Anomalous magnetic properties near Mott transition in Kagomé lattice Hubbard model

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Abstract

We investigate the characteristics of the metallic phase near the Mott transition in the Kagomé lattice Hubbard model using the cellular dynamical mean field theory. By calculating the specific heat and spin correlation functions, we demonstrate that the quasiparticles show anomalous properties in the metallic phase close to the Mott transition. We find clear evidence for the multi-band heavy quasiparticles in the specific heat, which gives rise to unusual temperature dependence of the spin correlation functions.

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Geometrical frustration has attracted much attention in the field of strongly correlated electron systems. The observation of heavy fermion behavior in the pyrochlore compound LiV 2 O 4 [1] and the discovery of superconductivity in the triangular lattice compound Na x CoO 2 · yH 2 O [2], the β-pyrochlore osmate KO 2 S 6 [3], etc. have stimulated intensive studies of frustrated electron systems. The Kagomé lattice (Fig. 1(a)) is another prototype of frustrated systems, which may be regarded as a two-dimensional analog of the pyrochlore lattice. It is suggested that a correlated electron system on the Kagomé lattice can be an effective model of Na x CoO 2 · yH 2 O [4]. The issue of electron correlations for the Kagomé lattice systems was addressed by using the FLEX approximation [5] and QMC method [6] in the metallic regime. In our recent paper [7], we have studied electron correlations in the Kagomé lattice Hubbard model, and found the first-order Mott transition at the Hubbard interaction $U/W \sim 1.37$ ($W$: band width).

In this paper, we focus on the anomalous properties around the Mott transition in the Kagomé lattice Hubbard model. We consider the standard Hubbard model with nearest-neighbor hopping $t$ ($> 0$) on the Kagomé lattice,

$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow},$

where $c_{i\sigma}^\dagger$ ($c_{j\sigma}$) creates (annihilates) an electron with spin $\sigma$ at site $i$. We use the band width $W = 6t$ as a unit of energy. In order to treat both effects of strong correlations and geometrical frustration, we employ the cellular dynamical mean field theory (CDMFT) [8]. In CDMFT, the original lattice is regarded as a super-lattice consisting of clusters, which is then mapped onto an effective cluster model via a standard DMFT procedure. Each unit cell of the Kagomé lattice has three sites labeled by 1, 2, and 3, as shown in Fig. 1(a). We thus end up with a three-site cluster model coupled to the self-consistently determined medium illustrated in Fig. 1(b), which is solved by using QMC method [9].

We now investigate the characteristics around the Mott transition at half filling. In Fig. 2, we show the temperature ($T$) dependence of the specific heat $C$ for several values of interaction strength. In the noninteracting case ($U = 0$), $C$
has a single hump structure. As \( U \) increases (\( U/W = 0.5, 1.0, 1.3 \)), sharp peaks are developed in the low-\( T \) regime due to low-energy spin excitations, while charge excitations feature the higher-\( T \) hump structure. In particular, in the strongly correlated metallic regime at \( U/W = 1.0 \) and 1.3, we clearly find the three different structures at low \( T \): the shoulder around \( T/W \sim 0.1 \), the peak at \( T/W \sim 0.06 \), and the other sharp peak at lower \( T \). These characteristic structures reflect the three bands in the Kagomé lattice electron system which consist of one flat and two dispersive bands. In the small-\( U \) region, the electrons near the Fermi surface are mainly renormalized and contribute to the low-energy excitations so that the low-\( T \) peak structure is indistinct. In the strong-\( U \) region (\( U/W = 1.0, 1.3 \)), the whole three bands including the two bands away from the Fermi surface are renormalized to participate in the formation of quasiparticles. Therefore, the three types of quasiparticles become all relevant for the low-energy excitations, resulting in the three distinct structures in \( C \). On the other hand, one can see the suppression of \( C \) at low \( T \) in the insulating phase (\( U/W = 1.5 \)). In our previous study [7], we found a dramatic change in spin excitation spectra at the Mott transition. The single hump structure splits into two peaks once the system enters the insulating phase, where the low-energy peak is mainly formed by the AF coupled electrons between adjacent sites while the high-energy one is due to almost free spin states created in a three-site cluster. As \( T \) decreases, the contribution of the high-energy spin excitations to \( C \) becomes small, resulting in the decrease of \( C \) at low \( T \).

By investigating the short-range spin correlations, we further find the anomalous magnetic properties in the metallic phase close to the Mott transition. Shown in Fig. 3 is the \( T \)-dependence of the nearest-neighbor spin correlation function \( \langle S_i^z S_{i+1}^z \rangle \) for several values of \( U/W \). \( \langle S_i^z S_{i+1}^z \rangle \) is always negative so that the spin correlation is antiferromagnetic (AF), which is a source of strong frustration on the frustrated Kagomé lattice. As \( T \) decreases, the nearest-neighbor AF spin correlation is enhanced gradually. In the insulating phase (\( U/W = 1.5 \)) the AF spin correlation becomes stronger with decreasing \( T \), as is expected. On the other hand, \( \langle S_i^z S_{i+1}^z \rangle \) in the metallic phase close to the Mott transition (\( U/W = 1.3 \)) shows a nonmonotonic \( T \)-dependence: the AF spin correlation is once enhanced and then suppressed with the decrease of \( T \). The unusual \( T \)-dependence results from the competition between the quasiparticle formation and the frustrated spin correlations, which may be characterized by two energy scales: the coherence temperature \( T_C \) and \( T_M \) characterizing the AF spin fluctuations. The AF correlation is developed around \( T \sim T_M \), which stabilizes localized moments and causes frustration in accordance with the monotonic enhancement of spin correlations in the insulating phase. On the other hand, when the system is in the metallic phase, electrons recover coherence in itinerant motion below \( T_C \). Therefore, the frustration is relaxed by itinerancy of electrons via the suppression of AF correlations at \( T < T_C \). Thus, the nonmonotonic \( T \)-dependence of \( \langle S_i^z S_{i+1}^z \rangle \) clearly demonstrates that the heavy quasiparticles are formed under the influence of strong frustration.

In summary, we have studied the Kagomé lattice Hubbard model by means of CDMFT combined with QMC. We have found some anomalous magnetic properties in the metallic phase close to the Mott transition. The calculation of the specific heat has demonstrated the formation of multi-band quasiparticles, which shows the unusual temperature dependence of the spin correlation function.

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References

[1] S. Kondo, et al., Phys. Rev. Lett. 78, 3729 (1997).
[2] K. Takada, et al., Nature (London) 422, 53 (2003).
[3] S. Yonezawa, et al., J. Phys.: Cond. Mat. 16, L9 (2004).
[4] W. Koshiba, et al., Phys. Rev. Lett. 91, 257003 (2003).
[5] Y. Imai, et al., Phys. Rev. B 68, 195103 (2003).
[6] N. Bulut, et al., Phys. Rev. Lett. 95, 037001 (2005).
[7] T. Ohashi, et al., Phys. Rev. Lett. 97, 066401 (2006).
[8] G. Kotliar, et al, Phys. Rev. Lett. 87, 186401 (2001).
[9] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. 56, 2521 (1986).