Mott transition in the Hubbard model on the anisotropic kagomé lattice: Variational cluster approach

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Abstract. We study the Mott transition and ferrimagnetism in the Hubbard model on the anisotropic kagomé lattice using the variational cluster approximation. The phase diagram of the model at half-filling and zero temperature is analyzed. We find that the ferrimagnetic phase rapidly grows as the geometric frustration is relaxed, and the Mott-insulating phase disappears in moderately frustrated region, indicating that the ferrimagnetic fluctuations stemming from the relaxation of the geometric frustration is enhanced by the electron correlations. In the metallic phase, heavy fermion behavior is observed and mass enhancement factor is computed. Enhancement of effective spatial anisotropy by the electron correlations is also confirmed in moderately frustrated region, and its effect on the heavy fermion behavior is examined.

1. Introduction

Electron systems with geometric frustration play an important role to reveal the nature of the Mott transition and physics related to it, e.g., heavy fermion behavior and spin liquids. When spatial anisotropy is introduced in systems with geometric frustration, the interplay between the spin fluctuations and Mott transition appears as a new feature and provides unique phenomena which take place neither in the unfrustrated nor fully frustrated systems. As for the kagomé lattice, the issues related to the anisotropy have been considered only recently. The Mott transition and magnetic properties near the transition have been studied using the cellular dynamical mean field theory [1], where the Mott transition point was analyzed and enhancement of spatial anisotropy and spin correlations were observed. Such enhancement may give rise to the extension of the ordered (ferrimagnetic) phase. Therefore, if the Mott transition itself persists without being veiled by the ferrimagnetic phase remains to be examined. Also, the effect of the enhanced anisotropy on the heavy fermion behavior is worth being studied. We investigate the ferrimagnetism and Mott transition on the anisotropic kagomé lattice using the variational cluster approximation (VCA) [2, 3, 4], which is formulated based on a rigorous variational principle and exactly takes into account the short-range correlations. We study the phase diagram at zero temperature and half-filling. We show that, in moderately frustrated region, the ferrimagnetic phase rapidly grows down to the metal-insulator phase boundary, and the Mott insulator (MI) phase disappears. In the metallic phase, heavy fermion behavior is observed and the mass enhancement of the quasiparticle is computed. Effective spatial anisotropy becomes
also larger due to the electron correlations, in agreement with the previous study [1]. This effect gives rise to an enhancement of the anisotropy of the effective masses of the quasiparticles.

2. The model and formalism
The Hamiltonian of the Hubbard model on the anisotropic kagomé lattice (see Fig. 1) reads

\[ H = -\sum_{i,j,\sigma} t_{ij} c_i^{\dagger} c_j + U \sum_i n_i^{\uparrow} n_i^{\downarrow} - \mu \sum_i n_i^{\sigma}, \]

where \( t_{ij} = t \) between the sites 1 and 2, 3 and \( t_{ij} = t' \) between the sites 2 and 3, \( U \) is the on-site Coulomb repulsion, and \( \mu \) is the chemical potential. The energy unit is set as \( t = 1 \) hereafter.

In our analysis, the 6- and 12-site clusters in Fig. 1(a) are used to set up the cluster Hamiltonian \( H' \). To study the ferrimagnetism, the Weiss field \( H_F = h_F \sum_i \text{sign}(i)(n_{i\uparrow} - n_{i\downarrow}) \) with \( \text{sign}(i) = -1 \) for the site 1 and \( \text{sign}(i) = 1 \) for the sites 2 and 3, is also included, and the Weiss field \( h_F \) and the chemical potential \( \mu' \) of the cluster Hamiltonian \( H' \) are treated as the variational parameters, where the latter should be included for the thermodynamic consistency [5]. The chemical potential of the system \( \mu \) is also adjusted so that the electron density \( n \) is equal to 1 within 0.1%, and the ground-state energies per site \( E = \Omega + \mu n \) are compared to determine which phase (ferrimagnetic or paramagnetic) is stable. The density of state is also calculated to examine the gap.

3. Results of calculation
In Fig. 2, we show the phase diagram at zero temperature and half-filling obtained using the 12-site cluster. In this region of \( t' \), the ferrimagnetic phase is an insulator since there is a gap, and the transition between the ferrimagnetic and paramagnetic (including MI) phases is a level crossing (first order). The critical interaction strength \( U_{\text{MI}} \) separating the MI and metallic phases is slightly smaller than the noninteracting band width \( W \), where \( W = 6 \) at \( t' = 1 \) and \( W = 4\sqrt{2} \approx 5.66 \) at \( t' = 0 \). The difference of \( U_{\text{MI}} \) between the 12-site and 6-site analysis is less than 20% of \( W \). The behavior of our \( U_{\text{MI}} \) according to the relaxation of the frustration is qualitatively consistent with the previous results [1], though our values for \( U_{\text{MI}} \) are relatively small compared to those in Ref. [1]. At present the origin of these discrepancies are not clear to us. As for the Mott transition, we could not find out the Mott insulator and paramagnetic metal coexisting region of \( U \) at half-filling within our two controlling parameters \( \mu \) and \( \mu' \). Detailed analysis of the Mott gap and double occupancy in Ref. [1] also shows that there are no indication of the discontinuity around the Mott transition, suggesting that the transition is continuous. In Ref. [1] this transition is reported to be first order. First-order Mott transitions are obtained in other models in the variational cluster approach with bath degrees of freedom and treating the hybridization between the bath sites and cluster sites as a variational parameter [7, 8]. In these analyses, the coexisting metal and insulator solutions, leading to the first-order transition, differ by the value of these hybridization parameters, and these situations will be similar to the case of Ref. [1]. Our analysis does not have bath degrees of freedom and technically this will be the origin of the difference. It remains to be clarified which is the correct picture.
Figure 2. Phase diagram of the Hubbard model on the anisotropic kagomé lattice at zero temperature and half-filling as a function of $t'$ and $U$ obtained by VCA, where the 12-site cluster is used (crosses and circles). Lines are guides to the eye.

4. Heavy fermion behavior

In Fig. 3, we show the spectral weight function $\rho(\omega, k)$ calculated using the 12-site cluster for solutions corresponding to (a), (b) the ferrimagnetic phase (up and down spin parts are plotted separately), (c) the MI phase, and (d) the metallic phase at $t' = 0.75$. In (a) and (b), the mean-field spin-density-wave (SDW) dispersion is also included (solid lines) to see its general features, where $M = 0.92$ in the mean-field solution while $M = 0.72$ in VCA. In (d), the noninteracting band structure is also plotted (solid lines) for comparison. In (d), we notice that the spectral function is consistent with the Fermi-liquid state and the interacting bands slightly shrink toward the Fermi surface, leading to heavy-fermion behavior. To study it in detail, we consider well below the MI transition line where Fermi-liquid natures are confirmed from the behavior of the spectral function and compute the mass enhancement factor $m^*/m$ along the $x$ and $y$ directions in $k$ space, where the $x$ direction corresponds to the direction of $t'$ hopping in real space. We also compute the ratio of the Fermi momenta in the $x$ and $y$ directions, $r = k_{yF}/k_{xF}$. As $t'$ decreases, the noninteracting Fermi surface slightly shrinks in the $x$ direction and slightly evolves in the $y$ direction [9], so $r$ is a measure of the anisotropy including the effect of the electron correlations.

Figure 3. (a) Spectral density at $t' = 0.75$, (b) $U = 8$ (ferrimagnetic state), (c) $U = 6$ (MI state), and (d) $U = 3$ (metallic state) along the dotted line in Fig. 1(b). The Lorentzian broadening with $\eta = 0.15t$ is used in all the cases. In (a) and (b), the solid lines are the mean-field SDW dispersion for the same values of $U$, $t'$ and $\mu$. In (d), the solid lines are the noninteracting band structure. In (a), (b), and (c) the peaks are scaled by 5 compared to (d).
In Fig. 4, we show $r$ and $m^*/m$ in the $x$ and $y$ directions as functions of $U$ for $t' = 1.0$, 0.8, and 0.6 in our lattice geometry for the 12-site cluster, to see general features about the effect of the electron correlations on these quantities. The rapid growth of $r$ at $t' = 0.6$ indicates that the effective anisotropy is enhanced due to the electron correlations in moderately frustrated region. The analysis of the effective anisotropy was also done in Ref. [1] by considering the renormalization of the hoping parameters and our results are qualitatively consistent with their analysis. As is shown in Fig. 4(b)~(d), the heavy fermion behavior is observed in all cases, and appears largely in moderately frustrated region.

Figure 4. (a) Ratio $r$ as a function of $U$ for $t' = 1.0$, 0.8, and 0.6. The two arrows indicate the value of $r$ for noninteracting band at $t' = 0.5$ ($r = 1.24$) and at $t' = 0.4$ ($r = 1.30$). (b)~(d) Mass enhancement factor $m^*/m$ in the $x$ and $y$ directions as functions of $U$ for (b) $t' = 1.0$, (c) $t' = 0.8$, and (d) $t' = 0.6$. The 12-site cluster is used.

5. Summary
In summary, we have investigated the ferrimagnetism and Mott transition on the anisotropic the kagomé lattice using VCA. The phase diagram at zero temperature and half-filling is determined. The ferrimagnetic phase rapidly grows in moderately frustrated region and the MI phase disappears there. In the metallic phase, heavy fermion behavior is studied and the mass enhancement is computed. Enhancement of spatial anisotropy due to the electron correlations is also observed for moderately frustrated region and its effect on the heavy fermion behavior is discussed. Thus, the interplay between the spin correlations and Mott transition is quantitatively studied above and below the metal-insulator transition.

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References
[1] Furukawa Y, Ohashi T, Koyama K, and Kawakami N, Phys. Rev. B 82, 161101 (2010).
[2] Sénéchal D et al., Phys. Rev. Lett. 84, 522 (2000); Phys. Rev. B 66, 075129 (2002).
[3] Pothoff M et al., Phys. Rev. Lett. 91 206402 (2003); Dahnken C et al., Phys. Rev. B 70, 2451100 (2004).
[4] Pothoff M, Eur. Phys. J. B 32, 429 (2003).
[5] Aichhorn M, Arrigoni E, Potthoff M, and Hanke W, Phys. Rev. B 74, 024508 (2006).
[6] Yamada A, Seki K, Eder R, and Ohta Y, Phys. Rev. B 83, 195127 (2011).
[7] Pothoff M, Eur. Phys. J. B 36, 335 (2003).
[8] Balzer M, Kyung M, Sénéchal D, Tremblay A M, Potthoff M, Eur. Phys. Lett. 85, 17002 (2009).
[9] Imai Y, Kawakami N, and Tsunetsugu H, Phys. Rev. B 68, 195103 (2003).