I. INTRODUCTION

After nearly two decades intense study of the anomalous properties of high-Tc superconductors (HTS), many important questions still remain open. Among others, the nonmagnetic impurities effect on the cuprates has attracted much attention. The nonmagnetic impurities have little effect on the superfluid density and the transition temperature, which can be understood well from Anderson theorem. However, for HTS, it is found that such impurities can cause a strong pair-breaking effect, implying that HTS have the unconventional, most likely d-wave pairing symmetry. So understanding of the effects of the nonmagnetic impurities on these materials provide us important information to understand the pairing mechanism in HTS.

Experimentally, scanning tunneling microscopy (STM) is an ideal technique for the study of such effects at the atomic scale. With the help of the high quality of the surface properties of the samples and the improvement of the experimental techniques, a great deal of reliable data have been obtained by different STM groups. It is found that away from the nonmagnetic impurity, the tunneling spectra show the typical asymmetric superconducting coherence peaks, and around the nonmagnetic impurity, strong intra-gap density of states peaks are induced at energies close to the Fermi level, and at the same time the superconducting coherence peaks are strongly suppressed.

Theoretically, it has been widely accepted that the essential physics of cuprates can be effectively described by the two-dimensional Hubbard model or its equivalent t-J model in the large U limit. Based on these models, especially the t-J-like models, a good deal of work has been carried out to study the nonmagnetic impurity effect on the cuprate superconductors. But as we know that in the t-J-like models, the virtual double occupancy is completely neglected, and this maybe leads not to describe the real detailed physics in these materials. In this case, Laughlin proposed a new idea “Gossamer superconductor” to describe the physics of the HTS. In the Gossamer superconductor, even for the half filling, it may be a superconductor because of the double occupancy. Stimulated by the Laughlin’s idea, Anderson and Ong proposed a new wave function to quantitatively explain the observed asymmetric tunneling conductivity in the STM within the Gutzwiller-Resonating valence Bond theory. They believed that the asymmetries are predicted not to exist within the Fermi liquid theory, and one needs to explain the STM results within the Gutzwiller projected mean-field-theory.

Following above ideas, in this paper, we study the nonmagnetic impurity effect in the cuprate superconductor within the two-dimensional t-t'-J-U model using the Gutzwiller-projected mean-field-theory (MFT) and the Bogoliubov-de Gennes theory. The order parameter (OP) are determined self-consistently and the LDOS is calculated numerically. We reproduced the main experimental results within our present theory. In the large U limit without electron double occupancy (EDO), far away from the local nonmagnetic impurity the LDOS shows asymmetric superconducting coherence peaks. While around the nonmagnetic impurity, a zero-energy resonance peak in the LDOS indeed appears when pushing the impurity potential into the unitary limit, and meanwhile the superconducting coherence peaks are strongly suppressed. We also find that with increasing the EDO d
which is directly modulated by Coulomb repulsion $U$, the OP gradually decreases and the resulting superconducting coherence peaks move to lower energies, while it is interesting to see the above zero-energy resonance peak begins to evolve into a double-peaked structure since a critical value $d_c$. These novel feathers of asymmetric or splitting of the resonance state near Fermi energy are qualitatively agreement with the STM experiments, and reveal the essential role played by the electron correlation in cuprate superconductors.

II. THE t-t′-J-U MODEL AND GUTZWILLER PROJECTED MEAN-FIELD APPROXIMATION

We start from the t-t′-J-U model on a square lattice \cite{25,26,27},

$$
H = -t \sum_{i\bar{j}\sigma} C_{i\sigma}^\dagger C_{i+\bar{j}\sigma} + t' \sum_{i\bar{j}\sigma} C_{i\sigma}^\dagger C_{i+\bar{j}\sigma}
+ \sum_{\bar{i}\sigma} S_{\bar{i}} \cdot S_{i+\bar{j}} - \mu \sum_{\bar{i}\sigma} C_{\bar{i}\sigma}^\dagger C_{\bar{i}\sigma} 
+ U \sum_{i\sigma} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i\sigma} U_i n_{i\sigma}
$$

where $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ is the electron creation (annihilation) operator, $S_{\bar{i}} = \frac{1}{2} \sum_{\sigma\sigma'} C_{\bar{i}\sigma}^\dagger \sigma \cdot \sigma' C_{\bar{i}\sigma}$ is spin operator with $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ as the Pauli matrices, $n_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma}$, $\mu$ is the chemical potential, and $U$ is the on-site Coulomb potential, which is introduced to partially impose the no-double-occupancy constraint for the strongly correlated system. In the limit $U \to \infty$, the model is reduced to the t-J model. The scattering potential from the single-site impurity is modeled by $U_i = U_0 \delta_{iI}$ with $I$ the index for the impurity site.

To study the Hamiltonian (1) with the Gutzwiller variational approach, we take the trial wave function $|\psi\rangle$ as

$$
|\psi\rangle = P_G|BCS(\Delta_{ij}),
$$

where $|BCS(\Delta_{ij})\rangle$ is the BCS mean-field solution, and $P_G$ is the Gutzwiller projection operator which is defined as

$$
P_G = \Pi_t[1 - (1 - g)\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}],
$$

here $g$ is a variational parameter which takes the value between 0 and 1. The choice $g = 0$ corresponds to the situation with no doubly occupied sites ($U \to \infty$), while $g = 1$ corresponds to the uncorrelated state ($U = 0$). With the help of the trial wave function and the Gutzwiller approximation \cite{25,26}, we can get a Gutzwiller renormalized hamiltonian \cite{27},

$$
H_{eff} = -g_t \sum_{i\bar{j}\sigma} C_{i\sigma}^\dagger C_{i+\bar{j}\sigma} - t' \sum_{i\bar{j}\sigma} C_{i\sigma}^\dagger C_{i+\bar{j}\sigma}
+ g_s \sum_{i\sigma} S_{i\sigma} \cdot S_{i+\bar{j}\sigma} + NUd
+ \sum_{i\sigma} U_i n_{i\sigma} - \mu \sum_{i\sigma} C_{i\sigma}^\dagger C_{i\sigma}
$$

where $g_t$ and $g_s$ are the renormalized factors in the Gutzwiller approximation,

$$
g_t = \frac{2(n_i - 2d_i)}{n_i(2 - n_i)} \left[ \sqrt{1 - n_i} + d_i + \sqrt{d_i} \right]^2
$$

$$
g_s = \left[ \frac{2(n_i - 2d_i)}{n_i(2 - n_i)} \right]^2
$$

with the electron number $n_i$, and the double occupancy number $d_i$ at the site i. Then using the mean-field approximation, we obtain a Bogoliubov-de Gennes (BdG) equation,

$$
\sum_j \left( H_{ij} F_{ij}^* - H_{ij}^* F_{ij} \right) \left( u_n^j \right)^* = E_n \left( u_n^j \right),
$$

with

$$
H_{ij} = -\sum_{\bar{\eta}} \left( g_t + \frac{3}{4} g_s J \chi_{ij} \right) \delta_{\bar{\eta},i+\bar{\eta}} + \sum_{\bar{\eta}} g_t \delta_{\bar{\eta},i+\bar{\eta}}
+ \left( U_i - \mu \right) \delta_{ij}
$$

$$
F_{ij} = -\sum_{\bar{\eta}} \frac{3}{8} g_s J \Delta_{ij} \delta_{\bar{\eta},i+\bar{\eta}}
$$

In the above equations, we have introduced the electron pairing OP and the bond OP,

$$
\Delta_{ij} = \langle C_{i\uparrow} C_{j\uparrow} - C_{i\downarrow} C_{j\downarrow} \rangle_0
$$

$$
\chi_{ij} = \langle C_{i\uparrow}^\dagger C_{j\uparrow} \rangle_0
$$

which can be determined self-consistently as,

$$
\Delta_{ij} = \frac{1}{2} \sum_n \left( v_{ij}^* v_{in} + v_{ij}^* v_{in} \right) \tanh \left( \frac{1}{2} \beta E_n \right)
$$

$$
\chi_{ij} = \sum_n \left| v_{ij}^* \right|^2 f(E_n) + \sum_n \left| v_{ij}^* \right|^2 [1 - f(E_n)]
$$

$$
n_i = \sum_n \left| v_{in}^* \right|^2 f(E_n) + \sum_n \left| v_{in}^* \right|^2 [1 - f(E_n)]
$$

and

$$
0 = \sum_{i,n} \left( \frac{\partial E_{i,n}}{\partial g_t} \frac{\partial g_t}{\partial d_i} + \frac{\partial E_{i,n}}{\partial g_s} \frac{\partial g_s}{\partial d_i} \right) + U,
$$

where $f(E) = 1/(e^{\beta E} + 1)$ is the Fermi-Dirac distribution function. In the numerical calculation, we construct a superlattice with the square lattice $Nx \times Ny$ as a unit supercell. As detailed in Ref. 7, this method can provide the required energy resolution for the possible resonant states. Throughout this paper, we take the size.
of the unit supercell \( N = 33 \times 33 \), the number of supercell \( N_c = 10 \times 10 \). Then we can solve numerically the BdG equation and carry out an iteration until the selfconsistent equations are satisfied. Hereafter, we set \( t = 1 \), \( t' / t = -0.3 \), \( J / t = 0.3 \) for the band structure corresponding to the doping \( \delta = 0.1 \). The impurity potential \( U_0 = 100t \) is in the unitary limit.

III. NUMERICAL RESULTS AND DISCUSSIONS

We firstly review the local electronic structure near a nonmagnetic impurity in the limit \( U \rightarrow \infty \), the model now is reduced to the \( t-t'-J \) model and no EDO is constraint. In Fig. 1, we plot the obtained OP. The spatial variation of the d-wave OP defined as

\[
\Delta_d(i) = \frac{1}{4} [\Delta_{(i,i+x)} + \Delta_{(i,i-x)} - \Delta_{(i,i+y)} - \Delta_{(i,i-y)}],
\]

It is shown that because of the presence of the nonmagnetic impurity, the OP is suppressed at the impurity site and recovers its bulk value over 2-3 lattice spacings.

Next we calculate the LDOS as,

\[
\rho_i(E) = -2 \sum_{n,k} \left[ |u_i^{n,k}|^2 f'(E_{n,k} - E) + |v_i^{n,k}|^2 f'(E_{n,k} + E) \right]
\]

where the prefactor 2 comes from the spin summation, and \( f'(E) = df(E)/dE \) is the derivation of the fermi distribution function \( f(E) \). The LDOS \( \rho_i(E) \) is proportional to the local differential tunneling conductance which can be measured in a scanning tunneling microscope/spectroscopy experiment, so we can compare our calculated LDOS with the STM results directly.

The LDOS spectra for different scattering potentials around the impurity site are plotted in Fig. 2. For the site which locates far away from the impurity in Fig. 2a, LDOS displays the typical "V"-shaped curve which has recovered the bulk DOS, by exhibiting a gaplike feature at the gap edges. And especially we find that under the present Gutzwiller-projector MFA, the LDOS shows the particle-hole asymmetry which have been observed by the STM measurement. At impurity site (not shown here), a single resonance state only appears at small scattering strength and is invisible with increasing \( U_0 \) due to the stronger impurity scattering. On the nearest-neighbor site of the impurity (N,N) as seen in Fig. 2b, it is shown that the superconducting coherence peaks are strongly suppressed, and quasiparticle resonance states at intragap energies are generated by a single nonmagnetic impurity. The details features are that for a moderately strong impurity \( U_0 = 3t \), the asymmetric resonance states behave to be a double-peaked structure with the \( \omega > 0 \) peak having the dominant spectral weight over the \( \omega < 0 \) peak. While increasing the impurity strength pushes the resonance peaks toward the Fermi level, so that in the unitary limit \( U_0 = 100t \), the resonance state occurs right on the Fermi energy, and only a single zero-energy resonance peak appears in the LDOS near the impurity. It is also shown that the effect of the impurity is completely localized. To see clearly this point, we plot the spatial variation of the LDOS at \( \omega/t = \pm 0.02 \) in the unitary limit in Fig. 3 where we can see that the impurity-induced resonance state is indeed localized around the impurity. All the present results are consistent with the experimental data and previous theoretical calculations.

We now turn to investigate the effect of the Coulomb repulsion \( U \) on the quasiparticle resonance states in the impurity scattering unitary limit. The average double occupation number \( d \) modulated by \( U \) has been studied by one of the authors where they found that \( d \) decreased linearly with increasing Coulomb repulsion \( U \) as shown in an insert in Fig. 4b. Thus we can directly investigate the effect of the EDO \( d \) on the LDOS. The spatial variation of d-wave OP with various \( d \) at \( T = 0 \) is self-consistently cal-

![FIG. 1: (Color online) The spatial variation of the d-wave order parameter \( \Delta_d \) for the parameter \( U_0 = 100t \) in the large \( U \) limit.](image1)

![FIG. 2: (Color online) The LDOS spectra for different scattering potentials \( U_0 \) near the impurity site in the large \( U \) limit at \( T = 0 \).](image2)
FIG. 3: (Color online) The spatial variation of the LDOS at $\omega/t = \pm 0.02$ in the unitary limit.

FIG. 4: (Color online) (a) The spatial variation of the d-wave OP with the EDO $d = 0.001, 0.01, 0.03$ at $T = 0$ and $U_0 = 100t$. (b) The d-wave OP as a function of $d$. Insert: the EDO $d$ as a function of $U$ from Ref. 29.

Calculated in Fig. 4a, which indicates that with increasing EDO $d$ (decreasing Coulomb repulsion $U$), the magnitude of order parameter gradually decreases seen in Fig. 4b. As a result, in Fig. 5 the corresponding position of the superconducting coherent peaks in LDOS move to the lower energies with increasing $d$, while a single zero-energy impurity resonance peak always survives for small value of $d$, and begins to evolve into a double-peaked structure with negative energy peak having the dominant spectral weight over the positive energy peak since a critical double occupancy $d_c = 0.01$. These novel feathers of asymmetric or splitting of the resonance state in the impurity scattering unitary limit near Fermi energy are qualitatively agreement with the STM experiments. Since the $d$ is modulated by the $U$, in the large $U$ limit, the no double occupation ($d=0$) constraint is satisfied for the strongly correlated electron systems. As $U$ decreases, the electron double occupation is permitted and the electron correlation becomes weaker, the evolution of quasiparticle resonance states shown above qualitatively describes the effect of the electron correlation interactions on the STM. With the variation of the electron onsite Coulomb interaction, the resonance states induced by the impurity would display different features, which in turn reflects the role played by electron correlation in various cuprate superconductors. In order to avoid the misunderstanding, we stress here again that the evolution of double-peaked resonance into a single one as shown in Fig. 2 just depends on the impurity potential strength $U_0$.

IV. SUMMARY

In conclusion, we have studied the LDOS around a nonmagnetic impurity in the cuprate superconductors within the Gutzwiller approximation and Bogoliubov-de Gennes theory. We reproduced the main related experimental results, that is, the asymmetric feature of the LDOS, and impurity induced resonance states which are approximately localized around the impurity. In addition, considering the effect of the Coulomb repulsion, we increase the EDO $d$ which is modulated by $U$, and find that the OP gradually decreases and the resulting superconducting coherence peaks move to lower energies, while a unitary impurity induced single zero-energy resonance peak always survives for small value of $d$, and begins to evolve into a double-peaked structure since a critical double occupancy $d_c$. These important feathers represent the essential role played by the electron correlations in cuprate superconductors.

Acknowledgments

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