DMFT study of the local correlation effects in quasi-periodic system

Nayuta Takemori and Akihisa Koga
Department of Physics, Tokyo Institute of Technology, Meguro, Tokyo 152-8551, Japan
E-mail: takemori@stat.phys.titech.ac.jp

Abstract. We study a two-dimensional Hubbard model on a Penrose lattice by means of the real-space dynamical mean-field theory. Calculating the renormalization factor and density of states at each site, we discuss local electron correlations on the quasi-periodic structure. It is found that the renormalized metallic state appears near the Mott transition in the Penrose lattice system. We also address a spatially-dependent renormalization characteristic of the quasi-periodic lattice.

1. Introduction
Since the discovery of quasicrystalline Al-Mn alloys [1], quasiperiodic systems have attracted considerable interest. One of the characteristic features of these systems is the existence of long-range order without translational symmetry, which should yield interesting low-temperature properties in the metallic quasicrystals [2, 3]. The tight-binding model on some quasiperiodic lattices has theoretically been studied and intrinsic properties such as the existence of the confined states and fractal dimensions, have been clarified [4, 5]. Recently, quantum critical behavior has been observed in the Tsai-cluster quasicrystal compounds Au51Al34Yb15, which stimulates further theoretical investigations on strong correlations in the quasiperiodic systems [7, 8].

In our previous paper[9], we have studied the half-filled Hubbard model on the Penrose lattice as an example of strongly correlated electron systems on the quasiperiodic lattice. We have clarified that nontrivial renormalizations depending on the local geometry appear when the system approaches the Mott transition point. However, it was not so clear how the edge of the system affects low temperature properties. Therefore, in this paper, we focus on the heavy metallic state around the Mott transition to discuss how the correlated metallic state is realized in the bulk and around the edge of the system. For this purpose, we study the two-dimensional Hubbard model on the Penrose lattice by means of the real-space dynamical mean-field theory (RDMFT). By calculating the renormalization factor and density of states at each site, we discuss site-dependent electron correlations in the Penrose lattice.

This paper is organized as follows. In Sec. 2, we introduce the model Hamiltonian and explain our theoretical approach. We discuss how the quasiperiodic structure affects local electron correlations around the Mott transition point at low temperatures in Sec. 3. Brief summary is given in Sec. 4.
Figure 1. (Color online) (a) Two-dimensional Penrose lattice. The lattice is composed of shaded (fat) and open (skinny) rhombuses. (b) Pentagon structures $P_\alpha$ and $P_\beta$. We label center sites in $P_\alpha$($P_\beta$) as A(B).

2. Model and Method

We consider the single-band Hubbard model on the Penrose lattice, which should be given by the following Hamiltonian

$$ H = -t \sum_{\langle i,j \rangle} (c_{i \sigma}^\dagger c_{j \sigma} + h.c.) + U \sum_i n_{i \uparrow} n_{i \downarrow}, \quad (1) $$

where $\langle i, j \rangle$ denotes the nearest neighbor site, $c_{i \sigma}^\dagger$($c_{i \sigma}$) is a creation (annihilation) operator of an electron at the $i$th site with spin $\sigma(=\uparrow, \downarrow)$ and $n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma}$. $t$ is the transfer integral between sites and $U$ is the Coulomb interaction. The vertex model on the Penrose lattice is bipartite, and its ground state is expected to be an antiferromagnetically ordered state when $U \neq 0$. Namely, the spontaneous staggered magnetization appears in the Heisenberg limit ($U/t \to \infty$) [11]. In contrast, electron correlations at finite temperatures may not be trivial. When $U = 0$, there appears an interesting density of states due to the local lattice geometry. There are many pentagon structures in the Penrose lattice, as shown in Fig. 1. Each central vertex has locally a five-fold rotational symmetry, which leads to a number of isolated confined states [4]. When the system is half-filled, the corresponding energy is located at the Fermi level and it may be difficult to treat electron correlations in the system. In addition, the spatial dependence of the renormalization is highly nontrivial in the quasi-periodic system since the coordination number ranges from 3 to 7 and the geometrical structure depends on the lattice site. Here, we consider the Penrose Hubbard model under the open boundary condition. The lattice is iteratively generated by applying the inflation rule to the pentagon structure composed of the five fat rhombuses.

In the paper, we use the RDMFT method, which allows us to obtain reliable results if spatially extended correlations are negligible. In fact, the method has successfully been applied to correlated particle systems such as surface [15], interface [16], fermionic atoms [17] and topological insulating systems [18]. In RDMFT, the lattice model is mapped to the effective impurity models dynamically connected to each "heat bath". The lattice Green’s function is
then obtained via the self-consistency condition imposed on these impurity problems. In the framework of RDMFT, the lattice Green’s function $G_{\text{lat}}$ is given in terms of the site-diagonal self-energies $\Sigma_i$ as

$$
G_{\text{lat}}^{-1}(i\omega_n) = 
\begin{pmatrix}
  i\omega_n + \mu - \Sigma_1 & -t & 0 & \cdots & -t \\
  -t & i\omega_n + \mu - \Sigma_2 & -t & \cdots & 0 \\
  0 & -t & i\omega_n + \mu - \Sigma_3 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  -t & 0 & 0 & \cdots & i\omega_n + \mu - \Sigma_N
\end{pmatrix}. 
$$

(2)

where $\mu$ is the chemical potential, $\omega_n = (2n + 1)\pi T$ is the Matsubara frequency, and $T$ is the temperature. The local Green’s function for the site $i$ is obtained from the diagonal part of the lattice Green’s function, $G_{\text{loc}}(i\omega_n) = G_{\text{lat}}^{-1}(i\omega_n)$.

To solve the effective impurity model for each site, we use the iterative perturbation theory (IPT) [19]. This method is based on the second order perturbation theory and is appropriate to describe the Mott transitions for a single-band Hubbard model with the particle-hole symmetry. Furthermore, this method has an advantage in efficiently evaluating the self-energy of the effective impurity model. The local self-energy is obtained by the effective medium $G^0_i$ for the $i$th site, as

$$
\Sigma_i(i\omega_n) = -(UT)^2 \sum_{lm} G^0_l(i\omega_l)G^0_m(i\omega_m)G^0_l(i\omega_n + i\omega_l - i\omega_m),
$$

(3)

$$
G^0_{i}^{-1}(i\omega_n) = G_{\text{loc}}^{-1}(i\omega_n) + \Sigma_i(i\omega_n).
$$

(4)

To discuss Mott transitions, we focus on the half-filled system, setting the chemical potential as $\mu = U/2$. We neglect ordered states such as density wave and magnetically ordered states, and consider the paramagnetic solution with $\langle n_{i\sigma} \rangle = 0.5$. In order to discuss local electron correlations, we calculate the following quantities, $z_i = [1 - \text{Im}\Sigma_i(i\omega_0)/\omega_0]^{-1}$, which can be regarded as the renormalization factors at finite temperatures. In the following, we use the transfer integral $t$ as the unit of the energy and treat the Penrose lattice with 4481 sites, where there are 444 independent sites under the five-fold rotational symmetry.

3. Results

In the paper, we focus on the correlated metallic state near the Mott transition point at low temperatures, applying the RDMFT method to the two-dimensional Penrose Hubbard model. It has been clarified that the Mott transition occurs in the system at a certain interaction $U_c = 12.82$, where local quantities such as the double occupancy and renormalization factor have jump singularities [9]. In addition, there is the other transition point $U'_c = 12.79$, where the local quantities for some sites have jump singularities. In fact, one finds in Fig. 2 (a) two jump singularities in some curves of the renormalization factors for the center sites of the pentagon structures. The density plots of the renormalization factors for all sites are shown in Fig. 2 (b). When $U = 12.75(< U'_c)$, the system is in the metallic state, where the two peak structures appear around $z \sim 0.03$ and 0.043. Once the transition occurs at $U = U'_c$, two peak structures are slightly changed, while the peak structure at $z = 0$ suddenly develops, as shown in Fig. 2 (b). This implies that strongly renormalized electrons ($z \sim 0$) are newly realized at the corresponding sites.

To clarify this phenomenon, we show in Fig. 3 the distribution of the renormalization factors in the Penrose lattice. When $U = 12.75$, the system is metallic, where a finite renormalization factor appears in the bulk. We find that at the edge sites with two connecting bonds and their nearest neighbor sites, the renormalization factors are almost zero. Increasing the interaction $U$
Figure 2. (a) Renormalization factors for A and B sites at $T = 0.02$. (b) Cross-section of the density plot of renormalization factors in the half-filled Penrose-Hubbard model at $T = 0.05$ when $U = 12.75$ and $U = 12.8$. The unit of energy is set to be $t$.

Figure 3. The distribution of the renormalization factors in the Penrose Hubbard model with (a) $U = 12.75$, (b) $U = 12.8$. The diameter of a circle on each vertices indicates the value of renormalization factors. The positions of $A_b$, $B_b$, $A_r$ and $B_r$ are explicitly shown. We note that $B_b$ is located at the center of the system. Beyond $U = U_c'$, the renormalization factors in the ring region with a certain thickness, which is bounded by the dashed lines shown in Fig. 3, are suddenly decreased, as shown in Fig. 3 (b). Therefore, we can say that the transition at $U = U_c'$ originates from the open boundary effect in the Penrose lattice. Further increase of the interaction leads to the Mott transition at $U = U_c$. In the case $U > U_c$, the renormalization factor for each site vanishes.

To clarify how the heavy metallic state is realized in the region $U < U_c$, we also show the local density of states for the bulk and ring regions, as shown in Fig. 4. First, we focus on the local density of states at a certain $A$ site in the bulk. When $U = 12.75$, the sharp quasi-particle peak appears in the density of states, as shown in Fig. 4 (a). Since the transition $U = U_c'$ little affects low temperature properties in the bulk, the density of states are not changed qualitatively. Increasing the interaction, the Mott transition occurs at $U = U_c$, and the quasiparticle peak at $\omega = 0$ vanishes. In contrast, different behavior appears in the ring region, as shown in Fig. 4 (b). It is found that the height of the peak structure at $\omega = 0$ is suddenly changed at $U = U_c'$. 
As shown in Fig. 4(b), which corresponds to behavior for the local renormalization factors.

To understand the nature of the intermediate regime \( (U'_{c} < U < U_{c}) \) more clearly, we show in Fig. 4 (c) the imaginary part of the self-energies for \( A_{b} \), \( A_{r} \), \( B_{b} \), and \( B_{r} \) sites, where the positions of \( A_{b} \), \( A_{r} \), \( B_{b} \), and \( B_{r} \) are explicitly shown in Fig. 3 (b). For the bulk region \( (A_{b} \) and \( B_{b} \)), the imaginary part of the self-energy little changes when the interaction \( U \) is changed from \( U = 12.75 \) to 12.8. Although a difference appears for the sites \( A_{r} \) and \( B_{r} \) in the ring region, the metallic behavior is not changed. Once \( U \) increases beyond \( U_{c} \), insulating behavior clearly appears in all sites. Therefore, we can say that the metal-insulator transition occurs only at \( U_{c} \) in this system. To clarify whether or not such low-temperature properties appear in the Hubbard model on a simple lattice, we perform similar calculations with the square lattice under the open boundary condition \( (39 \times 39 \text{ sites}) \). We do not find two singularities, but a single Mott transition at \( U \sim 13.9 \). Therefore, we believe that two singularities discussed above are not due to our numerical technique, but are characteristic of electron correlations on the Penrose lattice.
4. Summary
In summary, we have investigated the half-filled Hubbard model on the two-dimensional Penrose lattice, combining the RDMFT with the IPT. Computing the renormalization factor and density of states at each site, we have discussed in detail how the renormalized metallic state is realized near the Mott transition. It has been clarified that in a certain ring region, heavy metallic states characteristic of the Penrose-Hubbard model are realized in the case $U'_c < U < U_c$. It is interesting to study the effect of the defects and impurities in the strongly correlated electron systems on the quasiperiodic systems, which is now under consideration.

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