \frac{1}{A} \left[|k \downarrow; 0\rangle + \sum_q f_q |k - q \uparrow; q\rangle \right], \quad (9)$$

where $A = (1 + \sum_q |f_q|^2)^{1/2}$. Requiring $H|\Psi_k\rangle = E_k|\Psi_k\rangle$ and using the orthonormality of the basis,

we find

$$E_k = \epsilon_k + \frac{Js}{2} - \gamma J \left(\frac{s}{2N} \right)^{1/2} \sum_q f_q, \quad (10)$$

$$f_q \left[E_k - \epsilon_{k-q} + \frac{Js}{2} - \omega_q \right] = -\gamma J \left(\frac{s}{2N} \right)^{1/2} + \frac{J}{2N} \sum_q f_q. \quad (11)$$

It is obvious at this stage that for $\gamma \neq 0$, the Hartree energy $\epsilon_k + Js/2$ is not, in general, close to the exact eigenvalue E_k . A straightforward calculation gives

$$E_k = \epsilon_k - Js \left(\gamma^2 - \frac{1}{2} \right) + \frac{\gamma^2 Js}{1 + (J/2) \Lambda(k, E_k)}, \quad (12)$$

where

$$\Lambda(k, \omega) = \frac{1}{N} \sum_{\epsilon_{k-q} + \omega_q - Js/2 - \omega}. \quad (13)$$

The solutions of Eq. (12) may be classified as bound or scattering solutions. The bound state solution (there is only one for either sign of J) is characterized by the fact that $f_q = O(1/\sqrt{N})$ for every q and the coefficient of f_q in the left-hand side (LHS) of Eq. (11) is nonzero for all q . Thus the conduction electron magnetization

$$\frac{1}{2} \langle \sigma^z \rangle = -\frac{1}{2} \frac{1 - \sum_q |f_q|^2}{1 + \sum_q |f_q|^2}, \quad (14)$$

is $-1/2 + O(1)$ for the bound state.

The scattering solutions are, on the other hand, characterized by

$$E_k^{(q_0)} = \epsilon_{k-q_0} - Js/2 + \omega_{q_0} + e_{q_0}/N, \quad (15)$$

where e_{q_0}/N is a small energy shift. Thus the scattering states (there are N of them) have, essentially, the energy of a spin-up electron plus a magnon. Equations (15) and (11) require that

$$f_q = \begin{cases} O(1/\sqrt{N}), & q \neq q_0 \\ O(\sqrt{N}), & q = q_0 \end{cases}. \quad (16)$$

Thus the conduction-electron magnetization in the scattering states is $+1/2 - O(1/N)$. The electron in these states must be pictured as having essentially spin up. The electron spectral weight (see Secs. III and IV) contains contributions from both bound and scattering states and there is no *a priori* way to estimate their relative importance. We will show that in the case $J > 0$ (i.e., ferromagnetic coupling) the

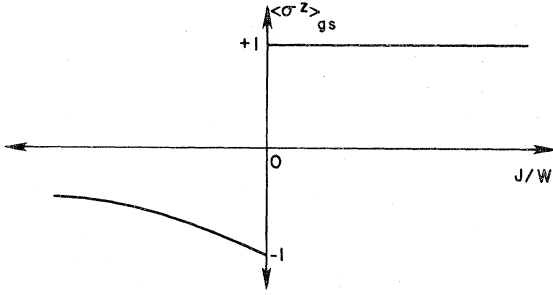


FIG. 1. Schematic illustration of the conduction-electron spin polarization in the lowest energy state for $J > 0$ (ferromagnetic coupling) and $J < 0$ (antiferromagnetic coupling of electron spin to lattice) showing discontinuity at $J = 0$, and screening for $J < 0$.

scattering states essentially exhaust the spectral weight whereas for $J < 0$ the bound state dominates. The qualitative aspects for an electron in or near the ground state are shown in Fig. 1. Perturbation theory in J would fail because of the discontinuities in the physical properties as J changes sign.

III. GREEN'S FUNCTION

In this section we calculate the one electron Green's function by a straightforward approach. We define the conventional (retarded) Green's functions as follows:

$$G_{\sigma}(k, \omega) = \int_0^{+\infty} dt e^{i\omega t} G_{\sigma}(k, t), \quad (17)$$

$$G_{\sigma}(k, t) = -i\theta(t) \langle 0 | \{a_{k\sigma}(t), a_{k\sigma}^{\dagger}(0)\} | 0 \rangle,$$

where ω is assumed to contain a small damping term ($\omega \equiv \omega + i0^+$). In addition, we find it expedient to introduce an anomalous (off-diagonal) Green's function L :

$$L_q(k, t) \equiv -i\theta(t) e^{-i\omega_q t} \langle q | \{a_{k+q\uparrow}(t), a_{k\downarrow}^{\dagger}(0)\} | 0 \rangle, \quad (18)$$

where $|q\rangle \equiv |\text{vac}\rangle S_q^- / \sqrt{2s} |\Phi\rangle$ and $|0\rangle \equiv |\text{vac}\rangle |\Phi\rangle$.

The up-spin Green's function is trivial to compute. On taking the time derivative of $G_{\uparrow}(k, t)$ we find

$$\left(i \frac{\partial}{\partial t} - \epsilon_k \right) G_{\uparrow}(k, t) = \delta(t) - \frac{J}{2\sqrt{N}} \sum_q (-i)\theta(t) \langle 0 | \{a_{k+q\uparrow} S_q^z(t), a_{k\uparrow}^{\dagger}\} | 0 \rangle - \frac{\gamma J}{2\sqrt{N}} (-i)\theta(t) \sum_q \langle 0 | \{a_{k+q\downarrow} S_q^-(t), a_{k\uparrow}^{\dagger}\} | 0 \rangle. \quad (19)$$

The third term on the RHS of Eq. (19) vanishes on using the property of the ferromagnetic ground state $\langle 0 | S_q^- = 0$. Hence we find

$$G_{\uparrow}(k, \omega) = \frac{1}{\omega - \epsilon_k + Js/2}. \quad (20)$$

This is precisely the result of the Hartree approximation as well.

In the case of spin down, the transverse terms are nontrivial. We find after taking a single time deriva-

tive

$$\left(i \frac{\partial}{\partial t} - \epsilon_k - \frac{Js}{2} \right) G_{\downarrow}(k, t) = \delta(t) - \gamma J \left(\frac{s}{2N} \right)^{1/2} \sum_q L_q(k, t). \quad (21)$$

The anomalous Green's functions are each of $O(1/\sqrt{N})$ in the thermodynamic limit, but their sum over all q is non-negligible. We proceed by taking the time derivatives of $L_q(k, t)$. The first time derivative gives rise to a vanishing inhomogeneous term and hence we proceed to the second derivative and find

$$\left(i \frac{\partial}{\partial t} - \omega_q \right)^2 L_q(k, t) = \delta(t) \langle q | \{ [a_{k+q\uparrow}, H], a_{k\downarrow}^{\dagger} \} | 0 \rangle + (-i)\theta(t) \langle q | \{ [[a_{k+q\uparrow}, H], H], a_{k\downarrow}^{\dagger} \} | 0 \rangle e^{-i\omega_q t}. \quad (22)$$

The inhomogeneous term is readily seen to be $\delta(t) [-\gamma J (s/2N)^{1/2}]$. The next term is expanded out and after taking the commutator with H we obtain a very long expression. We have found it possible to evaluate it exactly by using the following identities involving the Heisenberg operators $S^{\alpha}(t)$:

$$\langle q | S_p^z(t) = s\sqrt{N} \delta_{\vec{p}, 0} \langle q | - \frac{1}{\sqrt{N}} e^{i(\omega_q - \omega_{p+q})t} \langle p+q | \quad (23)$$

and

$$\langle q | S_{-p}^{-}(t) = e^{i\omega_q t} \sqrt{2s} \delta_{\vec{q}+\vec{p},0} \langle 0 | \quad (24)$$

Using these we find, after tedious algebra, the following expression for the Fourier transform of L :

$$\begin{aligned} \left[(\omega - \omega_q)^2 - \left(\epsilon_{k+q} - \frac{Js}{2} \right)^2 \right] L_q(k, \omega) = & - \left(\frac{s}{2N} \right)^{1/2} \gamma J + \frac{J}{2N} \sum_p L_p(k, \omega) \left(\epsilon_{k+q} + \epsilon_{k+p} + \omega_p - \omega_q + \frac{J}{2} + (\gamma^2 - 1)Js \right) \\ & - \gamma J \left(\frac{s}{2N} \right)^{1/2} G_1(k, \omega) \left(\epsilon_{k+q} + \epsilon_k - \omega_q + \frac{J}{2} \right). \end{aligned} \quad (25)$$

The exact solution of the problem rests on the observation that L_q can be expressed in terms of G_1 (and L_q) alone. In order to proceed further, we define a vertex function K_q through the relation

$$L_q(k, \omega) = -\gamma (J^2 s / 2N)^{1/2} G_1(k, \omega) K_q(k, \omega). \quad (26)$$

Combining with (21) we find

$$G_1^{-1}(k, \omega) = [\omega - \epsilon_k - Js/2 - \Sigma(k, \omega)]^{-1}, \quad (27)$$

$$\begin{aligned} \Gamma_q(k, \omega) - 1 - \frac{J}{2N} \sum_p \frac{\Gamma_p(k, \omega)}{\omega - \omega_p - \epsilon_{k+p} + Js/2} \\ = \frac{J}{2(\omega - \omega_q + \epsilon_{k+q} - Js/2)} \left(1 - \frac{1}{N} \sum_l \Gamma_l(k, \omega) + \frac{J}{2N} \sum_l \frac{\Gamma_l(k, \omega)}{\omega - \omega_l - \epsilon_{k+l} + Js/2} \right). \end{aligned} \quad (30)$$

On summing over q we find

$$\left(\frac{1}{N} \sum_q \Gamma_q(k, \omega) - 1 - \frac{J}{2N} \sum_q \frac{\Gamma_q(k, \omega)}{\omega - \omega_q - \epsilon_{k+q} + Js/2} \right) \left(1 + \frac{J}{2N} \sum_q \frac{1}{\omega - \omega_q + \epsilon_{k+q} - Js/2} \right) = 0. \quad (31)$$

The second bracket in the LHS is nonzero in general and the solution is seen to be $\Gamma_q(k, \omega) = \Gamma(k, \omega)$, i.e., independent of q . Therefore,

$$\Gamma(k, \omega) = \left(1 + \frac{J}{2} \Lambda(k, \omega) \right)^{-1}, \quad (32)$$

where Λ is given in (13). Combining with (29) and (28) we find

$$\Sigma(k, \omega) = -\gamma^2 \frac{J^2 s}{2} \frac{\Lambda(k, \omega)}{1 + (J/2)\Lambda(k, \omega)}. \quad (33)$$

Equation (33) combined with (27) and (26) essentially completes the formal solution of the Green's functions. It is seen that the equation $G_1^{-1}(k, \omega) = 0$

where the self-energy is given by

$$\Sigma(k, \omega) = \gamma^2 \frac{J^2 s}{2N} \sum_q K_q(k, \omega). \quad (28)$$

We can find an equation for K_q by combining Eqs. (25) and (26). It is convenient to factor out an energy denominator and define a reduced vertex function Γ_q through

$$K_q(k, \omega) = \frac{\Gamma_q(k, \omega)}{\omega - \omega_q - \epsilon_{k+q} + Js/2}, \quad (29)$$

where Γ_q obeys a linear integral equation

coincides with Eq. (12) and hence the Green's function has a branch cut at the scattering solutions and an isolated pole at the bound state.

In Secs. IV and V we evaluate the various integrals for a simple band structure and a simplified spin-wave dispersion.

IV. SIMPLE BAND STRUCTURE

In this section we introduce a simple parabolic electron band structure and parabolic spin-wave dispersion which enables us to carry out most of the required integrals analytically. The Brillouin zone is

further replaced by a sphere of radius q_m such that the volume is conserved. The spectra are then completely specified by the bandwidth W of the conduction electrons and the maximum magnon energy ω_m . This approximation is very good for states at the bottom of the conduction band and is expected to be reasonable throughout the range of relevant energies.

$$\Lambda(k, \omega) = \frac{1}{2} \sum_q \left[\frac{\omega_m W}{\omega_m + W} k^2 - \frac{Js}{2} - \omega - i0^+ + \left[\bar{q}(\omega_m + W)^{1/2} - \frac{\bar{k}W}{(\omega_m + W)^{1/2}} \right]^2 \right]^{-1} \quad (34)$$

In this equation we shift \bar{q} by an appropriate amount to eliminate the term linear in \bar{k} in the denominator and then restrict the new sum over q to $q < q_m$. This approximation is expected to be fair for values of $k \ll q_m$. We define a new variable

$$\nu_k = \omega + \frac{Js}{2} - \frac{\omega_m}{\omega_m + W} \epsilon_k \quad (35)$$

in terms of which we get

$$\Lambda(k, \omega) = \frac{1}{N} \sum_q \frac{1}{(W + \omega_m)q^2 - \nu_k - i\eta} \quad (36)$$

Separating into real and imaginary parts we find

$$\Lambda = \Lambda_1 + i\Lambda_2, \quad (37)$$

where

$$\Lambda_2(k, \omega) = \frac{3\pi}{2(W + \omega_m)^{3/2}} \nu_k^{1/2} \theta(\nu_k) \times \theta(W + \omega_m - \nu_k) \quad (38)$$

$\nu_k < 0$:

$$\Lambda_1(k, \omega) = \frac{3}{(W + \omega_m)} \left[1 - \frac{|\nu_k|^{1/2}}{(W + \omega_m)^{1/2}} \times \tan^{-1} \left(\frac{W + \omega_m}{|\nu_k|} \right) \right] \quad (39)$$

$\nu_k > 0$:

$$\Lambda_1(k, \omega) = \frac{3}{(W + \omega_m)} \left[1 - \frac{1}{2} \left(\frac{\nu_k}{W + \omega_m} \right)^{1/2} \times \ln \left(\frac{\sqrt{W + \omega_m} + \sqrt{\nu_k}}{|\sqrt{W + \omega_m} - \sqrt{\nu_k}|} \right) \right] \quad (40)$$

In terms of Λ_1 and Λ_2 we find the self-energy

$$\Sigma(k, \omega) = \Sigma_1 + i\Sigma_2, \quad (41)$$

$$\Sigma_1 = Js \gamma^2 \left[\frac{1 + \frac{J}{2} \Lambda_1}{\left(1 + \frac{J}{2} \Lambda_1 \right)^2 + \frac{J^2}{4} \Lambda_2^2} - 1 \right], \quad (42)$$

It fails at high energies because of neglect of the appropriate van Hove singularities—but that is of little consequence to the problem at hand.

We first address ourselves to the evaluation of $\Lambda(k, \omega)$ [Eq. (13)]. Writing $\epsilon_k = Wk^2$, $\omega_q = \omega_m q^2$ (i.e., momenta in units of the maximum wave vector q_m) we may write

and

$$\Sigma_2 = -\frac{J^2 s}{2} \gamma^2 \frac{\Lambda_2}{\left[1 + \frac{J}{2} \Lambda_1 \right]^2 + \frac{J^2}{4} \Lambda_2^2} \quad (43)$$

The spectral weight function is defined as

$$\rho_1(k, \omega) = -\frac{1}{\pi} \text{Im} G_1(k, \omega) \quad (44)$$

and is given as

$$\rho_1(k, \omega) = \frac{1}{\pi} \frac{0^+ - \Sigma_2(k, \omega)}{[0^+ - \Sigma_2(k, \omega)]^2 + \left[\omega - \epsilon_k - \frac{Js}{2} - \Sigma_1(k, \omega) \right]^2} \quad (45)$$

In terms of $\rho_1(k, \omega)$ the downspin quasiparticle picture can be given a quantitative meaning. It obeys the normalization condition

$$\int_{-\infty}^{+\infty} \rho_1(k, \omega) d\omega = 1 \quad (46)$$

and further, a density of states may be defined as

$$\rho_1(\omega) = \frac{1}{N} \sum_k \rho_1(k, \omega) \quad (47)$$

In Sec. V we present detailed numerical results for the various quantities listed above.

V. RESULTS

In this section we present the computational results for the down-spin density of states and the quasiparticle spectral weights for values of parameters that may be regarded as typical of the rare-earth chalcogenide family. We choose the parameters (Ref. 16):

$$J = 0.2 \text{ eV}, \quad W = 2 \text{ eV}, \quad \omega_m = 0.002 \text{ eV}, \quad s = \frac{7}{2} \quad (48)$$

The unit of energy is chosen by setting $|J| = 1$ (hence

$W = 10$, $\omega_m = 0.01$). The two cases $J = +1$ and $J = -1$ are discussed separately.

A. $J > 0$

This case is believed to be appropriate to several materials in the rare-earth chalcogenide family. In Fig. 2, we plot the spectral weight function for $k = 0$ (i.e., band bottom). Several features are worth noting about Fig. 2: the spectral weight is largely dominated by the broad peak located at approximately the Hartree value (the Hartree approximation yields a delta function at $\omega = \epsilon_k + Js/2$). The bound state lies above the band edge and has very little spectral weight since the area under the scattering state contribution almost saturates the sum rule, Eq. (46). It may, anyhow, be the artifact of our sharp cutoff at q_m . The scattering continuum extends down to the bottom of the spin-up conduction band implying that the total density of states of the down-spin band has a lower threshold than the Hartree value. The fact that the quasiparticle peak is fairly sharp (it has a width $\gamma_k = \gamma^2 J^2 / W \times \text{const}$) lends some meaning, however, to the Hartree approximation, although not at the lowest energies or temperature. We discuss this further in Sec. VIB.

In Fig. 3 we plot the spectral weight for a sequence of band energies ($\epsilon_k = 0, J, 3J$) to illustrate the qualitative trend. It is seen that the linewidths increase with increasing k which is related to the greater phase

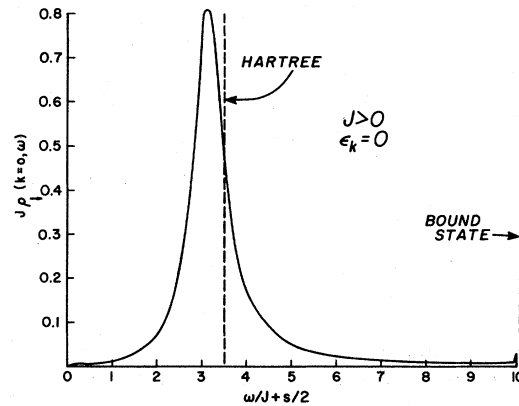


FIG. 2. Down-spin spectral weight for $k = 0$, $J > 0$. The Hartree approximation reproduces the peak position reasonably but predicts a delta function spectrum. The bound state above the conduction band in this case is irrelevant since there is very little area under it. The half-width of the distribution characterizes the rate at which a spin-down electron decays into spin up, with a magnon being emitted (see text).

space available for emission of a magnon. In all cases, the Hartree approximation does reasonably well in locating the peaks.

In Fig. 4 we present the total density of states for the down-spin band and compare with the up-spin band and the Hartree approximation. The remarkable feature is the nonvanishing density of states at

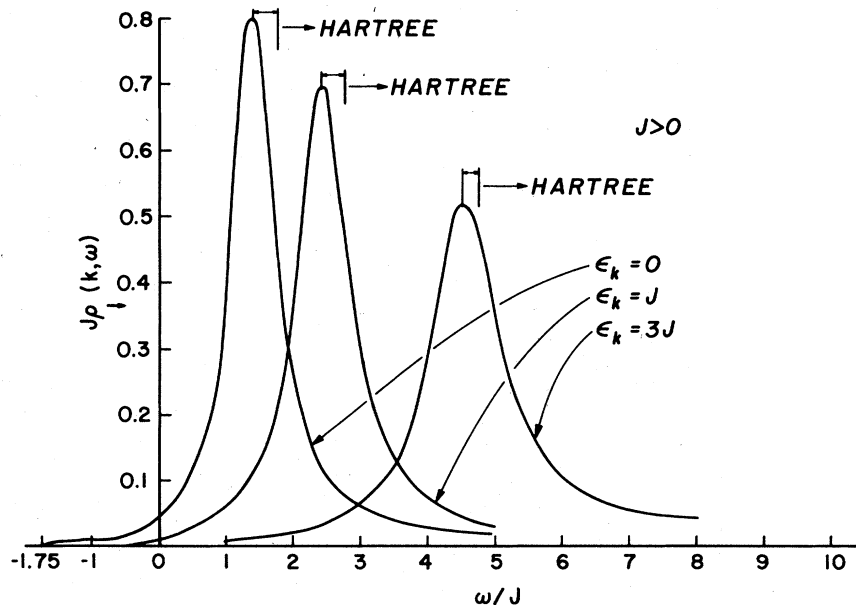


FIG. 3. Down-spin spectral weight for $J > 0$ at a series of values for $\epsilon_k/W (=0, J, 3J)$. The Hartree approximation is accurate in predicting the peak positions. The linewidths, i.e., decay rates increase with increasing ϵ_k/J .

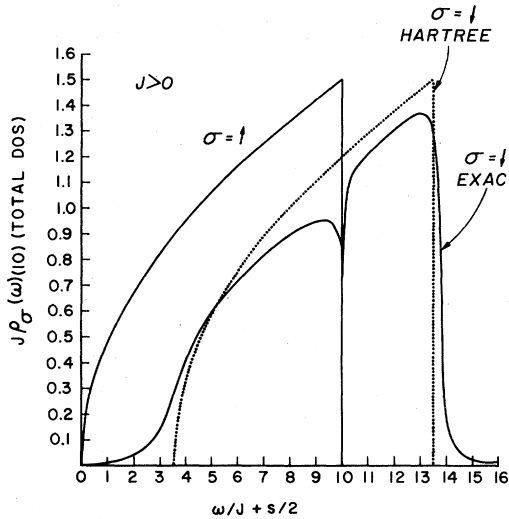


FIG. 4. Total density of states for spin-up and spin-down quasiparticles for $J > 0$ contrasted with the Hartree result. Notice that the down-spin density is nonzero where the Hartree approximation shows a spurious gap.

energies below the Hartree threshold. In fact, it is seen that there is no "gap" in the spectrum at all. Although at higher energies the Hartree density of states is fairly close to the exact result, it is only the lowest part of the spectrum which counts at low temperature and this part is never given correctly in the Hartree picture.

B. $J < 0$

In this case the up-spin band is pushed up and the down-spin band is lowered in energy. Figure 5 shows the quasiparticle spectral weight for $k = 0$ (i.e., states at the bottom of the band). In this case the bound state lies below the scattering states and in fact exhausts most of the spectral weight. We have introduced a small imaginary part to the frequency in order to display the spectrum, for in reality, the bound state is a δ function. The position of the peak lies below the Hartree value by a small amount which we denote by ϵ_B (the binding energy). The binding energy can in fact be found analytically in the weak coupling limit $|J| \ll W$ where we find

$$\epsilon_B = 1.5 \frac{J^2}{W}, \quad (49)$$

independent of k . This formula works reasonably for the binding energy at small k , for the parameters in Eq. (48).

To summarize, we find that scattering states dominate the spectral weight for ferromagnetic $J > 0$, and that the bound state dominates for antiferromagnetic

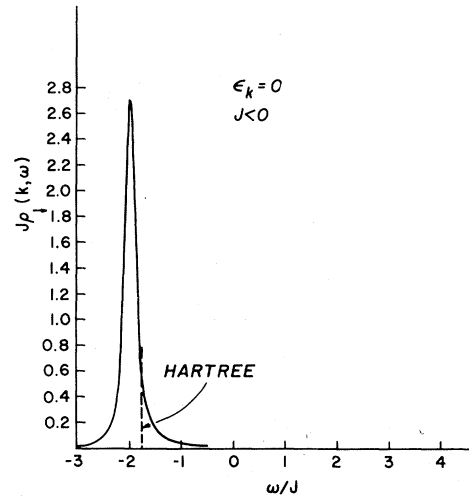


FIG. 5. Down-spin spectral weight for $J < 0$ for $k = 0$, corresponding to the polaronic state. The width of the peak is artificially produced by adding a small imaginary part to the frequency. In reality the bound state near -2 is a δ function and accounts for almost all the spectral weight. (Note change in vertical scale compared to Fig. 2.) In comparing this case ($J < 0$) with Fig. 2 ($J > 0$), note the three-fold change in vertical scale.

$J < 0$. In the former case $J > 0$, important for the chalcogenides, the spectral weight is roughly a Lorentzian peak of width $\propto \gamma^2 J^2 / W$ located at approximately the Hartree value for the energy.

VI. DISCUSSION AND CONCLUSIONS

A. Sum rules

It is easy to show (Ref. 16) that the spectral weight obeys several sum rules, one of which reads

$$\langle \omega \rangle_k \equiv \int_{-\infty}^{+\infty} \omega \rho_1(\vec{k}, \omega) d\omega = \epsilon_k + Js/2. \quad (50)$$

The analyticity of $G_1(k, \omega)$ in the upper half plane implies

$$G_1(k, \omega) \approx \frac{1}{\omega - \infty} + \frac{\langle \omega_k \rangle}{\omega^2} + O\left(\frac{1}{\omega^3}\right). \quad (51)$$

From our equation for $G_1(k, \omega)$ [Eqs. (27) and (33)], we see that Eq. (50) satisfied exactly [since $\Sigma(\omega) \approx_{\omega \rightarrow \infty} \gamma^2 J^2 s / \omega^2 + O(1/\omega^2)$]. Now it has been argued that since the bound state does not fulfill the sum rule, other states must lie beneath the bound state for $J > 0$. In fact, these states are precisely the scattering states discussed at length in Secs. II, IV, and V.

B. Meaning of a nonvanishing $\rho_1(k, \omega)$

We have seen in Secs. III, IV, and V that the nature of bound states is very different from those of scattering states. A nonvanishing $\rho_1(k, \omega)$ simply implies the existence of an eigenstate and we need to inquire further, whether it is an isolated peak or part of a continuum. In the present example we are fortunate in that the wave functions¹² as well as the spectral weights are available. Our main conclusion, in this regard, is that for a bound state (i.e., an isolated peak) a nonvanishing $\rho_1(k, \omega)$ is indicative of the existence and persistence of a down-spin state. However, in the case of scattering states a nonvanishing $\rho_1(k, \omega)$ does not imply a spin-down electron at all. From Eq. (14) we see that a scattering state yields $1/2 \langle \sigma^z \rangle = 1/2 - O(1/N)$ and hence, if the electron spin could be measured, as in a "gedanken" emission followed by a polarization analysis, we would find the spin to be up. This state contains just a small admixture of the spin-down state, sufficient to be an eigenstate of H .

It is natural to query, in connection with the above, the results of a gedanken wave-packet experiment. If we construct, at $t=0$, a pure spin-down state $e^{i\mathbf{k} \cdot \mathbf{r}} \chi_{\downarrow}^{(0)}$ such a state evolves under the Hamiltonian into one with spin down as well as spin up at a later time. The probability amplitudes at subsequent times are given in terms of a convolution with the Green's function which were calculated in Sec. II. The probability densities may be readily found to be

$$\rho_1(x, t) = \frac{1}{\Omega} |G_1(x, t)|^2, \quad (52)$$

$$\rho_1^q(x, t) = \frac{1}{\Omega} |L_q(x, t)|^2, \quad (53)$$

where ρ_1^q is conditional to emission of a magnon with wave vector q . Now, the analyticity of G in the upper half plane implies that we may write

$$G_1(k, t) \propto \int_{-\infty}^{+\infty} e^{+i\omega t} \rho_1(k, \omega) d\omega \quad (54)$$

and hence the scattering states correspond to $\rho_1(x, t) \propto e^{-2\gamma k t}$, i.e., a decay to the spin "up" configuration after a characteristic (life) time $W/\gamma^2 J^2$. Conservation of probability implies that at any time t , the space integrals over $[\rho_1(x, t) + \sum_q \rho_1^q(x, t)]$ nor-

malizes to unity, i.e., the down-spin electron gets converted to one with spin up and appropriate magnons are emitted. The number of lattice points the down spin transverses before converting to an up-spin state is of the order $(W/\gamma J)^2$. For typical values [Eq. (48)] this implies that for $J > 0$ a down-spin electron injected into the semiconductor would transverse ~ 100 lattice constants before converting to an up-spin state. This of course means that thin films would be partially "transparent" to spin-down electrons but bulk materials would not be. In conclusion we may view the criterion for validity of the Hartree picture as $(W/\gamma J) \ll \sqrt{L}$ when L is the length of the sample. Thus, the Hartree approximations *must* fail for bulk systems. For thin films and sandwiches, the physics is reasonably accounted for by the Hartree picture, as it is in the case of $J < 0$.

C. Relevance to photoemission experiments

In Sec. VIB above, we have elaborated in some detail, the physical significance of the down-spin spectral function in order to address the question of spin polarized photoemission. As mentioned in the Introduction, several experiments have established that electrons emitted from ferromagnetic EuO, EuS where $J > 0$ do not show the expected 100% spin polarization. But, electrons in the scattering states have in reality spin up, with a vanishingly small admixture of spin down. Hence the explanation must lie elsewhere; the possibility of surface paramagnetic impurities seems to be the most promising one,⁴ and effects of thermal fluctuations at $T > 0$ also should decrease the observed polarization. Finally, the photoemitted particles may not have had time to convert before being emitted from a thin film.

ACKNOWLEDGMENTS

B. S. Shastry would like to thank Professor David Edwards for a helpful conversation and for bringing some relevant papers to our attention. D. Mattis is grateful to the Physics Department at the ETH—to Dr. R. Schilling for reviving his interest in this problem, and to Dr. K. Hepp and Dr. W. Baltensperger for their gracious hospitality. This work has been supported in part by the AFOSR and NSF.

¹For a recent review see S. F. Alvarado, W. Eib, F. Neier, H. S. Siegmann, and P. Zurcher, in *Photoemission and Electronic Properties of Surfaces*, edited by B. Feuerbacher, B. Fitton, and R. F. Willis (Wiley, New York, 1978), p. 437.
²P. Wachter, *Crit. Rev. Solid State Sci.* **3**, 189 (1972).

³G. Busch, P. Junod, and P. Wachter, *Phys. Lett. A* **12**, 11 (1964).

⁴K. Sattler and H. C. Siegmann, *Phys. Rev. Lett.* **29**, 1565 (1972).

⁵N. Muller, W. Eckstein, W. Heiland, and W. Zinn, *Phys.*

- Rev. Lett. 29, 1651 (1972).
- ⁶E. Kisker, G. Baum, A. H. Mahan, W. Raith, and K. Schroder, Phys. Rev. Lett. 36, 982 (1976).
- ⁷E. Kisker, G. Baum, A. H. Mahan, W. Raith, and B. Reihl, Phys. Rev. B 18, 2256 (1978).
- ⁸F. Meier, P. Zurcher, and E. Kaldis, Phys. Rev. B 19, 4576 (1979).
- ⁹E. Kisker, W. Gudat, E. Kuhlmann, R. Clauberg, and M. Campagna, Phys. Rev. Lett. 45, 2053 (1980).
- ¹⁰T. Wolfram and J. Callaway, Phys. Rev. 127, 1605 (1962).
- ¹¹T. Wolfram and J. Callaway, Phys. Rev. 130, 45 (1963).
- ¹²S. Methfessel and D. C. Mattis, Handb. Physiol. 18, 389 (1968).
- ¹³R. M. Woolsey and R. M. White, Phys. Rev. B 1, 4474 (1970).
- ¹⁴Y. Izumov and M. V. Medvedev, Sov. Phys. JETP 32, 302 (1971).
- ¹⁵Y. Izumov, F. A. Kassan-Ogly, and M. V. Medvedev, J. Phys. (Paris) Suppl. 2-3 32, C1-1076 (1971).
- ¹⁶W. Nolting, Phys. Status Solidi B 96, 11 (1979); J. Phys. C 12, 3033 (1979); also, W. Nolting and A. M. Oles, Phys. Rev. B (in press).
- ¹⁷S. Allen and D. M. Edwards (unpublished); also S. Allen, Ph.D. thesis (Imperial College, London, 1981) (unpublished).