Electronic properties of the doped antiferromagnet on a kagomé lattice

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Abstract

Within the $t$-$J$ model, we study the electronic properties of the doped antiferromagnet on the kagomé lattice based on the framework of the self-consistent mean-field theory. At the half-filling, the spin-liquid ground-state energy per site of the kagomé antiferromagnet is $E_g/N_s J = -0.859$, which is in very good agreement with the numerical estimates. Away from the half-filling, the electron photoemission spectroscopy and density of states are discussed, and the results indicate that there is a gap in the normal-state of the system.

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It has been clear in the last decades that detailed understanding of the motion of the holes in a two-dimensional (2D) antiferromagnet is one of the central issues in the theory of strongly correlated electron systems, especially as it relates to the copper oxide superconductors [1]. This followed from the argument, made by many researchers [2], that the essential physics of the copper oxide materials is contained in 2D doped Mott insulators, obtained by chemically adding charge carriers to a strongly correlated antiferromagnetic (AF) insulating state, therefore the physical properties of these systems mainly depend on the extent of doping, and the regimes have been classified into the underdoped, optimally doped, and overdoped, respectively. The normal-state properties of the copper oxide materials in the underdoped and optimally doped regimes exhibit a number of anomalous properties in the sense that they do not fit in the conventional Fermi-liquid theory [3]. In particular, the unusual normal-state gap behavior [4], and the stripe order of holes and spins [5] are found in the underdoped regime. It is also shown from the experiments [6] that the highest superconducting transition temperature $T_c$ for the square lattice $CuO_2$ planes in the tetragonal structure in the optimally doped regime is reduced by the structure distortions of the $CuO_2$ planes in the orthorhombic structure in the underdoped regime, and the stripe order of holes and spins is closely related with this distortion of the lattice [5]. The spinon frustration is also induced due to the distortion of the lattice of the system. Motivated by the above experimental facts, we believe that the doped kagomé lattice antiferromagnet (KLA) is an attractive candidate for describing the distorted square $CuO_2$ planes since it has the same coordinate number with the square lattice. On the other hand, the doped KLA, which is the system with the geometric frustration as in the triangular lattice, is also of the theoretical interest in their own right, with many fascinating theoretical questions remaining unanswered. The undoped KLA has been extensively studied [7–10], and the results show that its ground-state is the novel quantum disordered spin-liquid state without the AF long-range-order (AFLRO). It is also believed that the undoped KLA involving only nearest-neighbor coupling is the unique model to display the quantum spin liquid ground-state [11]. Recognizing that these novel physics showed by the undoped KLA, a natural
question is what is the electronic properties with doping on this system.

The situation for the doped square lattice antiferromagnet (SLA) is a bit more advanced. Some physical properties of the doped SLA have been studied intensively by many researchers within the $t$-$J$ model [12], where the strong electron correlation manifests itself by the electron single occupancy local constraint, and therefore the crucial requirement is to impose this local constraint in analytical calculations [13]. Based on the charge-spin separation, it has been shown that a useful method to treat this local constraint is the fermion-spin theory [14]. The fermion-spin theory has been used to discuss the physical properties of the doped SLA [13], and the results are consistent with the experiments and numerical simulations. In this paper, we apply the fermion-spin approach [14] to study the physical properties of the doped KLA. Our results show that at the half-filling the ground-state of the kagomé Heisenberg antiferromagnet is the quantum spin liquid state with energy per site $E_g/N_sJ = -0.859$, which is in very good agreement with the numerical simulations [7–10]. Away from half-filling, the electron photoemission spectroscopy and density of states are discussed, and the results indicate that there is a gap in the normal-state of the system.

The simple way to visualize the kagomé lattice is to regard the triangular lattice as consisting of four sublattices and remove the spins on one of the sublattices, therefore there are three inequivalent sublattices $A$, $B$, and $C$ even without AFLRO, where the spins in $A$, $B$, and $C$ sublattices pointing to the vertices of an equilateral triangle are placed with no two nearest-neighbors pointing in the same direction, then the kagomé lattice structure is much more complicated than the square lattice. For convenience, the equilateral triangle $ABC$ is chosen as the cell as shown in Fig. 1, in this case the kagomé lattice is reduced as the triangular structure, then the position of the spin $s$ in the cell $i$ is specified by the vector $X_{is} = R_i + d_s$, with $s = A$, $B$, $C$, i.e., each cell contains three spins, while the lattice vector $R_i$ and the reciprocal lattice $K_j$ satisfy the relationship as $R_i \cdot K_j = 2\pi \delta_{ij}$. With the above definition, the 2D $t$-$J$ model on the kagomé lattice is described by the Hamiltonian as,

$$H = -t \sum_{i_s,\eta_s,\sigma} C_{i_s,\sigma}^{\dagger} C_{i_s+\eta_s,\sigma} + \text{h.c.} - \mu \sum_{i_s,\sigma} C_{i_s,\sigma}^{\dagger} C_{i_s,\sigma} + J \sum_{i_s,\eta_s} S_{i_s} \cdot S_{i_s+\eta_s}, \quad (1)$$
where $C_{i_s,\sigma}^\dagger C_{i_s,\sigma}$ are the electron creation (annihilation) operators, $S_{i_s} = C_{i_s,\sigma}^\dagger \sigma C_{i_s,\sigma}/2$ are spin operators with $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ as pauli operators, and $\mu$ is the chemical potential. The sum is over all sites $X_{i_s}$, and for each $X_{i_s}$, over the nearest-neighbor $\eta_s$. The Hamiltonian (1) is restricted to the sub-space where a given site cannot be occupied by more than one electron, i.e., $\sum_\sigma C_{i_s,\sigma}^\dagger C_{i_s,\sigma} \leq 1$. In the fermion-spin representation, $C_{i_s} = h_{i_s}^z S_{i_s} - C_{i_s} = h_{i_s}^z S_{i_s}^+ + \tilde{C}_{i_s} = h_{i_s}^z S_{i_s}^+$, where the spinless fermion operator $h_{i_s}$ keeps track of the charge (holon), while the pseudospin operator $S_{i_s}^+$ keeps track of the spin (spinon), the $t$-$J$ model (1) is decoupled within the mean-field approximation (MFA) as $H = H_t + H_J - 24Nt\chi\phi$ with

$$H_t = 2\chi t \sum_{i_s,\eta_s} h_{i_s+\eta_s}^+ h_{i_s} - \mu \sum_{i_s} h_{i_s}^+ h_{i_s},$$

(2a)

$$H_J = \frac{1}{2} J_{eff} \epsilon \sum_{i_s,\eta_s} (S_{i_s}^+ S_{i_s+\eta_s}^- + S_{i_s}^- S_{i_s+\eta_s}^+) + J_{eff} \sum_{i_s,\eta_s} S_{i_s}^z S_{i_s+\eta_s}^z,$$

(2b)

where $N$ is the number of cells, $J_{eff} = J[(1 - \delta)^2 - \delta^2]$, and $\epsilon = 1 + 2\epsilon/|J_{eff}|$. The nearest-neighbor spin bond-order amplitude $\chi$ and holon particle-hole parameter $\phi$ are defined as $\chi = \langle S_{i_s}^+ S_{i_s+\eta_s}^- \rangle$, $\phi = \langle h_{i_s}^+ h_{i_s+\eta_s}^- \rangle$, respectively. In the present mean-field case, the holon moves in the background of spinons, and the spinon’s behavior is described by the anisotropic Heisenberg model. Since there are three inequivalent sublattices $A$, $B$, and $C$ in the kagomé lattice system, then the one-particle spinon and holon two-time Green’s functions are defined as matrices,

$$D_{\lambda\eta}(k, t - t') = \begin{pmatrix}
D_{\lambda A}^{AA}(k, t - t') & D_{\lambda A}^{AB}(k, t - t') & D_{\lambda A}^{AC}(k, t - t') \\
D_{\lambda B}^{BA}(k, t - t') & D_{\lambda B}^{BB}(k, t - t') & D_{\lambda B}^{BC}(k, t - t') \\
D_{\lambda C}^{CA}(k, t - t') & D_{\lambda C}^{CB}(k, t - t') & D_{\lambda C}^{CC}(k, t - t')
\end{pmatrix},$$

(3)

where $\lambda = s, z, h$, $D_{\mu\nu}^{wz}(i_\mu - j_\nu, t - t') = \langle \langle S_{i_\mu}^z(t); S_{j_\nu}^z(t') \rangle \rangle$ and $D_{\mu\nu}^{wz}(i_\mu - j_\nu, t - t') = \langle \langle S_{i_\mu}^z(t); S_{j_\nu}^z(t') \rangle \rangle$ with $\mu, \nu = A, B, C$, are the spinon’s propagators, while $D_{h}^{wz}(i_\mu - j_\nu, t - t') = \langle \langle h_{i_\mu}(t); h_{j_\nu}(t') \rangle \rangle$ is the holon’s propagator. At the half filling, the $t$-$J$ model is reduced as Heisenberg model. Since the absence of the simple three sublattice magnetic order on KLA has been convincingly demonstrated by many researchers, then in the following discussions, we will study the holon moves in the disordered spin liquid state, where there is no AFLRO, i.e., $\langle S_{i_s}^z \rangle = 0$. In this case, the basic equation for the Green’s functions within
in discussions \cite{15}, the Green’s functions (3) is obtained as,

\[
D_{\lambda}(k, \omega) = \frac{1}{[\omega^2 - \omega_\lambda^2(k)][\omega^2 - \omega_\lambda^2(k)][\omega^2 - \omega_\lambda^2(k)]}
\]

where \(\Gamma^\xi(k, \omega)\) is the adjugate matrix of

\[
\Delta^\xi(k, \omega) = \begin{pmatrix}
\omega^2 - (Z_{\xi1} + Z_{\xi2}\gamma_{k1}) & Z_{\xi3}\gamma_{k4} - Z_{\xi2}\gamma_{k5} & Z_{\xi3}\gamma_{k6} - Z_{\xi2}\gamma_{k7} \\
Z_{\xi3}\gamma_{k4} - Z_{\xi2}\gamma_{k5} & \omega^2 - (Z_{\xi1} + Z_{\xi2}\gamma_{k2}) & Z_{\xi3}\gamma_{k8} - Z_{\xi2}\gamma_{k9} \\
Z_{\xi3}\gamma_{k6} - Z_{\xi2}\gamma_{k7} & Z_{\xi3}\gamma_{k8} - Z_{\xi2}\gamma_{k9} & \omega^2 - (Z_{\xi1} + Z_{\xi2}\gamma_{k3})
\end{pmatrix},
\]

with \(\xi = s, z\), and \(\Gamma^h(k, \omega)\) is the adjugate matrix of

\[
\Delta^h(k, \omega) = \begin{pmatrix}
\omega + \mu & -4\chi t\gamma_{k4} & -4\chi t\gamma_{k6} \\
-4\chi t\gamma_{k4}^* & \omega + \mu & -4\chi t\gamma_{k8} \\
-4\chi t\gamma_{k6}^* & -4\chi t\gamma_{k8}^* & \omega + \mu
\end{pmatrix},
\]

while,

\[
a^\xi(k) = \begin{pmatrix}
-2Z_{\xi1} & Z_{\xi5}\gamma_{k4} & Z_{\xi5}\gamma_{k6} \\
Z_{\xi5}\gamma_{k4}^* & -2Z_{\xi4} & Z_{\xi5}\gamma_{k8} \\
Z_{\xi5}\gamma_{k6}^* & Z_{\xi5}\gamma_{k8}^* & -2Z_{\xi4}
\end{pmatrix},
\]

and \(a^h = 1\), where \(Z_{s1} = 8J_{eff}^2[e^2(\alpha C + 1/2) + (\alpha C_{z} + 1/2)]\), \(Z_{s2} = 4J_{eff}^2(e^2\alpha\chi_{z} + \epsilon\alpha\chi)\), \(Z_{s3} = 4J_{eff}^2(\epsilon(\alpha C + \alpha C_{z} + 1) + 3(e^2\alpha\chi + \epsilon\alpha\chi_{z}) - (e^2\alpha\chi_{z} + \epsilon\alpha\chi)]\), \(Z_{s4} = 4J_{eff}(\epsilon\chi + \chi_{z})\), \(Z_{s5} = 4J_{eff}(\epsilon\chi_{z} + \chi)\), \(Z_{s1} = 16J_{eff}^2(\alpha C + 1/2)\), \(Z_{s2} = 8J_{eff}e\alpha\chi_{z}\), \(Z_{s3} = Z_{21}/2 + 2Z_{22}, Z_{s4} = 4J_{eff}\chi_{z}, Z_{s5} = Z_{s1}, \gamma_{k1} = \cos k_{y} + \cos(k_{y} - k_{x}), \gamma_{k2} = \cos k_{x} + \cos k_{y}, \gamma_{k3} = \cos k_{z} + \cos(k_{y} - k_{x}), \gamma_{k4} = (1 + e^{ik_{y}})/2, \gamma_{k5} = (e^{ik_{x}} + e^{(ik_{y} - k_{x})})/2, \gamma_{k6} = (1 + e^{ik_{y} - k_{x}})/2, \gamma_{k7} = (e^{-ik_{x}} + e^{ik_{y}})/2, \gamma_{k8} = (1 + e^{-ik_{x}})/2, \gamma_{k9} = (e^{-ik_{y}} + e^{(ik_{y} - k_{x})})/2\), and the order parameters \(C = \sum_{\eta_{z} \neq \eta_{z}'} \langle S_{i_{x} + \eta_{z}'} S_{i_{x} + \eta_{z}} \rangle\), \(\chi_{z} = 2\langle S_{i_{z} + \eta_{z}} S_{i_{z} + \eta_{z}} \rangle\), \(C_{z} = 2 \sum_{\eta_{z} \neq \eta_{z}'} \langle S_{i_{z} + \eta_{z}} S_{i_{z} + \eta_{z}} \rangle\), while \(\omega_{\lambda j}(k)\) is the solution of the determinant \(|\Delta_{\lambda}(k, \omega_{j})| = 0\). In order not to violate the sum rule \(\langle S_{i_{z}} S_{i_{z}}^\pm \rangle = 1/2\) in the case \(\langle S_{i_{z}}^\pm \rangle = 0\), the important decoupling parameter \(\alpha\) has been introduced in the above calculation, which can
be regarded as the vertex corrections \[15,17\]. With the help of the spectral representation of the correlation functions, the decoupling parameter \(\alpha\) and order parameters \(\chi, \chi_z, C, C_z\), \(\phi\), and chemical potential \(\mu\) can be determined by the seven self-consistent equations \[15\].

At the half-filling, the \(t-J\) model is reduced as the Heisenberg model, where \(\epsilon = 1\), \(\chi_z = \chi\), \(C_z = C\) in the rotational symmetrical case, and therefore \(D_z(k, \omega) = D_s(k, \omega)/2\). In this case, the disordered spin liquid ground-state energy per site is \(E_g/N_sJ = -0.859\). For comparison, some results of the ground-state energy of KLA obtained from the numerical simulations and the present theoretical result are listed in Table I, where we find that the present spin liquid energy seems to be closer to the extrapolated finite lattice results of Leung and Elser \[8\], only is more than 3\% higher than the best numerical estimates by Zeng and Elser \[7\], and is almost identical with that of the variational calculation by Sindzinger, Lecheminant and Lhuillier \[10\]. Therefore the accuracy of the present mean-field results at half-filling is confirmed. As a by-product, the Heisenberg antiferromagnet on the triangular lattice has been discussed, and the spin liquid energy per site is \(E_g/NJ = -0.966\), which is essentially identical to results obtained by Kalmeyer and Laughlin \[18\] and Lee and Feng \[19\] based on the resonating-valence-bond state.

Away from half-filling, we find that the phase separation, present in the doped SLA \[20\], is absent here. For discussing the physical properties of the electronic state of the doped KLA, we need to calculate the electron Green’s function \(G^{\mu\nu}(i\mu - j\nu, t - t') = \langle\langle C_{i\mu\sigma}^{\dagger}(t); C_{j\nu\sigma}(t')\rangle\rangle\), which is a convolution of the spinon Green’s function \(D_s(k, t - t')\) and holon Green’s function \(D_h(k, t - t')\) in the framework of the fermion-spin theory, and can be obtained at the mean-field level as,

\[
G^{\mu A}(k, \omega) = \frac{1}{N} \sum_{\mathbf{p}} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \frac{n_F(\omega') + n_B(\omega'')}{\omega + \omega' - \omega''} \begin{pmatrix}
A^{A\mu}_{h'}(p - k', \omega')\ A^{\nu A}_{h'}(p, \omega'') \\
A^{A\mu}_{h'}(p - k', \omega') A^{\nu A}_{s'}(p, \omega'') \\
A^{A\mu}_{h'}(p - k', \omega') A^{\nu A}_{s'}(p, \omega'')
\end{pmatrix},
\]

where \(A^{\mu\nu}_{h'}(k, \omega) = -2\text{Im}\ D^{\mu\nu}_{h}(k, \omega)\) and \(A^{\mu\nu}_{s'}(k, \omega) = -2\text{Im}\ D^{\mu\nu}_{s}(k, \omega)\) are the holon and spinon spectral functions, respectively, \(n_B(\omega)\) is the boson distribution function, while \(n_F(\omega)\) is the
fermion distribution function. From the Green’s function (8), we obtain the electron spectral function as

\[ A(k, \omega) = -2 \text{Im} G^{AA}(k, \omega) - 2 \text{Im} G^{BA}(k, \omega) - \text{Im} G^{CA}(k, \omega). \]

Although the structural distortions of the \( \text{CuO}_2 \) planes in the copper oxide materials in the underdoped regime, measured most conveniently by the copper-oxygen bond angles [6], are very complicated and materials dependent, the common feature is that the spin frustration has been introduced. This spin frustration is related to the variation of the electronic density of states at the Fermi energy [6]. Among the doped antiferromagnets the most helpful for discussing the effects of the spin frustration on the electronic properties due to the distortions of the square \( \text{CuO}_2 \) planes may be the doped KLA since, as mentioned above, it has the same coordinate number with the square lattice. We have performed the numerical calculation for the electron spectral function \( A(k, \omega) \) of the doped KLA, and the results at the doping \( \delta = 0.12 \) for the parameter \( t/J = 2.5 \) at the zero temperature is plotted in Fig. 2. In comparison with the results of the spectral function on the square lattice [15], it is shown that the structure of the spectroscopy on the kagomé lattice is much complicated than the square lattice. Moving in the momentum space in the direction of O point, the photoemission spectroscopy weight increases, while the inverse photoemission spectroscopy weight decreases. On the contrary, increasing momentum towards the M point, the situation is inversed. For the further understanding of the electronic state properties, we investigate the electron density of states \( \rho(\omega) \), which is closely related with the spectral function, and is given as \( \rho(\omega) = \frac{1}{N} \sum_k A(k, \omega) \). The results of \( \rho(\omega) \) with (a) the doping \( \delta = 0.12 \) and (b) the doping \( \delta = 0.06 \) for the parameter \( t/J = 2.5 \) at the zero temperature are plotted in Fig. 3, where the existence of the gap in the electron density of states is an important feature. It is also shown that the density of states is shifted towards smaller energies with increasing doped holes, and the total weight is reduced since the integral of the density of states up to the Fermi energy has to be equal to the number of electrons, therefore there is a tendency that the gap narrows with increasing dopings since some states appear in the gap upon dopings. These results are consistent with the experiments of the copper oxide materials in the underdoped regime [4]. In comparison with the results of the density of
states on the square lattice \[15\], we find that the electron density of states near the Fermi energy on the kagomé lattice is lower than these on the square lattice. Irrespective of the coupling mechanism responsible for the superconductivity in the copper oxide materials, the transition temperature \(T_c\) is usually related to the electronic density of states at the Fermi energy. Our results may interpret that the highest superconducting transition temperature \(T_c\) for the square lattice \(CuO_2\) planes in the tetragonal structure in the optimal doping is reduced by the structure distortions of the \(CuO_2\) planes in the orthorhombic structure in the underdoped regime \[6\], i.e., this observed decrease of \(T_c\) in the underdoped regime \[6\] is due to the split singularity of the electronic density of states with the gap and lower electronic density of states near the Fermi energy. Moreover, the present results also indicate that the existence of the normal state gap and decrease of the electronic density of state near Fermi energy is possibly induced by the distortions of the lattice (then the spinon frustration).

In summary, we have discussed the electronic properties of the doped KLA within the \(t-J\) model. In the self-consistent mean-field level, we show that the ground-state of the undoped KLA is the spin liquid state with the energy per site \(E_g/N_s J = -0.859\), which is consistent with the numerical simulations \[7–10\]. It is also indicated that there is the normal-state gap in the electronic density of states for the doped KLA.

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FIGURES

FIG. 1. The spin configuration of the sublattices A, B, and C on the kagomé lattice.

FIG. 2. Electron spectral function $A(k, \omega)$ of the $t$-$J$ model on the kagomé lattice within the self-consistent mean-field theory in the doping $\delta = 0.12$ for the parameter $t/J = 2.5$ at the temperature $T = 0$. Note that there is a gap in the electron spectroscopy.

FIG. 3. Electron spectral density of the $t$-$J$ model on the kagomé lattice in the doping (a) $\delta = 0.12$ and (b) $\delta = 0.06$ for the parameter $t/J = 2.5$. 
TABLES

TABLE I. A comparison of the ground-state energy per site for the antiferromagnetic Heisenberg model on the two-dimensional kagomé lattice.

| Authors                         | $E_g/N_s J$ | Method              |
|---------------------------------|-------------|---------------------|
| Zeng and Elser [7]              | −0.882      | Finite lattice      |
| Yang, Warman and Girvin [9]     | −0.788      | Variational Monte Carlo |
| Leung and Elser [8]             | −0.877      | Finite lattice      |
| Sindzingre, Lecheminant and Lhuillier [10] | −0.84      | Variational Monte Carlo |
| The present work                | −0.859      | Green’s function method |