Cluster Size Effects on Electronic Reconstruction in Quasiperiodic System

Ryu Shinzaki, Joji Nasu, and Akihisa Koga
Department of Physics, Tokyo Institute of Technology, Meguro-ku, Tokyo 152-8551, Japan
E-mail: koga@phys.titech.ac.jp

Abstract. We study the extended Anderson model on a two-dimensional Penrose lattice to discuss how the electronic reconstruction in the valence is realized at low temperatures. Making use of the real-space dynamical mean-field theory combined with the continuous-time quantum Monte Carlo method, we find that inhomogeneous electronic distribution appears at low temperatures. The system size dependence is also addressed.

Strong electron correlations in the rare-earth or actinide compounds have attracted great attention, where exotic low-temperature properties have been observed such as heavy fermion behavior [1, 2, 3], valence fluctuations [4, 5], and quantum critical behavior [6]. It has been understood that these interesting properties are attributed to the itinerancy of f electrons through the hybridization to conduction bands and strong electron correlations. Recently, intriguing phenomena have been observed in the Au – Al – Yb alloy [7]. The quasicrystal Au$_{51}$Al$_{34}$Yb$_{15}$, where Tsai-type clusters are arranged with quasiperiodic structure, exhibits the divergence in the magnetic susceptibility and the specific heat with unconventional critical exponents. This quantum critical behavior is contrast to heavy fermion behavior in the approximant Au$_{51}$Al$_{35}$Yb$_{14}$ with periodic structure. Furthermore, the ytterbium ions have intermediate valence [7, 8, 9], which should suggest that the quasiperiodicity and/or valence fluctuations play an essential role in understanding the exotic behavior of the quasicrystal Au$_{51}$Al$_{34}$Yb$_{15}$ [10, 11, 12].

In our previous study, we have considered strongly correlated electron systems on a two-dimensional Penrose lattice [13, 14, 15], making use of the real-space version of dynamical mean-field theory (R-DMFT) [16, 17, 18, 19]. In particular, we have discussed valence fluctuations inherent in the quasiperiodic lattice, by comparing with the results for the periodic lattice. However, it is still unclear whether or not such interesting behavior is realized even in the periodic system with a large unit cell. The first step to answer this fundamental and difficult question is to clarify how the system size affects the electronic reconstruction at low temperatures. To this end, we discuss low-temperature properties in distinct clusters.

We study the extended Anderson lattice model [13, 20, 21, 22, 23], which should be described by the following Hamiltonian,

\[ H = -t \sum_{\langle i, j \rangle, \sigma} c_{i \sigma}^\dagger c_{j \sigma} + V \sum_{i, \sigma} (c_{i \sigma}^\dagger f_{i \sigma} + \text{H.c.}) + \epsilon_f \sum_{i, \sigma} n_{i \sigma}^f + U_{ff} \sum_{i} n_{i \uparrow}^f n_{i \downarrow}^f + U_{cf} \sum_{i, \sigma, \sigma'} n_{i \sigma} c_{i \sigma'}^\dagger, \]  

(1)
where \( c_{i\sigma} (f_{i\sigma}) \) is an annihilation operator of a conduction electron \((f)\) electron with spin \( \sigma(=\uparrow, \downarrow) \). \( n_{i\sigma}^c (= c_{i\sigma}^\dagger c_{i\sigma}) \) and \( n_{i\sigma}^f (= f_{i\sigma}^\dagger f_{i\sigma}) \) are the number operators of the conduction and \( f \) electrons at the \( i \)th site, respectively. \( t \) is the hopping integral of the conduction electrons between the nearest-neighbor sites, \( V \) is the hybridization between the conduction band and \( f \) orbitals, and \( \epsilon_f \) is the energy level of the \( f \) orbitals. \( U_{ff} \) and \( U_{cf} \) are the repulsive interactions between the \( f \) electrons, and between the conduction and \( f \) electrons. We consider here the vertex model of the two-dimensional Penrose lattice \([13, 14, 15]\). In this lattice, sites are placed on the corner of the rhombuses and the coordination number \( Z \) ranges from three to seven except for the edge sites.

In the paper, we make use of the R-DMFT \([16]\). In the R-DMFT, the lattice Green’s function \( G_\sigma (i\omega_n) \) is assumed to be described by the site-diagonal selfenergy \( \Sigma_{i\sigma}(i\omega_n) \). This allows us to introduce the impurity models at each site, in which local electron correlations are taken into account properly. The noninteracting Green’s function of an effective bath at the \( i\)th site is determined as \( G_{\sigma}^{(i)} (i\omega_n)^{-1} = \left[ G_{\sigma}^{-1} (i\omega_n) \right]_{ii} + \sum_{\sigma'} \Sigma_{i\sigma}(i\omega_n) \). These self-consistent calculations are iterated until the Green’s functions are converged. In our study, we solve the impurity models by means of the continuous-time quantum Monte Carlo method based on the hybridization expansion \([24]\).

To discuss low temperature properties in the quasiperiodic lattice, we calculate the local quantities such as \( f \)-electron number \( \langle n_{i}^f \rangle \) and magnetic susceptibility \( \chi_l = \int_0^\beta d\tau \langle M_i^z(\tau) M_i^z\rangle_{\text{imp}} \), where \( M_i^z = n_{i^+}^c - n_{i^+}^c + n_{i^-}^f - n_{i^-}^f \) is the local magnetic moment operator. For simplicity, the total susceptibility is assumed to be given as \( \chi = \sum_i \chi_i / N \), where \( N \) is the total number of sites. Here, we use \( t \) as the unit of energy. We choose the parameters as \( U_{ff}/t = 20, U_{cf}/t = 5 \), and \( V/t = 0.2 \). The total electron number per site is fixed as \( \langle n^c \rangle + \langle n^f \rangle = 1.9 \), where \( \langle n^c \rangle = \sum_i \langle n_i^c \rangle / N \), and \( \langle n^f \rangle = \sum_i \langle n_i^f \rangle / N \). To discuss how the electronic reconstruction is realized in the quasiperiodic lattice, we treat different clusters with \( N = 86 \) and \( 601 \), which are generated in terms of the inflation-deflation rule \([25]\).

First, we discuss valence fluctuations in the larger cluster with \( N = 601 \). Figure 1(a) shows the \( f \)-level dependence of the valence \( \langle n_{i}^f \rangle \) when \( t/t = 0.2 \). We find that the increase of \( \epsilon_f \) decreases the valence from unity to zero without any singularities. Since the \( c - f \) spin correlations are not enhanced at the temperature (not shown), this indicates the crossover from the local moment state to mixed-valence state around \( \epsilon_f / t \sim -4 \), where the valence susceptibility \( \chi_v = -\Delta \langle n_i^f \rangle / \Delta \epsilon_f \) takes a maximum. We wish to note that the inhomogeneous electronic reconstruction appears in the crossover region \( \epsilon_f / t \sim -3 \) \([13, 15]\), which is characteristic of the

![Figure 1](image-url)
Figure 1(b) shows the density profiles for the local moment, crossover, and mixed-valence regions when $\epsilon_f/t = -6$, $-3$ and $-1$, respectively. In contrast to the cases of the local moment and mixed-valence regions, the valence distributes in a certain range when the system is in the crossover region. This implies the existence of the electronic reconstruction, which never appears in the periodic systems [13, 15].

To clarify how the electronic reconstruction inherent in a quasiperiodic lattice is realized, we show in Fig. 2(a) the density profiles of the valence at distinct temperatures in the systems with $N = 86$ and 601. At a high temperature $T/t = 7$, the electron valence is uniform in the lattice and $\langle n_f \rangle \sim 0.8$. In the case, we do not find any differences in the results for distinct clusters. Therefore, the quasiperiodic feature does not appear in the correlated electron systems at higher temperatures. However, the decrease of the temperature enhances site-dependent behavior, yielding the valence distribution. When $T/t = 0.75$, $\langle n_f \rangle$ distributes in a range $0.5 < \langle n_f \rangle < 0.7$. An important point is that the distributions for the clusters with $N = 86$ and 601 are slightly different from each other. This implies that the correlation length becomes longer with decrease of temperature, and thereby a large cluster, at least, with $N = 601$ sites is necessary to describe the electronic reconstruction correctly. Moreover, at lower temperatures, this behavior becomes more serious. In fact, the valence distribution in a larger cluster is quite different from the smaller one except for the peak around $\langle n_f \rangle \sim 0$. Therefore, a larger cluster may be necessary to describe the electronic reconstruction at lower temperatures more precisely.

In the Penrose lattice, sites are not equivalent to each other, but any cluster exists with a finite density, which is in contrast to the periodic system. Therefore, if the correlation length becomes longer with decreasing temperatures, the valence distributions are drastically changed [13]. In this sense, it should be hard to distinguish the properties of the periodic and quasiperiodic systems when the correlation length is shorter than the scale of its unit cell.

Finally, we consider how the magnetic response is affected by the system size and boundary effects. Figure 2 (b) shows the temperature dependence of the magnetic susceptibility $\chi$. In this parameter with $\epsilon_f/t = -3$, nonmonotonic behavior appears in the magnetic susceptibility, which is mainly reflected by the change in the number of valence [15]. Although the valence distribution strongly depends on the system size discussed above, the bulk magnetic susceptibility has little changed. This may imply that it is hard to see interesting electronic properties reflected by the quasiperiodic nature discussed above in terms of the bulk quantities.

In our work, only two different clusters with global fivefold rotational symmetry have been
dealt with due to numerical limitations. Although the systematic analysis for the cluster size, cluster shape, and/or boundary dependence have not been done, we have carefully examined local and bulk quantities in distinct clusters. We have then clarified that the cluster dependence becomes crucial with decreasing temperatures. This implies that, in the system with large valence fluctuations, the correlation length plays an important role and the effect of the cluster size and/or its shape should not be negligible at low temperatures. We have confirmed that in the Kondo region, the cluster size little affects low temperature properties (not shown) since the Kondo singlet is stabilized locally and the correlation length is very short. This is common to the physics in the strongly correlated electron systems with the periodic lattice. Therefore, low temperature properties characteristic of the quasiperiodic structure should appear when spin, orbital and/or valence fluctuations are enhanced.

In summary, we have investigated the extended Anderson model on the two dimensional Penrose lattice. Making use of the R-DMFT, we have calculated the $f$-electron number and bulk magnetic susceptibility. By comparing with the results with distinct clusters, it has been clarified that the correlation length becomes longer with decreasing temperatures and the electronic reconstruction appears inherent in the Penrose lattice.

Acknowledgments

We would like to thank N. Takemori for valuable discussions. Parts of the numerical calculations were performed in the supercomputing systems in ISSP, the University of Tokyo. This work was partly supported by the Grant-in-Aid for Scientific Research from JSPS, KAKENHI Grant Number 25800093, 16H01066 (A.K.), and 16K17747 (J.N.). The simulations have been performed using some of the ALPS libraries [26].

References

[1] Andres K, Graebner E J, and Ott R H: Phys. Rev. Lett. 35 (1975) 1779.
[2] Stewart R G: Rev. Mod. Phys. 56 (1984) 755.
[3] Satoh K, Fujita T, Maeno Y, Onuki Y, and Komatsubara T: J. Phys. Soc. Jpn. 58 (1989) 1012.
[4] Gschneidner A K and Eyring L: Handbook on the Physics and Chemistry of Rare Earths (1978)
[5] Manheimer A M and Parks D R: Phys. Rev. Lett. 42 (1979) 321.
[6] Doniach S: Physica B+C 91 (1977) 231.
[7] Deguchi K, Matsukawa S, Sato K N, Hattori T, Ishida K, Takakura H, and Ishimasa T: Nat. Mat. 11 (2012) 1013.
[8] Matsukawa S et al.: J. Phys. Soc. Jpn. 83 (2014) 034705.
[9] Watanuki T, Kashimoto S, Kawana D, Yamazaki T, Machida A, Tanaka Y, and Sato J T: Phys. Rev. B 86 (2012) 094201.
[10] Watanabe S and Miyake K: J. Phys. Soc. Jpn. 82 (2013) 083704.
[11] Andrade C E, Jagannathan A, Miranda E, Vojta M, and Dobrosavljević: Phys. Rev. Lett. 115 (2015) 036403.
[12] Otsubo J, Kusunose H: J. Phys. Soc. Jpn. 85 (2016) 073712.
[13] Takemura S, Takemori N, and Koga A: Phys. Rev. B 91 (2015) 165114.
[14] Takemori S and Koga A: J. Phys. Soc. Jpn. 84 (2015) 023701.
[15] Shimizaki R, Nasu J, and Koga A: J. Phys. Soc. Jpn. 85 (2016) 114706.
[16] Georges A, Kotliar G, Krauth W, and Rozenberg J M: Rev. Mod. Phys. 68 (1996) 13.
[17] Helmes R W, Costi T A, and Rosch A: Phys. Rev. Lett. 100, 056403 (2008).
[18] Snoek M, Tivvinidze I, Töke C, Byczuk K, and Hofstetter W: New J. Phys. 10, 093008 (2008).
[19] Koga A, Higashiyama T, Inaba K, Suga S, and Kawakami N, J. Phys. Soc. Jpn. 77, 073602 (2008); Phys. Rev. A 79, 013607 (2009).
[20] Onishi Y and Miyake K: J. Phys. Soc. Jpn. 69, 3955 (2000).
[21] Watanabe S, Inada M, and Miyake K: J. Phys. Soc. Jpn. 75 (2006) 043710.
[22] Kojima Y and Koga A: JPS Conf. Proc. 1 (2013) 012106.
[23] Shimizaki R, Nasu J, and Koga A: J. Phys.: Conf. Ser. 683 (2016) 012041.
[24] Werner P, Comanac A, de’ Medici L, Troyer M, and Millis J A: Phys. Rev. Lett. 97 (2006) 076405.
[25] Levine D and Steinhardt P J: Phys. Rev. Lett. 53, 2477 (1984).
[26] Bauer B et al.: J. Stat. Mech. Theory Exp. 2011 (2011) P05001.