

MAGNETISM AND FERROELECTRICITY

The Exact Spectrum of Fermi Quasiparticles in Kondo–Anderson Ferromagnetic Lattice

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Abstract—The spectrum of Fermi excitations of a nondegenerate ferromagnetic semiconductor at $T = 0$ with one electron present is investigated in order to describe the electronic structure of manganites with inclusion of strong electron correlations within the Anderson periodic model with s – d exchange interaction. Exact dispersion relations and the Green functions for different spin projections are found. The density-of-states function is calculated for different positions of the d level relative to the band bottom. © 2003 MAIK “Nauka/Interperiodica”.

1. INTRODUCTION

To investigate Kondo systems or systems with variable valence, such as $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ and $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$, a periodical Anderson model with s – d exchange is used in this work.

The interest in manganites stems from the fact that in these compounds the effect of colossal magnetic resistance is observed, whose maximum is reached at $x = 0.33$. In this case, the system can be considered a ferromagnetic [1] lattice of localized spins of Mn^{4+} ions with the electron configuration $3d^3$ (spin $S = 3/2$), into which some extra electrons of the corresponding concentration are added. These electrons can remain delocalized and interact with the lattice spins via exchange interaction of the Heisenberg type. As a result of possible hybridization, the electrons can become localized, forming a Mn^{3+} ion of $3d^4$ configuration at a lattice site. These two types of the electron state and two interactions are included in the Hamiltonian of the model, which is the periodical Anderson model with s – d exchange interactions.

This work is devoted to the specific case of a system containing one itinerant electron at $T = 0$. It is very important that, under these conditions, the problem turned out to have an exact solution. Formally speaking, this case corresponds to the lower limit of concentration, for which $x \rightarrow 0$ and the ground state of the localized spin subsystem of manganites is antiferromagnetic. Not aiming to describe this antiferromagnetic case, we only note that this exact solution is important for manganites in the range of parameters where the ground state of the localized spin subsystem is ferromagnetic ($x = 0.15$ – 0.40). If we take an approximate solution in this range and consider the concentration of carriers as a parameter, then tending this parameter to zero (with the localized spin subsystem frozen in the ferromagnetic ground state) will lead to our exact

solution. Thus, this solution may be useful for constructing and checking approximate solutions for the values of parameters corresponding to ferromagnetism in the localized spin subsystem.

This case is also a generalization of the problem of a magnetic polaron [2–4] with inclusion of hybridization interaction. Let us write the wave function of the $d^n s^m$ configuration as $|n, S, M; m, \sigma\rangle$, where S and M are the spin and its projection for a d^n ion, respectively; $m = 0$ or 1 is the number of s electrons per unit cell; and σ is the spin projection of an l electron. Then, in addition to the processes caused by the s – d exchange,

$$|n, S, S; 1, \downarrow\rangle \rightleftharpoons |n, S, S - 1; 1, \uparrow\rangle \quad (1)$$

we will have the processes due to hybridization

$$\begin{aligned} &|n, S, S; 1, \downarrow\rangle \\ &\rightleftharpoons |n + 1, S \pm 1/2, S - 1/2; 0\rangle \\ &\rightleftharpoons |n, S, S - 1; 1, \uparrow\rangle, \end{aligned} \quad (2)$$

$$|n, S, S; 1, \uparrow\rangle \rightleftharpoons |n + 1, S + 1/2, S + 1/2; 0\rangle, \quad (3)$$

which are included in this work. The plus and minus signs in Eq. (2) correspond to two possible values of the total spin on a site. In general, when the electron is localized, the spin of the site can take on the values $S' = S + 1/2$ and $S' = S - 1/2$. The corresponding cases are called the high-spin and low-spin cases. A solution for the low-spin case was obtained in [5]. In manganites, when the itinerant electron is localized, we have the high-spin case; the $3d^4$ configuration possesses spin $S' = 2$, which is used in this work. The excitations of quasiparticles with a definite spin projection, which are forbidden in the low-spin case, become allowed in the high-spin case. As a result, the one-particle density of states in the high-spin case radically differs from that in the low-spin case.

In Section 2, the model Hamiltonian is written out, necessary transformations are described, and the exact

results (dispersion relations and Green functions) are presented. In Section 3, we discuss the density of states calculated using the exact solution.

2. EXACT ONE-PARTICLE GREEN FUNCTIONS

Taking interactions into account, we write down the Hamiltonian of the model in the form

$$H = H_{0a} + H_{0d} - J \sum_f S_f \sigma_f + V \sum_{f\sigma} (d_{f\sigma}^\dagger a_{f\sigma} + \text{H.c.}). \quad (4)$$

Here, $H_{0a} = \sum_{k\sigma} \epsilon_k a_{k\sigma}^\dagger a_{k\sigma}$ describes delocalized states. The Hamiltonian H_{0d} describes localized states and generally can be written as

$$H_{0d} = \sum_{f,\lambda,\sigma} \epsilon_\lambda d_{f\lambda\sigma}^\dagger d_{f\lambda\sigma} + \sum_{\substack{\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4 \\ \sigma, \sigma'}} \langle \Gamma_1, \Gamma_2 | v | \Gamma_3, \Gamma_4 \rangle d_{\Gamma_1\sigma}^\dagger d_{\Gamma_2\sigma'}^\dagger d_{\Gamma_4\sigma}^\dagger d_{\Gamma_3\sigma}. \quad (5)$$

In the second term, the index Γ includes the site index f and the orbital index λ ; v is the Coulomb interaction.

Let us pass to the space of eigenstates of the Hamiltonian H_{0d} . Each of them is defined by three quantum numbers, namely, the number of electrons, the total spin, and its projection ($|n, S, M\rangle$), and has energy $E_{n,S,M}$. In this representation, H_{0d} can be written as

$$H_{0d} = \sum_{f,n,S,M} E_{n,S,M} X_f^{n,S,M; n,S,M} \quad (6)$$

where we used the Hubbard operators

$$X_f^{n_1, S_1, M_1; n_2, S_2, M_2} = |n_1, S_1, M_1\rangle \langle n_2, S_2, M_2|. \quad (7)$$

In the case of manganites, for half-integer projections of the total spin, the values of the other two quantum numbers are $n = 3$ and $S = 3/2$, while for integer projections we have $n = 4$ and $S' = 2$. Therefore, we will indicate only the projection of the total spin for the Hubbard operators:

$$X_f^{M_1, M_2} = |n_1, S_1, M_1\rangle \langle n_2, S_2, M_2|. \quad (8)$$

Since we have only two configurations of localized electrons on a site that differ in energy, the energy of the state $|n = 3, S = 3/2, M\rangle$ can be taken to be zero; the energy of the other state, $|n = 4, S' = 2, M'\rangle$, will be designated as Ω .

As a result, H_{0d} can be written as [6]

$$H_{0d} = \Omega \sum_f \sum_{M' = -S}^S X_f^{M', M'}. \quad (9)$$

For further calculations, we express all operators acting on the localized states in terms of the Hubbard operators. In this case, the components of the operators S_f have the form

$$S_f^Z = \sum_{M = -S}^S M X_f^{M, M} + \sum_{M' = -S}^S M' X_f^{M', M'}, \quad (10)$$

$$S_f^+ = (S_f^-)^\dagger = \sum_{M = -S}^S \gamma_S(M) X_f^{M+1, M} + \sum_{M' = -S}^S \gamma_S(M') X_f^{M'+1, M'}, \quad (11)$$

$$\gamma_S(M) = \sqrt{(S-M)(S+M+1)}. \quad (12)$$

The creation and annihilation operators for an electron on the localized d level can be written as

$$d_{f\uparrow}^\dagger = (d_{f\uparrow})^\dagger = \sum_M \sqrt{\frac{S+1+M}{2S+1}} X_f^{M+\frac{1}{2}, M}, \quad (13)$$

$$d_{f\downarrow}^\dagger = (d_{f\downarrow})^\dagger = \sum_M \sqrt{\frac{S+1-M}{2S+1}} X_f^{M-\frac{1}{2}, M}. \quad (14)$$

In calculating the densities of states of quasiparticles, we used the two-time retarded Green functions, while involve the creation and annihilation operators of the corresponding quasiparticles and the ferromagnetic ground state of the localized spin subsystem (thus, the ferromagnetic ordering in the localized spin subsystem, appearing due to spin exchange between manganese ions, is taken into account):

$$\begin{aligned} & \langle \langle a_{p\sigma}(t) | a_{p\sigma}^\dagger(t') \rangle \rangle \\ & = -i\theta(t-t') \langle FM | [a_{p\sigma}(t), a_{p\sigma}^\dagger(t')]_+ | FM \rangle. \end{aligned} \quad (15)$$

Here,

$$\theta(t) = \begin{cases} 1, & t > 0 \\ 0, & t < 0. \end{cases} \quad (16)$$

The matrix element is taken for the ferromagnetic ground state $|FM\rangle$ of the system in the absence of carriers. In this state, the energy band is empty: $a_{f\sigma}|FM\rangle = 0$ and each lattice site has spin S and the maximum spin projection, $S_f^Z|FM\rangle = S|FM\rangle$.

The equations of motion can be reduced to the set of equations:

$$\begin{bmatrix} E - \varepsilon_p + \frac{JS}{2} & -V \\ -V & E - \Omega \end{bmatrix} \begin{bmatrix} \langle \langle a_{p\uparrow} | a_{p\uparrow}^\dagger \rangle \rangle \\ \langle \langle X_p^{s, s+\frac{1}{2}} | a_{p\uparrow}^\dagger \rangle \rangle \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad (17)$$

from which we obtain a dispersion equation and an exact expression for the Green function (with spin up),

$$D_1(E) = E - \varepsilon_p - \frac{JS}{2} - \frac{V^2}{E - \Omega} = 0, \quad (18)$$

$$\langle \langle a_{p\uparrow} | a_{p\uparrow}^\dagger \rangle \rangle = D_1(E)^{-1}. \quad (19)$$

From Eqs. (17), it follows that the Green function $\langle \langle X_p^{s, s+\frac{1}{2}} | X_p^{s+\frac{1}{2}, s} \rangle \rangle$ corresponds to a localized quasiparticle with spin up. Analogous calculations for this function give

$$D_2(E) = E - \Omega - \frac{V^2}{E - \varepsilon_p + \frac{JS}{2}} = 0, \quad (20)$$

$$\langle \langle X_p^{s, s+\frac{1}{2}} | X_p^{s+\frac{1}{2}, s} \rangle \rangle = D_2(E)^{-1}. \quad (21)$$

For an itinerant and a localized quasiparticle with spin down, the corresponding set of equations is more complicated due to a larger variety of multiparticle processes [see Eqs. (1)–(3)], but at $T = 0$ and for one carrier, this set is also closed and allows an exact solution. It is significant that the ground state is assumed to be ferromagnetic in this case. The dispersion relation and the Green function (for an itinerant quasiparticle with spin down) are calculated exactly to be

$$D_3(E) = E - \varepsilon_p - \frac{JS}{2} + \frac{2V_1^2 JS - \frac{1}{2} J^2 S (E - \Omega) - V_1^2 (\Delta^{-1}(E) - J/2)}{(E - \Omega)(\Delta^{-1}(E) - J/2) - 2V_1^2 S} = 0, \quad (22)$$

$$\langle \langle a_{p\downarrow} | a_{p\downarrow}^\dagger \rangle \rangle = D_3(E)^{-1}. \quad (23)$$

For a localized quasiparticle with spin down, we have

$$D_4(E) = E - \Omega + \frac{2V_1^2 JS - 2V_1^2 S \left(E - \varepsilon_p - \frac{JS}{2} \right) - V_1^2 (\Delta^{-1}(E) - J/2)}{\left(E - \varepsilon_p - \frac{JS}{2} \right) (\Delta^{-1}(E) - J/2) - \frac{J^2 S}{2}} = 0, \quad (24)$$

$$\langle \langle X_p^{s, s-\frac{1}{2}} | X_p^{s-\frac{1}{2}, s} \rangle \rangle = D_4(E)^{-1}. \quad (25)$$

Here, the following notation is introduced:

$$\Delta(E) = \frac{1}{N} \sum_k \frac{1}{E - \varepsilon_k + \frac{JS}{2}}, \quad V_1 = \frac{V}{\sqrt{2S+1}}. \quad (26)$$

It should be noted that if we neglect the hybridization effects in Eqs. (19) and (23), by setting $V = 0$, then these equations will coincide exactly with the corresponding equations for a magnetic polaron [2–4] obtained for the case of a ferromagnetic saturated semiconductor, in particular, for EuO at $T = 0$ [7].

3. ONE-PARTICLE DENSITIES OF STATES

In order to illustrate the exact solution obtained, the density of states was calculated for each quasiparticle. Making the change of variables $\varepsilon_p = E'$, we write

$$n(E) = -\frac{1}{\pi N} \sum_p \text{Im} G(p, E + i0) = -\frac{1}{\pi} \int dE' n_0(E') \text{Im} G(E', E + i0). \quad (27)$$

In order to calculate the density of states for localized electrons, the relation between the Green functions

$\langle \langle d_{p\sigma} | d_{p\sigma}^\dagger \rangle \rangle$ and the functions $\langle \langle X_p^{s, s\pm\frac{1}{2}} | X_p^{s\pm\frac{1}{2}, s} \rangle \rangle$ needs to be established. Making use of the definition of the Green functions, Eqs. (13) and (14), and the fact that the projection of any localized spin in the ground state equals S , we obtain

$$\langle \langle d_{p\downarrow} | d_{p\downarrow}^\dagger \rangle \rangle = \sum_{M, M'} \sqrt{\frac{S+1-M}{2S+1}} \sqrt{\frac{S+1-M'}{2S+1}} \times \langle \langle X_p^{M, M-\frac{1}{2}} | X_p^{M-\frac{1}{2}, M'} \rangle \rangle = \frac{1}{2S+1} \langle \langle X_p^{s, s-\frac{1}{2}} | X_p^{s-\frac{1}{2}, s} \rangle \rangle. \quad (28)$$

The corresponding Green functions for a quasiparticle with spin up are

$$\langle \langle d_{p\uparrow} | d_{p\uparrow}^\dagger \rangle \rangle = \langle \langle X_p^{s, s+\frac{1}{2}} | X_p^{s+\frac{1}{2}, s} \rangle \rangle. \quad (29)$$

Numerical calculations were performed using the parameters characteristic of manganites: $J = 0.5$ eV, $V = 0.1$ eV, $W = 4$ eV, and $S = 3/2$.

We note that the parameters obtained from the adjustment to the experiment are dependent on the model. For example, in our case, W is the width of the bare band. The resulting band of quasiparticles, as will be seen further on, contains two bands; the lower one is narrow, with the narrow-band limit taking place for it [8], while the upper one is wide, with its width exceeding the exchange parameter J .

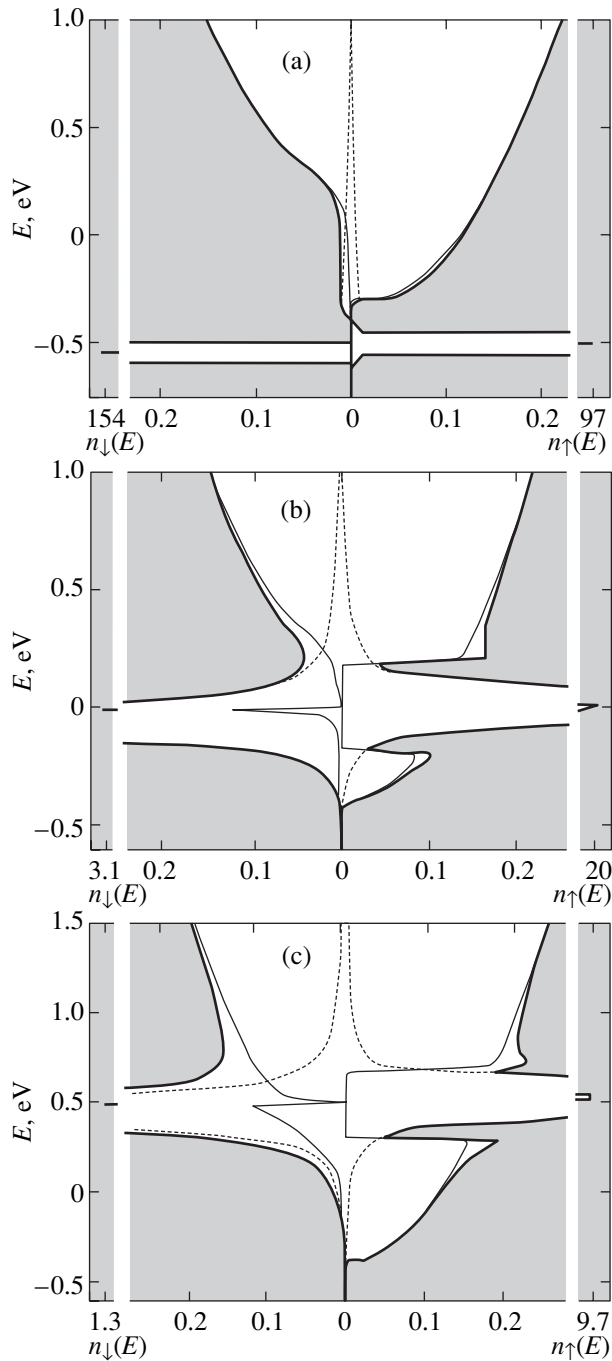


Fig. 1. Densities of states for Ω equal to (a) -0.5 , (b) 0 , and (c) 0.5 eV. The density of states with spin down is offset horizontally to the left and the one with spin up, to the right. Thin solid lines correspond to an itinerant quasiparticle, dashed lines to a localized quasiparticle, and thick solid lines to the total density for $J = 0.5$ eV, $V = 0.1$ eV, $W = 4$ eV, and $S = 3/2$.

For calculations, we used a quadratic dispersion law and the corresponding density of states

$$\varepsilon_x = \begin{cases} Wx^2, & x \in [-1, 1] \\ 0, & x \notin [-1, 1], \end{cases} \quad (30)$$

where $x = p/p_B$,

$$n_0(E) = \begin{cases} \frac{3}{2W} \sqrt{\frac{E}{W}}, & E \in [0, W] \\ 0, & E \notin [0, W]. \end{cases} \quad (31)$$

The localization energy Ω was chosen such that it fell in one of the three energy ranges into which the energy axis is divided by points $\pm JS/2 = \pm 0.375$ eV. For each value of Ω , the densities of states were calculated for itinerant and localized quasiparticles for both spin projections. The results are shown in Fig. 1.

Figure 1a shows the densities of states for $\Omega = -0.5$ eV. In this case, the localized level lies below the band. The band densities of states for both spin projections have the same form as in the $s-d$ model. The electrons with spin down exhibit a non-quasiparticle behavior in the region $(-JS/2, JS/2)$, which is a known effect characteristic of the $s-d$ model. The density of states of a localized quasiparticle for both spin projections has a narrow peak near the energy -0.5 eV. For both spin projections, there is a nonzero contribution near the conduction band bottom caused by hybridization.

This case (with the localized level lying below the band) resembles the situation in the $s-d$ model with a negative $s-d$ exchange parameter, where a deep discrete level appears corresponding to the band of spin-polaron states [3]. However, in this case, the localized level under the band has only an insignificant addition of polaron and band states, appearing due to hybridization, and consists mainly of the localized d -electron states.

Figure 1b presents the densities of states for $\Omega = 0$. Here, the situation is more complicated because the localized level crosses the band in the region of the Stoner gap $(-JS/2, JS/2)$. Hybridization effects are expressed in the blurring of the peaks of the densities of localized states.

For the spin up, in the region of the d level, there is a hybridization gap for an itinerant quasiparticle and a peak for a localized one. It should be noted that this does not happen in the low-spin case [5], because hybridization is impossible for this initial spin-up band state in this case. It is interesting to note that in the total density of states both effects are present; the peak of localized states dominates, but there are also dips (pseudogap) due to the hybridization gap.

Superposition of the localized level on the region of non-quasiparticle behavior (an itinerant quasiparticle with spin down) leads to the appearance of a narrow peak, above which a narrow pseudogap is observed. Nevertheless, localized d states dominate in the total density of states.

A qualitatively similar picture appears at $\Omega = +0.5$ eV (Fig. 1c). However, in this case, the localized level lies above the Stoner gap. The band density of states (with spin down) changes in the same way as at

$\Omega = 0$. A narrow gap and a less expressed peak under it are observed.

4. CONCLUSION

Thus, the exact dispersion relations and the Green functions at $T = 0$ obtained in this work describe one carrier moving on the background of the ferromagnetic ground state of a lattice. Two types of interaction, s - d exchange and hybridization, have been taken into account in the strong-correlation regime. This case corresponds to the lower limit of the concentration x . Although manganites are no longer ferromagnets at low x , the results obtained in this work should be reproduced by all solutions found for the ferromagnetism region ($x = 0.15$ – 0.40) in the limit of small concentrations and low temperatures.

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