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Mott transition of correlated electrons on the Kagomé lattice

Syunsuke Kuratani, Akihisa Koga and Norio Kawakami

Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan

E-mail: koga@tp.ap.eng.osaka-u.ac.jp

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Abstract

We investigate the stability of the metallic state in the Hubbard model on the Kagomé lattice at half filling. By means of the variational Monte Carlo simulations including onsite and nearest neighbour doublon–holon correlations, we clarify that the Mott transition occurs at $U_c \sim 11.5t$ in the system at zero temperature, which is consistent with the recent results obtained by the dynamical cluster approximation. The stability of the Mott insulating state is also addressed.

Strongly correlated electron systems on geometrically frustrated lattices have attracted current interest. One of typical examples is the transition-metal oxide $Na_xCoO_2{\cdot}yH_2O$($x \sim 0.35$, $y \sim 1.3$), which exhibits unconventional superconductivity below the critical temperature $T_c \sim 5$ K [1], stimulating further theoretical investigations [2–12]. One of the remarkable points is that if the hopping matrix elements via oxygen orbitals are properly taken into account, the system can be regarded as interpenetrating Kagomé lattices [13, 14]. Therefore, in recent years, there has been renewed interest in the effect of geometrical frustration in the Kagomé electron systems [13–17].

Motivated by this, we consider the effect of frustration on the Hubbard model on the Kagomé lattice (see figure 1(a)), which is composed of corner-sharing triangles. For simplicity, we adopt the decorated square lattice with some diagonal bonds, as shown in figure 1(b), which is topologically equivalent to the original one. The model Hamiltonian is explicitly described as

$$H = -t \sum_{(im,jn)\sigma} c^{\dagger}_{im\sigma} c_{jn\sigma} + U \sum_{im} c^{\dagger}_{im\uparrow} c_{im\uparrow} c^{\dagger}_{im\downarrow} c_{im\downarrow}, \tag{1}$$

where $c^{\dagger}_{im\sigma}(c_{im\sigma})$ is the creation (annihilation) operator of an electron at the ith unit cell together with a relative position $m(=1, 2, 3)$ with spin $\sigma(=\uparrow, \downarrow)$. t is the hopping integral

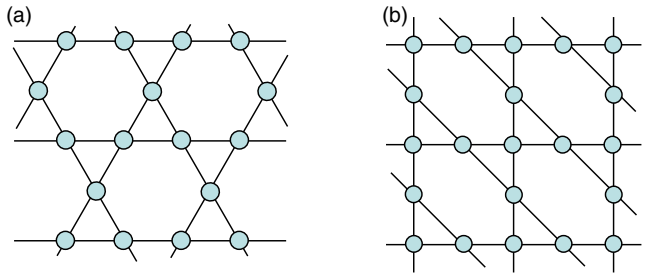

Figure 1. (a) Original Kagomé lattice and (b) decorated square lattice, which is topologically equivalent to (a).

(This figure is in colour only in the electronic version)

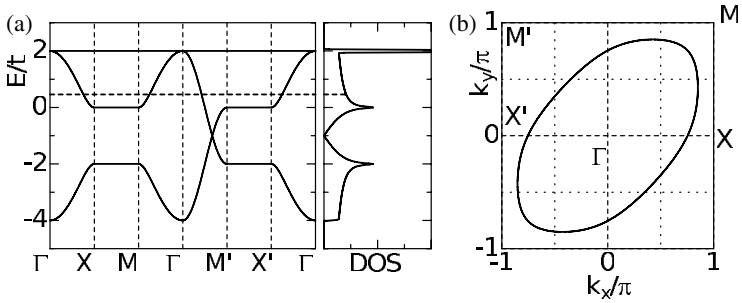

Figure 2. (a) Dispersion relations and the density of states (DOS) for the non-interacting case. (b) Fermi surface at half filling.

between the adjacent sites and U the Coulomb interaction. We diagonalize the non-interacting Hamiltonian in terms of the unitary transformation:

$$H_0 = \sum_{k\alpha\sigma} \epsilon_{k\alpha} a^{\dagger}_{k\alpha\sigma} a_{k\alpha\sigma}\,, \tag{2}$$

where $a_{k\alpha\sigma}$ ($a^{\dagger}_{k\alpha\sigma}$) is the annihilation (creation) operator. $\epsilon_{k\alpha}$ ($\epsilon_{k1} \leqslant \epsilon_{k2} \leqslant \epsilon_{k3}$) is the dispersion relation for the αth band, as shown in figure 2(a). The Fermi level is located in the dispersive band ($\alpha = 2$) at half filling, and thereby the paramagnetic metallic state is realized in the non-interacting case. On the other hand, in the large U limit, the Hubbard model equation (1) is reduced to the quantum Heisenberg model on the Kagomé lattice, where the non-magnetic ground state is realized [18–21]. Therefore, we restrict our discussion to the paramagnetic ground state expected naively.

To clarify how the introduction of the interaction affects the stability of the metallic state in the frustrated system, we make use of the variational Monte Carlo (VMC) method [22–24], where the lowest-energy state in a given parameter space can be determined. In comparison with other numerical methods, this method has an advantage in treating large clusters to discuss the ground state properties in the thermodynamic limit. For example, the quantum Monte Carlo simulations in general suffer from the minus sign problem and the path integral renormalization group method may have a difficulty in estimating physical quantities in the thermodynamic limit when the Coulomb interaction U is large. The VMC method has successfully been applied to various correlated electron systems such as frustrated systems [6, 25–29] and multi-orbital systems [30].

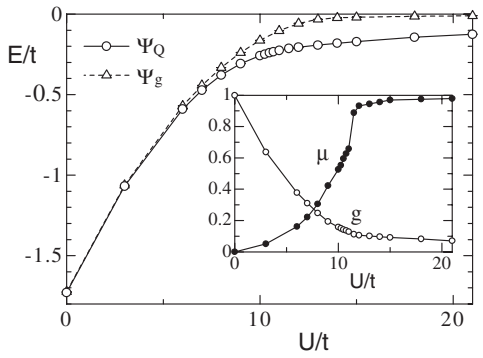

Figure 3. Ground state energy per site E/t as a function of the Coulomb interaction U. Solid (open) circles represent the optimum energy for the trial state equation (3) (equation (6)). The inset shows the optimum variational parameters for equation (6).

To apply the VMC method to the Hubbard model on the Kagomé lattice, we first consider a Gutzwiller type trial state [31] as

$$\Psi_g = \mathcal{P}_g \phi, \tag{3}$$

$$\mathcal{P}_g = \prod_{jm} \left[1 - (1-g)\, \hat{D}_{\mathbf{r}_{jm}} \right], \tag{4}$$

where $\hat{D}_{\mathbf{r}_{jm}} = n_{jm\uparrow} n_{jm\downarrow}$, g is a Gutzwiller factor for onsite correlations, and

$$\phi = \prod_{|k|>k_F,\sigma} a^{\dagger}_{k2\sigma} \prod_{k\sigma} a^{\dagger}_{k1\sigma} |0\rangle. \tag{5}$$

It is known that the Gutzwiller wave function describes the Mott transition in infinite dimensions [32], but not in low dimensions [24]. Therefore, it is necessary to take into account spatially extended electron correlations beyond onsite ones. To this end, we also consider another trial state including nearest-neighbour doublon–holon correlations [33–36] as

$$\Psi_Q = \mathcal{P}_Q \Psi_g, \tag{6}$$

$$\mathcal{P}_Q = \prod_{jm} \left[1 - \mu \hat{Q}_{jm} \right], \tag{7}$$

$$\hat{Q}_{jm} = \hat{D}_{\mathbf{r}_{jm}} \prod_{\boldsymbol{\tau}} \left[1 - \hat{H}_{\mathbf{r}_{jm}+\boldsymbol{\tau}} \right] + \hat{H}_{\mathbf{r}_{jm}} \prod_{\boldsymbol{\tau}} \left[1 - \hat{D}_{\mathbf{r}_{jm}+\boldsymbol{\tau}} \right], \tag{8}$$

where $\boldsymbol{\tau}$ runs over all the nearest-neighbour sites and $\hat{H}_{\mathbf{r}_{jm}} = (1-n_{jm\uparrow})(1-n_{jm\downarrow})$. By optimizing these trial states, we can discuss the role of onsite and intersite correlations in the system.

By performing the VMC simulations for each trial state, we obtain the ground state energy for the system ($N = 432$), as shown in figure 3. Needless to say, the energy obtained by the trial state Ψ_Q is always lower than that for Ψ_g. Note that the difference between their curves is changed, depending on the magnitude of the interaction. When U is small, the energies for both trial states are almost the same, where onsite correlations are relevant. On the other hand, the increase of the interaction U yields the energy gain in Ψ_Q, implying that intersite correlations are important for the ground state. Furthermore, we find a drastic change in the curves of the variational parameters for Ψ_Q, as shown in the inset of figure 3. At $U = 0$, the free electron states are realized, where $(g, \mu) = (1, 0)$. The introduction of the interaction first enhances the onsite electron correlations, resulting in the rapid decrease of g. Further increase

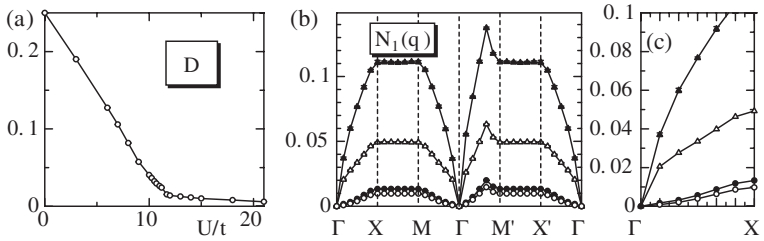

Figure 4. (a) The probability of doubly occupied states as a function of the Coulomb interaction U, (b) the lowest eigenvalues of the charge structure factor $N_1(\mathbf{q})$ for $U = 8, 10, 12$, and 15 from the top to the bottom, and (c) an enlarged view of the region around the Γ point.

of interaction enhances the doublon–holon correlations, where the corresponding parameter μ is changed. Note that the jump singularity appears in both parameters at $(U/t)_c \sim 11.5$, although that for g is very small. On the other hand, these anomalies do not appear in the small system ($N = 108$). Although a careful analysis of the size dependence is needed to determine the order of the transition in the thermodynamic limit, the existence of a weak first-order phase transition is naively expected, which is consistent with the result obtained by the dynamical cluster approach [17].

To reveal the nature of the transition, we calculate the physical quantities in terms of the optimized trial function Ψ_Q. In figure 4(a), we show the probability of the doubly occupied states $\langle D \rangle$, in which the statistical error for each point is almost negligible. In the non-interacting case ($U/t = 0$), the empty state, one-electron states with a spin, and doubly occupied states are equally realized, where $\langle D \rangle = 0.25$. The introduction of the Coulomb interaction decreases the probability of doubly occupied states, as shown in figure 4(a). Finally, the Mott transition occurs to the insulating phase with a small jump characteristic of the weak first-order transition. We also calculate the charge structure factor, which is defined as

$$N_{mn}(\mathbf{q}) = \sum_{ij} \left[\langle N_{im} N_{jn} \rangle - \langle N_{im} \rangle \langle N_{jn} \rangle \right] \mathrm{e}^{\mathrm{i}\mathbf{q}(\mathbf{r}_{im} - \mathbf{r}_{jn})}, \tag{9}$$

where $N_{im} = \sum n_{im\sigma}$, $\mathbf{r}_{im} = \mathbf{r}_i + \mathbf{d}_m$, $\mathbf{d}_1 = 0$, $\mathbf{d}_2 = \mathbf{x}/2$, and $\mathbf{d}_3 = \mathbf{y}/2$. In figure 4(b), we show the lowest eigenvalues of the charge structure factor $N_1(\mathbf{q})$. The singularity accompanied with the Mott transition appears in the vicinity of the Γ point (see also in figure 4(c)), where linear behaviour $N_q \sim q$ appears in the metallic phase ($U < U_c$), while quadratic behaviour $N_q \sim q^2$ appears in the Mott insulating phase ($U > U_c$). This implies that the Fermi surface vanishes due to the Mott transition. In addition, no sharp peak structure emerges in the spin structure factor (which is not shown here). Therefore, we can say that the transition drives the system to the Mott insulating state at the critical point $U = U_c$, which does not indicate instability to any magnetically ordered state, as far as the trial state equation (6) is concerned.

The present results are consistent with those obtained recently by the dynamical cluster approach with quantum Monte Carlo simulations [17]. It was claimed that a first-order transition with hysteresis occurs to the non-magnetic Mott insulating phase at the critical point $(U/t)_c \sim 8.4$, which is slightly different from our result, $(U/t)_c \sim 11.5$. Furthermore, it was suggested that anomalous behaviour in the spin correlation function shows up in the metallic state close to the Mott critical point as the temperature is varied. In contrast, we could not find such spin correlations at zero temperature. This may imply that the effect of frustration is not incorporated well in our treatment, which yields the slight difference for the critical points. Therefore, it is necessary to improve the trial state so as to describe the spin correlations more precisely, which is now under consideration.

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