Excitation spectra of the one-dimensional double-exchange model: An exact solution for one mobile electron

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Abstract. We study the one-dimensional double-exchange model with \( L \) localized spins and one mobile electron. We solve the Schrödinger equation analytically and obtain the energies and wave functions for all the eigenstates with spin \( S = (L - 1)/2 \) exactly. As an application, we compute the single-particle Green's function. We show that, for vanishing exchange interactions between localized spins, the single-particle spectrum is entirely incoherent and the lowest band has an infinite band mass, i.e., the single electron is localized due to its interaction with the spin excitations. The analysis of the wave function gives us a particularly simple ground state.

1. Introduction

Half-metallic ferromagnets [1] offer a unique opportunity for studying the electronic states of strongly correlated electron systems. Here, only the majority-spin (minority-spin) electrons form the Fermi surface with a gapped minority-spin (majority-spin) band and can couple with excitations of the spin (and possibly other) degrees of freedom of the system. In-gap states (or so-called nonquasiparticle states) in such half-metallic ferromagnets have attracted considerable attention in physics of strong electron correlations [1]. The states appear in the band gap of say spin-down band just above the Fermi level of say spin-up band due to the effects of electron correlations (see Fig. 1) and affect physical properties of the system. The origin of the in-gap states is beyond the one-electron band theory and their nature cannot be described by the Landau Fermi-liquid theory. So far, the appearance of the states has been understood in connected with spin polaron processes [1, 2, 3].

In this paper, we study such in-gap states using the simplest model for the half-metallic ferromagnets, which is constructed as follows. Suppose a double-exchange ferromagnet [4], where there are well localized electrons in the orbitals with energy \( -\varepsilon \) and on-site Coulomb repulsion \( U \), which are coupled, via the Heisenberg-type ferromagnetic exchange interaction \( J \), with conduction electrons in the noninteracting tight-binding band with hopping parameter \( t \) (see Fig. 1). Hereafter, we use the simplest double-exchange model [5, 6] defined in the limit of \( \varepsilon = U/2 \rightarrow \infty \) as given below, which retains the essential physics on the in-gap states.

We focus on this model in the case of one conduction electron because we can obtain an analytically exact solution for the energies and wave functions for all the eigenstates of the
Hamiltonian. We will thereby show that the single-particle Green’s function is entirely incoherent and the lowest band has an infinite band mass, i.e., the single electron is localized due to its interaction with the spin excitations.

2. Model

The double-exchange model is defined by the Hamiltonian

\[
\hat{H} = \hat{H}_0 + \hat{H}_J
\]

\[
\hat{H}_0 = -t \sum_{\langle ij \rangle \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.} \right)
\]

\[
\hat{H}_J = -J \sum_i \hat{S}_i \cdot \hat{\mathbf{S}}_i
\]

where \(\hat{c}_{i\sigma} (\hat{c}_{i\sigma}^\dagger)\) is the annihilation (creation) operator of an electron with spin \(\sigma\) in the conduction orbital at site \(i\). \(\hat{S}_i\) is the spin operator for the localized spin at site \(i\). \(\hat{S}_i\) is the spin operator of an electron in the conduction orbital at site \(i\) defined as \(\hat{S}_i = (1/2) \sum_\sigma \hat{c}_{i\sigma}^\dagger \sigma \hat{c}_{i\sigma}\) with the Pauli spin matrix \(\sigma\). \(\hat{H}_0\) represents the hopping of electrons between the conduction orbitals on nearest-neighbor sites \(\langle ij \rangle\) and \(\hat{H}_J\) represents the ferromagnetic \((J > 0)\) exchange interaction between an electron in the conduction orbital and the localized spin \(\hat{S}_i\) on the same site \(i\). We define the number operator of conduction electrons at site \(i\) as \(\hat{n}_i = \sum_\sigma \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}\). We assume the system of \(L\) unit cells, where each cell contains a conduction and a localized orbital. The ground state of the double-exchange model is known to be fully spin-polarized when there is a small number of conduction electrons [5, 6]. Without conduction electrons, the ground state is \(2^L\)-fold degenerate, one of which is the fully spin-polarized state. We take \(t = 1\) as the unit of energy unless otherwise stated.

3. Results of calculations

3.1. Single-particle spectra

To see the in-gap states, we first calculate the single-particle Green’s function for a single electron which is added to the fully spin-polarized (spin-up) state. We follow the method of Refs. [7, 8, 9, 10] to obtain the exact expression for the Green’s function when the added
electron is spin-down. The ground state $|\text{FM}\rangle$ is assumed to be with a full spin-up polarization without conduction electrons. The result obtained reads

$$G(k, \omega) = \frac{1}{G_0^{-1}(k, \omega - \frac{J}{4}) - \Sigma(\omega)}$$

where $G_0$ is the noninteracting Green’s function and $\Sigma(\omega)$ is the momentum-independent self-energy. The spectrum consists of two components: an incoherent continuum in the range $[-2t - \frac{J}{4}, 2t - \frac{J}{4}]$ and a single $\delta$-function-like peak at higher energy. The dispersive band corresponds to a spin polaron, i.e., the propagating electron is dressed by a magnon. This dressing leads to a modified dispersion with a bandwidth that strongly depends on $J$ and a significant reduction of the spectral weight. The single-particle spectrum at low-energies therefore is entirely incoherent and the lowest energy for each momentum is dispersionless so that the effective mass is infinite and the electron is localized due to its interaction with the spin excitations.

### 3.2. Wave function

In our model, the Dyson’s infinite sequence of equations terminates in the second order and thus the result is exact. This occurs because the addition of a spin-down electron yields only two types of states due to the spin rotational symmetry of the model; it is within the sector of the Hilbert space where the $z$-component of the total spin is $(L - 1)/2$. Hence, we can write the general form of the wave function as:

$$|\Psi(k, \omega)\rangle = \left[\alpha(k, \omega)c_{k\downarrow}^\dagger + \frac{1}{\sqrt{L}} \sum_q \beta(k, q, \omega)c_{k-q\uparrow}^\dagger \hat{S}_{q}^-\right]|\text{FM}\rangle.$$

The first term is the spin polaron state described by the usual Fermi liquid theory. The second term is the superposition of spin-up electron excitations and virtual magnons. Inserting Eq. (5) into the Schrödinger equation, we obtain the three equations for the coefficients:

$$\left(\omega - \epsilon_k - \frac{J}{4}\right)\alpha(k, \omega) = -\frac{J\gamma(k, \omega)}{2},$$

$$\left(\omega - \epsilon_{k-q} + \frac{J}{4}\right)\beta(k, q, \omega) = \frac{J}{2} [\gamma(k, \omega) - \alpha(k, \omega)],$$

$$\gamma(k, \omega) = \frac{1}{L} \sum_q \beta(k, q, \omega).$$

Adding the normalization condition to the above, we have four equations, which we can solve exactly. The solution (see Fig. 3) gives us the ground state properties with the polaron and magnon weight:

$$\alpha(k, \omega) \sim \frac{1}{\sqrt{L}},$$

$$\beta(k, q, \omega) \sim \sqrt{L}\delta_{k,q}.$$

The relation (7) means that we can neglect the polaron-state contributions to the ground state in thermodynamic limit. According to (8), the magnon momentum should be the same as the conduction electron momentum. This fact implies that the conduction electron minimizes its kinetic energy by transferring their momentum to a magnon and accumulate around zero momentum. As a result, the ground state is infinitely degenerate, and the effective mass becomes infinite. This degeneracy is lifted by adding the direct ferromagnetic exchange interaction between localized spins. Details of the calculations will be given elsewhere [11].
4. Summary

We have studied the one-dimensional double-exchange model with one conduction electron. We have obtained the analytically exact solution for the energies and wave functions for all the eigenstates of the Hamiltonian and have calculated the single-particle spectral function exactly. We have shown that the single-particle Green’s function at low energy is entirely incoherent and the electron has an infinite band mass, i.e., the single electron is localized due to its interaction with the spin excitations. We hope that the results presented in this paper will shed some light on the origin of the in-gap states in the half-metallic ferromagnets. Further details will be given elsewhere [11].

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