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Variational Monte Carlo study of magnetic correlations in bilayer *t-J* model

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Abstract We study the magnetic correlations in a t–J bilayer using Variational Monte Carlo (VMC) method, the variational wavefunction being the solution of the Hartree-Fock (HF) t-J Hamiltonian with antiferromagnetic (AF) order We calculate the spin-spin correlation functions and spin structure factors at half filling and slightly away from half filling The results show that, at half filling perfect antiferromagnetic long range order (AFLRO) exists which starts to diminish as soon as holes are introduced It is observed that the holes drastically reduce the interplanar spin correlations, whereas the effect on the planar correlations is rather small This is to be contrasted with the experimental results on the cuprates, which show that the AFLRO in the copper oxide planes gets completely destroyed even at a small hole concentration This is possibly due to the competition of AFLRO with the superconducting order, which has not been incorporated in our calculations We also examine the effect of the interplanar parameters *e g* the hopping integral t and exchange constant, $J_{\perp}$ on the magnetic correlations We find that $t_{\perp}$ reduces planar correlations while the effect of J is small

Keywords t-J model, VMC

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1. Introduction

High temperature superconductivity discovered in the cuprate compounds first in 1986 [1] has been a subject of very intense research for a variety of reasons [2] Experiments have shown that the parent (undoped) compounds of high-T_c superconductors are very good insulators with the spins of the Cu^{2+} ions ordered antiferromagnetically Upon doping with charge carriers (holes), the antiferromagnetic long range order (AFLRO) gets destroyed rapidly and the compounds show superconductivity with high transition temperatures. The basic feature in structure of the cuprate superconductors is the presence of copper oxide (CuO_2) layers intervened by other atoms (*e.g.* La, Ba *etc.*). The properties of the high-T_c

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superconductors are generally found to depend on the number of copper oxide layers present per unit cell. For example, the bilayer compounds (*e.g.* $YBa_2Cu_3O_{6+x}$) have a spin gap [3-5] which is absent in single layer compounds, also its transition temperature, T_c is higher as compared to the single layer ones [6, 7], *etc.*

Theoretically the *t-J* model have been shown to describe the properties of the high-T_c superconductors at least close to half filling reasonably satisfactorily. The model has been studied extensively using a variety of analytical and numerical techniques for two dimensional lattice. Application of numerical techniques, like the quantum Monte Carlo method is limited by the negative sign problem. On the other hand, analytical techniques can treat the constraint of no double occupancy in the *t-J* Hamiltonian only approaimately The Variational Monte Carlo (VMC) method is free from such problems, but it sensitively depends on the choice of the variational wavefunction. The VMC method has been used to study various phases of the *t-J* Hamiltonian, *viz.* antiferromagnetic, superconducting, metallic *etc.*, for two dimensional lattice. In this work, we use VMC study magnetic properties of the bilayer *t-J* model by taking the Hartree-Fock antiferromagnetic state as the variational wavefunction. However, away from half filling this wavefunction is not expected to be the true ground state. We leave the incorporation other degrees of freedom (superconducting) in the variational wavefunction, for a future investigation.

2. The model

The *t-J* Hamiltonian for a bilayered lattice can be written as

$$\mathcal{H} = -t\sum_{\langle i,j\rangle\sigma}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + H.c.\right) + J\sum_{\langle i,j\rangle}\left(S_i.S_j - \frac{1}{4}n_i n_j \right) - t_{\perp}\sum_{\langle\langle i,k\rangle\rangle\sigma}\left(c^{\dagger}_{i\sigma}c_{k\sigma} + H.c.\right)$$

$$+ J_{\perp}\sum_{\langle\langle i,k\rangle\rangle}\left(S_i.S_k - \frac{1}{4}n_i n_k \right) \qquad (1)$$

where t and J are the planar hopping and exchange integral respectively, while $t_{\perp}$ and $J_{\perp}$ are the corresponding interplanar parameters. $c_{i\sigma}$ $\left(c^{\dagger}_{i\sigma}\right)$ annihilates (creates) an electron of spin σ at site i. $\boldsymbol{S}_i$ is the spin operator at site i, given by $S^{\alpha}_i = \psi^{\dagger}_i\left(\frac{1}{2}\sigma_{\alpha}\right)\psi_i$, where $\psi_i = \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$ and σ_{α} $(\alpha = x, y, z)$ are the Pauli spin matrices. The summation indices $\langle i,j\rangle$ and $\langle\langle i,k\rangle\rangle$ indicate nearest neighbor pairs in the same plane and adjacent planes respectively. The Hamiltonian acts on a subspace of no doubly occupied sites.

3. The variational wavefunction

We take the following wavefunction with antiferromagnetic (AF) order as our variational ansatz for the ground state of the bilayer *t-J* Hamiltonian,

$$|\Psi_{\text{var}}\rangle = \mathcal{P}_G |\Psi_{AF}(\Delta)\rangle \tag{2}$$

where,

$$|\Psi_{AF}(\Delta)\rangle = \prod_{k<k_F} d^{\dagger}_{k\uparrow} d^{\dagger}_{k\downarrow} |0\rangle \tag{3}$$

$\mathcal{P}_G = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$ is the Gutzwiller operator which projects out the states with no doubly occupied site. The wavefunction $|\Psi_{AF}(\Delta)\rangle$ is the ground state of the Hartree-Fock (HF) antiferromagnetic Hamiltonian, given by

$$\mathcal{H}_{AF} = \sum_{\substack{k\sigma \\ (\varepsilon_k<0)}} \begin{bmatrix} c_k \\ c_{k+Q} \end{bmatrix}^{\dagger} \begin{bmatrix} \varepsilon_k & -\eta(\sigma)\Delta \\ -\eta(\sigma)\Delta & -\varepsilon_k \end{bmatrix} \begin{bmatrix} c_k \\ c_{k+Q} \end{bmatrix} \tag{4}$$

where $Q = (\pi, \pi, \pi)$ is the perfect nesting vector, $\varepsilon_k = -2t(\cos k_x + \cos k_y) - 2t_\perp \cos k_z$ is the free electron dispersion relation and $\eta(\sigma) = \pm 1$ for $\sigma = \uparrow, \downarrow$. Δ is proportional to the sublattice magnetization and is our variational parameter. The quasiparticle operators $d^{\dagger}_k$ are related to the electron operators by the following transformation,

$$\begin{bmatrix} d^{\dagger}_k \\ d^{\dagger}_{k+Q} \end{bmatrix} = \begin{bmatrix} \alpha_k & \eta(\sigma)\,\beta_k \\ -\eta(\sigma)\,\beta_k & \alpha_k \end{bmatrix} \begin{bmatrix} c^{\dagger}_k \\ c^{\dagger}_{k+Q} \end{bmatrix} \tag{5}$$

with

$$\alpha_k = \frac{1}{\sqrt{2}} \left(1 - \varepsilon_k / \sqrt{\varepsilon_k^2 + \Delta^2}\right)^{1/2} \tag{6}$$

$$\beta_k = -\frac{1}{\sqrt{2}} \left(1 + \varepsilon_k / \sqrt{\varepsilon_k^2 + \Delta^2}\right)^{1/2} \tag{7}$$

and k is such that $\varepsilon_k < 0$.

The variational wavefunction describes the Néel anti-ferromagnetic phase for nonzero Δ, while for $\Delta = 0$, it reduces to the singlet liquid state [9].

4. Numerical details

As with any variational calculation, we start by evaluating the energy expectation value

$$\langle \mathcal{H} \rangle = \frac{\langle \Psi_{\text{var}} | \mathcal{H} | \Psi_{\text{var}} \rangle}{\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle} \tag{8}$$

and optimizing the wavefunction with respect to the variational parameter Δ. The minimum energy thus found represents an upper bound to the true ground state energy of the system. For numerical evaluation of the expectation value, we write the expression as [10]

$$\langle \mathcal{H} \rangle = \sum P(R) \frac{\langle \Psi_{\text{var}} | \mathcal{H} | R \rangle}{C(R)} \tag{9}$$

where $|R\rangle = c_{r_1\uparrow} c_{r_2\uparrow} \ldots c_{r'_1\downarrow} c_{r'_2\downarrow} \ldots |0\rangle$ represents a configuration of the electrons in the real space representation of the wavefunction and C(R) is the weight of the configuration. The probability density for a configuration $|R\rangle$ is given by,

$$P(R) = \frac{|C(R)|^2}{\sum_{R'} |C(R')|^2} \tag{10}$$

In the Monte Carlo procedure, the summation over R is replaced by the importance sampling with weight $P(R)$, for which we use the Metropolis algorithm.

Simulations are performed on a lattice of size 10 × 10 × 2. In one Monte Carlo sweep (MCS) through the lattice, we attempt N_s (number of lattice sites) random moves which consists of moving an electron to an empty site and exchanging two antiparallel spins. The Monte Carlo update of the configurations, after each successful move, is done by using the inverse update method due to Ceperley *et al* [8]. For calculation of the expectation values of observables, we make measurements on configurations chosen from about 10,000 – 50,000 Monte Carlo sweeps after warming up the system for about 5,000 sweeps.

5. Results

The results shown here are for a lattice of size 10 × 10 × 2. As for the parameters, we choose values that are realized for various cuprate compounds, *e.g.* we take $J/t = 0.35$ and the interplanar parameters are varied from, $t_\perp/t = 0.05 - 0.20$ and $J_\perp/t = 0.05 - 0.35$.

First, we optimize the wavefunction with respect to the variational parameter, Δ for various values of interplanar parameters $(t_\perp, J_\perp)$, at half filling and slightly away from half filling. For one set of parameter value, *viz.* $(t_\perp/t, J_\perp/t) = (0.20, 0.10)$, we have carried out

the optimization to higher value of hole doping, in order to determine the stability of the antiferromagnetic phase against the singlet liquid state The results are shown in Figure 1 Our calculation shows that the antiferromagnetic phase yields lower energy upto 20% hole concentration in a bilayer for the chosen parameter values For comparison, we have also calculated the optimal parameter, $\tilde{\Delta}$ as a function of hole concentration, δ for a square lattice of size 10 x 10 and taking the value of J / t, to be the same as that for the bilayer. We found that in this case, the stability of the AF phase against the singlet liquid state, extends upto about 14% hole concentration which is lower than that for the bilayer This shows that interplanar couplings sustain the AF phase till larger values of hole doping

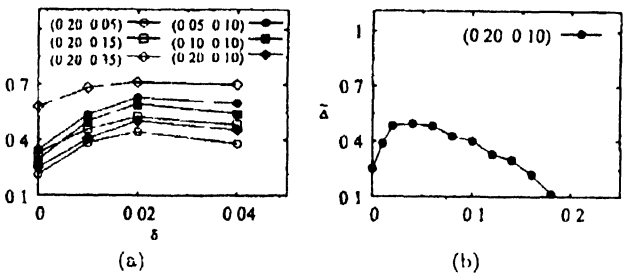


Figure 1. Optimal variational parameter Δ *versus* hole concentration δ For (a) different interplanar parameter values in the underdoped region and (b) for one value of the parameter set at all hole concentration The paired numbers inside bracket in the figures indicate the values of the parameters $(t, J_\perp)$

Next, we show results for spin-spin correlation function, $\langle S_i^z S_j^z \rangle$ calculated for the optimized wavefunction at various hole concentrations and for different parameter values Figure 2, shows the planar and interplanar spin correlations as a function of distance along the edge of a plane (x-direction), at and away from half filling for $(t_\parallel\ t, J_\perp\ t)$ equal to (0 20, 0 10) The figure shows that perfect antiferromagnetic long range correlations (Neel order) exist at half filling Moreover, the magnitude of planar and interplanar correlations are almost equal albeit with $J_\perp < J$ Away from half filling, as soon as holes are introduced, both planar and interplanar correlations get diminished This reduction is more prominent

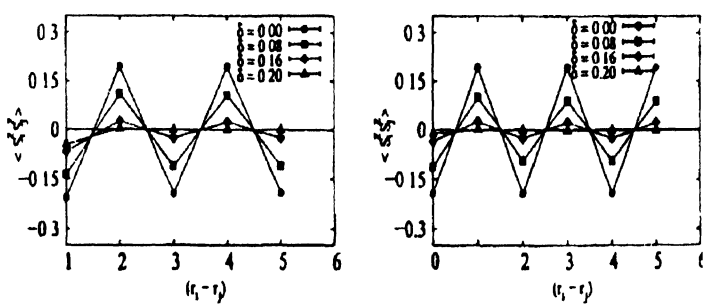
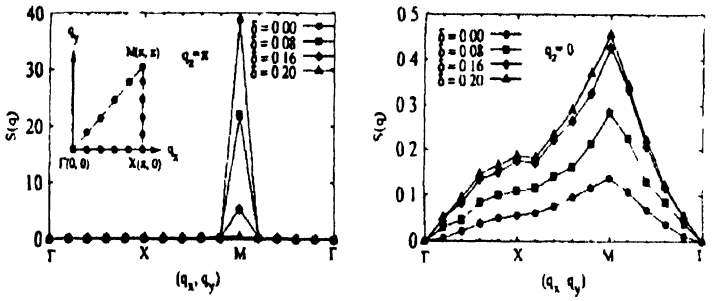


Figure 2. Spin spin correlation, $\langle S_i^z S_j^z \rangle$ as a function of distance $|r_i - r_j|$ along x-direction In (a) sites i and j belong to same plane, whereas in (b) i and j belong to different planes

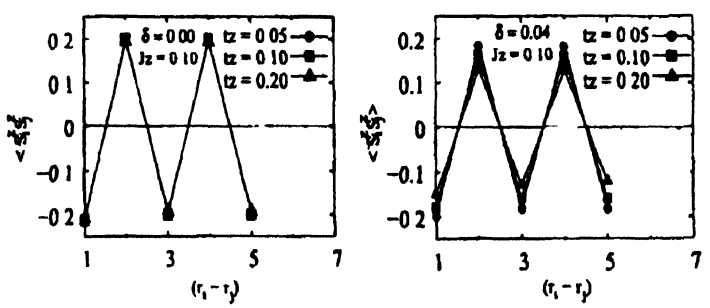
is case of the interplanar correlations This can be understood as follows Since $J_\perp < J$ the energy cost of disrupting a bond between two interplanar sites is less than that for a intraplanar bond So, the interplanar bonds of antiparallel spins are broken easily by the mobile holes. Another notable feature is that the magnitude of correlations at all distances get diminished uniformly by holes It does not decay appreciably with distance, except for the two larger hole concentrations shown in Figure, while planar correlations show a slow decay with distance. This result is to be contrasted with experimental results available for cuprates It is well known that the AFLRO in the copper oxide planes gets completely



(a) $q_z = \pi$ (b) $q_z = 0$

Figure 3. Spin structure factor $S(\boldsymbol{q})$ as a function of q, at various hole concentration δ The values of (q_x, q_y) on the horizontal axes are the points in the triangular path in q- space, shown in (a)

destroyed by as small as about 2% hole concentration, followed by the appearance of the superconducting phase. Our study here, where we consider a wavefunction only with antiferromagnetic order, shows that the holes alone are not effective in destroying long range correlations Thus we conclude that the AFLRO in the cuprate superconductors does not get destroyed, only due to the effects of mobile holes but possibly due to combined effects of holes and competition with other phases It may be mentioned that a number of phases are known to appear in the underdoped regime of high temperature superconductors [11]. These phases posses complex magnetic ordering and are found to be competing with each other. Further, the spin structure factors $S(\boldsymbol{q}) = (1/N)\,\Sigma_{i,j}\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}_{ij}} \langle S_i^z S_j^z \rangle$ as a function of $\boldsymbol{q}$, calculated at various hole concentrations



(a) $\delta = 0.00$ (b) $\delta = 0.04$

Figure 4. Spin spin correlation function, $\langle S_i^z S_j^z \rangle$ for different values of interplanar hopping parameter $t_\perp$, at and away from half filling

are shown in Figure 3. The sharp peaks at $\boldsymbol{q} = (\pi, \pi, \pi)$ are indications of the existence of antiferromagnetic long range order (AFLRO), which diminishes as one gos away from half filling There are also peaks in $S(q_x, q_y, 0)$ at $(\pi, \pi, 0)$ in the $S(\boldsymbol{q})$ *versus* $\boldsymbol{q}$ curves for $\eta = 0$ However, $S(q_x, q_y, 0)$ for all (q_x, q_y) increases with increasing hole concentration The increase in maximum in case of $S(\pi, \pi, 0)$ This is because of the reduction of interplanar antiferromagnetic correlations by the holes as remarked earlier

Finally, we examine the effects of interplanar coupling on the magnetic correlations in the bilayer Figure 4 shows the planar spin correlations along x-direction for different values of interplanar hopping parameter, $t_\perp$ As seen in the figure, $t_\perp$ plays no role at half filling as expected But away from half filling larger interplanar hopping reduces spin correlations in a plane Interplanar correlations (not shown here) are not effected by $t_\perp$ On the other hand the interplanar exchange constant, $J_\perp$ is found to have negligible effects on both the planar and interplanar correlations

6 Conclusion

We have studied the magnetic correlations in the Hartree-Fock antiferromagnetic wavefunction for a bilayer t-J model using VMC method We find that, perfect antiferromagnetic long range order exists at half filling Away from half filling, the magnitude of correlations decreases with increasing hole concentration, but the long range order survives upto much higher hole doping in comparison to the range of AF phase in cuprate superconductors We also find that, interplanar hopping reduces planar correlations while the effect of interplanar exchange is small

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