Functional renormalization group approach for extended Hubbard model in a triangular lattice

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Abstract.
The extended Hubbard model in an anisotropic triangular lattice is analyzed at quarter filling by the functional renormalization group (fRG) approach. We obtain the finite temperature phase diagram in the plane of nearest inter-site Coulomb interaction \(V_p\) and next-nearest Coulomb interaction \(V_c\). When \(V_p \approx V_c\), charge order does not occur down to the low temperature of \(0.1t_p\), where the \(t_p\) is the electron transfer between the nearest neighbor sites. We interpret the result using the random-phase approximation (RPA).

1. Introduction
The charge ordered and disordered system with strong electron correlation is one of the attractive issues in the recent transition metal oxides as well as the low dimensional organic salts. Above all, the charge order associated with the macroscopic electric polarization is an interesting topic. Since the charge order without the inversion symmetry is responsible for the macroscopic electric polarization, this kind of material is known as the electronic ferroelectricity [1]. Layered iron oxide \(\text{LuFe}_2\text{O}_4\) is a candidate for the electronic antiferroelectricity where the charge order of \(\text{Fe}^{2+}\) and \(\text{Fe}^{3+}\) in the paired triangular lattice produces the electric dipole moment [2]. Another example is \(\kappa-(\text{BEDT-TTF})_2\text{Cu}_2(\text{CN})_3\) [3, 4], in which the anomaly in the dielectric constant is observed in the experiment. This material is a 1/4 filled system, since the number of the hole carrier is 0.25 per BEDT-TTF molecule. It has a frustrated lattice structure, since two BEDT-TTF molecules form a dimer to constitute a triangular lattice. In the strong dimer coupling limit, one electron per dimer occupies the bonding orbital originated from the two molecule orbitals. From this point of view, studying the 1/4 charge order models in a triangular lattice is an interesting theoretical topic. In fact, several authors have studied the so-called 1/4 charge ordered models in a triangular lattice [5, 6, 7, 8, 9]. They showed the existence of competition of several charge ordered phases in an anisotropic triangular lattice with two kinds of the electron transfer and the inter-site Coulomb interactions. In the parameter region where there is strong competition, they expect some non-trivial phenomena such as the metallic phase or superconductivity.

In this paper, we present a theoretical study of the extended Hubbard model in an anisotropic triangular lattice at quarter-filling by weak coupling approach. We analyze the model by using the functional renormalization group (fRG) method. It is known that this method reproduces several static quantities in the Hubbard model calculated by the quantum Monte-Carlo simulation up to the intermediate coupling regime. We obtain the finite-temperature
phase diagram in the plane of the two inter-site Coulomb interactions. When there is strong competition among the two Coulomb interactions, the charge order does not occur down to the low temperature of $0.1t_p$, where the $t_p$ is the electron transfer between the nearest neighbor sites. We interpret the result using the random-phase approximation (RPA).

2. Model and method

We consider the extended-Hubbard model in a triangular lattice at quarter-filling. The Hamiltonian is given by

$$H = \sum_{\langle ij \rangle} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_i \uparrow n_i \downarrow + \sum_{\langle ij \rangle} V_{ij} n_i n_j,$$

where $c_{i\sigma}^\dagger$ is the electron creation operator with spin $\sigma$ at site $i$, and $n_i(=\sum_{\sigma} n_{i\sigma} = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma})$ is the number operator. We introduce the electron transfer $t_{ij}$, the on-site Coulomb interaction $U$, and the inter-site Coulomb interaction $V_{ij}$. We consider the square lattice with diagonal bonds along $[1\bar{1}]$ direction as shown in Fig. 1, which is equivalent to the triangular lattice. The transfer integral and the inter-site Coulomb interaction between the nearest neighbor sites along $[10]$ and $[01]$ directions are denoted by $t_p$ and $V_p$, respectively, and those along the $[1\bar{1}]$ direction are denoted by $t_c$ and $V_c$, respectively. It is obvious that this system is an isotropic triangular lattice when $t_p = t_c$ and $V_p = V_c$. We mainly report the result at $t_c = 0$.

We used the functional renormalization group (fRG) method [10, 11, 12, 13, 14]. The basic procedure of the fRG calculation is as follows: The susceptibility is expressed as a functional derivative of a generating functional of the green function. Let us consider an infinitesimal change in a certain parameter in a system. This parameter, termed a flow-parameter, determines the quadratic part of the action and remains independent in the remainder part of the action. By differentiating the generating functional of the green function with respect to the flow parameter, we can obtain the renormalization group equation, where the derivative of the generating functional is written as a functional of the generating functional. It is straightforward to rewrite this equation for the susceptibility by taking functional derivatives. Integrating the renormalization group equation from the bare-coupling regime, we can obtain the susceptibilities at strong correlated regime.

For numerical calculation, there are two major approximations: 1) two-loop truncation which neglects the two-loop contribution and 2) the static approximation, which neglects the Matsubara frequency dependence of the four-point vertex. These approximations are
partly justified because the neglected diagrams often have small contribution in phase volume even at intermediate coupling regime. The fRG method has the advantage of taking account of all Feynman diagrams at one-loop level and including full mode-couplings. In the present calculation, we adopt the temperature flow fRG [15], which is convenient for the finite temperature calculation.

Figure 2. Finite temperature phase diagram The number of discretization in the momentum space of the four point vertex function are taken to be 4 × 4 in (a) and 8 × 8 in (b). The charge ordering temperature is identified by divergence of the charge susceptibility. The metallic phase impies that there is no divergence in susceptibility nor vertex function down to $T = 0.1$. The parameter values are taken to be $t_c = 0$, $U = 10$ and $t_p = 1$.

3. Numerical results
In Fig. 2, we show the finite temperature phase diagram in the plane of $V_p$ and $V_c$. Other parameters are chosen to be $U = 10$ and $t_c = 0$ in a unit of $t_p$. The electron numbers per site are fixed to be 1.5. In this figure, we plot the temperature where the charge susceptibility diverges. The parameter region with $T = 0$ means that there is no divergence in the charge susceptibility nor the vertex function down to $T/t_p = 0.1$. In the regions of large $V_p$ limit or large $V_c$ limit, the charge ordered phase appears respectively, with the characteristic momentum of each charge ordered phase being mentioned later. The metallic phase is stable until large inter-site Coulomb interactions down to $T = 0.1t_p$ when $V_p \approx V_c$. The metallic state in the vicinity of the $V_p = V_c$ line becomes less stabilized as we increase the discretization number of four-point vertex, The global feature in the present results is consistent with the previous phase diagram at $T = 0$ obtained by the exact diagonalization method [16].

Next, we show the momentum dependence of the charge susceptibility in Fig. 3 for several parameter sets of $(V_c, V_p)$. The parameter values are chosen to be $(V_c = 5, V_p = 0)$ and $T/t_p = 0.017$ in (a), $(V_c = 6, V_p = 2)$ and $T/t_p = 2.03$ in (b), and $(V_c = 3, V_p = 4)$ and $T/t_p = 1.64$ in (c). In Fig. 3(a), the peak structures are seen in $(\pi, 0)$ and $(0, \pi)$ which corresponds to the so-called diagonal charge order, and the plateau appears along the line of $q_x + q_y = \pi$. In Fig. 3(b), in addition to the peaks in $(\pi, 0)$ and $(0, \pi)$, a new peak appears at about $(\pi/2, \pi/2)$ which corresponds to the horizontal charge order. In the case of $V_c > V_p$ as shown in Fig. 3(c), the peak position shifts to $(2\pi/3, 2\pi/3)$.

Now we interpret the result by the random-phase approximation (RPA). The charge
Figure 3. Momentum dependence of the charge susceptibility at $(V_c, V_p) = (5, 0)$ in (a), $(V_c, V_p) = (6, 2)$ in (b), and $(V_c, V_p) = (3, 4)$ in (c). Temperatures are chosen to be $T = 0.017$ in (a), 2.03 in (b) and 1.64 in (c). Other parameters are chosen to be $U = 10$, $t_c = 0$, and $t_p = 1$.

The charge susceptibility $\chi(q)$ in RPA is given by

$$\chi_c(q) = \frac{\chi_0(q)}{1 + [U + 2V(q)]\chi_0(q)}. \quad (2)$$

We introduce the bare charge susceptibility as

$$\chi_0(q) = -\sum_p \frac{n_f(\epsilon_p - \epsilon_{p+q})}{\epsilon_p - \epsilon_{p+q}}, \quad (3)$$

where $\epsilon_p = 2t_p[\cos(p_x) + \cos(p_y)] + 2t_c \cos(p_x + p_y)$ is the bare band dispersion, $n_f(q) = 1/[1 + \exp\{(\epsilon_q - \mu)/T\}]$ is the Fermi distribution function, and $V(q) = 2V_p[\cos(q_x) + \cos(q_y)] + 2V_c \cos(q_x + q_y)$ is the Fourier transform of the inter-site Coulomb interaction. The charge susceptibility is enhanced at the momentum where the denominator of Eq. (2) takes its minimum.

We have confirmed that, around $T/t_p = 1$, the momentum dependence of $\chi_0(q)$ is about 10% of its average value. Since this momentum dependence is weaker than that in the inter-site interaction $V(q)$, the wavenumbers where the denominator of Eq. (2) takes its minimum are governed by $V(q)$. Let us consider the following limit in the expression in Eq. (2). i) in $V_c = 0$, $V(q)$ takes its minimum at $q = (\pi, \pi)$. With increasing $V_c$ from $V_c = 0$, the minimum point of $V(q)$ remains at $q = (\pi, \pi)$ until a certain value of $V_c$ which is termed $V_c^*$. In the region of $V_c > V_c^*$, the minimum point shifts to an incommensurate wave number. ii) in the case of $V_p = V_c(\equiv V)$, $V(q)$ takes its minimum at $q = (\frac{2\pi}{3}, \frac{2\pi}{3})$, regardless of the value of $V$. iii) in $V_p = 0$, the momentum where $V(q)$ takes its minimum satisfies the condition $q_x + q_y = \pi$.

From the above considerations based on the momentum dependence of $V(q)$, the numerical results by fRG methods shown in Fig. 3(a) and (c) are consistent with the expectations from
the RPA expression. Large peak structures around \((\pi, 0)\) and \((\pi/2, \pi/2)\) in Fig. 3(b) may be due to the effects of \(\chi_0(q)\) and/or the renormalization.

4. Conclusion
To summarize, we have analyzed the extended Hubbard model in an anisotropic triangular lattice by using the functional renormalization group method. The finite-temperature phase diagram is obtained in the plane of the two inter-site Coulomb interactions, \(V_p\) and \(V_c\). In the limit of large \(V_p\) and \(V_c\), the charge order with the momentum of \(q = (\pi, \pi)\) and \(q = (\pi, 0)\) are realized respectively. When \(V_p \approx V_c\), the charge order does not occur down to the low temperature of 0.1\(T_p\). The obtained numerical results are interpreted by the random-phase approximation.

One possible extension of the present calculation is applying this method to the triangular lattice with the internal degree of freedom, such as the dimer degree of freedom at each site. Since some electronic ferroelectric materials such as \(\kappa-(BEDT-TTF)_{2}Cu_{2}(CN)_3\) are located near the boundary of the metal-insulator transition, this theoretical approach may provide supplemental information to that of the strong coupling approach in resolving the mechanism of ferroelectricity.

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5. References
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