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Magnetic correlations of the Hubbard model on frustrated lattices

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Abstract

In order to study the magnetic properties of frustrated metallic systems, we present quantum Monte Carlo data on the magnetic susceptibility of the Hubbard model on triangular and kagomé lattices. We show that the underlying lattice structure is important and determines the nature and the doping dependence of the magnetic fluctuations in these models.

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The discovery of superconductivity in $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ has generated new interest in frustrated interacting systems [1]. In cobaltates, cobalt and oxygen ions form a two-dimensional triangular network, and it has been shown that the triangular CoO_2 lattice consists of four coupled kagomé sublattices [2]. For this reason, we use Quantum Monte Carlo (QMC) simulations to investigate the magnetic properties of interacting systems on triangular and kagomé lattices [3]. The triangular Hubbard model was studied previously with the path-integral renormalization-group (RG) [4], the one-loop RG [5] and the fluctuation-exchange (FLEX) [6] approaches. The FLEX method was also used for studying the magnetic properties of the Hubbard model on the kagomé lattice [7].

In the following, we will see that the triangular Hubbard model has strong antiferromagnetic (AF) correlations near half-filling and at low temperatures, when the Coulomb repulsion U is of the order of the bandwidth. On the other hand, for weak U , the magnetic correlations saturate as $T \rightarrow 0$. The Hubbard model on the kagomé lattice also exhibits enhanced short-range AF correlations. In the doped case, we find that the short-range AF correlations are stronger for the kagomé than the triangular lattice.

This is interesting since the ground state of the spin- $\frac{1}{2}$ Heisenberg model has long-range order on the triangular lattice and it is disordered in the kagomé case. We note that it would be useful to investigate the possibility of superconductivity in metallic kagomé systems.

The Hubbard model is defined by

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}, \quad (1)$$

where t is the hopping matrix element between the nearest neighbor-sites, U is the on-site Coulomb repulsion, and μ is the chemical potential. Here, $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) annihilates (creates) an electron with spin σ at site i , and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. In the following, we will take $t < 0$ and consider $\langle n \rangle \geq 1.0$, which is the appropriate case for the cobaltates [2]. In obtaining the QMC data presented here, the determinantal QMC technique [8] was used.

For the triangular lattice, the magnetic susceptibility is defined by

$$\chi(\mathbf{q}) = \int_0^\beta d\tau \sum_{\ell} e^{-i\mathbf{q} \cdot \mathbf{r}_\ell} \langle m^z(\mathbf{r}_{i+\ell}, \tau) m^z(\mathbf{r}_i) \rangle, \quad (2)$$

where $m^z(\mathbf{r}_i) = c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}$ and $m^z(\mathbf{r}_i, \tau) = e^{H\tau} m^z(\mathbf{r}_i) e^{-H\tau}$. In the following, χ will be plotted in units of $|t|^{-1}$.

The kagomé lattice is a three-band model, since each unit cell consists of three sites. Hence, each lattice site on the kagomé lattice can be represented by the indices (ℓ, d)

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where ℓ is the unit-cell index and d denotes the atomic site in a particular unit cell. For the kagomé case, we define the magnetic susceptibility as

$$\chi_{dd'}(\mathbf{q}) = \int_0^\beta d\tau \sum_{\ell} e^{-i\mathbf{q}\cdot\mathbf{r}_\ell} \langle m_d^z(\mathbf{r}_{i+\ell}, \tau) m_{d'}^z(\mathbf{r}_i) \rangle, \quad (3)$$

where $m_d^z(\mathbf{r}_i) = c_{id\uparrow}^\dagger c_{id\uparrow} - c_{id\downarrow}^\dagger c_{id\downarrow}$, $c_{id\sigma}$ ($c_{id\sigma}^\dagger$) is the annihilation (creation) operator of an electron with spin σ at lattice site (i, d) and the summation is performed over the unit-cell locations. Diagonalizing the 3×3 matrix $\chi_{dd'}(\mathbf{q})$, we obtain $\chi_\alpha(\mathbf{q})$ which describes the three modes of the magnetic excitations on the kagomé lattice.

We first present results for the triangular lattice at half-filling. Fig. 1(a) shows $\chi(\mathbf{q})$ versus \mathbf{q} for $U = 4|t|$ on various size lattices as the temperature is lowered. Here, it is seen

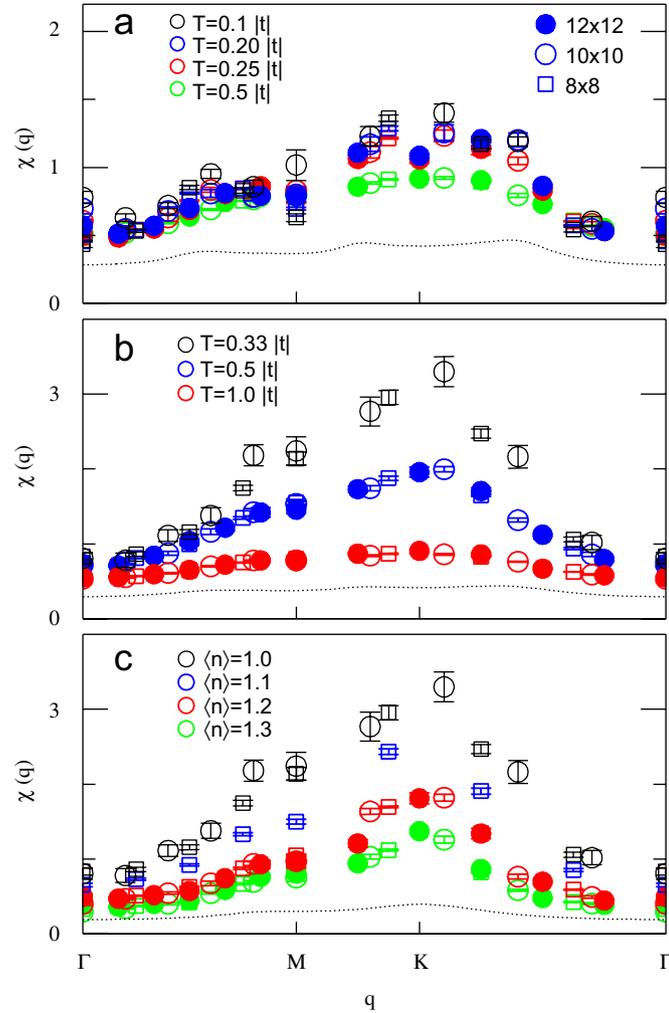


Fig. 1. Magnetic susceptibility $\chi(\mathbf{q})$ versus \mathbf{q} of the triangular Hubbard model. Here, \mathbf{q} is scanned along the path $\Gamma \rightarrow M \rightarrow K \rightarrow \Gamma$ in the BZ of the triangular lattice. The temperature evolution of $\chi(\mathbf{q})$ at half-filling is shown in (a) for $U = 4|t|$ and in (b) for $U = 8|t|$. In these figures, the dotted curves represent results for the noninteracting case at the lowest temperature used in that figure. The evolution of $\chi(\mathbf{q})$ versus \mathbf{q} with the electron density (n) is shown in (c) for $U = 8|t|$ and $T = 0.33|t|$. Here, the dotted curve represents the results for the noninteracting system at $\langle n \rangle = 1.3$ and $T = 0.33|t|$.

that $\chi(\mathbf{q})$ does not vary significantly with T , in particular for $0.25|t| \leq T \leq 0.17|t|$. For comparison, $\chi_0(\mathbf{q})$ for the noninteracting system at $T = 0.17|t|$ is shown by the dotted curve. Fig. 1(b) displays $\chi(\mathbf{q})$ versus \mathbf{q} for $U = 8|t|$ at half-filling, where we observe a large Stoner enhancement of the AF correlations. In contrast with the $U = 4|t|$ case, here, $\chi(\mathbf{q})$ at the K point grows rapidly with a Curie-like T dependence down to $0.33|t|$. However, it is not known whether $\chi(\mathbf{q})$ saturates at lower T for $U = 8|t|$. Fig. 1(c) shows the filling dependence of $\chi(\mathbf{q})$ for $U = 8|t|$ while T is kept fixed at $0.33|t|$. Here, we observe that the AF correlations decay monotonically with doping.

Next, we discuss the magnetic properties of the Hubbard model on the kagomé lattice. Fig. 2(a) shows QMC results on $\chi_\alpha(\mathbf{q})$ for $U = 4|t|$ and $T = 0.2|t|$ at half-filling. The top band ($\alpha = 1$) and the second band ($\alpha = 2$) involve strong

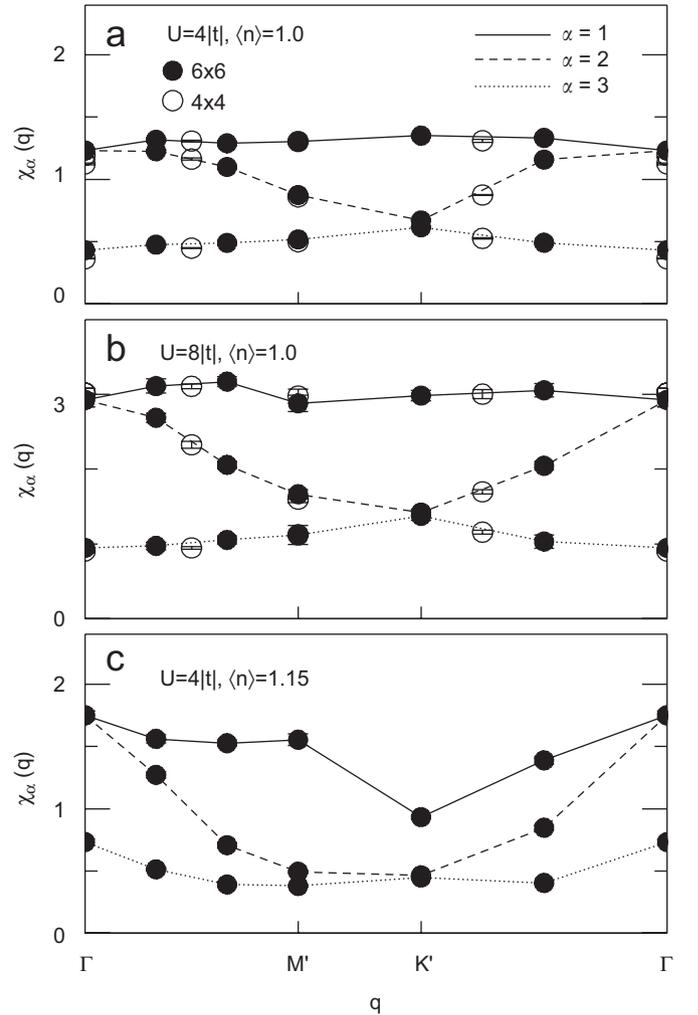


Fig. 2. Magnetic susceptibility $\chi_\alpha(\mathbf{q})$ versus \mathbf{q} for the Hubbard model on the kagomé lattice. Here, the three magnetic modes of $\chi_\alpha(\mathbf{q})$ are shown at each \mathbf{q} point, as \mathbf{q} is scanned along the path $\Gamma \rightarrow M' \rightarrow K' \rightarrow \Gamma$ in the first BZ of the kagomé lattice. Results on $\chi_\alpha(\mathbf{q})$ at half-filling are shown in (a) for $U = 4|t|$ and $T = 0.2|t|$ and in (b) for $U = 8|t|$ and $T = 0.33|t|$. These data have been obtained on lattices with 6×6 and 4×4 unit cells. In (c), results are shown for $\langle n \rangle = 1.15$ with $U = 4|t|$ and $T = 0.14|t|$.

short-range AF correlations. The third mode is weaker in magnitude. Fig. 2(b) shows $\chi_x(\mathbf{q})$ versus \mathbf{q} for $U = 8|t|$ and $T = 0.33|t|$ at half-filling. In Fig. 2(c), the QMC results are shown for $U = 4|t|$ and $T = 0.14|t|$ at $\langle n \rangle = 1.15$. In the doped case, we find that the near-neighbor AF correlations are stronger for the kagomé than the triangular lattice.

In this paper, we have presented QMC results on the magnetic correlations in the Hubbard model on the triangular and kagomé lattices. At the temperatures where these calculations were performed, we find, in both of these models, that the magnetic correlations grow rapidly as T decreases at half-filling for $U = 8|t|$, while they saturate when $U = 4|t|$. In addition, in the doped case, the low-frequency short-range AF correlations are stronger in the kagomé case than in the triangular case. This makes the interacting metallic systems with kagomé type of lattice

structures a promising field for studies of superconductivity.

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