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Charge and spin orderings in triangular t–J–V model with quarter filling: application to $Na_{0.5}CoO_2$

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Abstract
We investigated the ground state (GS) properties of the single-orbital t–J–V model in a quarter-filling two-dimensional triangular lattice with the slave-boson mean-field approach. We found that the charge ordering (CO) and spin ordering arising from the spin exchange interaction J competes with that from the inter-site Coulomb interaction V. For comparatively large J, the stable GS is insulating with striped CO and antiferromagnetic ordering, avoiding the homogeneous frustrated phase. Accompanying the insulating CO phase, a small insulating gap is opened. Within a reasonable J and V parameter region, our results are consistent with the recent neutron scattering experiments in $Na_{0.5}CoO_2$, which possibly elucidate its CO, magnetic and other GS properties.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Many properties of correlated electrons in transition-metal oxides and the layered organic compounds can be described by a single-orbital Hubbard model [1–5]. In the past several decades, huge efforts have been made to understand the ground state (GS) and various excited states properties of the single-orbital Hubbard model or t–J model so as to elucidate the rich phenomena and complicated phase diagrams in transition-metal oxides and other correlated electron compounds (for example, see [4]). In these systems, due to large on-site Coulomb interactions, the motion of an electron is strongly affected by the neighborhood electron occupations. In particular, in the strong Coulomb correlation regime, the low-energy physics of the single-orbital Hubbard model is equivalent to the single-orbital t–J model without the electron double occupation per site [6]. The t–J model is thought to describe the essential physics of the unusual normal and superconductivity in cuprates [5]. The entanglement of the strong electronic correlation with doping concentration, dimensionality, lattice geometric structure and external field results in the complexity and the rich properties of the t–J model. Among these factors, the properties of the t–J model in a two-dimensional triangular lattice are the most interesting, since the frustration and quantum fluctuations of the spins in the triangular geometry structure may lead to exotic phases, such as the resonating valence bond (RVB) phase [5, 7] or spin-liquid phase [8]. While Huse and Elser [9] showed that, in the homogeneous situation, the spins in a triangular lattice may adopt the 120° geometry to gain energy because of the competition between the classical potential and the quantum fluctuations or frustration effect.

On the other hand, the frustration effect can be avoided through the breaking of the translation invariance of the lattice. The correlated electrons may form a charge and spin ordered phase in proper doping, rather than be a uniform GS. Once the charge inhomogeneous distribution forms, the inter-site Coulomb interaction, V, is inevitably involved in the t–J model. The unusual ordered phases of the t–J–V model may be significantly distinct in different doping regions and different parameter ranges [10–14]. Within the Jastrow–Gutzwiller approach, Motrunich and Lee [10] showed that in

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the t–J–V model with $J = 0$, the $\sqrt{3} \times \sqrt{3}$ charge ordering is energetically favorable at $x = 0.7$ and 0.35 when V is strong; here $1 - x$ is the hole filling. Baskaran [11] argued that from $x = 1/4$ to 1/3, the charge ordering of the t–J–V model is the *Kagome* lattice. Zheng *et al* [12] suggested the formation of the honeycomb charge ordering of the t–J–V model at 2/3-filling and gave the phase diagram of this model in different parameter regions. In the large-N approximation, Bejas *et al* [13] showed that the t–J–V model allows a $\sqrt{3} \times \sqrt{3}$ charge ordering over a wide doping range when V is larger than a critical value V_c. Hassan and de' Medici [14] recently also found such a charge ordered GS in away from the half-filled extended Hubbard model in the limit of large U. However, to date, few studies have been reported, particularly on the charge and spin ordering configurations of the quarter-filling case. Thus, a further study on the quarter-filled t–J–V model is needed.

As a prototype example of the two-dimensional triangular compounds, layered unhydrated cobaltate Na_xCoO_2 has been studied for many years because of its potential applications in thermoelectric materials [15–17]. Recently, the discovery of superconductivity in $Na_xCoO_2{\cdot}yH_2O$ has aroused great interest in the t–J model on a two-dimensional triangular lattice [18]. Various experiments [15, 19, 20] and theoretical studies [21, 22] demonstrated that the electron correlation plays an important role in the electronic states of Na_xCoO_2, suggesting that the two-dimensional single-orbital t–J–V model could describe the GS properties of Na_xCoO_2. Experimentally, not only the hydrated Na_xCoO_2 exhibits unusual superconductivity, but also the phase diagram of Na_xCoO_2 displays many rich and interesting phases with the Na content x [23]. In the range $0.2 < x < 0.5$, the stable phase is Pauli paramagnetic (PM) metallic; while for $x > 0.5$, Na_xCoO_2 is a Curie–Weiss metal. The most interesting observation happens at $x = 0.5$, where a unique insulating state with $\sqrt{3} \times 1$ charge order and striped antiferromagnetic (AFM) spin ordering is found [24]. Obviously, such a charge and spin order is outside the theoretical expectations in the literature mentioned above. This raises a lot of questions, such as what the magnetic moments at inequivalent cobalt sites are, what the nature of the charge and spin ordering in the GS [23–26] is, and what role does Na ion ordering play in the phase diagram [23], etc. These require a more extensive study on the electronic properties, especially the charge and spin order parameters of the single-orbital t–J–V model in a two-dimensional triangular lattice at quarter filling, not only for better understanding the GS properties of $Na_{0.5}CoO_2$, but also for the essentials of the GS properties of the t–J–V model.

In this paper we present the slave-boson [27] mean-field solution for the quarter-filled t–J–V model in a two-dimensional triangular lattice, in order to understand the GS properties, in particular the magnetic and charge orderings of $Na_{0.5}CoO_2$. We find that different orders may compete with each other. For comparatively large J, due to the competition of the charge ordering from the inter-site Coulomb interaction V, the frustrated spin exchange coupling J leads to weak striped $\sqrt{3} \times 1$ charge order, and the GS of the system is insulating with AFM spin order; at the same time, a very small insulating gap is also found. The major results presented are applicable in accounting for the charge ordered and spin ordered GS in $Na_{0.5}CoO_2$. In the rest of the paper, we first describe the model Hamiltonian and its method in section 2. We then present the theoretical results of the charge and spin ordered GS of the triangular t–J–V model and discuss the possible relationship with $Na_{0.5}CoO_2$ in section 3. Section 4 is devoted to the summary.

2. Model Hamiltonian and formulae

We start from the single-orbital t–J–V model with quarter filling in a two-dimensional triangular lattice,

$$\hat{H} = -t \sum_{\langle ij\rangle\sigma} (P\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}P) + J \sum_{\langle ij\rangle} (\mathbf{S}_i \cdot \mathbf{S_j} - \tfrac{1}{4} n_i n_j) + \frac{V}{2} \sum_{\langle ij\rangle} n_i n_j - \mu \sum_{i\sigma} n_{i\sigma}, \quad (1)$$

where $\hat{c}^{\dagger}_{i\sigma}$ creates a 3d hole carrier with spin σ at the ith site, and $n_{i\sigma}$ is the corresponding hole occupation number. $\langle\cdots\rangle$ implies that only the nearest-neighbor hopping or interaction is taken into account. The operator P projects the double occupancy of the hole carrier; t, J, V denote the hopping integral between the nearest-neighbor sites, the spin–spin exchange interaction constant, and the nearest-neighbor hole–hole Coulomb repulsion interaction, respectively; μ is the chemical potential. Since the a_{1g} bandwidth W is about 1.5 eV in Na_xCoO_2 [28], throughout this paper, we take the hopping integral $t = 0.15$ eV with the tight-binding approximation $9|t| = W$ for two-dimensional triangular lattice.

This model can be used to describe the low-energy physics in Na_xCoO_2: the Co ions form a two-dimensional triangular lattice in the edge sharing CoO_6 octahedra with a crystalline field splitting of about 2.5 eV between higher e_g and lower t_{2g} orbitals [28]; under the triangular crystalline field, the three-fold t_{2g} orbitals further split into nondegenerate a_{1g} and twofold degenerate $e_{g'}$ orbitals. The Co ions have an electron configuration of $3d^{5+x}$ in Na_xCoO_2. The large crystalline field splitting and small Hund coupling in the Co 3d shell suggest that the Co ions have a low spin state and the a_{1g} hole carrier is dominant. The theoretical prediction [21, 22] of the dominant a_{1g} hole near the Fermi energy level E_F is also supported by the angle resolved photoemission spectroscopy (ARPES) experiments, where only the large a_{1g} cylinder Fermi surface was observed for a wide range of Na doping concentrations [19, 20], in contrast to the local density functional (LDA) band structure calculations [29]. The neutron scattering [24] and the electron diffraction experimental data [30] have shown that in quarter-filling $Na_{0.5}CoO_2$ the charges and spins form a stripe superlattice structure with four Co sites on Co–O layers, shown in figure 1, which implies the order parameter λ_c of the charge difference or disproportion between the Co(1) and Co(2) sites. Following the experimental denotation, we refer to $Co^{(3.5-\lambda_c/2)+}$ as the Co(2) site and to $Co^{(3.5+\lambda_c/2)+}$ as the Co(1) site. $\vec{Q}_c = (0, 1/2)$ is the modulation wavevector of charge ordering/disproportion.

When the electron correlation is so strong that high-energy double occupation is precluded, we can apply the

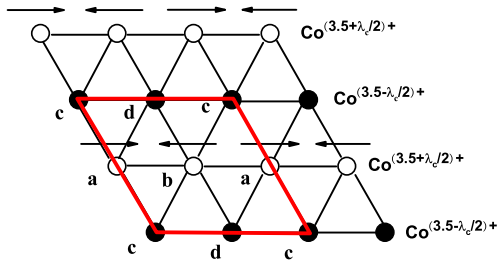

Figure 1. Schematic of the possible charge and spin arrangements of Co ions (a, b, c, d) in $Na_{0.5}CoO_2$. Hollow and solid circles denote Co(1) sites with spin directions and nonmagnetic Co(2) sites, respectively. The superlattice cell with charge and spin ordering is outlined with thick lines.

slave-boson ansatz to enforce the constraint. With the slave-boson transformation [27], the operators of hole carrier can be represented with fermion operators $f^{\dagger}_{i\sigma}$ ($f_{i\sigma}$) and bosonic operators b_i ($b^{\dagger}_i$), e.g. $\hat{c}^{\dagger}_{i\sigma} = b_i f^{\dagger}_{i\sigma}$, $\hat{c}_{i\sigma} = f_{i\sigma} b^{\dagger}_i$. The fermion operators and bosonic operators satisfy the constraints, $b^{\dagger}_i b_i + \sum_{\sigma} f^{\dagger}_{i\sigma} f_{i\sigma} = 1$. For the spin and charge configuration in figure 1, the slave-boson mean-field Hamiltonian becomes quadratic,

$$H_{\mathrm{SBMF}} = E_0 + \sum_{k\sigma} \begin{pmatrix} f^{\dagger}_{ka\sigma} & f^{\dagger}_{kb\sigma} & f^{\dagger}_{kc\sigma} & f^{\dagger}_{kd\sigma} \end{pmatrix} \begin{pmatrix} H_{aa} & H_{ab} & H_{ac} & H_{ad} \\ H_{ba} & H_{bb} & H_{bc} & H_{bd} \\ H_{ca} & H_{cb} & H_{cc} & H_{cd} \\ H_{da} & H_{db} & H_{dc} & H_{dd} \end{pmatrix} \begin{pmatrix} f_{ka\sigma} \\ f_{kb\sigma} \\ f_{kc\sigma} \\ f_{kd\sigma} \end{pmatrix} \tag{2}$$

with the constant E_0

$$E_0 = NJ \sum_{ll'\sigma} (n_{l\sigma} n_{l'\bar{\sigma}} - \delta_{ll'} n_{l\sigma} n_{l\bar{\sigma}}) - NV \sum_{ll'} (n_l n_{l'} - \delta_{ll'} n_l^2) \tag{3}$$

and the diagonal and off-diagonal matrix elements H_{ll} and $H_{ll'}$

$$H_{ll} = 2V \sum_{l'}^{l' \neq l} n_{l'} - 2J \sum_{l'}^{l' \neq l} n_{l'\bar{\sigma}}$$
$$H_{ll'} = -2t r_l r_{l'} \cos(\mathbf{k} \cdot \delta_{\mathbf{ll'}}) \tag{4}$$

etc; here l in r_l runs over the four inequivalent sublattices a, b, c, and d. $\delta_{\mathbf{ll'}} = \delta_{\mathbf{1,2,3}}$ refers to the three nearest-neighbor vectors from a to b sites, a to c sites, and a to d sites in figure 1. H_{SBMF} is now bilinear and could be diagonalized to obtain the following self-consistent equations of the electron occupation in equation (2) and the charge and spin order parameters λ_c and λ_s in equation (3),

$$\langle n^l_{i\sigma} \rangle = -\frac{1}{N\pi} \int_{-\infty}^{+\infty} \mathrm{Im} \sum_k G^l_{k\sigma}(\omega) f(\omega)\, \mathrm{d}\omega \tag{5}$$

$$\lambda_c = \sum_{\sigma} (\langle n^{c(d)}_{i\sigma} \rangle - \langle n^{a(b)}_{i\sigma} \rangle)$$
$$\lambda_s = \langle n^{a(b)}_{i\uparrow} - n^{a(b)}_{i\downarrow} \rangle, \tag{6}$$

where $G^l_{k\sigma}(\omega)$ is the diagonal retarded Green function for the sublattice l, and $f(\omega)$ the Fermi–Dirac distribution function. Obviously, one may choose different sublattices for different spin and charge ordered configurations, such as the homogeneous PM phase, $\sqrt{3} \times \sqrt{3}$ superstructure, etc.

On the other hand, these formulae become relatively simple in the homogeneous phase. For example, in the homogeneous FM or PM phase, within the slave-boson mean-field approach, the slave-boson mean-field Hamiltonian reads

$$H_{\mathrm{SBMF}} = \sum_{k\sigma} (\epsilon_k - 6Jn_{\bar{\sigma}} + 6Vn) f^{\dagger}_{k\sigma} f_{k\sigma} - 3NJ \sum_{\sigma} n_{\sigma} n_{\bar{\sigma}} - 3NVn^2 \tag{7}$$

with the renormalized tight-binding energy dispersion

$$\epsilon_k = -2tr^2(\cos\delta_1 + \cos\delta_2 + \cos\delta_3) - \mu, \tag{8}$$

where the empty probability is r^2 per site. Combining equations (1)–(8), we could obtain the electronic properties of the homogeneous PM or the ordered ground states, such as in figure 1. Furthermore, we could acquire the evolution of the order parameters with a variation of parameters J and V, and gain an insight for their different impacts on the ordered phase discussed. With the help of these results, we could address the unusual origin of the charge and spin ordering in $Na_{0.5}CoO_2$.

3. Theoretical results

3.1. Stability of the ordered phase

First of all, we find that when $J \geqslant 2V$, the charge and spin ordered phase is more stable than the homogeneous PM one, as can be seen from the dependence of the GS energy difference $\Delta E = E(\lambda_{c,s} \neq 0) - E(\lambda_{c,s} = 0)$ on the parameters J and V in figure 2. The energy difference ΔE always monotonously drops or rises with an increase of J or V, respectively. Consulting the numerical results in figure 2, we find that the strong AFM spin exchange interaction J is very essential in stabilizing the ordered state and in avoiding spin frustration in the triangular lattice. Interestingly, in addition to a phase transition from the homogeneous PM phase to the ordered state, there exists an inflexion at $J = V/2$ with an increase of J in the curves in figure 2(a). The implication of this inflexion will be discussed in the following text. With an increase of the inter-site Coulomb repulsion interaction V, a larger J value is needed to attain the charge and spin ordered state in figure 2(b). Thus, there is a phase transition from the ordered state to the homogeneous PM phase with an increase of V at a finite J, as shown in figure 2(b).

3.2. Evolution of spin and charge order parameters

As mentioned above, the larger the spin exchange interaction J and the smaller the inter-site Coulomb repulsion interaction V, the more stable the ordered state is. Quantitatively, we present the evolution of the charge and spin order parameters λ_c and λ_s with the variation of J and V in figures 3(a) and (b). For a specific inter-site Coulomb repulsion interaction V, the charge order is absent below a critical value J_c, but λ_s appears at a comparatively smaller J_s, which can be seen from the

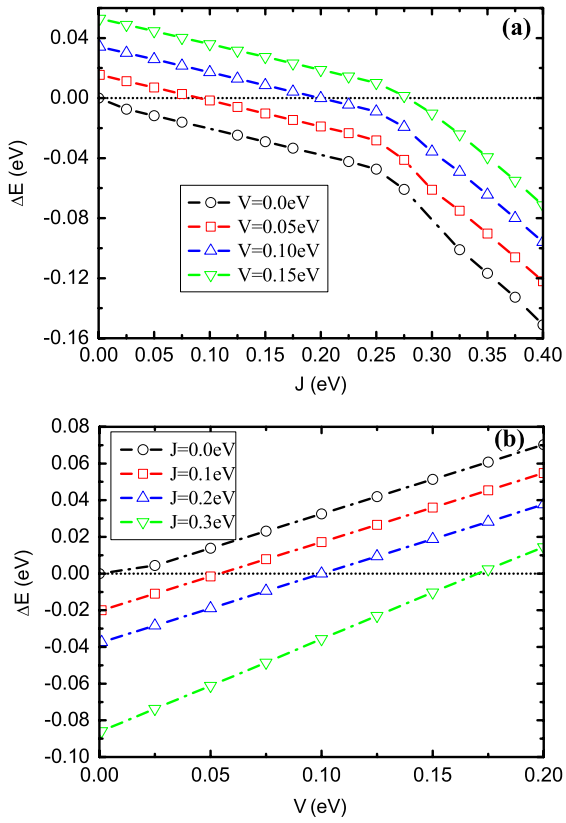

Figure 2. Dependence of the GS energy difference between the ordered and homogeneous PM states on the spin–spin interaction J (upper panel) and the inter-site Coulomb interaction V (lower panel).

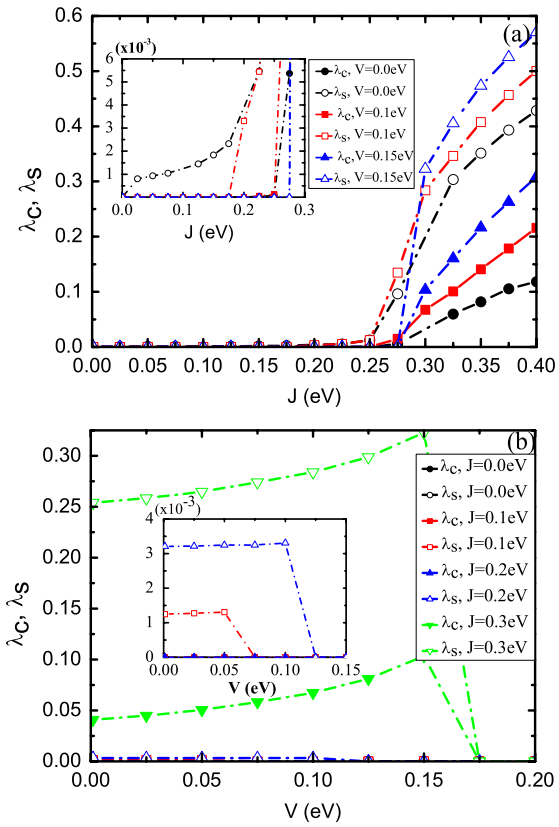

Figure 3. Dependence of the charge and spin order parameters on (a) spin–spin coupling J and (b) inter-site Coulomb interaction V. The insets show enlargements of the small J and V parameter regions, respectively.

insets of figures 3(a) and (b). When J is larger than J_c, λ_c and λ_s increase quickly with an increase of J. In fact, the formation of such a spin arrangement shown in figure 1 avoids the frustration, and it is very beneficial in reducing the GS energy of the triangular lattice. Therefore, λ_s emerges earlier than λ_c. By analyzing the critical values J_c for different V cases and the inflexions in figure 2(a), we can deduce that these inflexions correspond to phase transitions from system states with only spin order to ones with both charge and spin order.

Similarly, the dependence of λ_c and λ_s on V is shown in figure 3(b). For a relatively large J, λ_c and λ_s increase with an increase of the inter-site Coulomb repulsion V. However, a very large inter-site Coulomb interaction V destroys the ordered state and make this system re-enter the homogeneous PM phase or other ordered phases. In the present triangular lattice, when the inter-site hole–hole Coulomb repulsion V becomes very large, the inhomogeneous charge ordered phase is favorable in energy. The charge may be more localized and may avoid distributing too closely. In this case, one may expect the formation of more complicated charge ordered phases on a triangular lattice, such as a $\sqrt{3} \times \sqrt{3}$, a honeycomb or a *Kagome* charge ordering, etc. Moreover, different stable charge ordering phases may take place at different band fillings. The competition among these different charge ordered states in the large V region is interesting and deserves further study. In this paper, we find the configuration of $\sqrt{3}a \times a$ (here a is the triangular lattice parameter) charge order and $2a \times 2a$ for the AFM spin ordered state shown in figure 1 is the most stable within the comparatively larger spin exchange interaction J and a smaller inter-site Coulomb repulsion V parameter region. So our results are not affected by the competition of these complicated charge orderings in the large V region.

3.3. Density of states of quasi-particles

With the formation of the ordered state, the primary energy spectrum splits into four quasi-particle spectra $\omega_m(k)$, $(m = 1, 2, 3, 4)$. Also, from the retarded Green function in the reciprocal k-space, $G^l_{k\sigma}(\omega)$, one could get the total density of states (DOS) per site (or per superlattice), $\varrho(\omega) = -\frac{1}{N\pi}\,\mathrm{Im}\sum_{lk\sigma,\eta\to 0} G^l_{k\sigma}(\omega + \mathrm{i}\eta)$. The DOS for different spin exchange interactions J and inter-site Coulomb repulsion interactions V are shown in figure 4. From figure 4, we find that the spin exchange interaction J plays a key role in the DOS at E_F. At $J = 0.25$ and $V = 0.0$, the DOS exhibits a nonzero value at E_F, indicating that the GS is metallic.

On the contrary, at $J = 0.30$ and $V = 0.0$, the DOS at E_F vanishes and an insulating band gap of about 15 meV appears. However, under the present conditions, the charge disproportion λ_c between a and c sites in figure 1 is weak, $\sim$0.03. When $J = 0.30$ eV and $V = 0.15$ eV, the insulating

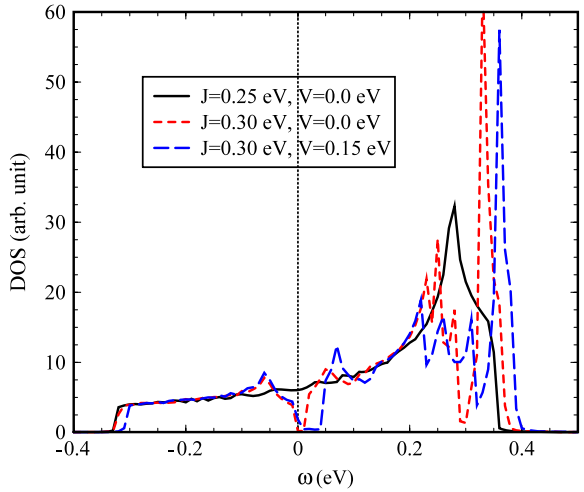

Figure 4. DOS for three sets of J, V parameters. The vertical line represents the Fermi energy level.

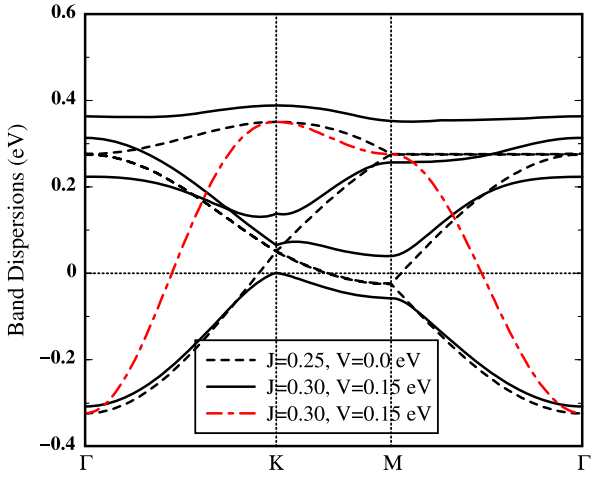

Figure 5. Band structures of ordered (solid line and dashed line) and homogeneous PM (dot-dashed line) states for different sets of J and V parameters. The horizontal line represents the Fermi energy level.

band gap of the system increases to about 50 meV with the order parameters $\lambda_c \sim 0.10$ and $\lambda_s \sim 0.32\ \mu_B$. Such a nonconventional charge ordering picture agrees quantitatively well with the recent nuclear magnetic resonance experiment in $Na_{0.5}CoO_2$, which suggested the charge distribution of $Co^{3.5\pm\delta}$ ($\delta < 0.2$) [31] on Co(1) and Co(2) sites. Simultaneously, the magnetic moment of Co(1) sites that we obtained, $\mu_{Co(1)} = \lambda_s \sim 0.32\ \mu_B$, is consistent with the experimental data from neutron scattering [24, 32].

3.4. Band structures of quasi-particles

Figure 5 shows the dependence of the band dispersion of the quasi-particle with the J and V interaction. We find that the homogeneous PM phase and the phase with only small spin ordering correspond to the metallic state.What is more interesting is that in the metallic state with only the spin ordering, two branches spectra of the quasi-particle cross each other near $E_F = 0$. Remarkably, an approximate Dirac-like linear dispersion appears in the vicinity of the K point, which arises from the three-fold symmetry of this system, just like that in the two-dimensional graphene [33]. When the spin exchange interaction J and inter-site Coulomb interaction V become large an insulating gap opens within two lower subbands in figure 5. The energy gap is about 50 meV for $J = 0.30$ eV and $V = 0.15$ eV. The formation of the insulating phase is a unique feature of the quarter-filling hole carriers in the band structures in the presence of a strong exchange interaction J between spins and Coulomb repulsion interaction between carriers. In detail, due to the formation of the charge and spin superstructure illustrated in figure 1, the a_{1g} band is split into four subbands in the reduced Brillouin zone, as shown in figure 5. The three upper subbands are pushed up above the Fermi surface and completely empty, whilst the lowest subband is fully occupied, hence the insulating gap opens. At this point, the hole occupations in a_{1g} orbitals are 0.552 at the a site and 0.448 at the c site. A slightly higher or lower carrier concentration unlikely leads to this insulating GS in the present ordered state.

In the present charge and spin ordered configuration, the charge difference between a and c sites is about 0.1, indicating a nonconventional charge order. Such a $(3.5 + \lambda_c/2)/(3.5 - \lambda_c/2)$ charge ordering picture agrees quantitatively well with the recent nuclear magnetic resonance experiment in $Na_{0.5}CoO_2$, which suggested the charge distribution of $Co^{3.5\pm\delta}$ ($\delta < 0.2$) [31] on Co(1) and Co(2) sites. Corresponding to the charge distribution, the spins on Co(1) sites AFM couple with each other along the horizontal rows, effectively showing a one-dimensional character. At the same time, the sublattice magnetic moment on the Co(1) site is about 0.32 μ_B, consistent with the experimental data, 0.3 μ_B, from the neutron scattering [24, 32]. It is worth emphasizing that the Na ion order [34, 35] is favorable for the formation of a $\lambda_c = 0.104$ charge order and a $\lambda_s = 0.32$ spin order. In the rows of nonmagnetic Co(2) sites, Na ions have positions just below or above the Co atoms. The positively charged Na ions contribute more electrons, thus stabilizing the nonmagnetic Co ions.

4. Concluding remarks

We have shown that the spin exchange interaction J and the inter-site Coulomb repulsion interaction V result in the stripe charge order and the AFM order in a quarter-filling t–J–V model on a two-dimensional triangular lattice, and which qualitatively interpret the GS properties in $Na_{0.5}CoO_2$. We also notice that the present spin and charge ordered phase is always stable as long as J is strong enough, even for the case without any inter-site Coulomb repulsion interaction, rather than the existence of a critical repulsion V_c in the t–U–V model with the Gutzwiller approach [36]. It indicates that the AFM superexchange interaction J plays a key role in establishing the AFM spin arrangement and the charge ordering to avoid spin frustration in the triangular lattice. In fact, the first-principles calculation on the parent material CoO_2 is a charge transfer insulator and the on-site Coulomb interaction is finite [37], which implies that the exchange interaction J in this system could be large.

From the experimental aspects of Na_xCoO_2 at $x = 0.5$, the Co(2) sites with less hole carriers have much smaller magnetic moments in or out of the CoO_2 plane, which align ferromagnetically or as an AFM [32, 38]. More interestingly, the recent NMR experiment by Ning *et al* [39] suggested that there also exists charge differentiation within Co(2) sites. All these experimental facts make the GS of $Na_{0.5}CoO_2$ more surprising and complicated. More recently, Yamakawa and Ono [40] proposed the possibility of the formation of charge, spin and orbital orderings in $Na_{0.5}CoO_2$. Hence, more research is needed to clarify whether the orbital degree of freedom is involved in the physical properties of Na_xCoO_2, in particular in $Na_{0.5}CoO_2$.

The SBMFA is now widely used in strongly correlated electron systems because it projects the high-energy double occupancy of carriers in the same orbit. The improvement of the SBMFA approach with respect to the Hartree–Fock approximation is considerable. However, the approach is expected to overestimate the charge and spin correlations and order parameters since the SBMFA is a saddle-point solution which enforces single occupancy only on average, and the boson fluctuations are not taken into account. It would be interesting to extend our results so as to consider the fluctuations of the boson fields via other techniques, e.g. the Gaussian fluctuation correction or the one-loop correction to the ground state energy, going beyond the simple mean-field approximation. While such a correction only renormalizes the groundstate properties [41], or is temperature dependent, the higher the temperature is, the more considerable the correction is [42, 43]. Thus we anticipate that it will not qualitatively affect our conclusions for the ground state at $T = 0$ K.

In summary, the two-dimensional triangular lattice t–J–V model behaves as a metallic phase for small J value. With an increase of spin–spin exchange interaction and inter-site Coulomb interaction, a very small insulating gap opens in the quarter-filling system, and the formation of charge disproportion and alternate rows AFM spin ordering avoids the frustration effect, thus giving an interpretation of the GS properties of $Na_{0.5}CoO_2$.

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