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Filling dependence of correlation exponents and metal-Mott insulator transition in strongly correlated electron systems*

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Using a universal relation between electron filling factor and ground state energy, this paper studies the dependence of correlation exponents on the electron filling factor of one-dimensional extended Hubbard model in a strong coupling regime, and demonstrates that in contrast to the usual Hubbard model ($g_c = 1/2$), the dimensionless coupling strength parameter g_c heavily depends on the electron filling, and it has a "particle–hole" symmetry about electron quarter filling point. As increasing the nearest neighbouring repulsive interaction, the single particle spectral weight is transferred from low energy to high energy regimes. Moreover, at electron quarter filling, there is a metal-Mott insulator transition at the strong coupling point $g_c = 1/4$, and this transition is a continuous phase transition.

Keywords: strong correlation, correlation effect, correlation exponent, correlation function

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Since the discovery of high T_c cuprate superconductors[1] and lots of quasi-one-dimensional new materials,[2] low dimensional strongly correlated electron systems have been extensively studied.[2−7] Now it is very successful in understanding of low energy behaviour of one-dimensional strongly correlated systems by applying powerful field theory methods, such as Bethe ansatz, conformal field theory and bosonization method, but for two-dimensional strongly correlated systems, the situation becomes more complex because of absence of an effective theory to treat the strong electron correlation effect.

The most simple model to describe one-dimensional strongly correlated electron systems is the Hubbard model, which can be exactly solved by Bethe ansatz[8] because of only considering an on-site electron–electron Coulomb interaction. Another simple model is the extended Hubbard model (EHM) which includes the on-site (U) and the nearest neighbour (V) electron–electron Coulomb interactions.

The EHM has a rich phase diagram, and it shows a variety of low energy physical behaviour for different U, V and electron filling factor.[9−12] For example, for large V and small U, it has phase separation,[10−12] in which one region is dominant by single particle, and another is dominant by particle pair. While, for large U and V, it has a long range static charge density wave order at electron quarter filling, in which there exists a gap in charge collective excitation spectrum.[13] While, because of absence of effective methods to treat the EHM in strong coupling regime, previous works mainly focused on weak coupling regime (small U and V)[9] and strong coupling regime with phase separation by numerical calculations.[10−12] Usual perturbation expansion methods are invalid for large U and V, and previous projection method for large U would introduce single particle occupation constraint which makes the problem to be more complex. Therefore, it is desirable to find a simple and effective analytic method to treat the EHM in strong coupling regime for any electron filling.

In one-dimensional uniform (no phase separation) electron systems, the charge and spin freedoms of electrons are generally separated, and the charge part of the systems can be independently re-modeled by a spinless fermion system with the same particle number. If charge collective excitation spectrum is gapless, there exists a universal relation between ground state energy and electron filling factor, which can be used to directly determine a dimensionless coupling strength

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parameter g_c if knowing the renormalized velocity of charge collective excitation modes. This universal dependence of the ground state energy on the electron filling factor completely comes from the contribution of the charge part, in this way it can be obtained by studying the equivalent spinless fermion system.

In this paper, using the universal relation between the ground state energy and the electron filling factor, we study the electron filling factor dependence of the parameter g_c of the EHM in strong coupling regime, and demonstrate that, in contrast to usual large U Hubbard model where[14−18] $g_c = 1/2$, the parameter g_c heavily depends upon the electron filling factor, and it has a "particle–hole" symmetry about the quarter filling of electrons. At the electron quarter filling, the system has a metal-Mott insulator transition in the strong coupling regime, and in the Mott insulator region, the system has a long range static charge density wave order where a gap appears in the charge collective excitation spectrum. Generally, except some special electron fillings, the velocity of spin collective excitation modes is renormalized by the repulsive Coulomb interactions, whereas the SU(2) symmetry of electron spin rotation enforces the renormalized parameter g_s^* to be equal to one, $g_s^* = 1$. Therefore, the correlation exponents of the EHM in strong repulsive interaction regime are completely determined by the parameter g_c.

The Hamiltonian of the EHM is

$$H = -t\sum_{i\sigma}\left\{c_{i\sigma}^{\dagger}c_{i+1\sigma} + c_{i\sigma+1\sigma}^{\dagger}c_{i\sigma}\right\} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{i} n_i n_{i+1}, \quad (1)$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) are the creation (annihilation) operators of an electron with spin σ (of value $\uparrow$ or $\downarrow$) at a lattice site x_i, $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$ is the electron number operator, and $n_i = n_{i\uparrow} + n_{i\downarrow}$. As $U = V = 0$, the non-interacting electron spectrum is $\varepsilon_k = -2t\cos(2ak)$, and its Fermi surface is composed of two points (Fermi levels), $\pm k_{\rm F}$, where $\hbar k_{\rm F}$ is the Fermi momentum. In general, the low energy physical property of the system is determined by the electron states near two Fermi levels $\pm k_{\rm F}$, thus the energy spectrum can be linearized around the Fermi levels $\pm k_{\rm F}$, and electron operators can be written as, $c_{n\sigma} = \sqrt{a}(\,{\rm e}^{{\rm i}k_{\rm F}x}\psi_{R\sigma}(na) + {\rm e}^{-{\rm i}k_{\rm F}x}\psi_{L\sigma}(na))$. In the continuum limit, the bosonic representations of right-(left) moving electron operators $\psi_{R(L)\sigma}(x)$ are[9,19−21] $\psi_{R(L)\sigma}(x) = (1/2\pi\alpha)^{1/2}\,{\rm e}^{-{\rm i}\Phi_{R(L)\sigma}(x)}$, where the boson fields satisfy the relations, $\partial_x\Phi_{R(L)\sigma} = \pm 2\pi\rho_{R(L)\sigma}(x)$, where $\rho_{R(L)\sigma}(x) = \psi_{R(L)\sigma}^{\dagger}(x)\psi_{R(L)\sigma}(x)$ are the density operators of the right- and left-moving electrons. On the other hand, the bosonic representation of the Hamiltonian can be written as two parts, $H = H_c + H_s$, in this way the charge (H_c) and spin (H_s) freedoms of electrons are completely separated (choosing $\hbar = 1$),

$$H_c = \frac{v_c}{4\pi}\int {\rm d}x\left\{\frac{1}{g_c}(\partial_x\Phi_{-c}(x))^2 + g_c(\partial_x\Phi_{+c}(x))^2\right\} + \frac{V_U}{2\pi^2\alpha^2}\int {\rm d}x\cos(2\Phi_{-c}(x) + (G - 4k_{\rm F})x), \quad (2)$$

$$H_s = \frac{v_s}{4\pi}\int {\rm d}x\left\{\frac{1}{g_s}(\partial_x\Phi_{-s}(x))^2 + g_s(\partial_x\Phi_{+s}(x))^2\right\} + \frac{V_B}{2\pi^2\alpha^2}\int {\rm d}x\cos(2\Phi_{-s}(x)), \quad (3)$$

where $\Phi_{\pm c}(x) = [\Phi_{R\uparrow}(x) + \Phi_{R\downarrow}(x) \pm (\Phi_{L\uparrow}(x) + \Phi_{L\downarrow}(x))]/2$, $\Phi_{\pm s}(x) = [\Phi_{R\uparrow}(x) - \Phi_{R\downarrow}(x) \pm (\Phi_{L\uparrow}(x) - \Phi_{L\downarrow}(x))]/2$, $V_U = V_B = aU + 2aV\cos(2ak_{\rm F})$, α is a momentum cutoff inversely proportional to bandwidth of the system, and a is the lattice constant ($G = 2\pi/a$). If the system is uniform (no phase separation), the Hamiltonians $H_{c(s)}$ in Eqs. (2) and (3) are valid for any repulsive interactions $U, V > 0$, the velocities $v_{c(s)}$ of charge and spin collective modes and the parameters $g_{c(s)}$ depend on the electron filling factor and the interaction potentials U and V. In general, exact dependence of the $v_{c(s)}$ and $g_{c(s)}$ on the interaction strength and the electron filling factor is unknown, but for small U and V (i.e., U/t, $V/t \ll 1$), we have the following relations, $g_c^2 = 2\pi v_{\rm F}/(2\pi v_{\rm F} + 2(V_2 + V_1))$, $g_s^2 = 2\pi v_{\rm F}/(2\pi v_{\rm F} + 2(V_2 - V_1))$, $V_1 = aU + 2aV$, $V_2 = 2aV(1 - \cos(2ak_{\rm F}))$, and $v_{c(s)} = v_{\rm F}/g_{c(s)}$, where $v_{\rm F}$ is the non-interacting electron Fermi velocity.

For the repulsive interactions, U, $V > 0$, the Umklapp scattering V_U-term is important only at $4k_{\rm F} = G$ (half filling), in which it opens a gap in the charge collective excitation spectrum. However, the backward scattering V_B-term is irrelevant for $U > 2V > 0$, where the potential V_B is renormalized to zero in the low energy limit. Hereafter, we only consider the case of $U > 2V > 0$, and electron filling factor $n = N_{\rm e}/N < 1$, where $N_{\rm e}$ is the total electron number, and N is the number of lattice sites of the system, in this way the V_U and V_B terms can be safely neglected. Under these conditions, the Hamiltonians of the charge and spin parts in Eqs. (2) and (3) can be rewritten as,

$$H_i = \frac{v_i}{4\pi}\int {\rm d}x\left\{\frac{1}{g_i}(\partial_x\Phi_{-i}(x))^2 + g_i(\partial_x\Phi_{+i}(x))^2\right\}, \quad (4)$$

where $i = c$, s.

At $V = 0$, the bosonization representation of usual Hubbard model is restored, in which the parameter[14,15] g_s is written down $g_s = 1$ as keeping SU(2) symmetry of spin rotation of the Hubbard model for any non-zero repulsive interaction U. However, as $U > 2V > 0$, the Hamiltonian of the spin part H_s is completely equivalent to that of a Hubbard model with effective on-site interaction $U_{\rm eff} = (V_1 - V_2)/a = U + 2V\cos(2ak_{\rm F}) > 0$, thus it is reasonable to assume that the $g_s = 1$ is also valid for the EHM with $U > 2V > 0$. With the bosonization representation of the electron operators, the charge density–density and spin–spin correlation functions can be written down,

$$\langle n(x)n(0)\rangle = \frac{g_c}{(\pi x)^2} + \frac{A\cos(2k_{\rm F}x)}{x^{1+g_c}},$$
$$\langle \hat{s}(x)\cdot\hat{s}(0)\rangle = \frac{1}{(\pi x)^2} + \frac{B\cos(2k_{\rm F}x)}{x^{1+g_c}}. \quad (5)$$

While, according to electron Green function, the momentum distribution function n_k and single electron density of states $n(\omega)$ can be written as

$$n_k - n_{k_{\rm F}} \sim {\rm sgn}(k_{\rm F} - k)|k_{\rm F} - k|^{\alpha}, \quad n(\omega) \sim |\omega|^{\alpha}, \quad (6)$$

where $\alpha = (g_c + 1/g_c - 2)/4$, and A and B are model-dependent constants.

The parameter g_c can be generally determined by the universal relation between ground state energy $E_{\rm g}$ and the electron filling factor n,

$$\frac{a}{N}\frac{\partial^2 E_{\rm g}(n)}{\partial n^2} = \frac{\pi}{2}\frac{v_c}{g_c}. \quad (7)$$

In general, an analytic expression of g_c by U, V, and n is unknown because this model cannot be exactly solved, whereas in some special cases, if we rigorously obtain the ground state energy $E_{\rm g}$ and the renormalized velocity v_c of the charge collective modes, the parameter g_c can be directly determined by the above equation, then the asymptotic behaviour of correlation functions can be obtained. Equation (7) has been extensively used to determine the correlation exponents of strongly correlated electron systems.[10,11,14,15,22,23]

In strong on-site repulsive interaction limit ($n < 1$), V/U, $2t/U \ll 1$, the probability of two electrons occupied the same site goes to zero, the EHM reduces to usual t–J model with the nearest neighbouring repulsive interaction V which is unfavourable to the $J(\sim t^2/U)$ term and puts the states of nearest neighbouring sites occupied by electrons to high energy levels. We do not use this extended t–J model to study the low energy behaviour of the system in the strong coupling regime because single electron occupation constraint makes the problem more complex. In the large U limit, the system is equivalent to a spinless fermion system with the Hamiltonian

$$H_f = -t\sum_i \left\{f_i^{\dagger}f_{i+1} + f_{i+1}^{\dagger}f_i\right\} + V\sum_i n_{fi}n_{fi+1}, \quad (8)$$

where $f_i^{\dagger}$ (f_i) is the creation (annihilation) operator of a fermion at lattice site i, $n_{fi} = f_i^{\dagger}f_i$ is the fermion number operator, and $\sum_i n_{fi} = N_{\rm e}$. The relation between electron operator $c_{i\sigma}$ and the fermion operator f_i is unknown, now the fermion operator only describes the charge degree freedom of the electrons, while the Hamiltonians H_f (Eq. (8)) and H_c (Eq. (2)) should have the same ground state energy for large repulsive interaction U. In the continuum limit, the bosonic representation of the Hamiltonian H_f can be written as

$$H_f = \frac{v_f}{4\pi}\int {\rm d}x\left\{g(\partial_x\Phi_+(x))^2 + \frac{1}{g}(\partial_x\Phi_-(x))^2\right\} + \lambda\int {\rm d}x\cos(2\sqrt{2}\Phi_-(x) + (G - 4k_{\rm F}^f)x + 2ak_{\rm F}^f), \quad (9)$$

where

$$\Phi_{\pm}(x) = [\Phi_R(x) \pm \Phi_L(x)]/\sqrt{2},$$
$$\partial_x\Phi_{R(L)}(x) = \pm 2\pi\rho_{R(L)}(x),$$
$$g = \left(\frac{1-\gamma}{1+\gamma}\right)^{1/2},$$
$$\gamma = (1 - \cos(2ak_{\rm F}^f))V/\pi\hbar v_{\rm F}^f,$$
$$v_f = \sqrt{1-\gamma^2}v_{\rm F}^f, \quad \lambda = 2aVD_0^2/(2\pi\hbar v_{\rm F}^f)^2,$$

where $v_{\rm F}^f$ is the fermion's Fermi velocity, and $\hbar k_{\rm F}^f$ is the fermion's Fermi momentum. The last term comes from the four-fermion interaction, $\psi_{fR}^{\dagger}(x)\psi_{fL}(x)\psi_{fR}^{\dagger}(x+a)\psi_{fL}(x+a)$ + h.c., which can be safely neglected as $4k_{\rm F}^f \neq G$ because it becomes an oscillating term. At quarter electron filling, one has the relation, $4k_{\rm F}^f = G = 2\pi/a$, the last term opens a gap in the charge collective excitation modes for strongly repulsive interaction $g < 1/2$ (i.e., $V > 2t$).

Under the following condition:

$$g_c = \frac{g}{2}\frac{v_c}{v_f}, \quad (10)$$

the Hamiltonian H_f in Eq. (9) is equivalent to H_c in Eq. (4) for any repulsive interaction V as $n \neq 1/2$. At $V = 0$, according to relation in Eq. (10), one obtains $g = 1$, $v_c = v_f$ and $g_c = 1/2$, which are the same as

the results of Refs. [14–[18]. If one can calculate the parameter g by the Hamiltonian H_f (Eq. (8)), the low energy behaviour of the EHM in large U limit can be determined with Eqs. (10), (5) and (6).

In the case of $n < 1/2$, and $2t/V < 1$, the probability of two or more fermions occupied the nearest neighbouring sites goes to zero. Therefore, as a good approximation for large repulsive interaction V, the system can be seen as equivalent to the $N_{\rm e}$ spinless fermions moving at $N - N_{\rm e}$ lattice sites ($N_{\rm e}$ is a macro quantity), the ground state energy $E_{\rm g}^f(n)$ and the renormalized velocity can be easily obtained,

$$\begin{aligned} v_f &= 2at \sin\left(\frac{n\pi}{1-n}\right), \\ E_{\rm g}^f(n) &= t - \frac{2tN}{\pi}(1-n)\sin\left(\frac{n\pi}{1-n}\right). \end{aligned} \quad (11)$$

With these relations and Eq. (7), the dependence of the parameter g_c on the electron filling n ($< 1/2$) can be written down in the strong coupling regime,

$$g_c = \frac{1}{2}(1-n)^2, \quad (12)$$

where the relation $v_c/v_f = 1/(1-n)$ is used.[24]

In the case of $1/2 < n < 1$ and $2t/V \ll 1$, the system is equivalent to the $N - N_{\rm e}$ spinless quasiparticles ("holes") moving at $N_{\rm e} - 1$ lattice sites ($N_{\rm e}$ is a macro quantity). Thus, under these conditions, the ground state energy and the renormalized velocity can be written down,

$$\begin{aligned} v_c &= 2at \sin\left(\frac{1-n}{n}\pi\right), \\ E_{\rm g}^f(n) &= t - \frac{2ntN}{\pi}\sin\left(\frac{1-n}{n}\pi\right), \end{aligned} \quad (13)$$

which can be used to determine the dependence of g_c on the electron filling n, $g_c = n^2/2$. If one defines a "hole" filling factor, $n_{\rm h} = (N - N_{\rm e})/N = 1 - n$, the parameter g_c can be written as a symmetric form in the strong coupling regime,

$$g_c = \begin{cases} \dfrac{1}{2}(1-n)^2, & 0 < n < \dfrac{1}{2}, \\ \dfrac{1}{2}(1-n_{\rm h})^2, & \dfrac{1}{2} < n < 1, \end{cases} \quad (14)$$

which is one of our central results. The most prominent feature of Eq. (14) is that the parameter g_c has a "particle–hole" symmetry about the point $n = 1/2$, and it strongly depends on the electron filling factor n. This feature originates from the nearest neighbouring repulsive interaction V, while in usual Hubbard model ($V = 0$) the parameter $g_c = 1/2$ as $2t/U \ll 1$, independent of the electron filling factor $n(< 1)$. Equation (14) can be taken as a criterion for numerical calculations in the strong coupling limit, because it only depends upon the electron/hole filling factor.

At the electron quarter filling, $n = 1/2$, the system can be reduced to an anisotropic spin -1/2 Heisenberg chain under Jordan–Wigner transformation. According to the exact solution of the Heisenberg model, one can obtain the following expression of the dimensionless coupling parameter,[25,26]

$$g_c = \frac{1}{2 + \dfrac{4}{\pi}\arcsin\left(\dfrac{V}{2t}\right)}. \quad (15)$$

This relation is valid only for $V \leq 2t$. However, for $V \geq 2t$, it is shown[13] that there exists a gap in the electron spectrum, and the system has a long range static charge density wave order in the zero temperature limit, $n_{fi} = (1/2)[1 - (-1)^i]$. According to Eqs. (14) and (15), in the large U limit, the parameter g_c of the EHM is less than 1/2, and the exponent α of the electron momentum distribution and density of states in Eq. (6) is larger than 1/8, i.e., $\alpha = (g_c + 1/g_c - 2)/4 > 1/8$, this means that the single particle spectral weight is transferred from low energy to high energy regimes, and the decay of the charge density–density and spin–spin correlation functions (5) near $2k_{\rm F}$ becomes slow as the repulsive interaction potential V increases.

On the other hand, at the electron quarter filling, $n = 1/2$, the Hamiltonian (9) is the same as that of the fermion representation of the standard quantum sine-Gordon model. As $g > 1/2$, the λ-term is irrelevant, and the charge excitation spectrum is gapless. While, as $g < 1/2$, it becomes relevant, and it will open a gap in the charge excitation spectrum. Therefore, there takes place a metal-Mott insulator transition at $g = 1/2$. At $n = 1/2$, the Hamiltonian (9) can be rewritten down by an anti-bosonization transformation with a set of new fermion fields $\psi_{R(L)}(x)$,

$$\begin{aligned} & H_f \\ &= -{\rm i}\hbar\tilde{v}_{\rm F}\int {\rm d}x \left\{\psi_R^\dagger(x)\partial_x\psi_R(x) - \psi_L^\dagger(x)\partial_x\psi_L(x)\right\} \\ &\quad - \int {\rm d}x\Big\{\tilde{V}\rho_R(x)\rho_L(x) + \Delta[\psi_R^\dagger(x)\psi_L(x) \\ &\quad + \psi_L^+(x)\psi_R(x)\Big\}, \end{aligned} \quad (16)$$

where $16g^2 = (1+\Gamma)/(1-\Gamma)$, $v_f = \sqrt{1-\Gamma^2}\tilde{v}_{\rm F}$, $\Gamma = \tilde{V}/2\pi\hbar\tilde{v}_{\rm F}$, $\Delta = 2\pi\hbar\tilde{v}_{\rm F}\lambda/D_0$, and D_0 is the bandwidth of the system. Obviously, Δ is a mass

parameter, and at $\tilde{V} = 0$, the fermion spectrum is $\omega^2 = (\tilde{v}_{\rm F}k)^2 + \Delta^2$. The fermion attractive interaction does not destroy the stability of the system, and it only suppresses the mass parameter Δ, i.e., Δ decreases as $\tilde{V}$ increases. Using the eigenfunctional theory,[27−30] by self-consistent solution of the equation of the parameter Δ, we can write down the charge excitation gap near $g = 1/2$,

$$\Delta = \begin{cases} 0, & g \geq 1/2, \\ \dfrac{16g(1-2g)(1+4g)^2}{(1+16g^2)^2} D_0, & g \leq 1/2 \end{cases} \tag{17}$$

which is one of our central results. Obviously, the metal-Mott insulator transition takes place at $g = 1/2$, and this transition is a continuous phase transition. The dependence of the charge excitation gap on the electron interaction strength is completely consistent with the exact solution of the sine-Gordon model.[31−34]

In conclusion, by studying the electron filling factor dependence of the parameter g_c of one-dimensional EHM in the strong coupling regime, it is demonstrated that in the large U limit, in contrast to usual Hubbard model where $g_c = 1/2$, the dimensionless coupling parameter g_c heavily depends on the electron filling factor n, and it has the "particle–hole" symmetry about the point $n = 1/2$. Away from the electron quarter filling, the parameter g_c decreases as the repulsive interaction potential V increases, this means that the single particle spectral weight is transferred from low energy to high energy regimes, while as $V \to \infty$ it goes to a non-zero constant which only depends on electron filling factor. At the electron quarter filling, there takes place the metal-Mott insulator transition at the strong coupling point $g_c = 1/4$, and this transition is a continuous phase transition.

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