Exact wave functions and excitation spectra of the one-dimensional double-exchange model with one mobile electron

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Abstract. Motivated by recent studies of the in-gap (or nonquasiparticle) states in the half-metallic ferromagnets, we study the one-dimensional double-exchange model with one mobile electron. We solve the Schrödinger equation analytically and obtain the energies and wave functions for all the eigenstates exactly. As an application, we compute the single-particle Green's function. We show that 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. Implication on the observed in-gap states in the half-metallic ferromagnets is considered.

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 where many-body effects lead only to renormalization of the quasiparticle parameters. So far, the appearance of the states has been understood in connected with spin polaron processes: the low-energy excitations of spin-down electrons, which are forbidden for half-metallic ferromagnets in the band picture, turn out to be possible as superpositions of the excitations with virtual magnons of the spin-up electrons [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). When there are conduction electrons in the tight-binding band, the system can
be fully spin-polarized due to the double-exchange mechanism \[4\], resulting in a large exchange splitting in the band structure, which leads to the situation of the half-metallic ferromagnet where only the spin-up conduction electrons have the Fermi surface. Hereafter, we use the simplest double-exchange model \[6, 5\] defined in the limit of \( \varepsilon = U/2 \to \infty \) as given below, which retains the essential physics on the in-gap states.

![Diagram showing the band structure and the Fermi level.](image)

**Figure 1.** (Left) Schematic representation of the single-particle density of states of a half-metallic ferromagnetic state of the double-exchange model. (Right) Schematic representation of the double-exchange model.

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 and thus we can calculate exactly the experimentally measurable physical quantities \[7, 8, 9\], such as single-particle spectral function, which helps us to understand the nature of the in-gap states in the half-metallic ferromagnets. 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. We thus have a similar phenomenon as in spin-charge separation.

**2. Model**

The double-exchange model is defined by the Hamiltonian

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

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

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

where \( \hat{c}_{i,\sigma} (\hat{c}^\dagger_{i,\sigma}) \) is the annihilation (creation) operator of an electron with spin \( \sigma \) in the conduction orbital at site \( i \). \( \hat{\mathbf{s}}_i \) is the spin operator for the localized spin at site \( i \), \( \hat{\mathbf{S}}_i \) the spin operator of an electron in the conduction orbital at site \( i \) defined as \( \hat{\mathbf{s}}_i = (1/2) \sum_{\alpha \beta} \hat{c}^\dagger_{i,\alpha} \sigma_{\alpha \beta} \hat{c}_{i,\beta} \) 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 $\hat{n}_i = \sum_\sigma \hat{c}^{\dagger}_i \hat{c}_i$. 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 [6, 5]. 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.

![Figure 2](image)

**Figure 2.** Calculated single-particle spectral function $A(k,\omega)$. Thickness of the color is in proportion to the spectral weight. Origin of energy $\omega$ is taken to be $-J/4$.

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. When the added electron is spin-up, the calculation of the Green’s function is trivial since it is a one-body problem. We follow the method of Refs. [10, 11, 12, 13] to obtain the exact expression for the Green’s function when the added electron is spin-down. We assume the ground state $|FM\rangle$ with a full spin-up polarization without conduction electrons. Then, there are only two types of states: the bare electron state $c^\dagger_{k\downarrow}|FM\rangle$ and an electron+magnon state $c^\dagger_{k-q\uparrow}\hat{S}^{-}_{q}|FM\rangle$, where $c^\dagger_{k\sigma}$ is the Fourier transform of $c^\dagger_{i\sigma}$. Details of the calculations will be given elsewhere [14].

Results for the spectral function are shown in Fig. 1. The spectrum consists of two components: an incoherent continuum in the range $[-2t-J/4,2t-J/4]$ 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.
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 thus have a similar phenomenon as in spin-charge separation [15]: an incoherent spectral function. 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 [14].

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References
[1] Katsnelson M I, Irkhin V Y, Chioncel L, Lichtenstein A I and de Groot R A 2008 Rev. Mod. Phys. 80 315.
[2] Edwards D M and Hertz J A 1973 J. Phys. F: Met. Phys. 3 2191.
[3] Irkhin V Y and Katsnelson M I 2006 Phys. Rev. B 73 104429.
[4] Zener C 1951 Phys. Rev. 82 403.
[5] Yunoki S, Hu J, Malvezzi A L, Moreo A, Furukawa N and E. Dagotto 1998 Phys. Rev. Lett. 80 845.
[6] Dagotto E, Yunoki S, Malvezzi A L, Moreo A, Hu J, Capponi S, Poilblanc D and Furukawa N 1998 Phys. Rev. B 58 6414.
[7] Tsuijoka T, Mizokawa T, Okamoto J, Fujimori A, Nohara M, Takagi H, Yamaura K and Takano M 1997 Phys. Rev. B 56 R15509.
[8] Huang D J, Tjeng L H, Chen J, Chang C F, Wu W P, Chung S C, Tanaka A, Guo G Y, Lin H-J, Shyu S G, Wu C C and Chen C T 2003 Phys. Rev. B 67 214419.
[9] Kurmaev E Z, Moewes A, Butorin S M, Katsnelson M I, Finkelstein L D, Nordgren J and Tedrow P M 2003 Phys. Rev. B 67 155105.
[10] Shastry B S and Mattis D C 1981 Phys. Rev. B 24 5340.
[11] Nolting M, Reddy G G, Ramakanth A, Meyer D 2001 Phys. Rev. B 64 155109.
[12] Berciu M and Sawatzky G A 2009 Phys. Rev. B 79 195116.
[13] Berciu M 2009 Physics 2 55.
[14] Nakano K, Eder R and Ohta Y, 2011 in preparation.
[15] Eder R, Ohta Y and Maekawa S 1995 Phys. Rev. Lett. 74 5124.