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Ferromagnetism and metal-half-metal-insulator transitions in a frustrated periodic Anderson-like organic polymer



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ABSTRACT

The ferromagnetism and quantum phase transitions of a periodic Anderson-like organic polymer, in which the next-nearest-neighboring hopping results in frustration, are investigated by means of many-body Green's function theory. It is found that the ground state lies in half-metallic and paramagnetic metallic states for weak and relatively strong frustrations, respectively. At finite temperatures, a ferromagnetic order and two different ferromagnetic phases are unveiled. In a magnetic field, in addition to 1/3 magnetization plateau, it presents three cusps and three critical fields indicating metal-half-metal and half-metal-insulator transitions, respectively, which are closely related to the energy bands controlled by the field.

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1. Introduction

Since the organic polymers have versatile structures and chemical properties, they are potentially wider useful than inorganic materials. Heeger et al. [1–3] discovered the conducting organic polymers, which has kicked off intensive studies, paving a new way to adopt organic polymers or oligomers in realizing various functions as molecular-electronics or spintronics devices like organic molecular diodes [4,5] or spin-valves [6,7]. Specially, the design of organic polymers to realize ferromagnetism is becoming increasingly realistic. Theoretically, the chains containing five membered rings (as a building block) with side groups have been explored and shown ferromagnetism or half-metal, wherein with the electron densities above half-filling, the on-site repulsive interactions permitted to differ on individual sites are employed to tune a bare dispersive band structure such that it develops a flat band [8,9]. Experimentally, several quasi-one-dimensional (1D) organic ferromagnets have been synthesized such as poly-BIPO [10], p-NPNN [11] and poly(9,10-anthryleneethynylene) [12] with pendant radicals. Ovchinnikov [13] firstly proposed an idea to obtain organic ferromagnet, which is the synthesis of alternate hydrocarbon with high-spin ground state, where the π -electrons along the main zigzag chain were considered to be itinerant, while the unpaired electrons on the side radicals were regarded as a delocalized or totally localized case. Indeed, this has to do with

ferrimagnetism, which has been demonstrated in our previous work [14]. At one time, the SSH and Hubbard models [2,15–17] were proposed to describe this quasi-1D conjugated organic polymer considered as a delocalized π -electron system, where the orbitals of successive carbon atoms overlap, giving rise to charge mobility along the backbone of the polymer chain. Later on, Wang [18] studied the ground state properties of this conjugated organic polymer using the exact diagonalization technique, which is developed as a periodic Anderson-like model. In this system, the conduction electrons with uncorrelated orbitals which reside in the main zigzag chain form a conduction sea, while a correlated localized f orbital locates at the side radical R. Due to the f electrons are strongly localized, while the conduction electrons form a conduction sea distribute throughout the system, which presents a Fermi liquid [19] coupling with localized spins, two interactions compete for dominance [19,20]. One interaction is the Kondo coupling, which happens as the spin of localized f electron is screened by the conduction orbital ($l,2$), favoring a nonmagnetic singlet state; the other is the superexchange, i.e., the indirect non-convulsively ferromagnetic RKKY interaction of the two contiguous localized spins mediated by conduction sea, which tends to stabilize a magnetically ordered phase. As we know, the Kondo coupling $J_K \sim V^2/U$ [21] reflects that the behavior of the system is controlled by two parameters: the hybridization V and the Hubbard repulsion U . Thus, the competition between Kondo coupling and RKKY interaction is attributed to the consequence of interplay between Coulomb interaction and hybridization.

However, if the next-nearest-neighboring site connected by organic ligand through chemical means, resulting in frustration,

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which would also destroy the magnetic order, it will demonstrate the competition between the frustration, Kondo coupling and RKKY interaction, making an important impact on magnetic order. In weak frustration, the ground state lies in a half-metal state, whereas it goes into a paramagnetic metal state in strong frustration. At finite temperatures, the frustration and the Kondo coupling may induce different ferromagnetic phase transitions. In addition, as an external magnetic field is turned on, apart from the 1/3 magnetization plateau, the metal-half-metal and half-metal-insulator transitions will happen. Furthermore, the spin channel controlled by magnetic field manifests an excellent application in organic spin filter.

The frustration which can be carried out by chemical means, will give rise to the emergence of ferromagnetism rather than the sole ferrimagnetism. Herein, we shall explore the ferromagnetism and thermodynamic properties of this frustrated periodic Anderson-like organic polymer by means of many-body Green's function theory in an external magnetic field. In the forthcoming section, we will present the model Hamiltonian and give an outline of the Green's function method. In Section 3, the energy bands, the magnetization, the susceptibility and the specific heat will be calculated; the temperature-induced phase diagrams will be explored; and the hole excitations, which are closely related to the thermodynamic behaviors, will also be discussed. Finally, we draw a conclusion in Section 4.

2. Model Hamiltonian and theoretical method

The Hamiltonian for the quasi-1D frustrated periodic Anderson-like chain model as illustrated in Fig. 1 in an external magnetic field is written as

$$H = H_c + H_f + H_{cf} + H_h \quad (1)$$

Here, the term H_c describes the conduction electrons of the main zigzag chain with uncorrelated orbitals,

$$H_c = -t \sum_{l,\sigma} (c_{1,l,\sigma}^+ c_{2,l,\sigma} + c_{2,l,\sigma}^+ c_{1,l+1,\sigma} + hc) - t_0 \sum_{l,\sigma} (c_{1,l,\sigma}^+ c_{1,l+1,\sigma} + c_{2,l,\sigma}^+ c_{2,l+1,\sigma} + hc), \quad (2)$$

where t is the hopping integral between the nearest-neighboring conduction orbitals, t_0 is the hopping integral between the next-nearest-neighboring conduction orbitals, reflecting the magnitude of frustration, $c_{\eta,l,\sigma}^+$, $c_{\eta,l,\sigma}$ ($\eta = 1, 2$) denote the creation and annihilation operators with spin $\sigma = \uparrow, \downarrow$ for the conduction electrons and $n_{l,\sigma}^\eta = c_{\eta,l,\sigma}^+ c_{\eta,l,\sigma}$ is the number operator in the conduction orbital.

The term H_f describes the correlated localized f orbital,

$$H_f = \sum_{l,\sigma} \varepsilon_f f_{l,\sigma}^+ f_{l,\sigma} + U \sum_l n_{l,\uparrow}^f n_{l,\downarrow}^f \quad (3)$$

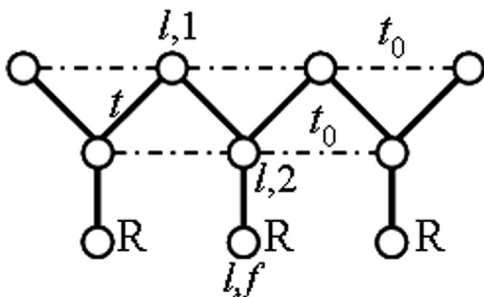


Fig. 1. Schematic illustration of a quasi-one-dimensional frustrated periodic Anderson-like organic polymer chain model.

where $f_{l,\sigma}^+$, $f_{l,\sigma}$ are the creation and annihilation operators for the localized f electrons in the side radical R, $n_{l,\sigma}^\eta = f_{l,\sigma}^+ f_{l,\sigma}$ is the number operator in the localized f orbital, ε_f is the bare energy of the localized f orbital, and U denotes the f orbital electron–electron Coulomb repulsion. The next term H_{cf} depicts the hybridization between the conduction orbital ($l, 2$) and the localized f electron,

$$H_{cf} = V \sum_{l,\sigma} (c_{2,l,\sigma}^+ f_{l,\sigma} + hc), \quad (4)$$

where V is the hybridization strength.

The last term H_h in Eq. (1) expresses the Zeeman splitting in an external magnetic field,

$$H_h = -\frac{\hbar}{2} \sum_l \sum_{\eta=1,2,f} (n_{l,\uparrow}^\eta - n_{l,\downarrow}^\eta) \quad (5)$$

where $h = g\mu_B B$ is the reduced magnetic field (Zeeman energy).

Now, we employ the equations of motion method to calculate the retarded Green's function [14,22–25] for the electrons, which is defined as

$$G_{ij}^a(t_1 - t_2) = \langle \langle a_{i,\sigma}(t_1); b_{j,\sigma}^+(t_2) \rangle \rangle = -i\theta(t_1 - t_2) \langle [a_{i,\sigma} b_{j,\sigma}^+ + a_{j,\sigma}^+ b_{i,\sigma}] \rangle, \quad (6)$$

($a, b = c_1, c_2, f$)

where the subscripts i and j number the lattice sites. After the time Fourier transformation, the Green's function is put into the equation of motion,

$$\omega \langle \langle a_{i,\sigma}; b_{j,\sigma}^+ \rangle \rangle = \langle [a_{i,\sigma}, b_{j,\sigma}^+] \rangle + \langle \langle [a_{i,\sigma}, H]; b_{j,\sigma}^+ \rangle \rangle. \quad (7)$$

By performing the equation of motion analogous to Eq. (7) for the high-order Green's function $\langle \langle [a_{i,\sigma}, H]; b_{j,\sigma}^+ \rangle \rangle$, the higher-order Green's function will appear on the right side, resulting in an infinite set of coupled equations. In terms of Wick's theorem, we adopt the decoupling scheme for the four-operator Green's functions [26],

$$\langle \langle A^+ B C; D^+ \rangle \rangle \approx \langle A^+ B \rangle \langle \langle C; D^+ \rangle \rangle - \langle A^+ C \rangle \langle \langle B; D^+ \rangle \rangle. \quad (8)$$

Herein, it is noted that the Green's functions are diagonal in spin space $G_{ij}^{\sigma\sigma'} = G_{ij}^\sigma \delta_{\sigma\sigma'}$.

For further Fourier transformation into k -space, the Green's function reads as

$$G_{ij}^\sigma = \frac{1}{N} \sum_k g^\sigma(k, \omega) e^{ik(i-j)}. \quad (9)$$

The integral of the wavevector k extends over the first Brillouin zone. Accordingly, the momentum space Green's function $g^\sigma(k, \omega)$ behaves as a function of wave vector k and the elementary excitation spectrum $\omega = \omega(k)$. Associated with the standard spectral theorem, the correlation function of the product of the electron operators can be expressed as

$$\langle b_{j,\sigma}^+ a_{i,\sigma} \rangle = \frac{i}{2\pi N} \sum_k e^{ik(i-j)} \int \frac{g^\sigma(k, \omega + i0^+) - g^\sigma(k, \omega - i0^+)}{e^{\beta\omega} + 1} d\omega, \quad (10)$$

where $\beta = 1/k_B T$, k_B is the Boltzmann's constant, and T is the absolute temperature.

The spin density (sublattice magnetization) at one site is defined as

$$\langle S_{n,l}^z \rangle = \frac{1}{2} (\langle n_{l,\uparrow}^\eta \rangle - \langle n_{l,\downarrow}^\eta \rangle), \quad (\eta = 1, 2, f). \quad (11)$$

Then the average magnetization of the unit cell M and the magnetic susceptibility χ are obtained as follows:

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