Physics Procedia
Volume 75, 2015, Pages 245–251
20th International Conference on Magnetism

Correlation Effects in One-Dimensional Quasiperiodic Anderson-Lattice Model

Fuyuki Matsuda *, Masaki Tezuka, and Norio Kawakami

Kyoto University, Kitashirakawa, Sakyo, Kyoto 606-8502, Japan

Abstract
We consider the one-dimensional (1D) quasiperiodic Anderson-lattice model, which has quasiperiodically ordered impurities. The sites with an f-orbital are ordered as a "Fibonacci word", one way to form 1D quasiperiodic orderings. To treat the correlation effect precisely, we use the density matrix renormalization group (DMRG) method. We show that the spin correlation function in the quasiperiodic system gives a characteristic pattern. Also, by analyzing the f-electron number and its fluctuation, we find that a valence transition, which usually occurs in the periodic Anderson model when the on-site interorbital interaction is large, is not sharp in the quasiperiodic system. Finally, we discuss the properties of the quasiperiodic Anderson-lattice model, comparing them against the Anderson-lattice model with randomly located f-orbitals. We find that the quasiperiodic Anderson-lattice model has a similar property to the periodic Anderson model for spin correlation, but also has a similar property to the Anderson-lattice model with randomly located f-orbitals for the valence fluctuation.

Keywords: Anderson-lattice model, Quasiperiodicity, DMRG

1 Introduction

Quasicrystals are solids which have a long-range order called quasiperiodicity but do not possess lattice periodicity. Since the discovery of quasicrystals in alloys[1], numerous researches have been conducted for quasicrystals, and many intriguing properties of quasicrystals have been found[2, 3, 4]. A question comes up naturally: Are there any properties which are peculiar to quasicrystals?

Recently, one answer to this question has been suggested. Deguchi et al.[5] have argued that they observed quantum critical phenomena of the Au-Al-Yb quasicrystal. In this quasicrystal, the magnetic susceptibility and the electronic specific heat coefficient diverge as $T \to 0$ due to the strongly correlated 4f electrons of the Yb atoms. Interestingly, this quantum critical phenomenon is robust against hydrostatic pressure. Moreover, quantum criticality has not been

*fuyuki.matsuda@scphys.kyoto-u.ac.jp

Selection and peer-review under responsibility of the Scientific Programme Committee of ICM 2015

doi:10.1016/j.phpro.2015.12.030

observed in the crystalline approximant of the quasicrystal material. The effects of quasiperiodicity in this system are still being discussed[6, 7, 8], so it is necessary to reveal the effects of quasiperiodicity in heavy fermion systems.

Besides such rapid progress in research of heavy-fermion quasicrystals, one dimensional (1D) quasiperiodic systems have also attracted a lot of attention. 1D quasiperiodic systems can be realized in various platforms, for instance, optical waveguides[9], ultracold atoms in optical lattices[10, 11], and so on. In the recent studies of ultracold atoms, the Anderson-lattice model, which have *c*-orbital and *f*-orbital in each sites, has been proposed[12, 13]. Thus, we naturally expect that 1D correlated quasiperiodic systems would provide some insights for a deeper understanding of the correlated quasicrystal systems.

As described above, there are several studies on 2D or 3D heavy-fermion quasicrystals, but no previous work about them in 1D to the best of our knowledge. In this paper, in order to understand the effects of quasiperiodicity in heavy fermion systems, we construct and analyze the minimal model for heavy-fermion based quasicrystals which we call 1D quasiperiodic Anderson lattice model (QPALM). In this model, the sites with an *f*-orbital are ordered as "Fibonacci word", which is known as a method to construct 1D quasiperiodic orderings. To treat the correlation effect precisely, we use the density matrix renormalization group (DMRG) method. We calculate the spin correlation of *f*-orbital fermions, and show that characteristic patterns appear in the spin correlation plot of the QPALM induced by the RKKY interaction. Also, we show that a valence transition in the QPALM is not as sharp as in the periodic Anderson model (PAM) when the on-site interorbital interaction is large. Finally, we compare the properties of the QPALM and the Anderson lattice model with randomly located *f*-orbitals (RfALM).

2 Model and Method

2.1 Model

We consider a quasiperiodic Anderson lattice model described by the Hamiltonian

$$\begin{aligned}\hat{\mathcal{H}} &= \sum_{j\sigma}\epsilon_{\mathrm{f}}\hat{f}^{\dagger}_{j\sigma}\hat{f}_{j\sigma}+\sum_{<i,i'>\sigma}t\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i'\sigma}+\sum_{j\sigma}(V\hat{f}^{\dagger}_{j\sigma}\hat{c}_{j\sigma}+V^{*}\hat{c}^{\dagger}_{j\sigma}\hat{f}_{j\sigma}) \\ &\quad +U_{\mathrm{c}}\sum_{i}(\hat{n}^{\mathrm{c}}_{i\uparrow}-1/2)(\hat{n}^{\mathrm{c}}_{i\downarrow}-1/2)+U_{\mathrm{f}}\sum_{j}(\hat{n}^{\mathrm{f}}_{j\uparrow}-1/2)(\hat{n}^{\mathrm{f}}_{j\downarrow}-1/2)+U_{\mathrm{fc}}\sum_{j}\hat{n}^{\mathrm{f}}_{j}\hat{n}^{\mathrm{c}}_{j}\end{aligned} \tag{1}$$

where $\hat{c}_{i\sigma}(\hat{c}^{\dagger}_{i\sigma})$ annihilates (creates) a fermion at *c*-orbital of site $i \in \mathrm{I}(\equiv \{1, 2, \ldots, N\})$ with spin $\sigma =\uparrow$ or $\downarrow$, $\hat{f}_{j\sigma}(\hat{f}^{\dagger}_{j\sigma})$ annihilates (creates) a fermion at *f*-orbital of site $j \in \mathrm{J}(\subset \mathrm{I})$ with spin $\sigma =\uparrow$ or $\downarrow$, and $\hat{n}^{\mathrm{c}}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$, $\hat{n}^{\mathrm{f}}_{j\sigma} = \hat{f}^{\dagger}_{j\sigma}\hat{f}_{j\sigma}$, $\hat{n}^{\mathrm{c}}_{i} = \hat{n}^{\mathrm{c}}_{i\uparrow} + \hat{n}^{\mathrm{c}}_{i\downarrow}$, $\hat{n}^{\mathrm{f}}_{j} = \hat{n}^{\mathrm{f}}_{j\uparrow} + \hat{n}^{\mathrm{f}}_{j\downarrow}$ are number operators. Here, t denotes the hopping integral between *c*-orbitals of nearest-neighbor sites, which we take it as a unit of other parameters. V is the hybridization of the *c*-orbital and the *f*-orbital, U_{c} and U_{f} respectively represent the on-site interaction of *c*-orbital and *f*-orbital, and U_{fc} represents the Coulomb repulsion between the *f*-orbital and the *c*-orbital on the same site. In our model, only a part of sites have an *f*-orbital, and these sites are ordered as "Fibonacci word", the sequence of binary digits formed by repeated concatenation.

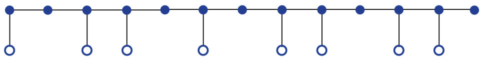

Figure 1: Sketch of our lattice system. Filled circles correspond to *c*-orbitals and open circles correspond to *f*-orbitals.

2.2 Method

Fibonacci words can be generated as follows: Let $S_0 = A$, $S_1 = AB$. Now $S_n = S_{n-1}S_{n-2}$ (the concatenation of two strings) for $n = 2, 3, \ldots$. Then we have $S_2 = ABA$, $S_3 = ABAAB$, $S_4 = ABAABABA$, and so on. The length of each Fibonacci word is a Fibonacci number. We take the total site number as a Fibonacci number, and only sites corresponding to the letter A have an *f*-orbital. For example, for $L = 8$, $\mathrm{J} = \{1, 3, 4, 6, 8\}$.

In 1D systems, the density-matrix renormalization group (DMRG) method is known as an excellent tool to analyze the ground-state properties. In this study, we calculate the spin correlation $\left\langle \hat{S}^{\mathrm{f}}_{z,j}\hat{S}^{\mathrm{f}}_{z,j'}\right\rangle$, the number of *f*-fermions $\left\langle \hat{n}^{\mathrm{f}}_{j}\right\rangle$, and the *f*-orbital density correlation $\left\langle \hat{n}^{\mathrm{f}}_{j}\hat{n}^{\mathrm{f}}_{j'}\right\rangle$ of each site using the ALPS application [14, 15]. From these results, we plot the average of *f*-electrons $\langle n_{\mathrm{f}}\rangle$ and the n_{f} fluctuation $\langle n_{\mathrm{f}}\rangle^2 - \left\langle n_{\mathrm{f}}^2\right\rangle$.

3 Results

In this section, we present the numerical results for the ground state. First, we consider the $U_{\mathrm{fc}} = 0$ case, and show that a characteristic pattern appears in the spin correlations plot. Next, we analyze the effect of a non-zero U_{fc}, which is important for a valence transition of the extended periodic Anderson model, pointed out by Watanabe et al. in previous researches[16]. Finally, we compare the properties of QPALM and RfALM.

3.1 Spin Correlations

First, we consider the spin correlations for the $U_{\mathrm{fc}} = 0$ case. In the usual PAM, the RKKY interaction makes the spin correlations strong when the repulsive interaction U_{f} is sufficiently large. In the case of half-filling, the system has antiferromagnetic order. In the PAM which is under the condition of $\epsilon_{\mathrm{f}} \ll 0 \ll \epsilon_{\mathrm{f}} + U_{\mathrm{f}}$, the system would be in an antiferromagnetic phase. However, in the QPALM, the system is not in an antiferromagnetic phase, but it is expected that the spin correlation is most important for low energy region because of RKKY interaction. In our calculation, we take $\epsilon_{\mathrm{f}} = -5, V = 1, U_{\mathrm{c}} = 1, U_{\mathrm{f}} = 10, U_{\mathrm{fc}} = 0$, and parameters satisfy the above condition. Our results in Fig. 2 shows a typical example for the system in the above condition. Figure 2 (left) shows the spin correlation function of the QPALM, whose filling is near half-filling. Unlike the PAM, the system is not in an antiferromagnetic phase, but there are locally ferromagnetic blocks in the system, with antiferromagnetic interaction with their neighboring blocks. When the *c*-band is half-filled, the RKKY interaction is antiferromagnetic for neighboring *f*-sites, and ferromagnetic for every other *f*-sites. This interaction makes the above-mentioned block structure.

Since QPALM is almost periodic, we can tune the Fermi wavelength and make the QPALM antiferromagnetic by changing the filling. Figure 2 (right) shows such an example with π/k_{F} almost equal to the average distance between neighboring *f*-orbital sites. We can check the

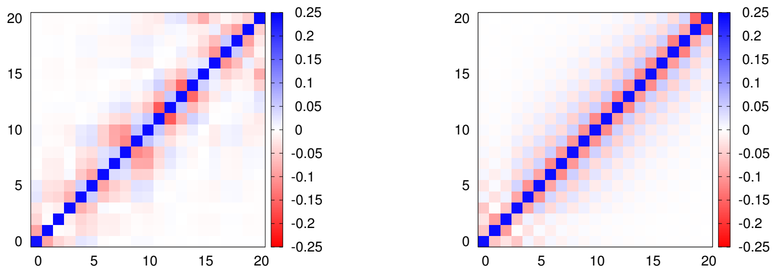

Figure 2: (Color online) Spin correlation function of *f*-electrons $\langle \hat{S}^{\mathrm{f}}_{z,j}\hat{S}^{\mathrm{f}}_{z,j'}\rangle$ of quasiperiodic Anderson-lattice model. $\hat{S}^{\mathrm{f}}_{z,j}$ is defined by $\hat{S}^{\mathrm{f}}_{z,j} = (\hat{n}^{\mathrm{f}}_{j\uparrow} - \hat{n}^{\mathrm{f}}_{j\downarrow})/2$. Here, the system size is $L = 55$ which includes 34 *c*-sites and 21 *f*-sites, $\epsilon_{\mathrm{f}} = -5, V = 1, U_{\mathrm{c}} = 1, U_{\mathrm{f}} = 10, U_{\mathrm{fc}} = 0$. Spin correlation function for $N_\uparrow = N_\downarrow = 28(\simeq L/2)$ ($N_\uparrow = N_\downarrow = 21$) is plotted in the left (right) panel, respectively.

antiferromagnetic phase from its checkered pattern. We note that this kind of pattern cannot be observed if the *f*-sites are randomly located.

3.2 Valence Transition

Next, we consider the PAM. If ϵ_{f} is low enough energetically, the ground state becomes Kondo state, and n_{f} becomes unity. On the contrary, if ϵ_{f} is high enough, all of fermions flow out to the *c*-band, and no fermion is left in the *f*-orbital. From these considerations, there must be an crossover of n_{f} when we change the value of ϵ_{f}. However, finite U_{fc} stabilises the intermediate phase, which is called the mixed valence state. When U_{fc} is sufficiently large, a first-order valence transition occurs between the Kondo state and the mixed valence state, which is shown in previous studies[16]. Figure 3 (left) shows the *f*-electron number $\langle n_{\mathrm{f}}\rangle$ and the valence fluctuation $\langle n_{\mathrm{f}}\rangle^2 - \langle n_{\mathrm{f}}^2\rangle$ as a function of ϵ_{f} for the periodic Anderson model for $U_{\mathrm{fc}} = 8$. Under the condition of $\epsilon_{\mathrm{f}} \ll 0 \ll \epsilon_{\mathrm{f}} + U_{\mathrm{f}}$, each *f*-site must have exactly one electron. In the case of $\epsilon_{\mathrm{f}} \lesssim U_{\mathrm{fc}}$, the mixed-valence state will be stabilized. We choose other parameters to investigate the phase transition between these two phases by taking $V = 0.1, U_{\mathrm{c}} = 0, U_{\mathrm{f}} = 100, U_{\mathrm{fc}} = 8$. We note that our calculation is focused on the parameter region around this phase transition, so we show the results as a typical example by fixing the parameters except ϵ_{f}. There are two sharp peaks in the valence fluctuation plot, and the left peak corresponds to the first-order valence transition. The result is consistent with the above discussion.

Now, we discuss the result for the QPALM. Figure 3 (middle) shows $\langle n_{\mathrm{f}}\rangle$ and $\langle n_{\mathrm{f}}\rangle^2 - \langle n_{\mathrm{f}}^2\rangle$

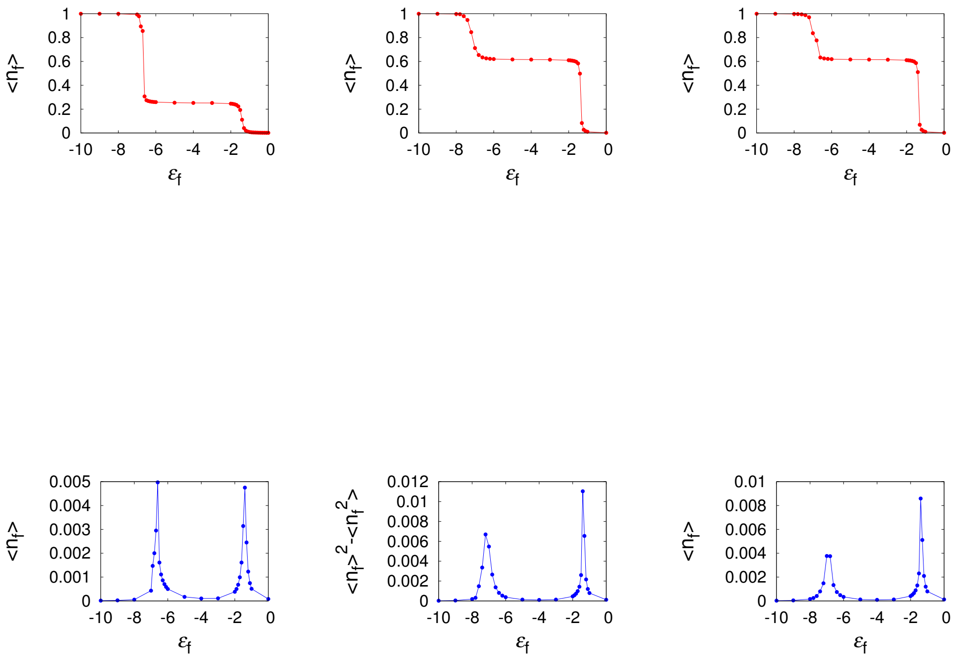

Figure 3: (Color online) The f-electron number and the valence fluctuation as a function of $\epsilon_{\rm f}$ for the periodic Anderson model (left), the quasiperiodic Anderson-lattice model (middle), and the Anderson-lattice model with randomly located f-sites (right) for $V = 0.1$, $U_{\rm c} = 0$, $U_{\rm f} = 100$, $U_{\rm fc} = 8$. System size and particle number are (left) $L = 32$ (16 c-sites, 16 f-sites), $N_\uparrow = N_\downarrow = 16$, (middle) and (right) $L = 34$ (21 c-sites, 13 f-sites), $N_\uparrow = N_\downarrow = 17$, respectively.

as a function of $\epsilon_{\rm f}$ of the QPALM for $U_{\rm fc} = 8$. The results of PAM is consistent with previous studies[16], which showed a sharp peak in valence fluctuation. Compared with the results of the PAM, the first-order valence transition in the QPALM is not as sharp, and the peak of the valence fluctuation is wider. This is consistent with the previous research, which showed that the robustness of the quantum criticality comes from the overlap of critical regimes at each site[6].

3.3 Comparison between quasiperiodic model and random model

In order to discuss the effect of quasiperiodicity on the valence transition, we analyze the RfALM. The results are shown in Fig. 3 (right). In this system, the first-order valence transition point is unsharpened, and the peak of the valence fluctuation is widened compared with PAM. It is hard to distinguish between QPALM and RfALM from these results. This suggests that the quasiperiodicity does not play an important role in the context of the valence transition and the valence fluctuation. However, we note that it is possible that the quasiperiodicity causes unexpected effects from other types of fluctuations.

4 Summary and Discussion

In this paper, we have analyzed the QPALM by DMRG calculation. The system shows the characteristic pattern in the plot of the spin correlation function, and its structure depends on the filling of the system. The appearance of the repeated pattern of the spin correlation function in the QPALM bears similarity to the behavior of periodic systems. We have studied the f-electron number and the valence fluctuation as a function of ϵ_{f} in the PAM, QPALM, and RfALM. The behaviour obtained for the PAM is consistent with previous studies[16]. The novelty of our study is the precise calculation of QPALM and RfALM using DMRG. We have found that a valence transition in the QPALM is not sharp as in the PAM. Finally, we have compared properties of the QPALM and the RfALM. The properties of the valence transition in the QPALM resembles that in the RfALM. Consequently, the QPALM has a similar property to the PAM for spin correlation, but also has a similar property to RfALM for the valence fluctuation. This characteristic nature of QPALM may lead to novel intriguing phenomena inherent in quasiperiodic systems. This issue is under consideration.

5 Acknowledgments

This work was in part supported by JSPS KAKENHI Grants No. 26870284 (M.T.), No. 25400366, and No. 15H05855 (N.K.). FM thanks JSPS for the support from a Research Fellowship for Young Scientists.

References

[1] D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn. Metallic phase with long-range orientational order and no translational symmetry. *Phys. Rev. Lett.*, 53:1951–1953, Nov 1984.

[2] Luca Bindi, Paul J Steinhardt, Nan Yao, and Peter J Lu. Natural quasicrystals. *science*, 324(5932):1306–1309, 2009.

[3] Stefan Förster, Klaus Meinel, René Hammer, Martin Trautmann, and Wolf Widdra. Quasicrystalline structure formation in a classical crystalline thin-film system. *Nature*, 502(7470):215–218, 2013.

[4] Natalie A Wasio, Rebecca C Quardokus, Ryan P Forrest, Craig S Lent, Steven A Corcelli, John A Christie, Kenneth W Henderson, and S Alex Kandel. Self-assembly of hydrogen-bonded two-dimensional quasicrystals. *Nature*, 507(7490):86–89, 2014.

[5] Kazuhiko Deguchi, Shuya Matsukawa, Noriaki K Sato, Taisuke Hattori, Kenji Ishida, Hiroyuki Takakura, and Tsutomu Ishimasa. Quantum critical state in a magnetic quasicrystal. *Nature Materials*, 11(12):1013–1016, 2012.

[6] Shinji Watanabe and Kazumasa Miyake. Robustness of quantum criticality of valence fluctuations. *Journal of the Physical Society of Japan*, 82(8):083704, 2013.

[7] V. R. Shaginyan, A. Z. Msezane, K. G. Popov, G. S. Japaridze, and V. A. Khodel. Common quantum phase transition in quasicrystals and heavy-fermion metals. *Phys. Rev. B*, 87:245122, Jun 2013.

[8] Shinichi Takemura, Nayuta Takemori, and Akihisa Koga. Valence fluctuations and electric reconstruction in the extended anderson model on the two-dimensional penrose lattice. *Phys. Rev. B*, 91:165114, Apr 2015.

[9] Yaacov E. Kraus, Yoav Lahini, Zohar Ringel, Mor Verbin, and Oded Zilberberg. Topological states and adiabatic pumping in quasicrystals. *Phys. Rev. Lett.*, 109:106402, Sep 2012.

[10] L Fallani, JE Lye, V Guarrera, C Fort, and M Inguscio. Ultracold atoms in a disordered crystal of light: Towards a bose glass. *Phys. Rev. Lett.*, 98(13):130404, 2007.

[11] Giacomo Roati, Chiara DfErrico, Leonardo Fallani, Marco Fattori, Chiara Fort, Matteo Zaccanti, Giovanni Modugno, Michele Modugno, and Massimo Inguscio. Anderson localization of a non-interacting bose–einstein condensate. *Nature*, 453(7197):895–898, 2008.

[12] B. Paredes, C. Tejedor, and J. I. Cirac. Fermionic atoms in optical superlattices. *Phys. Rev. A*, 71:063608, Jun 2005.

[13] M. Nakagawa and N. Kawakami. Laser-induced Kondo effect in ultracold alkaline-earth fermions. *ArXiv*: 1506.02947, June 2015.

[14] B Bauer, LD Carr, HG Evertz, A Feiguin, J Freire, S Fuchs, L Gamper, J Gukelberger, E Gull, S Guertler, et al. The alps project release 2.0: open source software for strongly correlated systems. *Journal of Statistical Mechanics: Theory and Experiment*, 2011(05):P05001, 2011.

[15] AF Albuquerque, F Alet, P Corboz, P Dayal, A Feiguin, S Fuchs, L Gamper, E Gull, S Gürtler, A Honecker, et al. The alps project release 1.3: Open-source software for strongly correlated systems. *Journal of Magnetism and Magnetic Materials*, 310(2):1187–1193, 2007.

[16] Shinji Watanabe, Masatoshi Imada, and Kazumasa Miyake. Superconductivity emerging near quantum critical point of valence transition. *Journal of the Physical Society of Japan*, 75(4):043710, 2006.