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Influence of the modulated hopping on the one-dimensional interacting electron system

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ABSTRACT

By introducing a modulation parameter (ξ), we study the one-dimensional correlated system with modulated hopping, on-site (U) and nearest-neighbor (V) repulsions in the weak-coupling regime. The induced three-body attraction changes topology of the conventional phase diagram. Besides the usual CDW and SDW phases, a BSDW phase exists for $|U - 2V| < 8t\xi^2/\pi$. In the absence of V, an insulator–metal transition takes place, and the TS phase is realized for $\xi > \sqrt{\pi U/8t}$. Phenomenologically, the general quantum phase diagram including insulating and superconducting phases is discussed.

1. Introduction

The study of low-dimensional systems and electron correlation continues to be an important subject in condensed matter. The one-dimensional Hubbard model is suggested to be an appropriate candidate for describing properties of low-dimensional strongly correlated electron systems. The Hubbard model describes spin-1/2 electrons which may hop between sites and interact with each other via on-site potential. At half filling, its low-energy excitation is exactly charge-spin separable. For all values of on-site repulsion, the ground state is a Mott-insulator, exhibiting a critical spin-density-wave (SDW) state. This behavior is caused by Umklapp scattering in the weak-coupling picture while it is caused by an effective Heisenberg exchange in the strong-coupling regime. The Hubbard model has a long history of research and is relevant to a wide variety of quasi-one-dimensional materials, such as polymers [1], strontium cuprates [2] and the charge transfer salt TTF-TCNQ [3]. Nevertheless, the extensions of the Hubbard model with inter-site interactions are believed to give rise to much more complicated dynamics. A simple extension is the conventional Hubbard model with a nearest-neighbor repulsion (V) (hereafter the t-U-V model) [4]. Much effort has been devoted to its ground state phase diagram at half filling [5–19]. For a long time, it was widely accepted that the phase diagram of the t-U-V model consists of two phases, the SDW phase for $U > 2V$ and CDW (charge-density-wave) phase for $U < 2V$. Such a common viewpoint had not been changed until Nakamura pointed out that a bond-charge-density-wave (BCDW) state exists at $U \simeq 2V$ in between the SDW and CDW phases for small to intermediate values of U and V [12]. Such an astonishing argument triggers increased interest in the t-U-V model [13–19]. Quite a few works reconfirmed numerically existence of the BCDW state. However, there is disagreement about the position of the tricritical point, which was reported to range from $U_c \simeq 1.5$ to $U_c \simeq 5$ (with $V_c \simeq U_c/2$).

To clarify the emergent BCDW phase, the extra interactions were considered. Nakamura claimed that the correlated hopping (X) enhances a dimerized phase [12]. This argument was reinforced by Japaridze's work, where the on-bond interaction (W) joins together [20]. Huang et al. proposed that the additional antiferromagnetic spin coupling (J) induces a BCDW phase [21]. On the other hand, the t-U-V model can be generalized by modifying the hopping term instead of the interaction terms. In this letter we will treat such a one-dimensional interacting electron system, and the model Hamiltonian considered is given by

$$H = -t\sum_{j,\alpha}(\bar{c}^{\dagger}_{j,\alpha}\bar{c}_{j+1,\alpha} + h.c.) + U\sum_{j} n_{j\uparrow}n_{j\downarrow} + V\sum_{j} n_j n_{j+1}, \quad (1)$$

with the deformation operators being

$$\bar{c}_{j,\alpha} = c_{j,\alpha}(1 - \xi n_{j,\bar{\alpha}}), \quad (2)$$

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where the introduced parameter ξ modulates the hopping matrix element. For $\xi = 0$, the conventional t-U-V model is recovered. When $\xi = 1$, the double occupancy state is completely excluded. Therefore, it is sufficient to define $0 < \xi < 1$. However, one immediately observes that the modulated hopping terms will induce extra two-body and three-body interactions. Below, we will examine influence of the modulated hopping on the ground-state phase diagram of the Hamiltonian (1). We restrict our consideration to small values of repulsive interactions ($U/t, V/t \ll 1$) and small modulation parameter ($\xi \ll 1$), where the weak-coupling theory armed with the bosonization and RG techniques can be safely applied. As will be shown, in the absence of V, an insulator–metal transition takes place at $\xi_c = \sqrt{\pi U/8t}$, and the triplet-superconducting (TS) phase is realized for $\xi \geq \xi_c$. In the presence of U and V, the induced three-body interaction breaks an accidental symmetry between the backscattering and the Umklapp processes at $U = 2V$, separating the synchronized Gaussian and spin-gap transition into two branches in between a bond-spin-density-wave (BSDW) phase is realized. The corresponding ground-state phase diagram contains three insulating phases, characterized by the CDW phase for $2V - U > 8t\xi^2/\pi$, the BSDW phase for $|2V - U| < 8t\xi^2/\pi$, and the SDW phase for $U - 2V > 8t\xi^2/\pi$. We have not found the controversial BCDW phase.

2. Weak-coupling theory analysis

We rewrite the Hamiltonian (1) in terms of the defined deformation operators (2) as

$$H = H_{tUV} + H_{t\xi} + H_{t\xi^2}, \tag{3}$$

with the components

$$H_{tUV} = -t\sum_{j,\alpha}(c^\dagger_{j,\alpha}c_{j+1,\alpha} + h.c.) + U\sum_j n_{j,\uparrow}n_{j,\downarrow} + V\sum_j n_j n_j, \tag{4}$$

$$H_{t\xi} = t\xi\sum_{j,\alpha}[c^\dagger_{j,\alpha}c_{j,\alpha}(n_{j,\bar{\alpha}} + n_{j+1,\bar{\alpha}}) + h.c.], \tag{5}$$

$$H_{t\xi^2} = -t\xi^2\sum_{j,\alpha}(c^\dagger_{j,\alpha}c_{j+1,\alpha}n_{j,\bar{\alpha}}n_{j+1,\bar{\alpha}} + h.c.). \tag{6}$$

Here, the H_{tUV} part describes the familiar t-U-V model. The $H_{t\xi}$ and $H_{t\xi^2}$ terms denote the induced two-body and three-body interactions, respectively. The minus in the $H_{t\xi^2}$ term represents the attraction, compensating the excessive repulsion in the $H_{t\xi}$ term. It is interesting to notice that these induced interactions are proportional to ξ and ξ^2, respectively. Therefore, when $\xi \ll 1$, all the induced interactions can be treated as perturbations.

In one dimension, the bosonization approach is a powerful tool to analyze interacting electrons. The 1D low-energy excitation spectrum is linearized around left (L) and right (R) Fermi points ($\pm k_F$) and the operator $c_{j,\alpha}$ is rewritten as $c_{j,\alpha} \to \sqrt{a}\sum_{r=L,R}\psi_{r,\alpha}(x)$, with $\psi_{r,\alpha}(x)$ annihilating a fermion of spin α on the branch $r = L/R$. These chiral fermion fields can be described by boson operators $\varphi_{L/R,\alpha}$ via the standard formula [22]

$$\psi_{L,\alpha}(x) = \frac{1}{\sqrt{2\pi a}}e^{-i\sqrt{4\pi}\varphi_{L,\alpha}(x)},$$
$$\psi_{R,\alpha}(x) = \frac{1}{\sqrt{2\pi a}}e^{i\sqrt{4\pi}\varphi_{R,\alpha}(x)}. \tag{7}$$

We define a pair of conjugate scalar fields $\phi_\alpha(x)$ and $\theta_\alpha(x)$,

$$\phi_\alpha(x) = \varphi_{L,\alpha}(x) + \varphi_{R,\alpha}(x), \tag{8}$$

$$\theta_\alpha(x) = \varphi_{L,\alpha}(x) - \varphi_{R,\alpha}(x), \tag{9}$$

and introduce their linear combinations,

$$\phi_{c/s}(x) = \frac{\phi_\uparrow(x) \pm \phi_\downarrow(x)}{\sqrt{2}}, \qquad \theta_{c/s}(x) = \frac{\theta_\uparrow(x) \pm \theta_\downarrow(x)}{\sqrt{2}}, \tag{10}$$

describing the charge (c) and spin (s) degrees of freedom, respectively. Thus, the bosonized version of the Hamiltonian (1) describing low-energy states acquires the form $H = H_c + H_s$, with

$$H_c = \frac{v_F}{2\beta_c}\int dx[(\partial_x\phi_c)^2 + \beta_c^2(\partial_x\theta_c)^2] + \frac{g_{3\perp}}{2a\pi^2}\int dx\cos(\sqrt{8\pi\beta_c}\phi_c), \tag{11}$$

$$H_s = \frac{v_F}{2\beta_s}\int dx[(\partial_x\phi_s)^2 + \beta_s^2(\partial_x\theta_s)^2] + \frac{g_{1\perp}}{2a\pi^2}\int dx\cos(\sqrt{8\pi\beta_s}\phi_s). \tag{12}$$

Here we have defined the Luttinger parameters

$$\beta_c \simeq 1 + \frac{g_c}{4\pi t}, \qquad \beta_s \simeq 1 + \frac{g_s}{4\pi t}. \tag{13}$$

v_F is the Fermi velocity, and at half filling $v_F = 2ta$. The small bare coupling constants read

$$g_c = \frac{8\xi^2}{\pi}t - U - 6V, \tag{14}$$

$$g_s = g_{1\perp} = \frac{8\xi^2}{\pi}t + U - 2V, \tag{15}$$

$$g_{3\perp} = \frac{8\xi^2}{\pi}t - U + 2V. \tag{16}$$

The relation $g_s = g_{1\perp}$ comes from the spin SU(2) symmetry.

In obtaining expressions (11) and (12), we discard the strongly irrelevant charge-spin term which has higher scaling dimensionality in the weak-coupling limit, as in other works [20,23–28]. In this case, the charge and spin modes exactly separate. Within this approximation, the model can be analyzed by the standard "g-ology" technique. To this end, we examine the relative importance of these couplings by the RG analysis in the weak-coupling regime. The low-energy properties of the system are described by pairs of RG equations for the effective coupling constants Γ_i [25,27]

$$\frac{d\Gamma_c(l)}{dl} = -\Gamma_{3\perp}^2(l), \qquad \frac{d\Gamma_{3\perp}(l)}{dl} = -\Gamma_c(l)\Gamma_{3\perp}(l), \tag{17}$$

$$\frac{d\Gamma_s(l)}{dl} = -\Gamma_{1\perp}^2(l), \qquad \frac{d\Gamma_{1\perp}(l)}{dl} = -\Gamma_s(l)\Gamma_{1\perp}(l), \tag{18}$$

where we have performed the scale transformation of the cutoff $a \to ae^{dl}$, with l being length scale. The dimensionless running coupling constants $\Gamma_i(0) = g_i/2\pi ta$. These scaling equations determine the RG flow diagram, shown in Fig. 1.

Depending on the constructed RG diagram, we can directly investigate influences of the Umklapp- and the backward-scattering, which drive the charge-gap and spin-gap transitions, respectively, if they are relevant. We first consider the spin channel. The spin SU(2) symmetry guarantees that the RG flows are exactly along the separatrix $\Gamma_s = \Gamma_{1\perp}$, and hence the spin excitation is determined only by signs of the bare coupling g_s. For $g_s > 0$, $\Gamma_{1\perp}(l)$ tends to zero with increasing l. The spin channel describes gapless excitation ($\Delta_s = 0$), and one obtains a free phase field ϕ_s. For $g_s < 0$, $|\Gamma_{1\perp}(l)|$ grows with increasing l. When the length scale arrives at the correlation length λ_s, $\Gamma_{1\perp}(l)$ flows to a strong coupling fixed-point $\Gamma^*_{1\perp}(l \to \ln\lambda_s) = -\infty$. In this context, the expectation value of the spin field is pinned at $\langle\phi_s\rangle = 0$ so that the system gains the energy. This indicates that the spin-gap transition takes place at