Variational study of the neutron resonance mode in the cuprate superconductors

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A Gutzwiller-type variational wave function is proposed for the neutron resonance mode in the cuprate superconductors. An efficient re-weighting 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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\textbf{INTRODUCTION}

The \((\pi, \pi)\) resonance mode observed by neutron scattering in the cuprate superconductors is among the most prominent phenomena in these systems\cite{1, 2, 3, 4}. Below the superconducting transition temperature \(T_c\), a sharp peak is observed in the spin fluctuation spectrum around \((\pi, \pi)\). 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\cite{3, 4, 5, 6, 7, 8, 9, 10}. Among these theories, the 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 Bogoliubov quasiparticles in the superconducting state, is the most popular. In this theory, the dynamical spin susceptibility is given by

\begin{equation}
\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - U(q)\chi_0(q, \omega)},
\end{equation}

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 at the best, 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. An effort to combine the more microscopic slave Boson mean field theory and the RPA theory in the \(t-J\) model\cite{1} 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, \(\int dq d\omega S(q, \omega) = (1-x)^2\), 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 capture 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 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.
THE SINGLE MODE APPROXIMATION

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

$$H = H_t + H_v + H_J,$$

$$H_t = -t \sum_{<i,j>,\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c.),$$

$$H_v = -t' \sum_{<i,j>,\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c.),$$

$$H_J = J \sum_{<i,j>} (\hat{S}_i \cdot \hat{S}_j - \frac{1}{4} n_in_j).$$  \hspace{1cm} (2)

Here $\hat{c}_{i\sigma}$ is the constrained electron operator satisfying the constraint $\sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \leq 1$. $\sum_{<i,j>}$ and $\sum_{<<i,j>>}$ represent the sum over nearest neighboring(NN) and next nearest neighboring(NNN) sites. Here we take $t' = -0.25$ to describe hole doped system. The exchange term is fixed at $t = \frac{1}{2}$.

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

$$\int dq d\omega S(q, \omega) = (1 - x)^3 \frac{3}{4},$$  \hspace{1cm} (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 $\left| \Psi_G \right\rangle$, which satisfy 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

$$\left| \Psi_g \right\rangle = P_N P_G \left| d - \text{BCS} \right\rangle$$

$$= P_G \sum_{i,j} a(i - j) \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\uparrow} \frac{\sum_{\sigma} \Delta_{\sigma}^2}{\xi_k} \left| 0 \right\rangle$$  \hspace{1cm} (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, $a(i - j) = \sum_k \frac{1}{\xi_k} e^{ik(r_i - r_j)}$ is the real space wave function of the Cooper pair with $\frac{\Delta_{\sigma}}{\xi_k} = \sqrt{\xi_k^2 + \Delta_k^2}$. $\xi_k$ and $\Delta_k$ are given by

$$\xi_k = -2(\cos k_x + \cos k_y) - 4t'u \cos k_x \cos k_y - \mu_v,$$

$$\Delta_k = 2\Delta_v(\cos k_x - \cos k_y),$$  \hspace{1cm} (5)

in which $t'u, \mu_v, \Delta_v$ are variational parameters to be determined by the optimization of the ground state energy with respect to the $t - J$ model. We note $t'u, \mu_v, \Delta_v$ 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 $(\pi, \pi)$ resonance mode, we adopt the single mode approximation of the form

$$|\Psi_Q^0 \rangle = S^+_Q |\Psi_g \rangle,$$  \hspace{1cm} (6)

in which $S^+_Q$ is the creation operator of the spin density excitation at $Q = (\pi, \pi)$. As the variational ground state satisfy 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

$$E_Q = \frac{\langle \Psi_Q^0 | H | \Psi_Q^0 \rangle - E_g}{\langle \Psi_Q^0 | S^+_Q S^-_Q | \Psi_Q^0 \rangle},$$  \hspace{1cm} (7)

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

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

Using the commutation relation

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

$$[\hat{c}_{i,\sigma}, S^+_j] = \delta_{ij} \delta_{\sigma,\uparrow} \hat{c}_{i,\uparrow},$$  \hspace{1cm} (9)

in which $\hat{c}_{i,\sigma}^\dagger$ 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

$$E_Q = -\frac{\langle \Psi_Q^0 | H | \Psi_Q^0 \rangle - \frac{\Delta_v}{2} \langle \Psi_g | H_j | \Psi_g \rangle}{\langle \Psi_Q^0 | S^+_Q S^-_Q | \Psi_Q^0 \rangle}.$$  \hspace{1cm} (10)

It is interesting to note that the $H_Q$ 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 of $E_Q$ is due to the rapid decrease of the spin structure factor as a function of doping which overcompensates the increase of the absolute
proximation energy directly from Eq.(7). At half filling, the spin structure factor calculated from $|\Psi_g\rangle$ scales superlinearly with the number of lattice site $N_s$ ($M_{Q}^2 = \langle \Psi_g | S_Q^z S_Q^z | \Psi_g \rangle / \langle \Psi_g | \Psi_g \rangle \propto N_s^2$) as a result of the long range correlation induced by the Gutzwiller projection\[13\]. However, the kinetic and exchange energy is by definition proportional to $N_s$. Thus Eq. must approach zero at half filling as $N_s \to \infty$. 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).

THE 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

$$|\tilde{\Psi}_Q\rangle = \sum_k \phi_k \gamma_k^\dagger \gamma_{Q-k}^\dagger |d - \text{BCS}\rangle,$$

in which $\phi_k$ describe the relative motion of the two quasiparticles $\gamma_k^\dagger$ and $\gamma_{Q-k}^\dagger$ within the bound state. $|d - \text{BCS}\rangle$ denotes the BCS mean field ground state and $\gamma_k^\dagger$ 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 $\phi_k$ as the variational parameter to be determined by optimization of energy.

$$|\Psi_Q\rangle = P_N P_G |\tilde{\Psi}_Q\rangle = \sum_k \phi_k |k, Q\rangle,$$

in which

$$|k, Q\rangle = P_N P_G \gamma_k^\dagger \gamma_{Q-k}^\dagger |d - \text{BCS}\rangle.$$  

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

$$|\Psi^0_Q\rangle = P_N P_G S_Q^\dagger |d - \text{BCS}\rangle = \sum_k P_N P_G \gamma_k^\dagger \gamma_{k+Q}^\dagger c_{k,\downarrow} |d - \text{BCS}\rangle$$

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

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

$$E_Q = \frac{\langle \Psi_Q | H_{t-J} | \Psi_Q \rangle}{\langle \Psi_Q | \Psi_Q \rangle} = \frac{\sum_{k,k'} \phi_k^* H_{k,k'} \phi_{k'}}{\sum_{k,k'} \phi_k^* C_{k,k'} \phi_{k'}}$$

in which

$$H_{k,k'} = (k, Q) H_{t-J} (k', Q)$$

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.
is the matrix element of the \( t - J \) Hamiltonian in the basis \( |k, Q \rangle \) and
\[
O_{k,k'} = \langle k, Q | k', Q \rangle \tag{17}
\]
denotes the overlap integral between these non-orthogonal basis function (note that \( \gamma_{k}^\dagger \gamma_{k'}^\dagger |d - \text{BCS} \rangle \) form a orthogonal basis set before the Gutzwiller projection).

The problem of minimizing \( E_Q \) respect to the set of variational parameters \( \phi_k \) now reduces to solving the following generalized eigenvalue problem
\[
\sum_{k'} O_{k,k'} \phi_{k'} = \lambda \sum_{k'} O_{k,k'} \phi_{k'} \tag{18}
\]
It is easily seen that the optimized energy \( E_Q \) is given by the lowest eigenvalue \( \lambda \) of the above generalized eigenvalue problem.

The above optimization procedure can also be interpreted as re-diagonalizing the \( t - J \) Hamiltonian in the subspace spanned by the set of non-orthogonal basis function \( |k, Q \rangle \). With this understanding in mind, we can even construct variationally the full spin fluctuation spectrum as follows
\[
S(Q, \omega) = M^2_Q \sum_{n,k,k'} |\phi_k^0 \phi_{k'}^* O_{k,k'} \phi_k^0| \delta(\omega - (E_n - E_g)) \tag{19}
\]
in which \( \phi_k^0 \) denotes the n-th eigenvector of the generalized energy problem with the eigenvalue \( E_n, E_g \) denotes the variational ground state energy (here we assume that \( \phi_k \) and \( \phi_k^0 \) are so chosen that both \( |\Psi_Q \rangle \) and \( |\Psi_Q^0 \rangle \) are normalized). As \( \phi_k^0 \) forms a orthonormal basis with respect to the overlap matrix \( O_{k,k'} \), i.e., \( \sum_{k,k'} \phi_k^0 \phi_{k'}^* O_{k,k'} \phi_{k'}^m = \delta_{n,m} \), we have
\[
\int d\omega S(Q, \omega) = M^2_Q \sum_{n,k,k'} |\phi_k^0 \phi_{k'}^* O_{k,k'} \phi_k^0|^2 = M^2_Q \sum_{k,k'} O_{k,k'} \phi_k^0 \phi_{k'}^0 \tag{20}
\]
in which we have used the fact that
\[
\sum_{n,k} \phi_k^0 \phi_{k}^* O_{k,k} \phi_{k}^0 = \delta_{k_1,k_2} \tag{21}
\]
which can be derived from the orthonormality of the eigenvectors of the generalized eigenvalue problem Eq.(18),
\[
\sum_{k,k'} \phi_k^0 \phi_{k'}^* O_{k,k'} \phi_{k'}^m = \delta_{n,m} \tag{22}
\]
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 \( \phi_k \) 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 \( \phi_k = \phi_k^0 = \phi_k^0 \)). 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.

THE RE-WEIGHTING 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 \( |k, Q \rangle \), \( H_{k,k'} \) and the overlap matrix element \( O_{k,k'} \). This can be done in principle by the variational Monte Carlo(VMC) method. For example, to evaluate \( \frac{H_{k,k'}}{O_{k,k'}} = \langle k, Q | H_{k,k'} | k', Q \rangle \), we first expand \( |k, Q \rangle \) in an orthogonal basis \( |R_i \rangle \), i.e.,
\[
|k, Q \rangle = \sum_{R_i} \psi_k(R_i) |R_i \rangle \tag{23}
\]
where \( \psi_k(R_i) \) is the wave function of \( |k, Q \rangle \) in this basis. Then we have
\[
\frac{H_{k,k'}}{O_{k,k'}} = \frac{\sum_{R_i} |\psi_k(R_i)|^2 \frac{H\psi_k(R_i)}{\psi_k(R_i)}}{\sum_{R_i} |\psi_k(R_i)|^2} \tag{24}
\]
in which
\[
H\psi_k(R_i) = \sum_{R_i'} \langle R_i | H | R_i' \rangle \psi_k^*(R_i') \psi_k(R_i) \tag{25}
\]
Then we sample the basis space \( |R_i \rangle \) with the weight \( |\psi_k(R_i)|^2 \) and do the sum with the standard VMC technique\[12\].

The above procedure, though straightforward, is very inefficient. In our problem, there are \( N^2 \) Hamiltonian matrix elements \( H_{k,k'} \) and \( N^2 \) overlap matrix elements \( O_{k,k'} \) to be evaluated. For lattice of reasonable size, say, \( 14 \times 14 \), the number of the matrix elements to be evaluated would exceed 40000 even take into account the
Hermitian property of $H_{k,k'}$ and $O_{k,k'}$. 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,

$$
\frac{O_{k,k'}}{O_{k,k}} = \frac{\sum R_i \psi_k (R_i)^2 \psi_k (R_i)}{\sum R_i |\psi_k (R_i)|^2}
$$

(26)

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

$$
\frac{O_{k,k'}}{O_{k,k}} = \frac{\sum_{R_i} W(R_i) \psi_k (R_i)^2 \psi_k (R_i)}{\sum_{R_i} W(R_i) |\psi_k (R_i)|^2}.
$$

(27)

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

$$
\frac{O_{k,k'}}{O_{k,k} + O_{k',k}} = \frac{\sum_{R_i} W(R_i) \psi_k (R_i)^2 \psi_k (R_i)}{\sum_{R_i} W(R_i)}.
$$

(28)

The combined weight samples symmetrically between $\psi_k (R_i)$ and $\psi_k' (R_i)$ 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 $O_{k,k'}$. Here we sample the combined weight of all the $N_s |\psi_k (R_i)|^2$: $W(R_i) = \sum_k |\psi_k (R_i)|^2$. The calculation is done as follows:

$$
\frac{O_{k_1,k_2}}{\sum_k O_{k,k}} = \frac{\sum_{R_i} W(R_i) \psi_k (R_i) \psi_k (R_i)}{\sum_{R_i} W(R_i)}.
$$

(29)

To sample $W(R_i)$, we note that

$$
W(R_i) = |\psi_k (R_i)|^2 \sum_k |\psi_k (R_i)|^2
$$

(30)

And

$$
\frac{\psi_k^* (R_i) \psi_k (R_i)}{W(R_i)} = \frac{\psi_k^* (R_i) \psi_k (R_i)}{\sum_k |\psi_k (R_i)|^2}.
$$

(31)

in which $\psi_k$ 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 $\frac{O_{k_1,k_2}}{\sum_k O_{k,k}}$ is the $N_s$ ratio between basis functions $\psi_k (R_i)$ and $\psi_k (R_i)$. As the different basis functions are all Slater determinant differing with each other 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

$$
\frac{H_{k_1,k_2}}{\sum_k O_{k,k}} = \frac{\sum_{R_i} W(R_i) \psi_k^* (R_i) \times H \psi_k (R_i)}{\sum_{R_i} W(R_i)}.
$$

(32)

where $H \psi_k (R_i) = \sum_{R_j} (H_{ij} |R_j | \psi_k (R_j))$. Following the same reasoning, we arrive at

$$
\frac{\psi_k^* (R_i) \times H \psi_k (R_i)}{W(R_i)} = \frac{\psi_k^* (R_i)}{\sum_k |\psi_k (R_i)|^2} \times \frac{H \psi_k (R_i)}{\sum_k |\psi_k (R_i)|^2}.
$$

(33)

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

Thus the re-weighting 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.

### NUMERICAL RESULTS

To calculate the energy of the neutron resonance mode, we first optimize the variational parameters $t'_{i,j}$, $\mu$, $\Delta_n$ as a function of doping for the ground state. The calculation is done on a $14 \times 14$ lattice with periodic-antiperiodic boundary condition. We choose $t_f = \frac{1}{2}$ and $t_{1,2} = -0.25$ 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 Fig.2 and Fig.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

$$
\Delta = \sqrt{\frac{1}{N_s} \sum_i <\hat{\Delta}_i \hat{\Delta}^+_i + R_{j,j'}>}
$$

(34)

in which $\hat{\Delta}_i = (c_{i+x+y}c_{i,y} - c_{i-x,y}c_{i+x+y}) - (c_{i+y,x}c_{i,t} - c_{i+y,x}c_{i+y,x})$ is the Cooper pair annihilation operator at site $i$, $R_{j,j'}$ 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 Hamil-
tonian matrix elements $H_{k,k'}$ and the overlap matrix elements $O_{k,k'}$. 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 $W(R_i)$. The accept ratio is tuned to be $1/2$. 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 $H_{k,k'}$ and $O_{k,k'}$, 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.

Fig.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%[14]. 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 0.3$t$
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$_2$Cu$_3$O$_{6.93}$[1].

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 $(\pi, \pi)$, namely the incommensurate spin fluctuation spectrum, is now under investigation.

We have also devised a very efficient re-weighting 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 of 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 optimally doped system[4] and would imply the breakdown of the $T_c = E_r$ linear scaling in the overdoped regime.

**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 $(\pi, \pi)$, namely the incommensurate spin fluctuation spectrum, is now under investigation.

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**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.

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 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. The would imply a breakdown of the scaling in the overdoped regime.

Fig. 6 shows the relative and absolute spectral weight 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 $Q = (\pi, \pi)$,

$$W = \frac{\langle \psi_Q^2 | \psi_Q \rangle^2}{\langle \phi_Q^2 | \psi_Q \rangle^2}. \quad (35)$$

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 of both the magnetic structure factor and the relative spectral weight. The relative spectral weight of the resonance mode decrease 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.
In our theory, the monotonic increase of the mode energy eventually cut off at about twice the maximal superconducting gap when the mode transfers all of its weight into the particle-hole continuum. To exhibit a non-monotonic 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 for the increase of the peak density at the optimal doping, 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 \( YBa_2Cu_3O_7 \). 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, 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, 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 off diagonal long range order (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 lose 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 of doping, the normal state signal becomes stronger and stronger and the enhancement due to superconductivity becomes less and less prominent.

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 of 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, 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 re-weighting technique to simulated wave function composed of N linearly superposed Slater determinants, an algorithm whose potential application is obviously far beyond the high-Tc issue.

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