Variational study of the neutron resonance mode in the cuprate superconductors

Tao Li[1] and Fan Yang[2]
[1]*Department of Physics, Renmin University of China, Beijing 100872, People's Republic of China*
[2]*Department of Physics, Beijing Institute of Technology, Beijing 100081, People's Republic of China*
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A Gutzwiller-type variational wave function is proposed for the neutron resonance mode in the cuprate superconductors. An efficient reweighting technique is devised to perform variational Monte Carlo simulation on the proposed wave function which is composed of linearly superposed Gutzwiller projected Slater determinants. The calculation, which involves no free parameter, predicts qualitatively correct behavior for both the energy and the spectral weight of the resonance mode as functions of doping.

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I. INTRODUCTION

The (π,π) resonance mode observed by neutron scattering in the cuparte superconductors is among the most prominent phenomena in these systems.[1–4] Below the superconducting transition temperature T_c, a sharp peak is observed in the spin-fluctuation spectrum around (π,π). The mode is found to have close correlation with superconductivity of the system. For example, the mode energy, which is temperature independent, is found to scale linearly with T_c as a function of doping. At the same time, the intensity of the mode is found to have the similar temperature dependence as the superfluid density.

Much theoretical efforts have been devoted to the understanding of the origin of the neutron resonance mode and its correlation with superconductivity.[5–11] Among these theories, the random-phase approximation (RPA)-like theory, which takes the resonance mode as a spin-one bound state in the particle-hole channel (spin exciton) induced by the residual attractive interaction between the Bogliubov quasiparticles in the superconducting state, is the most popular. In this theory, the dynamical spin susceptibility is given by

$$\chi(q,\omega)=\frac{\chi_0(q,\omega)}{1-U(q)\chi_0(q,\omega)}, \tag{1}$$

here $\chi_0(q,\omega)$ is the bare spin susceptibility of the BCS superconducting state determined by both the band dispersion and the gap function. $U(q)$ is the phenomenological RPA correction factor chosen to fit the experimental data. In the RPA theory, the superconducting gap sets a natural energy scale for the resonance mode below which the mode is stable. At the same time, when the system approaches the antiferromagnetic ordering instability under RPA correction, the mode will evolve into the Goldstone mode of the ordered state and its energy will approach zero. Thus, the energy of the resonance mode in the RPA theory is determined by both the magnitude of the superconducting gap and the strength of the antiferromagnetic correlation.

Although the RPA theory can account for some aspects of the neutron resonance mode, it is to a large extent, a phenomenological theory. The band dispersion of the quasiparticle and the RPA correction factor $U(q)$, on which the result of RPA calculation depends sensitively on, are subjected to fine tuning. Some attempts had been made to apply the RPA theory at a more microscopic level and had received some success.[7,8] However, a direct application of the RPA theory for the slave Boson mean-field theory of the t-J model[8] has resulted in too large a doping range ($0<x<0.2$, x is doping concentration) in which the system is unstable with respect to antiferromagnetic ordering. At the same time, neither the phenomenological RPA theory nor the RPA correction on the slave Boson mean-field theory of the t-J model respects the local-spin sum rule of the t-J model, $\int dqd\omega S(q,\omega)=(1-x)\frac{3}{4}$, as a result of their neglect of the no double-occupancy constraint of the t-J model.

In this paper, we propose a variational description for the neutron resonance mode with a Gutzwiller projected wave function. Our approach can be taken as the generalization of the usual RPA theory into the Hilbert space satisfying the no double occupancy constraint of the t-J model. The approach has the virtual that it is parameter free: the RPA correction is automatically done through the variational procedure. We also devise an efficient algorithm to do Monte Carlo simulation on the variational wave function we proposed. Numerical calculation shows that our variational description of the neutron resonance mode captures its basic characteristics very well.

The paper is organized as follows. In the next section, we introduce the variational ground state and present the result of the single-mode approximation (SMA) on which the result of our variational calculation would compare to. We then introduce our variational wave function for the neutron resonance mode and the numerical technique to do Monte Carlo simulation on it. Then we present our numerical results and offer a discussion on the results. Finally, we conclude this paper with some further problems to be addressed in the future.

II. SINGLE-MODE APPROXIMATION

We take the t-J model as the basic model to describe the physics of high-T_c superconductors

$$H=H_t+H_{t'}+H_J,$$

$$H_t=-t\sum_{\langle i,j\rangle,\sigma}(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma}+\text{H.c.}),$$

$$H_{t'} = -t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{H.c.}),$$

$$H_J = J\sum_{\langle i,j\rangle}\left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}n_i n_j\right). \tag{2}$$

Here $\hat{c}_{j,\sigma}$ is the constrained electron operator satisfying the constraint $\Sigma_\sigma \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma} \leq 1$. $\Sigma_{\langle i,j\rangle}$ and $\Sigma_{\langle\langle i,j\rangle\rangle}$ represent the sum over nearest-neighboring and next-nearest-neighboring (NNN) sites. Here we take $\frac{t'}{t} = -0.25$ to describe hole-doped system. The exchange term is fixed at $\frac{J}{t} = \frac{1}{3}$.

The no double-occupancy constraint $\Sigma_\sigma \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma} \leq 1$ is crucial for the spin dynamics of the system. With this constraint, the electron behaves like mobile $s = \frac{1}{2}$ spin rather than usual free electron. More quantitatively, the spin structure factor in the t-J model satisfies the following local-spin sum rule:

$$\int dq d\omega S(q,\omega) = (1-x)\frac{3}{4} \tag{3}$$

in any physical state, here x is hole density. When the constraint is relaxed, as is done in slave Boson mean-field theory or phenomenological RPA theory, the spin fluctuation would be strongly suppressed and no such sum rule would apply.

To satisfy the local-spin sum rule of the t-J model, the variational ground state, on which to construct the variational excitations, must respect the no double-occupancy constraint. The Gutzwiller projected d-wave BCS state,[12–15] which satisfies the no double-occupancy constraint and for long has been known as an excellent variational description of the ground state of the system, is the most natural choice for this purpose.

Thus our variational ground state is given by

$$|\Psi_g\rangle = P_N P_G |d-\text{BCS}\rangle = P_G\left(\sum_{i,j} a(i-j)c^{\dagger}_{i,\uparrow}c^{\dagger}_{j,\downarrow}\right)^{N/2}|0\rangle, \tag{4}$$

in which P_N is the projection operator into the subspace with N electrons and P_G is the Gutzwiller projection operator into the subspace of no double occupancy, $a(i-j) = \Sigma_{\text{k}} \frac{v_{\text{k}}}{u_{\text{k}}} e^{ik(r_i - r_j)}$ is the real-space wave function of the Cooper pair with $\frac{v_{\text{k}}}{u_{\text{k}}} = \frac{\Delta_{\text{k}}}{\xi_{\text{k}} + E_{\text{k}}}$. Here, $E_{\text{k}} = \sqrt{\xi^2_{\text{k}} + \Delta^2_{\text{k}}}$, ξ_{k}, and Δ_{k} are given by

$$\xi_{\text{k}} = -2(\cos k_x + \cos k_y) - 4t'_v \cos k_x \cos k_y - \mu_v,$$

$$\Delta_{\text{k}} = 2\Delta_v(\cos k_x - \cos k_y), \tag{5}$$

in which t'_v, μ_v, Δ_v are variational parameters to be determined by the optimization of the ground-state energy with respect to the t-J model. We note t'_v, μ_v, Δ_v are just variational parameters, rather than real NNN hoping term, real chemical potential, and real superconducting gap.

Now we construct the spin excitation on the variational ground state. As a first approximation to (π,π) resonance mode, we adopt the single-mode approximation of the form

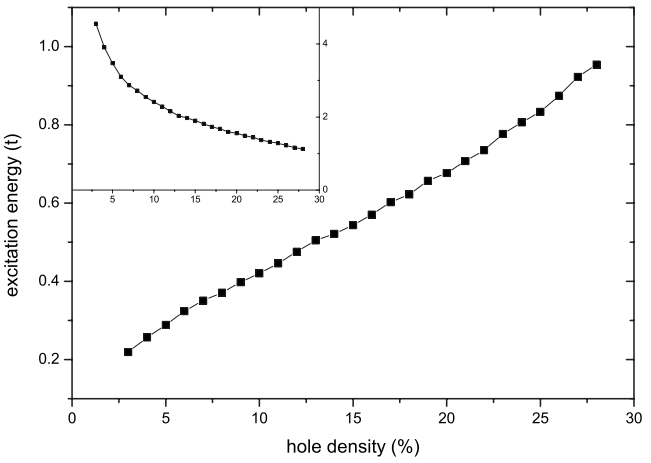

FIG. 1. The resonance energy determined from the single-mode approximation as a function of doping. The inset shows the structure factor at $Q=(\pi,\pi)$ (divided by the number of lattice sites, N_s) as a function of doping.

$$|\Psi^0_Q\rangle = S^+_Q|\Psi_g\rangle, \tag{6}$$

in which S^+_Q is the creation operator of the spin-density excitation at $Q=(\pi,\pi)$. As the variational ground-state satisfies the no double-occupancy constraint, the spin-excitation spectrum is guaranteed to obey the local-spin sum rule.

The single-mode approximation is a good approximation when the spin-fluctuation spectrum is dominated by the contribution form the resonance mode. The excitation energy in the single-mode approximation can be calculated in the standard way

$$E_Q = \frac{\langle\Psi^0_Q|H|\Psi^0_Q\rangle}{\langle\Psi^0_Q|\Psi^0_Q\rangle} - E_g, \tag{7}$$

where E_g denotes the ground-state energy. Assuming that $H|\Psi_g\rangle = E_g|\Psi_g\rangle$, we have

$$E_Q = \frac{1}{2}\frac{\langle\Psi_g|[S^-_Q,(H,S^+_Q)]|\Psi_g\rangle}{\langle\Psi_g|S^-_Q S^+_Q|\Psi_g\rangle}. \tag{8}$$

Using the commutation relation

$$[\hat{c}^{\dagger}_{i,\sigma}, S^+_j] = -\delta_{ij}\delta_{\sigma,\downarrow}\hat{c}^{\dagger}_{i,\uparrow},$$

$$[\hat{c}_{i,\sigma}, S^+_j] = \delta_{ij}\delta_{\sigma,\uparrow}\hat{c}_{i,\downarrow}, \tag{9}$$

in which $\hat{c}^{\dagger}_{i,\sigma}$ is the constrained electron-creation operator at site i and S^+_j is spin-lifting operator at site j, the mode energy in the single-mode approximation can be shown to be given by

$$E_Q = \frac{-\langle\Psi_g|H_t|\Psi_g\rangle - \frac{8}{3}\langle\Psi_g|H_J|\Psi_g\rangle}{\langle\Psi_g|S^-_Q S^+_Q|\Psi_g\rangle}. \tag{10}$$

It is interesting to note that the $H_{t'}$ term of the Hamiltonian does not contribute when $Q=(\pi,\pi)$.

The mode energy calculated from Eq. (10) is shown in Fig. 1. Two things are to be noted here. First, E_Q increases monotonically with doping, consistent with observation in

the underdoped regime. Second, E_Q approaches zero at half filling in the thermodynamic limit. The monotonic increase in E_Q is due to the rapid decrease in the spin-structure factor as a function of doping which overcompensates the increase in the absolute value of the kinetic energy and the exchange energy. The second is, in fact, a reflection of the Goldstone theorem. At half filling, the spin-structure factor calculated from $|\Psi_g\rangle$ scales superlinearly with the number of lattice site N_s ($M_Q^2=\langle\Psi_g|S_Q^-S_Q^+|\Psi_g\rangle/\langle\Psi_g|\Psi_g\rangle\propto N_s^{4/3}$) as a result of the long-range correlation induced by the Gutzwiller projection.[14] However, kinetic and exchange energies are by definition proportional to N_s. Thus E_Q must approach zero at half filling as $N_s\rightarrow\infty$. This is to be compared with the mean-field prediction that $M_Q^2\propto N_s$ at all doping which imply that E_Q remains finite even at half filling. Thus the Gutzwiller projection in our wave function plays a key role to recover the correct trend of the mode energy as a function of doping.

The mode energy calculated by the single-mode approximation is, in fact, the center of gravity of the spin fluctuation spectrum at $Q=(\pi,\pi)$ and thus overestimates the energy of the resonance mode which lies at the bottom of the spin-fluctuation spectrum. In fact, the single-mode approximation we adopted above has nothing to say about the very existence of the resonance mode. This is especially clear at large doping when the mode energy predicted by Eq. (10) stretches into the particle-hole continuum. Thus, although the single-mode approximation gives correctly the trend of the mode energy as a function of doping, it is too crude to give a quantitative answer on both the mode energy and mode weight.

It should be noted that the energy calculated from Eq. (10) with the variational ground state is only a approximation to the single-mode approximation energy (as we have made the assumption that $H|\Psi_g\rangle=E_g|\Psi_g\rangle$). Thus, although Eq. (10) is by definition positive definite, the true single-mode approximation energy can be negative when the system become unstable with respect to magnetic ordering at $Q=(\pi,\pi)$. We will encounter this situation below when we calculate the single-mode approximation energy directly from Eq. (7).

III. PROJECTED SPIN-EXCITON WAVE FUNCTION

In the RPA theory, the resonance mode is interpreted as a spin exciton: a spin-one particle-hole bound state below the superconducting gap induced by the residual interaction between the Bogliubov quasiparticles. The wave function for the spin exciton can be generally written as

$$|\tilde{\Psi}_Q\rangle=\sum_{\mathrm{k}}\phi_{\mathrm{k}}\gamma_{\mathrm{k}\uparrow}^{\dagger}\gamma_{Q-\mathrm{k}\uparrow}^{\dagger}|d-\mathrm{BCS}\rangle, \tag{11}$$

in which ϕ_{k} describes the relative motion of the two quasiparticles $\gamma_{\mathrm{k}\uparrow}^{\dagger}$ and $\gamma_{Q-\mathrm{k}\uparrow}^{\dagger}$ within the bound state. $|d-\mathrm{BCS}\rangle$ denotes the BCS mean-field ground state and $\gamma_{\mathrm{k}\uparrow}^{\dagger}$ denotes the creation operator for the Bogliubov quasiparticles.

As we have shown, the mean-field state fails to satisfy the local-spin sum rule. For this reason, we project the spin-exciton wave function Eq. (11) into the subspace of no double occupancy to construct a variational wave function for the resonance mode with ϕ_{k} as the variational parameter to be determined by optimization of energy.

$$|\Psi_Q\rangle=P_NP_G|\tilde{\Psi}_Q\rangle=\sum_{\mathrm{k}}\phi_{\mathrm{k}}|\mathrm{k},Q\rangle, \tag{12}$$

in which

$$|k,Q\rangle=P_NP_G\gamma_{\mathrm{k}\uparrow}^{\dagger}\gamma_{Q-\mathrm{k}\uparrow}^{\dagger}|d-\mathrm{BCS}\rangle. \tag{13}$$

We note that the wave function of the single-mode approximation can also be cast into the form of Eq. (12), i.e.,

$$\begin{aligned}|\Psi_Q^0\rangle&=P_NP_GS_Q^+|d-\mathrm{BCS}\rangle\\&=\sum_{\mathrm{k}}P_NP_Gc_{\mathrm{k}+Q,\uparrow}^{\dagger}c_{\mathrm{k},\downarrow}|d-\mathrm{BCS}\rangle\\&=\sum_{\mathrm{k}}\phi_{\mathrm{k}}^0|\mathrm{k},Q\rangle,\end{aligned} \tag{14}$$

in which $\phi_{\mathrm{k}}^0=u_{\mathrm{k}+Q}v_k$. Here we have used the fact that S_Q^+ commute with both P_N and P_G.

The variational parameters ϕ_{k} can be determined by minimizing the energy of $|\Psi_Q\rangle$ with respect to the t-J Hamiltonian. The variational energy is given by

$$E_Q=\frac{\langle\Psi_Q|H_{t\text{-}J}|\Psi_Q\rangle}{\langle\Psi_Q|\Psi_Q\rangle}=\frac{\sum_{\mathrm{k},\mathrm{k}'}\phi_{\mathrm{k}}^*H_{\mathrm{k},\mathrm{k}'}\phi_{\mathrm{k}'}}{\sum_{\mathrm{k},\mathrm{k}'}\phi_{\mathrm{k}}^*O_{\mathrm{k},\mathrm{k}'}\phi_{\mathrm{k}'}}, \tag{15}$$

in which

$$H_{\mathrm{k},\mathrm{k}'}=\langle k,Q|H_{t\text{-}J}|k',Q\rangle \tag{16}$$

is the matrix element of the t-J Hamiltonian in the basis $|k,Q\rangle$ and

$$O_{\mathrm{k},\mathrm{k}'}=\langle k,Q|k',Q\rangle \tag{17}$$

denotes the overlap integral between these nonorthogonal basis function (note that $\gamma_{\mathrm{k}\uparrow}^{\dagger}\gamma_{Q-\mathrm{k}\uparrow}^{\dagger}|d-\mathrm{BCS}\rangle$ form a orthogonal basis set before the Gutzwiller projection).

The problem of minimizing E_Q respect to the set of variational parameters ϕ_{k} now reduces to solving the following generalized eigenvalue problem:

$$\sum_{\mathrm{k}'}H_{\mathrm{k},\mathrm{k}'}\phi_{\mathrm{k}'}=\lambda\sum_{\mathrm{k}'}O_{\mathrm{k},\mathrm{k}'}\phi_{\mathrm{k}'}. \tag{18}$$

It is easily seen that the optimized energy E_Q is given by the lowest eigenvalue λ of the above generalized eigenvalue problem.

The above optimization procedure can also be interpreted as rediagonalizing the t-J Hamiltonian in the subspace spanned by the set of nonorthogonal basis function $|k,Q\rangle$. With this understanding in mind, we can even construct variationally the full spin-fluctuation spectrum as follows:

$$S(Q,\omega)=M_Q^2\sum_{n,\mathrm{k},\mathrm{k}'}|\phi_{\mathrm{k}}^{n*}O_{\mathrm{k},\mathrm{k}'}\phi_{\mathrm{k}'}^0|^2\delta[\omega-(E_n-E_g)], \tag{19}$$

in which ϕ_{k}^n denotes the nth eigenvector of the generalized eigenvalue problem with the eigenvalue E_n, E_g denotes the variational ground-state energy (here we assume that ϕ_{k} and ϕ_{k}^0 are so chosen that both $|\Psi_Q\rangle$ and $|\Psi_Q^0\rangle$ are normalized). As ϕ_{k}^n forms a orthonormal basis with respect to the overlap

matrix $O_{\mathrm{k,k}'}$, i.e., $\Sigma_{\mathrm{k,k}'}\phi_{\mathrm{k}}^{n*}O_{\mathrm{k,k}'}\phi_{\mathrm{k}'}^{m}=\delta_{n,m}$, we have

$$\int d\omega S(Q,\omega) = M_Q^2 \sum_n \left| \sum_{\mathrm{k,k}'} \phi_{\mathrm{k}}^{n*} O_{\mathrm{k,k}'} \phi_{\mathrm{k}'}^{0} \right|^2 = M_Q^2 \sum_{\mathrm{k,k}'} \phi_{\mathrm{k}}^{0*} O_{\mathrm{k,k}'} \phi_{\mathrm{k}'}^{0} = M_Q^2, \tag{20}$$

in which we have used the fact that

$$\sum_{n,\mathrm{k}} \phi_{\mathrm{k}_1}^{n*} O_{\mathrm{k}_2,\mathrm{k}} \phi_{\mathrm{k}}^{n} = \delta_{\mathrm{k}_1,\mathrm{k}_2}, \tag{21}$$

which can be derived from the orthonormality of the eigenvectors of the generalized eigenvalue problem Eq. (18),

$$\sum_{\mathrm{k,k}'} \phi_{\mathrm{k}}^{n*} O_{\mathrm{k,k}'} \phi_{\mathrm{k}'}^{m} = \delta_{n,m}. \tag{22}$$

Thus our variational construction of the spin-fluctuation spectrum respects the local-spin sum rule of the t-J model.

Our variational scheme for the resonance mode has the advantage that it involves no tunable parameter: the parameters in $|\Psi_g\rangle$ is determined by optimizing the ground-state energy and the spin-exciton wave function ϕ_{k} is determined by solving the generalized eigenvalue problem. The RPA correction is thus automatically taken into account in our formalism.

From the above discussion, we know the single-mode approximation can be taken as a special case of the projected spin-exciton wave function (with $\phi_{\mathrm{k}}=\phi_{\mathrm{k}}^0=u_{\mathrm{k}}v_{Q-\mathrm{k}}$). Thus by construction, the resonance energy calculated from Eq. (18) should be lower than that calculated from single-mode approximation. In fact, the mode energy calculated from the single-mode approximation gives the center of gravity of the spin-fluctuation spectrum while the resonance mode lies at the bottom of the spectrum. As the single-mode approximation already reproduces the correct trend for the mode energy as a function of doping in the underdoped regime, we can even expect our variational scheme to produce quantitatively reasonable result.

IV. REWEIGHTING TECHNIQUE

To calculate the energy of the resonance mode, we should first evaluate the matrix element of the Hamiltonian in the set of strongly correlated basis functions $|k,Q\rangle$, $H_{\mathrm{k,k}'}$, and the overlap matrix element $O_{\mathrm{k,k}'}$. This can be done, in principle, by the variational Monte Carlo (VMC) method. For example, to evaluate $\frac{H_{\mathrm{k,k}'}}{O_{\mathrm{k,k}}}=\frac{\langle k,Q|H_{t\text{-}J}|k',Q\rangle}{\langle k,Q|k,Q\rangle}$, we first expand $|k,Q\rangle$ in an orthogonal basis $|R_i\rangle$, i.e.,

$$|k,Q\rangle = \sum_{R_i} \psi_{\mathrm{k}}(R_i)|R_i\rangle, \tag{23}$$

where $\psi(R_i)$ is the wave function of $|k,Q\rangle$ in this basis. Then we have

$$\frac{H_{\mathrm{k,k}'}}{O_{\mathrm{k,k}}} = \frac{\sum_{R_i} |\psi_{\mathrm{k}}(R_i)|^2 \frac{H\psi_{\mathrm{k}'}(R_i)}{\psi_{\mathrm{k}}(R_i)}}{\sum_{R_i} |\psi_{\mathrm{k}}(R_i)|^2}, \tag{24}$$

in which

$$H\psi_{\mathrm{k}'}(R_i) = \sum_{R_{i'}} \langle R_i|H|R_{i'}\rangle \frac{\psi_{\mathrm{k}'}(R_{i'})}{\psi_{\mathrm{k}}(R_i)}. \tag{25}$$

Then we sample the basis space $|R_i\rangle$ with the weight $|\psi_{\mathrm{k}}(R_i)|^2$ and do the sum with the standard VMC technique.[13]

The above procedure, though straightforward, is very inefficient. In our problem, there are N_s^2 Hamiltonian matrix elements $H_{\mathrm{k,k}'}$ and N_s^2 overlap matrix elements $O_{\mathrm{k,k}'}$ to be evaluated. For lattice of reasonable size, say, 14×14, the number of the matrix elements to be evaluated would exceed 40 000 even take into account the Hermitian property of $H_{\mathrm{k,k}'}$ and $O_{\mathrm{k,k}'}$. This is very time consuming. At the same time, the naive approach has the drawback that it involves large statistical error in the simulation. This can be seen as follows:

$$\frac{O_{\mathrm{k,k}'}}{O_{\mathrm{k,k}}} = \frac{\sum_{R_i} |\psi_{\mathrm{k}}(R_i)|^2 \frac{\psi_{\mathrm{k}'}(R_i)}{\psi_{\mathrm{k}}(R_i)}}{\sum_{R_i} |\psi_{\mathrm{k}}(R_i)|^2}. \tag{26}$$

Thus, when the node of $\psi_{\mathrm{k}}(R_i)$ and $\psi_{\mathrm{k}'}(R_i)$ do not coincide with each other, we will run into trouble when we sample $\psi_{\mathrm{k}}(R_i)$ around its node as the fluctuation of $\frac{\psi_{\mathrm{k}'}(R_i)}{\psi_{\mathrm{k}}(R_i)}$ becomes large. A way to reduce the statistical error caused by the fluctuation of $\frac{\psi_{\mathrm{k}'}(R_i)}{\psi_{\mathrm{k}}(R_i)}$ is to sample the combined weight $\mathcal{W}(R_i)=|\psi_{\mathrm{k}}(R_i)|^2+|\psi_{\mathrm{k}'}(R_i)|^2$ rather than $|\psi_{\mathrm{k}}(R_i)|^2$,

$$\frac{O_{\mathrm{k,k}'}}{O_{\mathrm{k,k}}} = \frac{O_{\mathrm{k,k}'}}{O_{\mathrm{k,k}}+O_{\mathrm{k}',\mathrm{k}'}} \Big/ \frac{O_{\mathrm{k,k}}}{O_{\mathrm{k,k}}+O_{\mathrm{k}',\mathrm{k}'}}. \tag{27}$$

Now the calculation of $\frac{O_{\mathrm{k,k}'}}{O_{\mathrm{k,k}}+O_{\mathrm{k}',\mathrm{k}'}}$ can be done as

$$\frac{O_{\mathrm{k,k}'}}{O_{\mathrm{k,k}}+O_{\mathrm{k}',\mathrm{k}'}} = \frac{\sum_{R_i} \mathcal{W}(R_i) \frac{\psi_{\mathrm{k}}^*(R_i)\psi_{\mathrm{k}}(R_i)}{\mathcal{W}(R_i)}}{\sum_{R_i} \mathcal{W}(R_i)}. \tag{28}$$

The combined-weight samples symmetrically between $\psi_{\mathrm{k}}(R_i)$ and $\psi_{\mathrm{k}'}(R_i)$ and avoids the fluctuation caused by their uncommon nodes. Thus the statistical error is much reduced.

The above technique can be easily generalized to calculate all the N_s^2 overlap matrix elements $O_{\mathrm{k,k}'}$. Here we sample the combined weight of all the N_s $|\psi_{\mathrm{k}}(R_i)|^2$: $\mathcal{W}(R_i)=\Sigma_{\mathrm{k}}|\psi_{\mathrm{k}}(R_i)|^2$. The calculation is done as follows:

$$\frac{O_{\mathrm{k}_1,\mathrm{k}_2}}{\sum_{\mathrm{k}} O_{\mathrm{k},\mathrm{k}}} = \frac{\sum_{R_i} \mathcal{W}(R_i) \frac{\psi^*_{\mathrm{k}_1}(R_i)\psi_{\mathrm{k}_2}(R_i)}{\mathcal{W}(R_i)}}{\sum_{R_i} \mathcal{W}(R_i)}. \tag{29}$$

To sample $\mathcal{W}(R_i)$, we note that

$$\mathcal{W}(R_i) = |\psi_{\mathrm{k}_0}(R_i)|^2 \sum_{\mathrm{k}} \left| \frac{\psi_{\mathrm{k}}(R_i)}{\psi_{\mathrm{k}_0}(R_i)} \right|^2 \tag{30}$$

and

$$\frac{\psi^*_{\mathrm{k}_1}(R_i)\psi_{\mathrm{k}_2}(R_i)}{\mathcal{W}(R_i)} = \frac{\left(\frac{\psi_{\mathrm{k}_1}(R_i)}{\psi_{\mathrm{k}_0}(R_i)}\right)^* \frac{\psi_{\mathrm{k}_2}(R_i)}{\psi_{\mathrm{k}_0}(R_i)}}{\sum_{\mathrm{k}} \left| \frac{\psi_{\mathrm{k}}(R_i)}{\psi_{\mathrm{k}_0}(R_i)} \right|^2}, \tag{31}$$

in which ψ_{k_0} is one basis function arbitrarily chosen from the N_s basis functions. From this transformation, we see all we need to calculate in order to evaluate $\frac{O_{\mathrm{k}_1,\mathrm{k}_2}}{\Sigma_{\mathrm{k}} O_{\mathrm{k},\mathrm{k}}}$ is the N_s ratio between basis functions $\frac{\psi_{\mathrm{k}}(R_i)}{\psi_{\mathrm{k}_0}(R_i)}$. As the different basis functions are all Slater determinant differing with each other by at most in a pair of quasiparticle excitations, such ratio is easy to calculate using the inverse updating technique for Fermion determinant. More importantly, the calculation of all the N_s^2 overlap matrix elements can be done in a single Monte Carlo simulation: the algorithm is highly parallelized.

The calculation of the Hamiltonian matrix elements can be done similarly. We have

$$\frac{H_{\mathrm{k}_1,\mathrm{k}_2}}{\sum_{\mathrm{k}} O_{\mathrm{k},\mathrm{k}}} = \frac{\sum_{R_i} \mathcal{W}(R_i) \frac{\psi^*_{\mathrm{k}_1}(R_i) \times H\psi_{\mathrm{k}_2}(R_i)}{\mathcal{W}(R_i)}}{\sum_{R_i} \mathcal{W}(R_i)}, \tag{32}$$

where $H\psi_{\mathrm{k}_2}(R_i) = \Sigma_{R_j} \langle R_i | H_{t\text{-}J} | R_j \rangle \psi_{\mathrm{k}_2}(R_j)$. Following the same reasoning, we arrive at

$$\frac{\psi^*_{\mathrm{k}_1}(R_i) \times H\psi_{\mathrm{k}_2}(R_i)}{\mathcal{W}(R_i)} = \frac{\left(\frac{\psi_{\mathrm{k}_1}(R_i)}{\psi_{\mathrm{k}_0}(R_i)}\right)^* \frac{H\psi_{\mathrm{k}_2}(R_i)}{\psi_{\mathrm{k}_0}(R_i)}}{\sum_{\mathrm{k}} \left| \frac{\psi_{\mathrm{k}}(R_i)}{\psi_{\mathrm{k}_0}(R_i)} \right|^2}. \tag{33}$$

Thus the calculation of the Hamiltonian matrix elements involves the evaluation of the ratio $\frac{H\psi_{\mathrm{k}_2}(R_i)}{\psi_{\mathrm{k}_0}(R_i)}$. The calculation of this ratio, though numerically more demanding, is still highly parallelized.

Thus the reweighting technique developed here not only reduce considerably the statistical error involved in the Monte Carlo simulation but also highly parallelize the calculation of the overlap and Hamiltonian matrix elements, reducing their calculation from the order of N_s^2 to a single Monte Carlo simulation.

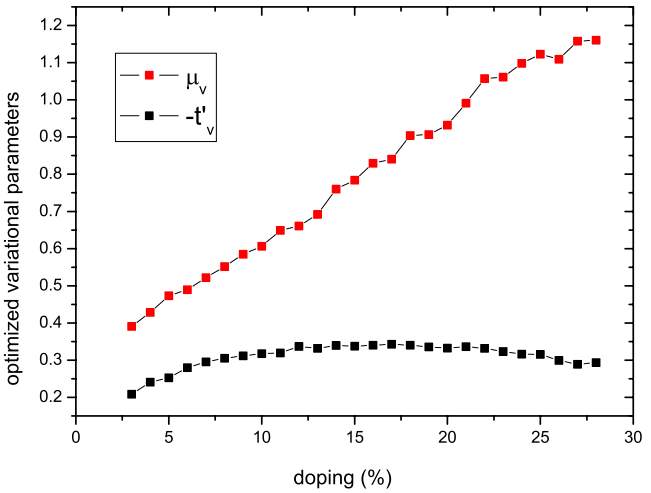

FIG. 2. (Color online) The optimized variational parameters as a function of doping.

V. NUMERICAL RESULTS

To calculate the energy of the neutron resonance mode, we first optimize the variational parameters t_v', μ_v, and Δ_v as a function of doping for the ground state. The calculation is done on a 14×14 lattice with periodic-antiperiodic boundary condition. We choose $\frac{J}{t} = \frac{1}{3}$ and $\frac{t'}{t} = -0.25$ in the t-J model to describe a hole-doped cuprate. The results of the optimized variational parameters as a function of doping are shown in Figs. 2 and 3.

We note the superconducting region determined by the variational approach for the t-J model is considerably larger than that observed in experiments. In Fig. 3, we plot the off-diagonal long-range order (ODLRO) calculated from the optimized variational ground state. The ODLRO is defined as

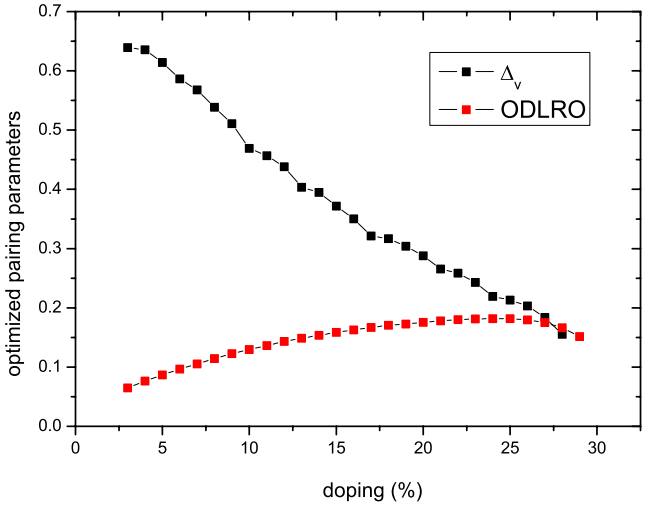

FIG. 3. (Color online) The optimized pairing parameters as a function of doping and the off-diagonal long-range order calculated from the variational ground state.

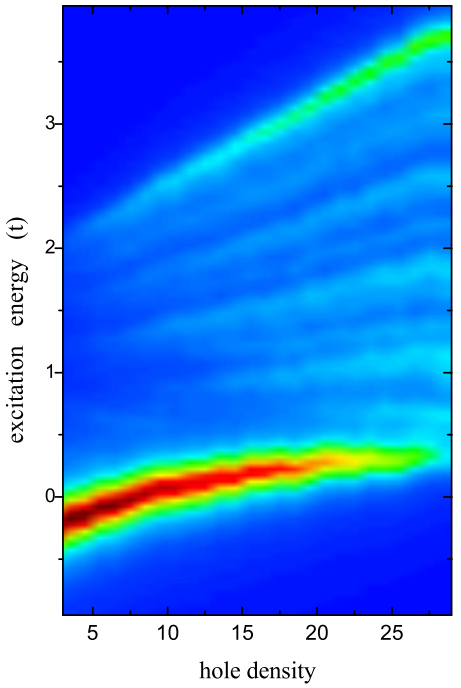

FIG. 4. (Color online) The spin-fluctuation spectrum at $q=(\pi,\pi)$ as a function of excitation energy and doping determined from the variational calculation. The calculation is done on a 14 $\times$ 14 lattice. The delta function peaks of the spectrum are broadened into Lorentzian peaks with a width of $0.1t$.

$$\Delta = \sqrt{\frac{1}{N_s}\sum_i \langle \hat{\Delta}_i \hat{\Delta}^{\dagger}_{i+R_M} \rangle}, \tag{34}$$

in which $\hat{\Delta}_i=(c_{i+x,\downarrow}c_{i,\uparrow}-c_{i+x,\uparrow}c_{i,\downarrow})-(c_{i+y,\downarrow}c_{i,\uparrow}-c_{i+y,\uparrow}c_{i,\downarrow})$ is the Cooper pair annihilation operator at site i, R_M is the largest distance on the finite lattice. We find the ODLRO reaches its maximal around $x\approx 26\%$. We will take this doping concentration as an estimate of the location of the optimal doping in the following discussion.

After obtaining the variational parameters of the ground state we are now ready to calculate the Hamiltonian matrix elements $H_{\mathrm{k,k}'}$ and the overlap matrix elements $O_{\mathrm{k,k}'}$. This is the most heavy part of our numerical calculation. In our calculation, we have sampled more than two and a half million configurations with the weight $\mathcal{W}(R_i)$. The accept ratio is tuned to be $\frac{1}{2}$. The statistical error is found to be smaller than the fluctuation caused by the finite-size effect in our calculation.

When we get the matrix elements $H_{\mathrm{k,k}'}$ and $O_{\mathrm{k,k}'}$, we solve the generalized eigenvalue problem Eq. (18) and calculate the physical quantities that we are interested in. First we show the spin-fluctuation spectrum calculated in this variational approach in Fig. 4. We see the spectrum consists of both a coherent peak and a continuum of incoherent spin fluctuation. The coherent peak at the bottom of the spectrum is nothing but the neutron resonance mode in our variational description.

Figure 5 shows the mode energy as a function of doping. We find the mode energy becomes negative below a critical doping around $x=7.5\%$. A negative excitation energy indicates magnetic instability of the system. The critical doping so determined is close but slightly lower than that determined by assuming directly a magnetic order in the variational ground state, which is about 10%.[15] In whole doping range in which the mode has nonzero spectral weight, the mode energy is a monotonically increasing function of doping and reaches about $0.3t$ before it loses its weight and merges into the particle-hole continuum at about $x=29\%$. If we take $t=0.25$ eV as is usually done in the literature, we get the maximum of the mode energy to be about 75 meV, about a factor of 1.8 larger than that observed in optimally doped $YBa_2Cu_3O_{6.93}$.[1]

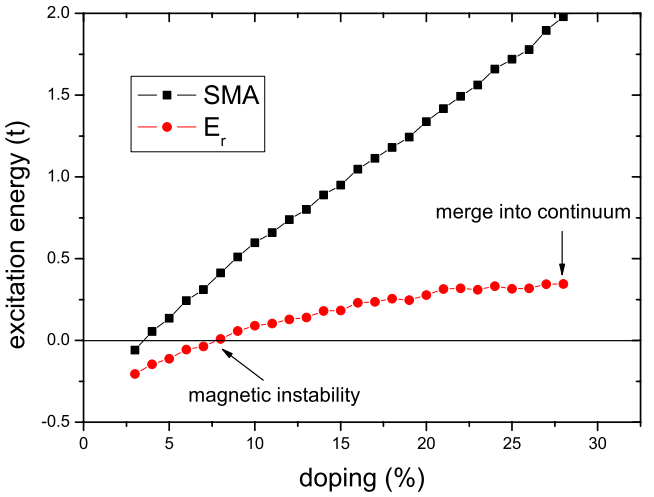

FIG. 5. (Color online) The mode energy determined by our variational approach as a function of doping as compared with the result of SMA.

In our theory, the mode energy increases monotonically with doping. This is consistent with experiments in the underdoped regime but may have inconsistency with experiment in the overdoped regime, where experiment reported

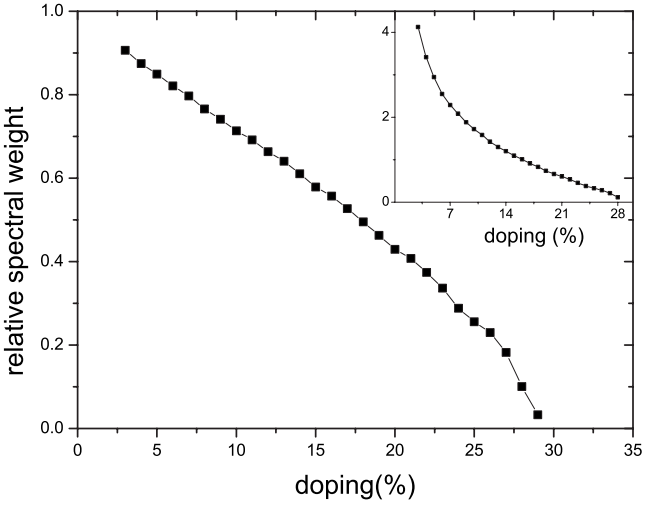

FIG. 6. The relative spectral weight of the resonance mode as a function of doping. The inset shows the result of the absolute spectral weight.

evidence of a weak-resonance mode with an energy slightly lower than that of the optimally doped system.[4] If we take the doping at which the ODLRO reaches maximum ($x=26\%$) as the optimal doping, then the resonance mode will survive in the slightly overdoped regime with an energy higher than that of the optimal doped system. This would imply a breakdown of the linear scaling between the mode energy and T_c in the slightly overdoped regime.

Figure 6 shows the relative and the absolute spectral weights of the resonance mode calculated from our theory. The relative spectral weight is defined as the proportion of the mode intensity to the total spectral weight at $Q=(\pi,\pi)$,

$$W=\frac{|\langle\Psi_Q^0|\Psi_Q\rangle|^2}{\langle\Psi_Q^0|\Psi_Q^0\rangle}. \tag{35}$$

The absolute spectral weight is defined as the product of the relative spectral weight and the spin-structure factor divided by N_s. The absolute spectral weight decreases rapidly with doping as a result of the decrease in both the magnetic structure factor and the relative spectral weight. The relative spectral weight of the resonance mode decreases from unity at half filling down to zero at about $x=29\%$. The unity of the relative spectral weight come from the long-range correlation of spin at half filling and indicates that the resonance mode can be connected smoothly to the Goldstone mode in the magnetic ordered state.

VI. DISCUSSION

In this paper, we proposed a variational theory for the neutron resonance mode in the cuprate superconductors. Our theory has the virtue that it involves no free parameter and thus has much larger predictive power than the phenomenological RPA treatment of the spin fluctuation. In our theory, the RPA correction is automatically taken into account by the variational procedure which reduces to solving a generalized eigenvalue problem. More importantly, our variational approach builds in the no double-occupancy constraint and thus satisfies the local-spin sum rule of the t-J model. This is of vital importance for a correct description of the spin dynamics of cuprates. Our approach has the further advantage that it provides a physical transparent understanding of the resonance mode as a spin exciton in the physical subspace of no double occupancy.

Our approach can also be taken as diagonalizing the Hamiltonian in a truncated subspace with the same quantum number as the excitation discussed and can be used to calculate the full spectrum rather than the coherent excitation only. It is important to note this truncated subspace exhaust the spectral weight for the relevant sum rule, indicating the relevance of the spectrum calculated in this way. An effort to apply the current approach to calculate the spin-fluctuation spectrum at momentum other than (π,π), namely, the incommensurate spin-fluctuation spectrum, is now under investigation.

We have also devised a very efficient reweighting technique to tackle the numerical problem of simulating the variational wave function composed of N linearly superposed Slater determinants. The key for the efficiency of the algorithm is the observation that the Slater determinants involved in our wave function differ with each other by at most a pair of quasiparticle excitations. Obviously this technique can be applied in a much larger literature than simulating the physics of cuprates.

As we have found in the single-mode approximation, the center of gravity of the spin-fluctuation spectrum increases monotonically with doping as a result of the rapid decrease in the spin-structure factor at $Q=(\pi,\pi)$. We find the resonance mode, which lies at the bottom of the spin-fluctuation spectrum, inherits this monotonic behavior, probably for the same reason. As we have mentioned above, this may have potential conflict with the report of weak-resonance mode in the overdoped sample with an energy lower than that of the optimal doped system[4] and would imply the breakdown of the T_c-E_r linear scaling in the overdoped regime.

In our theory, the monotonic increase in the mode energy eventually cutoff at about twice the maximal superconducting gap when the mode transfers all of its weight into the particle-hole continuum. To exhibit a nonmonotonic behavior before merging into the particle-hole continuum, it is necessary for the superconducting gap to decrease faster with doping than that predicted by the present variational calculation. This is not at all impossible. However, since there is no generally reason to believe the T_c-E_r linear scaling to hold in the overdoped regime and the mode weight become very small in the overdoped regime, we think the mode energy in the overdoped regime is a problem subjected to fine tuning.

The mode energy at the optimal doping ($x=26\%$) as calculated from our approach is about $0.3t$ and is a factor of 1.8 larger than that observed in optimally doped $YBa_2Cu_3O_{6.93}$. At the same time, the variational theory predicts a considerably larger value of optimal doping than observed in experiments ($x=16\%$). It is likely that these two problems and the problem of the T_c-E_r linear scaling to hold in the overdoped regime are related with each other. However, it is not clear to what extent should we attribute these disagreements with experiment solely to the limitation of the variational approach we have adopted rather than the intrinsic properties of the t-J model.

Finally, we discuss the relation between the resonance mode and the superconductivity. As many other theories of the resonance mode,[5,8,10] our theory also predicts that the resonance mode becomes stronger and stronger with decreasing doping and evolves smoothly into the Goldstone mode of the ordered state at half filling. On the other hand, in the phenomenological SO(5) theory of cuprates,[11] in which the mode is understood as a pseudo-Goldstone mode accompanying breaking of an SO(5) symmetry between the d-wave superconducting order and the antiferromagnetic order, the mode intensity is predicted to be proportional to the ODLRO of the system. Thus the theory predicts that the mode intensity should decrease when we increase temperature or decrease doping and disappear out of the superconducting dome. On the experimental side, the resonance mode is observed to loss weight with increasing temperature and to disappear in the normal state at optimal doping. In slightly underdoped sample, a broadened and weak signal is observed above T_c. With further decrease in doping, the normal-state

signal becomes stronger and stronger and the enhancement due to superconductivity becomes less and less prominent.[1–3]

In our theory, we only consider the zero-temperature case. At finite temperature, both quasiparticle excitations and collective fluctuation of the superconducting order parameter will be thermally excited. The latter excitation is believed to be especially important around the superconducting transition point. We believe both of these thermal excitations are responsible for the decrease in the mode intensity with increasing temperature. The doping dependence of the mode intensity is more subtle. Here the relevant question is why the superconductivity-related enhancement of the mode intensity becomes smaller and smaller with decreasing doping. In the very underdoped regime, the electron correlation (Mott physics) is greatly enhanced. We believe the Mott physics is at work in reducing the superconductivity-related enhancement of the mode intensity in the very underdoped regime. It is interesting to note that in the RVB picture, in which the spins of the system form a liquid-like state composed of resonating spin singlet pairs, the electron-correlation effect manifests itself as quantum fluctuation of the superconducting order parameter.

In all, apart from some subtle issues mentioned above, our variational approach capture the gross feature of the neutron resonance mode and provides the first truly microscopic understanding of this important phenomena in the high-temperature superconductors. As a by product of this research, we developed a very efficient reweighting technique to simulated wave function composed of N linearly superposed Slater determinants, an algorithm whose potential application is obviously far beyond the high-T_c issue.

ACKNOWLEDGMENTS

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