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CHARGE AND SPIN GAPS IN THE DIMERIZED HUBBARD MODEL*

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By using the bosonization and renormalization group methods, we have studied the low energy physical properties in the one-dimensional dimerized Hubbard model. The formation of charge and spin gaps is investigated both for the half-filled electron band and away from the half-filled band. The scaling laws of the charge and spin gaps with the dimerization parameterΔ and the repulsive interaction strength U are obtained.

Keywords: dimerized hubbard model, charge and spin gaps
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I. INTRODUCTION

Quasi-one-dimensional organic conductors, such as TTF-TCNQ or Bechgard salts $(TMTSF)_2X$ and $(TMTTF)_2X$, have attracted much research attention during last two decades.[1] Due to their various broken symmetry ground states at low temperature and unusual electronic properties of the normal states, they are under intensive research both in experiments and theories, and some problems still remain controversial.[2−4]

It is believed that the interaction between electrons plays an important role in the physical properties of those low-dimensional systems.[2] As is well known, the one-dimensional (1D) interacting fermion systems show non-Fermi liquid behaviors, the collective low energy excitations are spin and charge density waves, and they are described by the Luttinger liquid theory which gives more distinct physical properties than that of the normal Fermi liquid,[5,6] and the quasi-one-dimensional organic conductors give concrete examples of the Luttinger liquid.

As the coupling with the periodic lattice is involved, 1D metal exhibits Peierls instability, the lattice shows periodic distortion with the wave vector equal to twice the Fermi wave vector $2k_F$, and it opens an energy gap in the electronic spectrum at the Fermi surface.[7] The Umklapp scattering process caused by interaction between electrons can also generate an energy gap in the excitations of charge density wave.

In this paper we shall study the spin gap and charge gap formation in those quasi-one-dimensional systems. Based on the dimerized Hubbard model, which takes into account both the dimerization of the lattice and the on-site Coulomb repulsive interaction between electrons, we investigate the scale relations of charge gap(m_ρ) and spin gap(m_σ) with the dimerization parameter Δ and the on-site interaction strength U.

II. THE DIMERIZED HUBBARD MODEL AND ITS BOSONIZD FORM

In the adiabatic approximation, the effective Hamiltonian of 1D interacting electron system coupled to a crystal lattice can be described by the dimerized Hubbard model with the Hamiltonian[4]

$$H = \sum_i t(1+\delta_i)[c^+_{i\sigma}c_{i+1\sigma} + h.c.] + U\sum_i n_{i\uparrow}n_{i\downarrow} + \frac{K}{2}\sum_i \delta_i^2 \,, \qquad (1)$$

where $c_{i\sigma}(c^+_{i\sigma})$ denote annihilation(creation) operators for electrons at site i, δ_i are local lattice distortions induced by Peierls transition, K the lattice elastic constant and U is the on-site repulsive interaction strength. At half filling, the lattice distortion $\delta_i = (-1)^i\delta$ with the parameter δ being a constant for the dimerized chain. The constant term of the elastic energy density $1/2\ K\delta^2$ will be omitted in the following consideration. We shall approach this Hamiltonian by Abelian bosonization method.[8,9] In the continuum limit, the effective Hamiltonian in terms of boson fields is given as[10,11]

$$H = H_\rho + H_\sigma + H_{\rm dim}, \qquad (2)$$

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$$H_\rho = v_\rho \int \mathrm{d}x \frac{1}{2}\left[K_\rho \Pi_\rho^2(x) + \frac{1}{K_\rho}(\partial_x \phi_\rho)^2\right] + \frac{U_{\mathrm{um}}}{2\pi^2\epsilon^2}\int \mathrm{d}x \cos(\sqrt{8\pi}\phi_\rho + qx), \quad (3)$$

$$H_\sigma = v_\sigma \int \mathrm{d}x \frac{1}{2}\left[K_\sigma \Pi_\sigma^2(x) + \frac{1}{K_\sigma}(\partial_x \phi_\sigma)^2\right], \quad (4)$$

$$H_{\mathrm{dim}} = \frac{\Delta}{\pi\epsilon}\int \mathrm{d}x \cos\sqrt{2\pi}\phi_\rho \cos\sqrt{2\pi}\phi_\sigma, \quad (5)$$

where $\phi_\rho(x), \phi_\sigma(x)$ are boson fields for the charge and spin degrees of freedom of electrons, respectively; $\Pi_\rho(x), \Pi_\sigma(x)$ are their conjugate momentums. The coupling term H_{dim} of charge and spin fields is caused by the dimerization, with $\Delta = 4t\delta$. The $U_{\mathrm{um}}-$term is the Umklapp term of electron-electron interaction, the initial values of $U_{\mathrm{um}} = U$, and the parameter defined by $q = 4k_F - 2\pi$ measures the deviation from the half-filling case. The Tomonaga-Luttinger parameters K_ρ and K_σ determine the long distance properties of the system, and their initial values are given by $K_\rho = \dfrac{1}{\sqrt{1+2U/\pi v_F}}$ and $K_\sigma = 1$, with $v_F = 2t\sin(\pi n/2)$, where n is filling factor.[10] The values of charge and spin density wave velocity are $v_\rho = v_F\sqrt{1+2U/\pi v_F}$ and $v_\sigma = v_F\sqrt{1-2U/\pi v_F}$ respectively.

Ⅲ. AT HALF-FILLED BAND OF ELECTRONS

We first consider the half-filling case with $k_F = \pi/2a$, hence the parameter $q = 0$. To derive the renormalization group(RG) equations for various coupling constants of the effective Hamiltonian, we utilize the operator product expansion(OPE) technique of the conformal quantum field theory. The charge field ϕ_ρ and the spin field ϕ_σ satisfy the following OPE of $U(1)$ Guassian model[12,13]

$$e^{i\alpha\phi_\nu(x,\tau)}e^{-i\alpha\phi_\nu(0,0)} \sim \frac{i\alpha}{|z|^{\alpha^2K_\nu/2\pi-2}}\left(\frac{\partial_z\phi_\nu(0,0)}{\bar z} + \frac{\partial_{\bar z}\phi_\nu(0,0)}{z}\right) + \frac{1}{|z|^{\alpha^2K_\nu/2\pi}} - \frac{\alpha^2}{|z|^{\alpha^2K_\nu/2\pi-2}}\partial_z\phi_\nu(0,0)\partial_{\bar z}\phi_\nu(0,0) - \frac{\alpha^2}{2|z|^{\alpha^2K_\nu/2\pi}}(z^2(\partial_z\phi_\nu)^2 + \bar z^2(\partial_{\bar z}\phi_\nu)^2) + \cdots \quad (6)$$

with $\nu = \rho, \sigma$; and $z = x + iv_\rho\tau, \bar z = x - iv_\rho\tau$ for the charge field ϕ_ρ, and $z = x + iv_\sigma\tau, \bar z = x - iv_\sigma\tau$ for the spin field ϕ_σ. By using the above OPE formulae, we can derive the RG equations

$$\frac{\mathrm{d}\Delta}{\mathrm{dln}b} = [2 - (K_\rho/2 + K_\sigma/2)]\Delta, \quad (7)$$

$$\frac{\mathrm{d}U_{\mathrm{um}}}{\mathrm{dln}b} = (2 - 2K_\rho)U_{\mathrm{um}}, \quad (8)$$

$$\frac{\mathrm{d}K_\rho}{\mathrm{dln}b} = -\frac{K_\rho^2}{v_\rho^2}[U_{\mathrm{um}}^2 + \Delta^2 f_2(\frac{v_\sigma}{v_\rho})], \quad (9)$$

$$\frac{\mathrm{d}K_\sigma}{\mathrm{dln}b} = -\frac{K_\sigma^2}{v_\sigma^2}\Delta^2 f_1(\frac{v_\rho}{v_\sigma}), \quad (10)$$

with

$$f_1(\mu) = \int_0^\pi \frac{\mathrm{d}\theta}{(\cos^2\theta + \mu^2\sin^2\theta)^{K_\rho/2}}, \quad (11)$$

$$f_2(\mu) = \int_0^\pi \frac{\mathrm{d}\theta}{(\cos^2\theta + \mu^2\sin^2\theta)^{K_\sigma/2}}. \quad (12)$$

Now we will discuss the charge and spin gaps in different cases of the interaction strength U of electrons.

(a) $U = 0$, and $K_\rho(0) = K_\sigma(0) = 1$

In the absence of Coulomb interaction of electrons, the Hamiltonian of the model is exactly solvable. The charge gap m_ρ and the spin gap m_σ are given by

$$m_{\rho,\sigma} \propto \Delta \quad (13)$$

for small Δ. This result can also be obtained from the scaling equation(7)

$$\frac{\mathrm{d}\Delta}{\mathrm{d}\ln b} = \Delta. \quad (14)$$

The energy difference between the dimerized system ($\Delta \neq 0$)and the system with no lattice distortion ($\Delta = 0$) can also be calculated exactly

$$\Delta E_0^e = E_0^e(\Delta) - E_0^e(0) \propto -\frac{\Delta^2}{32\pi t}\ln\frac{16t}{\Delta} - \frac{\Delta^2}{64\pi t}, \quad (15)$$

where the logarithmic correction is due to the nonlinear dispersion of elementary excitation. We see

that the electronic part energy of the ground state decreases by dimerization. In the adiabatic approximation, the elastic energy increases with dimerization, $\Delta E_0^{\rm elastic} \propto \Delta^2$. Thus the total amount of change of ground state energy $\Delta E_0 = \Delta E_0^{\rm el} + \Delta E_0^{\rm elastic} < 0$ for small dimerization parameter Δ, implying the ground state of the system is a dimerized state in the case of $U = 0$.

(b) $U > 0$, and $K_\rho(0) < 1, K_\sigma(0) = 1$

When the electrons have on-site repulsive interaction ($U > 0$), there are two mechanisms for generating charge gap, one is the Umklapp scattering from electron-electron interaction with strength $U_{\rm um}$, the other is the dimerization term. In the following, we will consider the charge gap and spin gap in the two limit cases of the interaction strength U and the dimerization parameter Δ.

(i) $U \gg \Delta$

In this case the charge gap due to $U_{\rm um}$-term opens prior to the spin gap formation. After the charge gap formation, $K_\rho = 0$ and $K_\sigma = 1$. The scaling equation (7) becomes

$$\frac{{\rm d}\Delta}{{\rm d}\ln b} = \frac{3}{2}\Delta \ . \tag{16}$$

Thus the spin gap for small Δ is given as

$$m_\sigma \propto \Delta^{2/3} \ . \tag{17}$$

It is well known that in the spin-Peierls transition systems the spin gap scales with the dimerization parameter as $\Delta^{2/3}$ by the Cross-Fisher theory,[14] which is based on the anti-ferromagnetic Heisenberg chain model. Since the Hubbard model can be mapped to the Heisenberg chain model in the large U limit, our result is consistent with that of the Cross-Fisher theory. The charge gap m_ρ of this system is given by the Mott-Hubbard gap of 1D Hubbard model.[15]

The energy of interacting electrons with dimerization is lowered compared with that of no dimerization system, with $\Delta E_0^e \propto -\Delta^{4/3}$. Hence $\Delta E_0^e + \Delta E_0^{\rm elastic} < 0$ for small Δ, the dimerized ground state is favored.

(ii) $U \ll \Delta$

In this case , the $\Delta-$term is a relevant interaction with scaling dimension $K_\rho/2 + 1/2$. This dimension is smaller than that of the Umklapp term, which has the scaling dimension $2K_\rho$, hence the interaction Δ increases more rapidly than $U_{\rm um}$ under RG transformation. The charge gap is dominantly determined by the $\Delta-$ term. Thus the Umklapp interaction term is negligible. From the scaling equation(7) and the initial value $K_\sigma = 1$, we obtain the spin and charge gaps as follows

$$m_{\rho,\sigma} \propto \Delta^{\frac{2}{3-K_\rho}} \ , \tag{18}$$

where $K_\rho = \frac{1}{\sqrt{1+2U/\pi v_F}}$. The electronic energy $\Delta E_0^e \propto -\Delta^{4/(3-K_\rho)}$. Since $1/2 < K_\rho < 1$ for repulsive interaction,[10] it follows that $\Delta E_0^e + \Delta E_0^{\rm elastic} < 0$. The ground state is a dimerized state.

It should be noted that the charge gap formation is due to Umklapp scattering term and the dimerization term, while the spin gap is only contributed from the dimerization term. As the on-site interaction strength U increases from the limit $U \ll \Delta$ to $U \gg \Delta$, the charge gap initially depends on Δ and finally on U, this is a kind of cross-over phenomena. The spin gap is mainly dependent on the parameter Δ in all the cases.

IV. AWAY FROM HALF-FILLED BAND

We now discuss the spin gap and charge gap formation in the system with the electronic band away from half-filling. In this case, the Umklapp interaction term will be absent in the low energy effective Hamiltonian. Hence the RG equations of various coupling constants reduce to

$$\frac{{\rm d}\Delta}{{\rm d}\ln b} = [2 - (K_\rho/2 + K_\sigma/2)]\Delta \ , \tag{19}$$

$$\frac{{\rm d}K_\rho}{{\rm d}\ln b} = -\frac{K_\rho^2}{{v_\rho}^2}\Delta^2 f_2(\frac{v_\sigma}{v_\rho}) \ , \tag{20}$$

$$\frac{{\rm d}K_\sigma}{{\rm d}\ln b} = -\frac{K_\sigma^2}{v_\sigma^2}\Delta^2 f_1(\frac{v_\rho}{v_\sigma}) \ , \tag{21}$$

where K_ρ is a function of the interaction strength U and the filling factor n, and can be calculated as in Ref.[10]. The scaling equation(19) can be written as

$$\frac{{\rm d}\Delta}{{\rm d}\ln b} = (3/2 - K_\rho/2)\Delta \ . \tag{22}$$

The charge and spin gaps for small Δ are

$$m_{\rho,\sigma} \propto \Delta^{\frac{2}{3-K_\rho}} \ . \tag{23}$$

The energy of interacting electrons $\Delta E_0^e \propto -\Delta^{4/(3-k_\rho)}$. Since $1/2 < K_\rho < 1$ for the 1D Hubbard model with repulsive interaction away from half-filling, we see that the total amount of energy changed by dimerizing effect in the ground state is $\Delta E_0 < 0$. The ground state is dimerized.

V. CONCLUSIONS

In this paper we have studied the charge and spin gaps formation in 1D dimerized Hubbard model

by bosonization and renormalization group technique. The dimerizing effect will introduce coupling between the charge and spin degrees of freedom in this interacting electron system, and contribute to the formation of charge and spin gaps. The charge gap can also be generated by Umklapp scattering of electrons at half-filling. We have obtained the scaling relations of the charge and spin gaps with the dimerization parameter Δ and the interaction strength U, and found that in the adiabatic approximation of the lattice vibration, the system is always in a dimerized state both for the half-filled electron band or away from the half-filled band. In further work, it seems important to consider the quantum lattice fluctuation effects in this system.

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