Electronic structure of the vortex lattice of *d*-, $d+is$-, and $d_{x^2-y^2}+id_{xy}$-wave superconductors

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On the basis of the self-consistent Bogoliubov-de Gennes equations and a tight-binding lattice model, we investigate the quasiparticle spectrum of vortex-lattice state in pure *d*-, mixed $d+is$, and $d_{x^2-y^2}+id_{xy}$-wave superconductors. For a *d*-wave case, the local density of states (LDOS) at the vortex core shows a multipeak structure, and the positions of peaks as well as the width of splitting between peaks are sensitively dependent on both the magnetic-field strength and the orientation of the vortex lattice. For the mixed $d+is$- and $d_{x^2-y^2}+id_{xy}$-wave pairing states, we observe a double-peak structure of the local density of states at vortex center, where the two peaks are asymmetrically situated around the Fermi energy. By taking into account the matrix-element effect, the local density of states appears to be qualitatively consistent with the scanning-tunneling-microscopy experimental data.

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I. INTRODUCTION

In recent years, a number of experimental evidences have demonstrated that the dominant pairing state of high-T_c superconductors has a $d_{x^2-y^2}$ symmetry.[1,2] Many investigations have been stimulated in clarifying the nature of electronic structure in the vortex state of *d*-wave superconductors because such an issue is important in understanding various static and transport properties in the mixed state of high-T_c materials. In the vortex state of conventional *s*-wave superconductors, Caroli, de Gennes, and Matricon[3] predicted the existence of discrete quasiparticle excitations localized around the vortex core long ago, which was observed later by scanning-tunneling-microscopy (STM) experiment on $NbSe_2$.[4] On the other hand, in the *d*-wave case, due to the existence of four nodes of the superconducting gap, it was argued[5] that the low-lying quasiparticle states around the vortex core are delocalized with wave functions extending along the nodal directions. Numerical studies on both electronic structure of the vortex lattice within a tight-binding lattice model[6] and an isolated vortex line in a continuum model[5] in the framework of Bogoliubov-de Gennes (BdG) theory[7] demonstrated that the local density of states in the vortex core has a broad featureless peak centered around zero energy in contrast to the clearly resolved bound-state structure[8–10] in *s*-wave cases, indicating that the vortex-core quasiparticle states between *d*-wave and *s*-wave superconductors are essentially different. However, the STM measurements on $YBa_2Cu_8O_{7-\delta}$ (YBCO)[11] and $Bi_2Sr_2CaCu_2O_8$ (BSCCO)[12] found that the tunneling conductance at vortex center does not exhibit the broad peak around the Fermi energy as theoretically expected and a double-peak splitting symmetrically around zero bias is revealed.

The discrepancy has intrigued significant theoretical effort to reconcile the theory with experimental observation. In the framework of a weak coupling mean-field approach, Franz and Tesanović[5] proposed a magnetic-field-induced mixed $d_{x^2-y^2}+id_{xy}$ ($\Delta_{xy}/\Delta_{x^2-y^2}\simeq 0.17$) state and studied the tunneling conductance of a single vortex in the very low field region to qualitatively explain the experimental data. On the other hand, Yasui and Kita[13] investigated the quasiparticle spectrum of the pure *d*-wave vortex-lattice state by employing a Landau-level-expansion method in solving the BdG problem. In intermediate magnetic field, they found clear double-peak structure of the spectrum for systems with short coherent length ($k_F\xi \leqslant 5$) and the splitting is found to be proportional to the field strength. Furthermore, they found that mixing of a small value of d_{xy}- or *s*-wave component ($\Delta_{xy}/\Delta_{x^2-y^2}\simeq 0.06$) has little effect on the tunneling spectra. Triggered by the above-mentioned seemingly contradicting theories, the actual effect of the finite field and the mixed $d+is$ and $d_{x^2-y^2}+id_{xy}$ (will be called $d+id'$-wave later) pairing state on the spectrum of quasiparticle excitation is studied in this work by numerical diagonalization of the BdG equation established on a 2D lattice. First, we perform a study on the square-vortex-lattice state of a pure *d*-wave superconductor at finite magnetic field ranging from 14–32 T (where the lattice constant of the underlying lattice is chosen as 5 Å) with $k_F\xi \simeq 1$. Around zero energy, both broad peak[5] and double-peak[13] structure of the local density of states (LDOS) at the vortex core are revealed for some specific parameters. However, generally speaking, we find that the LDOS at the core has multipeak splitting with the single-broad peak and double-peak structure as its two specific examples. Moreover, as the field varies, there is no simple proportional relation between the splitting width and field strength; on the contrary, the peak position and its splitting width are sensitively dependent on both the field and the orientation of vortex lattice, which indicates that the experimental data might not be simply understood only in terms of a pure *d*-wave superconductor at finite magnetic fields. Second, we take the mixing of *s*- or d_{xy}-wave component into consideration. The time-reversal-symmetry-breaking $d+id'$ state was first invoked by Laughlin[14] to explain the experimental observation of a plateau in thermal conductivity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ at finite fields,[15] and later addressed within Ginzburg-Landau (GL) theory at low-field[16] and high-field region[17] through field-induced phase transition. Applying the BdG theory, we study the vortex-lattice structure of a $d+is$- and a $d+id'$-wave state that are favorable at finite fields with $\Delta_s/\Delta_d \lesssim 0.4$ and $\Delta_{d'}/\Delta_d \lesssim 0.2$. We find a double-peak structure of the LDOS at the vortex core asymmetrically located with respect to zero energy. One peak corresponds to vortex-bound state as in s-wave superconductors and the other corresponds to the coherent peak at the gap edge of the subdominant s- or d_{xy}-wave component. Employing the matrix-element effect,[18] an approximately symmetric double-peak structure can be observed, which is qualitatively consistent with experimental data.

II. MODEL AND BASIC EQUATIONS

In this work, we adopt an extended Hubbard model on a two-dimensional (2D) lattice with nearest-neighbor (NN) hopping and onsite, nearest-neighbor, and/or next-nearest-neighbor (NNN) pairing interactions to model the decoupled CuO_2 layers of high-T_c cuprates. The model Hamiltonian is expressed as

$$H=-\sum_{\langle i,j\rangle\sigma} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}-\mu\sum_{i\sigma} n_{i\sigma}-V_0\sum_{i} n_{i\uparrow}n_{i\downarrow} -\frac{V_1}{2}\sum_{\langle i,j\rangle\sigma\sigma'} n_{i\sigma}n_{j\sigma'}-\frac{V_2}{2}\sum_{\langle\langle i,j\rangle\rangle\sigma\sigma'} n_{i\sigma}n_{j\sigma'}. \quad (1)$$

Here $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$ is the electron number operator for spin σ on site i, $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote NN and NNN pairs in the lattice, respectively. μ is the chemical potential. The hopping integral is written as

$$t_{ij}=t\exp\left[-\frac{i\pi}{\Phi_0}\int_{\mathbf{r}_i}^{\mathbf{r}_j}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}\right],$$

with $\mathbf{A}(\mathbf{r})$ the vector potential and $\Phi_0=hc/2e$ the superconducting flux quantum. V_0, V_1, $V_2>0$ are onsite, NN, and NNN attractive potentials, which give rise to the pairing in the s-wave, $d_{x^2-y^2}$-wave, and d_{xy}-wave channel, respectively. With appropriate setting of the values of V_0, V_1, and V_2, s-, $d_{x^2-y^2}$, mixed $d+is$, or $d+id'$-wave superconducting instability can be reached. By applying the self-consistent mean-field (MF) approximation and performing the Bogoliubov transformation,[6,7] diagonalization of the Hamiltonian (1) can be achieved by solving the following BdG equations:

$$\sum_j \begin{pmatrix} H_{i,j} & \Delta_{i,j} \\ \Delta^{*}_{i,j} & -H^{*}_{i,j}\end{pmatrix}\begin{pmatrix} u_n(\mathbf{r}_j) \\ v_n(\mathbf{r}_j)\end{pmatrix}=E_n\begin{pmatrix} u_n(\mathbf{r}_i) \\ v_n(\mathbf{r}_i)\end{pmatrix}, \quad (2)$$

where u_n, v_n are the Bogoliubov quasiparticle amplitudes with corresponding eigenvalue E_n and

$$H_{i,j}=-\delta_{i+\tau,j}t_{ij}-\delta_{ij}\mu,$$

with $\tau=\pm\hat{\mathbf{x}},\pm\hat{\mathbf{y}}$ are unit vectors; therefore, according to $\delta_{i+\tau,j}$, only NN sites hopping will be taken into consideration. The mean-field pairing potential is defined as

$$\Delta_{i,j}=\delta_{ij}\Delta_0(\mathbf{r}_i)+\delta_{i+\tau,j}\Delta(\mathbf{r}_i,\mathbf{r}_{i+\tau}),$$

where

$$\Delta_0(\mathbf{r}_i)=-V_0\langle c_{i\downarrow}c_{i\uparrow}\rangle=V_0\sum_n u_n(\mathbf{r}_i)v^{*}_n(\mathbf{r}_i)\tanh\left(\frac{E_n}{2k_BT}\right),$$

$$\Delta(\mathbf{r}_i,\mathbf{r}_{i+\tau})=-V_{1,2}\langle c_{i\downarrow}c_{i+\tau\uparrow}\rangle=\frac{V_{1,2}}{2}\sum_n [u_n(\mathbf{r}_i)v^{*}_n(\mathbf{r}_{i+\tau}) +u_n(\mathbf{r}_{i+\tau})v^{*}_n(\mathbf{r}_i)]\tanh\left(\frac{E_n}{2k_BT}\right),$$

with $\tau=\pm\hat{\mathbf{x}},\pm\hat{\mathbf{y}}$ for the NN sites pairing and $\tau=\pm\hat{\mathbf{x}}\pm\hat{\mathbf{y}}$ for the NNN sites pairing case. The $d_{x^2-y^2}$-wave and d_{xy}-wave pairing potential is given by

$$\Delta_{x^2-y^2}(\mathbf{r}_i)=[\Delta_{\hat{x}}(\mathbf{r}_i)+\Delta_{-\hat{x}}(\mathbf{r}_i)-\Delta_{\hat{y}}(\mathbf{r}_i)-\Delta_{-\hat{y}}(\mathbf{r}_i)]/4,$$

$$\Delta_{xy}(\mathbf{r}_i)=[\Delta_{\hat{x}+\hat{y}(\mathbf{r}_i)}+\Delta_{-\hat{x}-\hat{y}}(\mathbf{r}_i)-\Delta_{\hat{x}-\hat{y}}(\mathbf{r}_i)-\Delta_{-\hat{x}+\hat{y}}(\mathbf{r}_i)]/4, \quad (3)$$

where

$$\Delta_{\tau}(\mathbf{r}_i)=\Delta(\mathbf{r}_i,\mathbf{r}_{i+\tau})\exp\left[-\frac{i\pi}{\Phi_0}\int_{\mathbf{r}_i}^{\mathbf{r}_{i+\tau}}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}\right].$$

In this paper, we will study square-vortex-lattice configurations with two different kinds of orientation, where the NN vortices are aligned along the [100] or [110] direction of the underlying crystal lattice (in the following, we denote the former configuration as "I" and the latter "II"). To study vortex-lattice states, we employ the *magnetic* unit cell that accommodates two vortices, i.e., one electronic flux quantum $\phi_0=hc/e$ (two superconducting flux quanta $2\Phi_0$). Commonly, the primitive translation vectors of the magnetic unit cell are $\mathbf{R}_x=aN_x\hat{\mathbf{x}}$ and $\mathbf{R}_y=aN_y\hat{\mathbf{y}}$, where a is the lattice constant and will be taken as unity in the following discussion. Applying the theory of magnetic translation group,[19] the quasiparticle amplitude u_n and v_n can be expressed as magnetic Bloch states (eigenfunctions of the subgroup of the magnetic translation group)

$$u^{\mathbf{k}}_n(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})\tilde{u}^{\mathbf{k}}_n(\mathbf{r}),$$

$$v^{\mathbf{k}}_n(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})\tilde{v}^{\mathbf{k}}_n(\mathbf{r}), \quad (4)$$

which are labeled by the quasimomentum $\mathbf{k}$. $u^{\mathbf{k}}_n$ and $v^{\mathbf{k}}_n$ have the following translation properties:

$$\begin{pmatrix} u^{\mathbf{k}}_n(\mathbf{r}+\mathbf{R}) \\ v^{\mathbf{k}}_n(\mathbf{r}+\mathbf{R})\end{pmatrix}=\exp(i\mathbf{k}\cdot\mathbf{R})\begin{pmatrix} u^{\mathbf{k}}_n(\mathbf{r})\exp(i\chi(\mathbf{r},\mathbf{R})/2) \\ v^{\mathbf{k}}_n(\mathbf{r})\exp(-i\chi(\mathbf{r},\mathbf{R})/2)\end{pmatrix}, \quad (5)$$

where $\mathbf{R}=\mathbf{m}\mathbf{R}_x+n\mathbf{R}_y$ is magnetic translation vector. The phase factor $\chi(\mathbf{r},\mathbf{R})$ has an identical form despite the specific choice of gauge. Within the Landau gauge where $\mathbf{A}^L(\mathbf{r})=(0,Hx,0)$ and the symmetric gauge with $\mathbf{A}^S(\mathbf{r})=\mathbf{H}\times\mathbf{r}/2=(-Hy,Hx,0)/2$, we have

$$\chi^{L(S)}(\mathbf{r},\mathbf{R})=\frac{2\pi}{\Phi_0}\mathbf{A}^{L(S)}(\mathbf{R})\cdot\mathbf{r}+2mn\pi. \quad (6)$$

From Eqs. (3)–(6), one can readily find that $\Delta_{x^2-y^2}(\mathbf{r}_i)$ [and $\Delta_{xy}(\mathbf{r}_i)$] has the following translation property: $\Delta_{x^2-y^2}(\mathbf{r}_i+\mathbf{R})=\Delta_{x^2-y^2}(\mathbf{r}_i)\exp[i\chi(\mathbf{r},\mathbf{R})]$.

For convenience of numerical calculation, we choose the Landau gauge to deal with the square-vortex-lattice configuration I and the symmetric gauge to deal with configuration II. In both cases, the magnetic field is approximated to be uniform, which is appropriate for type-II high-T_c superconductors at finite fields. Substituting Eq. (4) into the BdG Eq. (2), the original vortex-lattice problem changes into an eigensystem defined within one single magnetic unit cell,

$$\sum_j \exp(i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_i))\begin{pmatrix} H_{i,j} & \Delta_{i,j} \\ \Delta^*_{i,j} & -H^*_{i,j}\end{pmatrix}\begin{pmatrix}\tilde{u}^{\mathbf{k}}_n(\mathbf{r}_j)\\ \tilde{v}^{\mathbf{k}}_n(\mathbf{r}_j)\end{pmatrix}=E^{\mathbf{k}}_n\begin{pmatrix}\tilde{u}^{\mathbf{k}}_n(\mathbf{r}_i)\\ \tilde{v}^{\mathbf{k}}_n(\mathbf{r}_i)\end{pmatrix}, \tag{7}$$

together with the appropriate boundary conditions derived from Eq. (5),

$$\begin{pmatrix}\tilde{u}^{\mathbf{k}}_n(\mathbf{r}+\mathbf{R})\\ \tilde{v}^{\mathbf{k}}_n(\mathbf{r}+\mathbf{R})\end{pmatrix}=\begin{pmatrix}\tilde{u}^{\mathbf{k}}_n(\mathbf{r})\exp(i\chi(\mathbf{r},\mathbf{R})/2)\\ \tilde{v}^{\mathbf{k}}_n(\mathbf{r})\exp(-i\chi(\mathbf{r},\mathbf{R})/2)\end{pmatrix}. \tag{8}$$

For the vortex lattice with $M_x\times M_y$ number of magnetic unit cells, the magnetic wave vector $\mathbf{k}=2\pi(m_x,m_y)/(aN_{x,y}M_{x,y})$, with $m_{x,y}=0,1,...,M_{x,y}-1$, is defined in the first magnetic Brillouin zone. Similarly, we obtain $\Delta_0(\mathbf{r}_i)$ and $\Delta_\tau(\mathbf{r}_i)$ expressed by $\tilde{u}^{\mathbf{k}}_n$ and $\tilde{v}^{\mathbf{k}}_n$,

$$\Delta_0(\mathbf{r}_i)=V_0\sum_{\mathbf{k},n}\tilde{u}^{\mathbf{k}}_n(\mathbf{r}_i)\tilde{v}^{\mathbf{k}*}_n(\mathbf{r}_i)\tanh\left(\frac{E^{\mathbf{k}}_n}{2k_BT}\right),$$

$$\Delta_\tau(\mathbf{r}_i)=\frac{V_{1,2}}{2}\sum_{\mathbf{k},n}[\tilde{u}^{\mathbf{k}}_n(\mathbf{r}_i)\tilde{v}^{\mathbf{k}*}_n(\mathbf{r}_{i+\tau})e^{-i\mathbf{k}\cdot\tau}+\tilde{u}^{\mathbf{k}}_n(\mathbf{r}_{i+\tau})\tilde{v}^{\mathbf{k}*}_n(\mathbf{r}_i)e^{i\mathbf{k}\cdot\tau}]\tanh\left(\frac{E^{\mathbf{k}}_n}{2k_BT}\right).$$

With the above boundary conditions, the resulting quasiparticle spectrum is obtained by repeated diagonalization of the BdG equations and iteration of the pairing potential until sufficient accuracy is achieved (in the present work, the maximum relative error of the pairing potential is controlled $\leqslant 1\%$).

Once the BdG Eqs. (7) is solved self-consistently, the quasiparticle-excitation spectrum can be obtained. The local density of states (LDOS) is given by

$$\rho(\mathbf{r}_i,E)=-\frac{1}{M_xM_y}\sum_{\mathbf{k},n}[|\tilde{u}^{\mathbf{k}}_n(\mathbf{r}_i)|^2f'(E^{\mathbf{k}}_n-E)+|\tilde{v}^{\mathbf{k}}_n(\mathbf{r}_i)|^2f'(E^{\mathbf{k}}_n+E)], \tag{9}$$

where $f(E)$ represents the usual Fermi distribution function. In the following sections, the electronic structure of the vortex-lattice state in d-, $d+is$-, and $d+id'$-wave superconductors will be studied.

III. LDOS OF PURE *d*-WAVE VORTEX LATTICE

For convenience of later comparison, the electronic structure of the vortex-lattice state of a pure d-wave superconductor is studied at first. The size of the magnetic unit cell is $N_La\times 2N_La$ for the Landau gauge corresponding to a magnetic field $H^L=\Phi_0/(2N_L^2a^2)$ and $N_sa\times N_sa$ for the symmetric gauge corresponding to a magnetic field $H^s=\Phi_0/(N_s^2a^2)$, where N_L and N_s are both integers. $\mu/t=-1$, which gives rise to a band filling factor $\langle n\rangle\simeq 0.62$. To get the d pairing instability, V_1 will be taken as positive and V_0, $V_2=0$. We use $V_1/t=3.0$, $\mu/t=-1.0$. This set of parameter values results in $\Delta_d/t=0.368$ and $T_c^d/t=0.569$. The coherent peak of the d-wave order parameter is at $\Delta_{\max}/t\simeq 1.1$. From the BCS formula $\xi=\hbar v_F/\pi\Delta_{\max}\sim E_F/\pi\Delta_{\max}k_F$, we have $k_F\xi\simeq 1$.

First we give the LDOS of the pure $d_{x^2-y^2}$-wave vortex lattice in Fig. 1, which is proportional to the differential tunneling conductance of the STM experiments. We find that the azimuthally averaged LDOS of the intervortex sites far from the vortex center behaves like that of the homogeneous zero-field case. At about $\pm 1.1t$, there are coherence peaks corresponding to the superconducting gap edge $\Delta_{\max}$, while around $\pm 1.8t$ there are peaks reflecting the Van Hove singularity of the band.[6] There are no bound states localized around the vortex core of pure d-wave superconductors, which is consistent with the results of the BdG study of both an isolated vortex[5] and vortex lattice[6,20] at low magnetic fields while is in contrast with those of s-wave vortex problems.[3,8–10] We have studied the variation of LDOS at vortex core with magnetic field by changing the magnetic unit cell size. The results are shown in Fig. 1. We find that besides broad resonant peak centered near the zero energy [see Figs. 1(a2), 1(a3), and 1(b5)], which was pointed out in Refs. 5, 6, 20, there are also peak splittings where their width and position exhibit significant dependence on both the magnetic field and vortex-lattice arrangement. This multiple-peak feature of the spectrum line is clearly different from the broad featureless resonant peak reported in Ref. 5 and the fine details observed in the single-vortex study,[5] which were contributed to possible finite-size effect. We find that these peaks correspond to subbands generated by the overlap among the low-lying vortex-core quasiparticle resonant states of different vortices. Figure 2 shows the quasiparticle subband spectra in the first magnetic Brillouin zone of vortex lattice I and II for the magnetic-field strength $H^L=\Phi_0/(324a^2)$ and $H^S=\Phi_0/(338a^2)$. It can be seen that although the applied field is approximately the same for these two configurations the dispersion differs with each other largely. From Fig. 2(b) a cluster of subbands ranging from $0.05t$ to $0.15t$ gives rise to the double-peak splitting of LDOS at the Fermi surface as shown in Fig. 1(b2), while the nearness or even crossing of the subbands in Fig. 2(a) results in a broad peak with only weak oscillations, as seen in Fig. 1(a2). Similar sensitivity of subband spectrum to the field strength is also found, which leads to the large variation of LDOS with changing field strength, as seen in Fig. 1. Such a strong field effect has also been pointed out in Ref. 21 in a non-self-consistent solution of the BdG Hamiltonian by

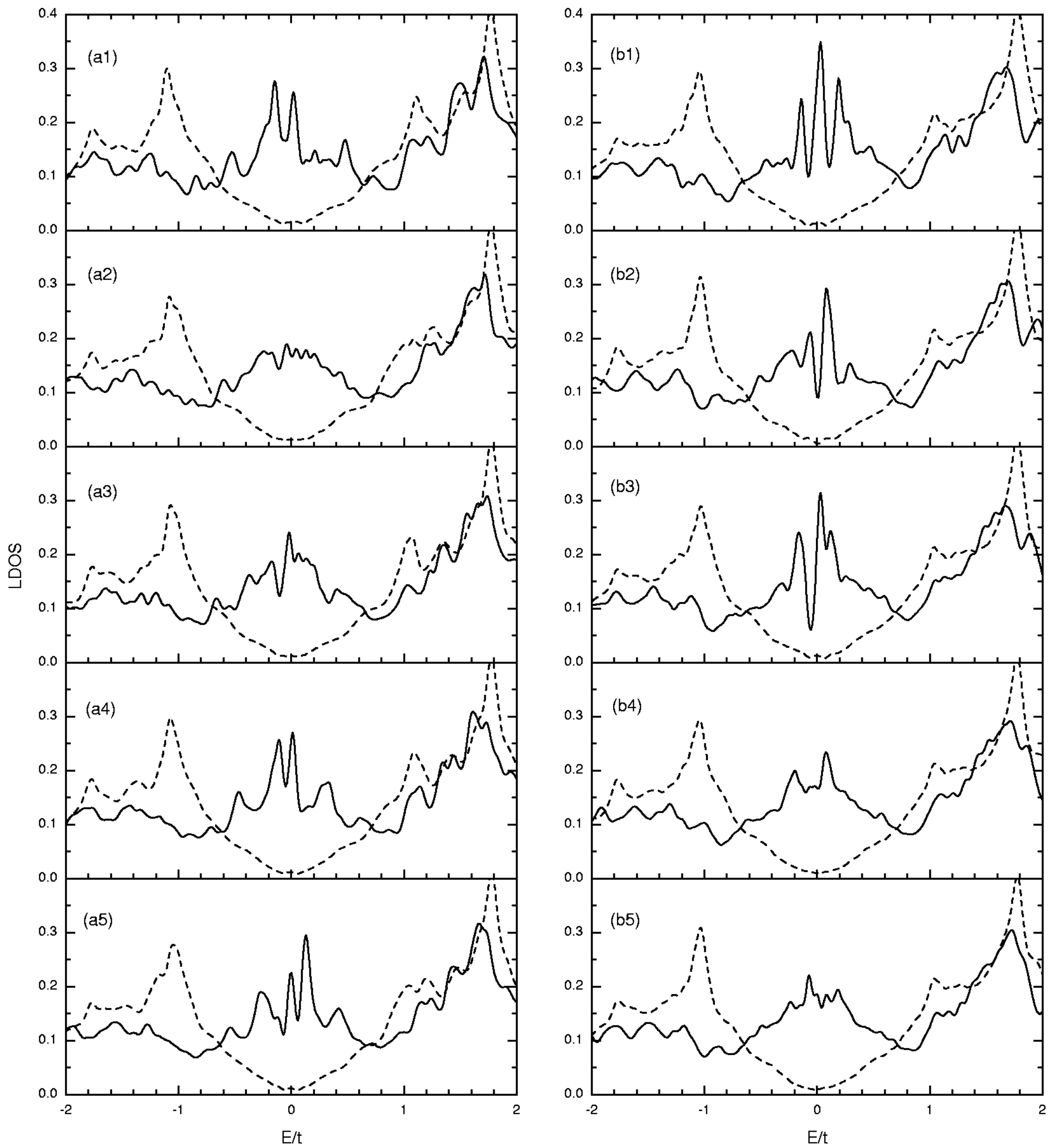

FIG. 1. LDOS at the center of vortex (solid line) and spatially averaged LDOS of the intervortex sites (dashed line) at $T=0$. Left: vortex-lattice configuration I; from (a1) to (a5) the magnetic unit cell sizes are 16×32, 18×36, 20×40, 22×44, and 24×48. Right: vortex-lattice configuration II; from (b1) to (b5) the magnetic unit cell sizes are 24×24, 26×26, 28×28, 30×30, and 32×32.

means of Franz-Tesanovic singular gauge transformation.[22] For the reason that the wave functions of the low-lying resonant states are extended mainly along the nodal directions where $\Delta_d(\mathbf{k})$ vanishes, strong interference effect[21] of these states causes the remarkable oscillation of the spectra with even slight change of the field (accordingly, magnetic unit cell size) and vortex arrangement.

For specific field strength and vortex-lattice configuration, such as in Figs. 1(b2) and (b3), the LDOS might be qualitatively consistent with the double-peak structure of the tunneling conductance observed in experiments[11,12] and a self-consistent BdG analysis of the quasiparticle spectrum of *d*-wave vortex lattice within a continuum model employing a Landau-level expansion method.[13] However, the sensitivity of the details of the peak structure to the field and vortex-core arrangement indicates that the experimentally observed double-peak structure at the vortex core might *not* be in close connection with the vortex subbands if we further take into account the fact that the experimentally observed vortex-core states do not show any dependence on the applied magnetic field in the range from 1 to 6 T (Ref. 24) and the vortex lattice of real high-T_c cuprates seem more like disordered vortex glass without long range order.[11]

In the following section, we invoke the mixed $d+is$ and $d+id'$ paring states to address the double-peak structure of the LDOS at vortex core, which is shown to be insensitive to the field variation and the orientation of vortex lattice.

IV. LDOS OF MIXED $d+is$- AND $d+id'$-WAVE VORTEX LATTICE

In this section, the electronic structure of the vortex lattice state of the $d+is$-wave ($d+id'$-wave) superconductor is studied. Almost all parameters are the same as those in the

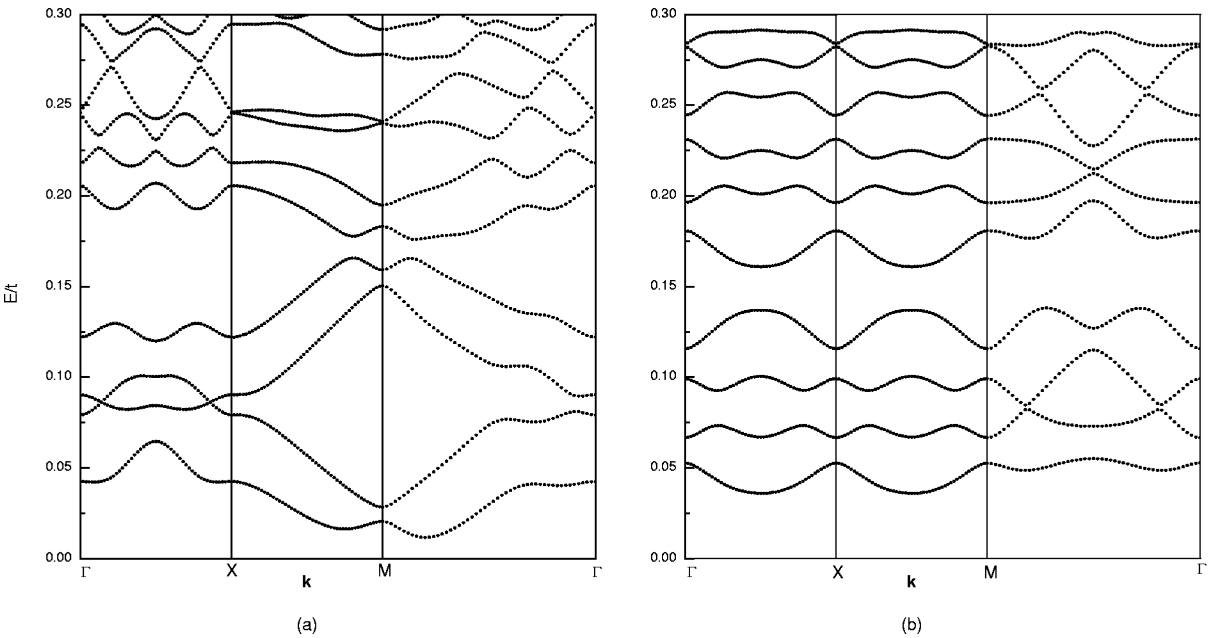

FIG. 2. Quasiparticle subband spectrum for the two square-vortex-lattice configuration. (a): configuration I with magnetic unit cell size 18 and (b): configuration II with magnetic unit cell size 26.

above mentioned pure d-wave case, except that both V_1 and V_0 (V_2) are taken as positive while V_2 (V_0) as zero to get the $d+is$ ($d+id'$) pairing instability. In Fig. 3, we present the phase diagram of the superconducting states within our tight-binding model with $\mu/t=-1$ and $T=0$ for the homogeneous case. As the relative magnitude of V_1 and V_0 (V_2) varies, different pairing states might be realized and the mixed $d+is$ wave ($d+id'$-wave) state exists in a relatively narrow parameter region as shown in Fig. 3. To study the vortex-lattice state of the mixed-pairing phase when a uniform magnetic field is applied along the z axis of lattice, we choose $V_1/t=3.0$, $\mu/t=-1.0$, and $V_0/t=2.4$, 2.5 for the $d+is$ phase and $V_2/t=2.0$, 2.1, 2.2 for the $d+id'$ phase. From Fig. 3, we find that these values of V_0 and V_2 are close to the lower transition line that separates the pure $d_{x^2-y^2}$ state with the mixed $d+is$ or $d+id'$ phases and, therefore, pure d-wave pairing state is favorable at zero field and will give rise to $\Delta_d/t=0.368$ and negligibly small ($\sim 10^{-4}t$) s-wave or d_{xy}-wave components as our numerical calculation shows.

However, when a moderate magnetic field is applied in the vortex-lattice state, nonzero s-wave or d_{xy}-wave pairing potential is generated due to the finite magnetic field ($H_{c1} \ll H \ll H_{c2}$), which is consistent with the result of Ref. 13. In Table I, we list the values of the pairing potentials for a few sets of parameter values, showing that the s- and d'-wave components are small compared with the dominant d-wave order parameter ($\Delta_s/\Delta_d \lesssim 0.4$ and $\Delta_{d'}/\Delta_d \lesssim 0.2$). This field-induced phase transition was first proposed by Laughlin[14] for $d_{x^2-y^2}+id_{xy}$ superconductors and later addressed within the framework of the GL theory at both low (near zero field)[16] and high ($H \simeq H_{c2}$)[17] field. At low temperatures where STM experiment is carried out, the previous theory chose a larger pairing interaction that gave rise to a result that $d+id'$ phase

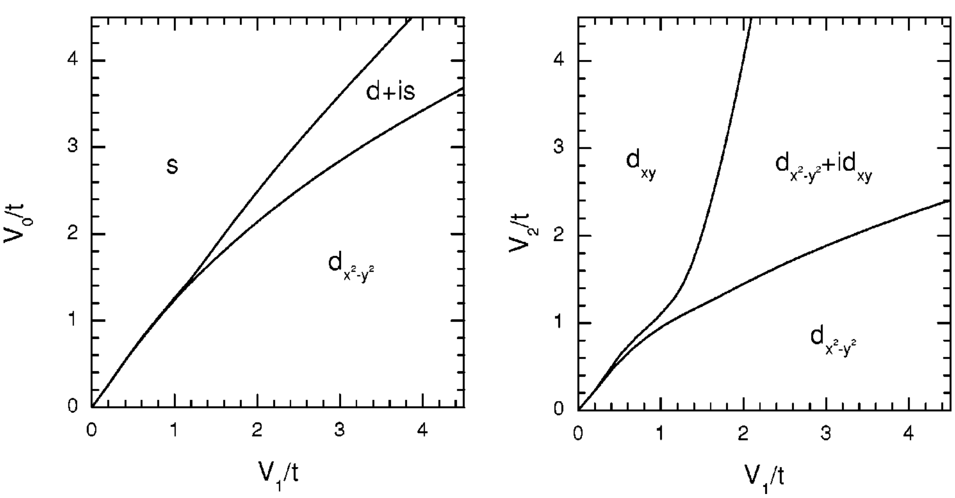

FIG. 3. Phase diagram of the pairing states at zero field. The parameters are $\mu/t=-1$ and $T=0$.

TABLE I. The magnitude of the $d_{z^2-y^2}$, s, and d_{xy} wave order parameters averaged in a magnetic unit cell for a few sets of parameter values. Other parameters are fixed with $T=0$, $\mu/t=-1$, and $V_1/t=3.0$. The number with superscript "I" denotes the corresponding values for square-vortex lattice aligned along the [100] direction with the magnetic unit cell size 20×40 [$H=\Phi_0/(400a^2)$] and that with "II" for the $\pi/4$ tilted square-vortex lattice with the magnetic unit cell size 28×28 [$H=\Phi_0/(392a^2)$].

V_0/t	$\Delta_{x^2-y^2}/t$	Δ_s/t
2.4	0.362^{I}, 0.361^{II}	0.090^{I}, 0.081^{II}
2.5	0.356^{I}, 0.355^{II}	0.154^{I}, 0.153^{II}
V_2/t	$\Delta_{x^2-y^2}/t$	Δ_{xy}/t
2.0	0.364^{I}, 0.362^{II}	0.022^{I}, 0.034^{II}
2.1	0.362^{I}, 0.360^{II}	0.050^{I}, 0.056^{II}
2.2	0.360^{I}, 0.358^{II}	0.073^{I}, 0.075^{II}

even exists at zero magnetic field,[5] which was inconsistent with the experimental observation, while in our calculation, pure $d_{x^2-y^2}$ phase is preferable when $H=0$. Therefore, our results do not seem to contradict with a possible mixed $d+id'$ pairing phase suggested by the thermal conductivity experiment on $Bi_2Sr_2CaCu_2O_8$ at finite magnetic fields[15] and the pure $d_{x^2-y^2}$ phase hinted by the low-temperature STM data at zero field.[23]

In Fig. 4, we show the spatial variation of the $|\Delta_{x^2-y^2}|$ and $|\Delta_s|$ for the two vortex-lattice orientations of the mixed $d+is$-wave superconducting phase. The results indicate clearly a twofold symmetry, while in the $d+id'$-wave case we find fourfold symmetric structure (not shown here), which is consistent with the GL numerical analysis.[25,26] Furthermore, small components of higher order, such as $s_{x^2-y^2}$ or s_{xy} is also induced around the vortex center. In Fig. 5, we give the LDOS at the vortex core in the $d+is$-wave pairing state. In such a model it can be clearly seen that a subgap opens and a double-peak structure exists with minimum at the Fermi energy, which is qualitatively consistent with experimental data. Such a structure is insensitive to vortex-lattice configuration and magnetic field, which indicate that it originates from the fully gapped feature of the $d+is$ state. However, the particle-hole symmetry is broken, with the peak below E_F lying farther away and having smaller spectral weight than the peak above E_F. $E_+/|E_-|\simeq0.5$, $|E_-|/\Delta_{\max}\simeq1/7$ when $V_0/t=2.4$ and increases to $E_+/|E_-|\simeq0.6$ and $|E_-|/\Delta_{\max}\simeq1/5$ when $V_0/t=2.5$ as shown in Fig. 5. By examining the position of the peaks in Fig. 5 and the subband spectrum in Fig. 6, we find that the peak at negative energy E_- actually coincides with the coherent peak at the s-wave gap edge ($\Delta_s^g\simeq0.15$, 0.20 for $V_0=2.4$, 2.5, respectively), while that at positive energy E_+ corresponds to the localized vortex-core state as in a pure s-wave superconductor.[10] However, different from s-wave vortex-bound states,[8,10,13] there is only one closely coupled pair of low-lying subbands within the the s-wave gap, originating from the two vortices in each magnetic unit cell; therefore, the peak of LDOS around zero bias does not change in energy as a function of increasing distance from the vortex center. Moreover, these subbands exhibit considerable dispersion showing that the overlapping of the localized core

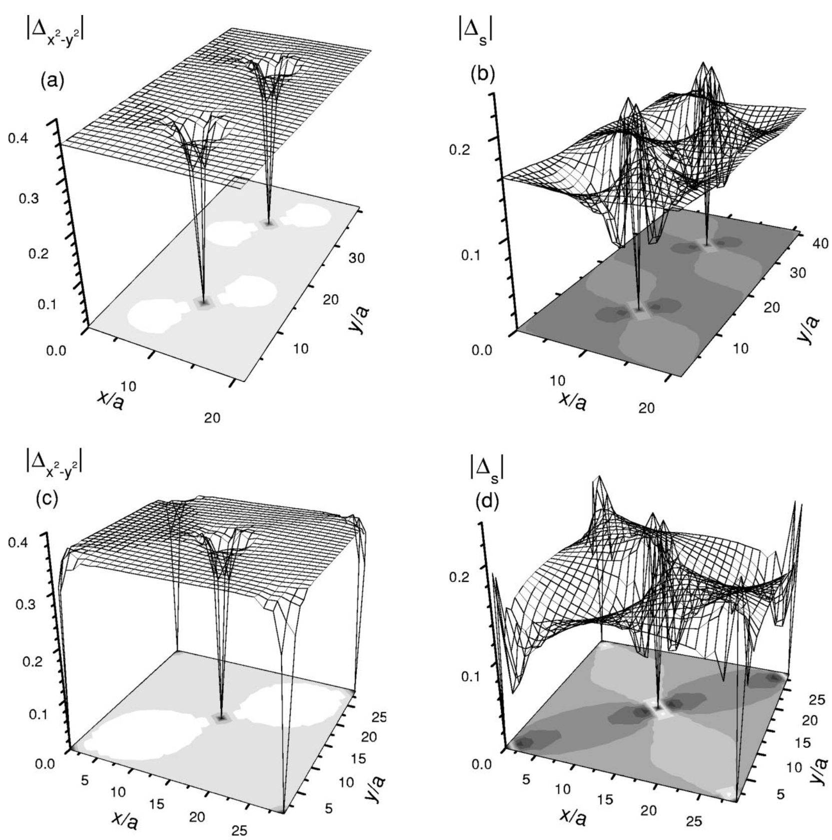

FIG. 4. Spatial distribution of $|\Delta_{x^2-y^2}|$ (a), (c) and $|\Delta_s|$ (b), (d) for the two square-vortex-lattice configurations. The parameters are $\mu/t=-1$, $T=0$, $V_1/t=3.0$, and $V_0/t=2.5$. (a) and (b) correspond to vortex-lattice configuration "I," while (c) and (d) correspond to configuration "II."

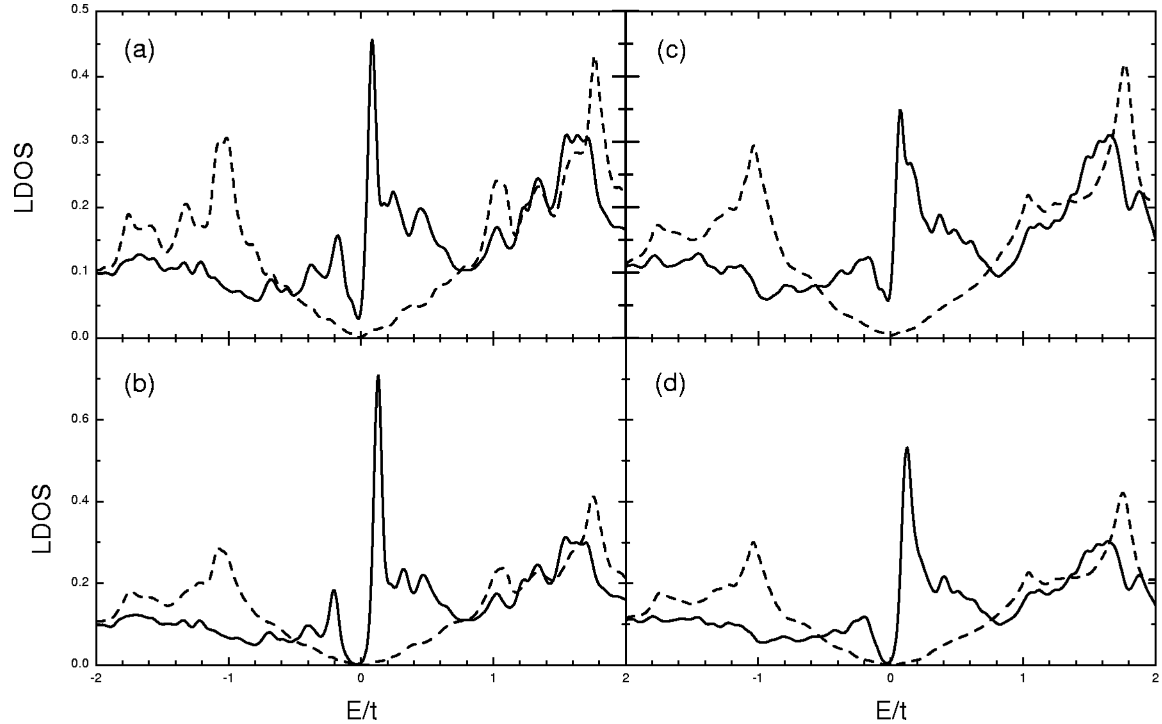

FIG. 5. LDOS at the center of vortex (solid line) and spatially averaged LDOS of the intervortex sites (dashed line) at $T=0$. (a), (b): vortex-lattice configuration I; (c), (d): vortex-lattice configuration II with $V_0/t=2.4$, 2.5, respectively. The magnetic unit cell sizes are 20 $\times 40$ for vortex-lattice configuration I and 28×28 for configuration II.

states of adjacent vortices is quite large. We attribute the large dispersion of the subbands to the smallness of the *s*-wave component, which results in long coherent length characterizing the attenuation of the vortex-bound state. According to the rough estimation in Ref. 10, the coherent length $\xi_s=\hbar v_F/\pi\Delta_s^g\sim 20a$, $15a$ for $V_0/t=2.4$, 2.5, respectively. For the magnetic unit cell size 20 as in Fig. 6, ξ_s is comparable with intervortex distance; therefore, this explains the dispersion of the low-lying subbands and its flattening when Δ_s^g increases [compare Fig. 6(a) with Fig. 6(b)].

Figure 5 also shows that the spatially averaged LDOS of intervortex sites does *not* exhibit gap structure opened at

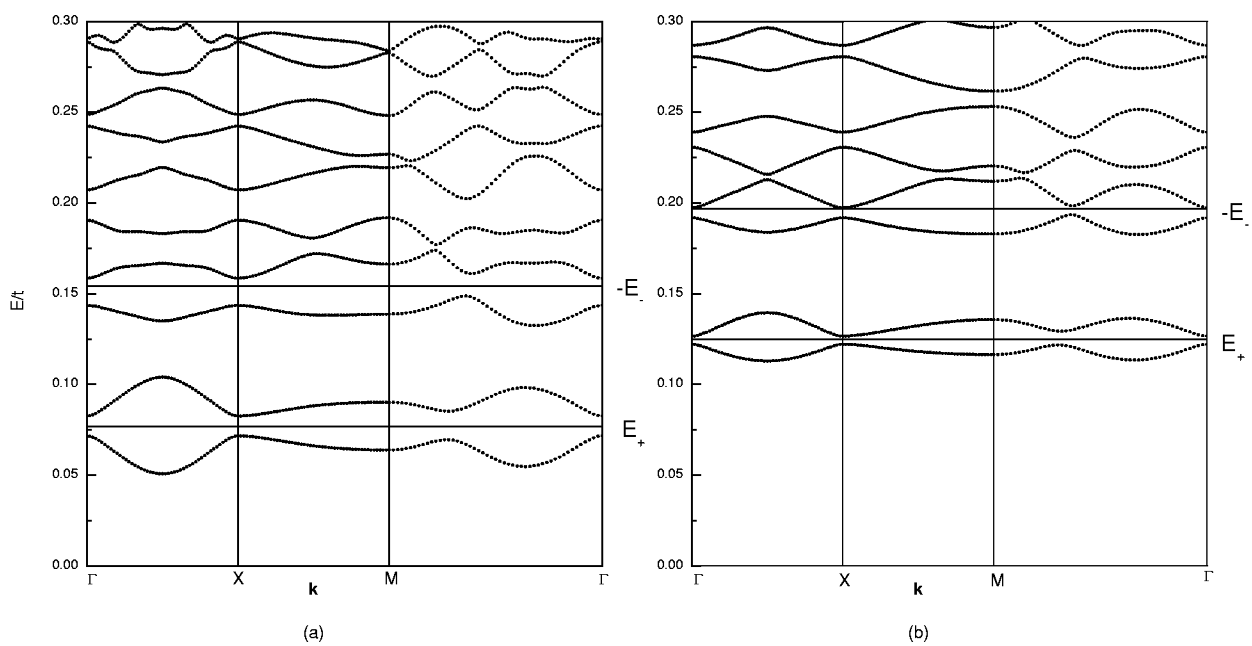

FIG. 6. Quasiparticle subband spectrum for the square-vortex-lattice configuration I with magnetic unit cell size 20×40. (a): $V_0=2.4$ and (b): $V_0=2.5$. The solid lines show the positions of LDOS peaks at the vortex core. The temperature is chosen as $0.02t$.

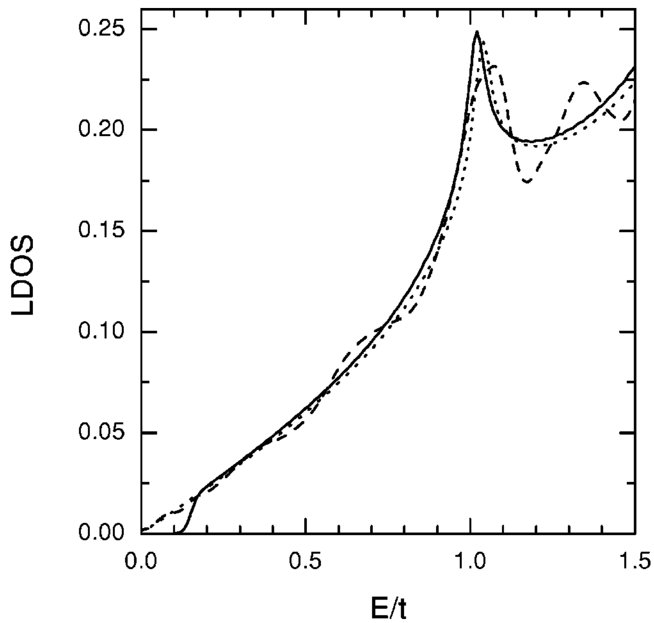

FIG. 7. Density of states of mixed $d+is$-wave pairing phase in homogeneous case, with $\Delta_d/t=0.36$ and $\Delta_s/t=0.15$ (solid line). Spatially averaged LDOS of intervortex sites of square-vortex-lattice configuration I with magnetic unit cell size 20×40 for $d+is$-wave state with $V_0/t=2.4$ (dashed line). Density of states of pure d-wave phase in homogeneous case with $\Delta_d/t=0.37$ (dotted line).

$\pm\Delta_s^g$ near E_F expected for $d+is$-wave pairing phase. Again, we employ the considerable dispersion of the low-lying subband within Δ_s^g to explain this effect. That is, the long attenuation length of the vortex-core state makes the wave function of the quasiparticle *leak* out of the vortex center and, therefore, makes contribution to the LDOS at intervortex sites, which can partially close the expected gap as far as Δ_s^g is small compared to the dominant d-wave component. The thermally broadening effect will help this effect further. Detailed comparison of the spatially averaged LDOS's of intervortex sites for mixed $d+is$-wave phase at finite magnetic fields with that at zero field is shown in Fig. 7 where the density of state of a pure d-wave superconductor at zero field is also given. Near E_F, the averaged LDOS in vortex-lattice state clearly differs from that of homogeneous case and behaves more like that of a pure d-wave superconductor at zero field when $T/t=0.02$ ($T/T_c\simeq0.035$). This implies that even if $d+is$-wave pairing phase does exist in the vortex phase it might be difficult to distinguish it from the pure d-wave phase by examining the LDOS far away from the vortex cores.

Similar results have also been found in the mixed $d+id'$-wave phase. The LDOS's at the vortex core for $V_2/t=2.0$, 2.1, 2.2 have been given in Fig. 8(a). With increasing pairing interaction V_2, E_+ and $|E_-|$ rise due to larger d_{xy}-wave component relative to approximately constant

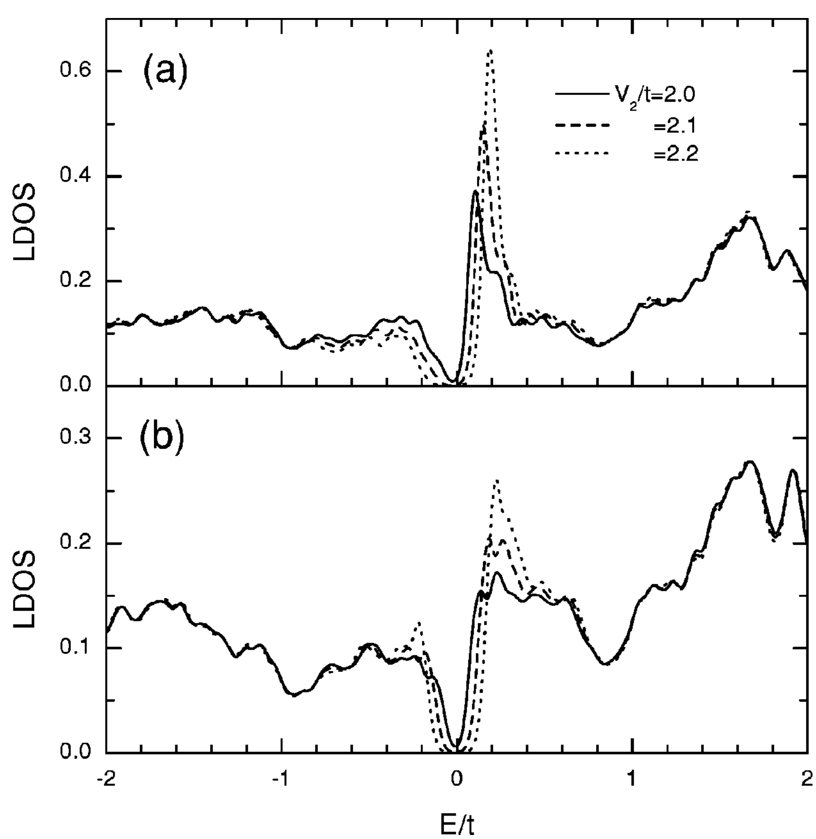

FIG. 8. LDOS at the center of vortex for the mixed $d+id'$. wave pairing state in the square-vortex-lattice configuration II with $V_2/t=2.0,2.1,2.2$. The magnetic unit cell size is 28 ×28. (a): without blocking effect; (b): with blocking effect

$\Delta_{x^2-y^2}$ as shown in Table I. Combining with the result of mixed $d+is$-wave state, we find that the main discrepancy between our theory and experimental data lies in the fact that in our model the double peaks locate asymmetrically with respect to E_F. We now employ the matrix-element effect[18] of the possible intermediate layer (for example, BiO layer in $Bi_2Sr_2CaCu_2O_{8+\delta}$) lying between the STM tip and the CuO layer being probed to resolve such a discrepancy. The blocking effect was proposed by Zhu, Ting, and Hu[18] to explain the impurity state of BiSrCaCuO. It was pointed out that due to the blocking of the Bi atom right above the Cu atom, the experimentally measured LDOS at a Cu site is actually a sum of the contribution of its NN sites in the CuO_2 plane. Therefore, we have

$$\tilde{\rho}(\mathbf{r}_0,E)=\sum_{\delta}\rho(\mathbf{r}_0+\delta,E), \quad (10)$$

where $\mathbf{r_0}$ denotes the position vector of the vortex-core site and δ its four NN sites. The modified LDOS is shown in Fig. 8(b). In comparison with Fig. 8(a), it can be seen that after taking into account the matrix-element effect E_+ keeps almost unchanged while E_- moves close to E_+ and an approximate particle-hole symmetry is recovered. The mechanism is that: according to the analysis of the vortex-bound state of s-wave superconductor,[8–10] the lowest-lying core state (with eigenenergy E_+) has largest spectral weight at the vortex-center site while its time-reversal counterpart (with eigenenergy $-E_+$) has zero spectral weight. Therefore, at the vortex-center site the particle-hole asymmetry is maximum; however, at its NN sites, both states ($\pm E_+$) have finite spectral weight showing the feature of particle-hole symmetry as seen in Fig. 8(b). For the mixed $d+is$-wave pairing state, the conclusion is the same. We find that when $V_0/t=2.5$ for the $d+is$-wave phase $E_+/\Delta_{\max}\simeq 1/8$ and $V_2/t=2.2$ for the $d+id'$-wave phase $E_+/\Delta_{\max}\simeq 1/5$, which is qualitatively consistent with experimental data.[11,12]

V. CONCLUSION

In this paper, the quasiparticle spectrum of pure d-wave, mixed $d+is$-wave, and $d+id'$-wave superconductors have been studied in the vortex-lattice state subject to a uniform magnetic field perpendicular to the underlying 2D discretized lattice. We discussed the square vortex lattice with two types of orientations with respect to the underlying finite-size lattice. The self-consistent BdG equations are solved numerically.

For the d-wave pairing state, the quasiparticle spectrum shows that no bound states are revealed, being consistent with previous results.[5,6] The LDOS at vortex core has a multipeak structure. By changing the magnetic field, we find that the peak positions and the width of peaks between peaks vary largely without a simple relation between the field strength and splitting of peaks. The LDOS at the vortex center exhibits obvious difference for two orientations of the square vortex lattice we study. The sensitivity of LDOS to the field and vortex arrangement is attributed to the interference effect of the wave function of quasiparticle state of adjacent vortices. Since the vortices in high-T_c materials may not be regularly distributed, the double-peak structure observed experimentally would not be explained by merely including the field effect on pure d-wave superconductors.

For the mixed $d+is$ and $d+id'$ pairing, we chose the parameters in such a way that pure d-wave phase is stablized at zero field while the mixed $d+is$ and $d+id'$ are favorable at finite fields. Vortex-bound state weakly localized around the vortex core is shown to be insensitive to both strength of field and vortex-lattice orientation. Due to the weakness of the subdominant s- or d_{xy}-wave component relative to the dominant $d_{x^2-y^2}$-wave pairing potential, the vortex-bound state has a characteristic length comparable with vortex-vortex distance, which form one vortex-core quasiparticle subband. Accordingly, the LDOS at the vortex center has an asymmetric double-peak structure, where the peak corresponding to the vortex-core quasiparticle subband has a positive energy and the other peak corresponding to the coherent peak has a negative energy. The positions of both peaks are proportional to the magnitude of the s- or d_{xy}-wave component. By employing the matrix-element effect[18] proposed to deal with the intermediate layer between the STM tip and the superconducting CuO_2 layer, we find that the double peak can locate symmetrically around the Fermi level, which is qualitatively consistent with STM observations.

It is natural to ask that whether the particle-hole symmetry of the tunneling conductance at the vortex core observed in STM experiments on both YBCO[11] and BSCCO[12] is intrinsic for high-T_c cuprates or just a feint related to the existence of an intermediate layer, which might have nontrivial influence on STM measurements. Further STM experiments are needed to clarify this issue.

At present, there are still no concrete experimental evidences of the bulk generation of the subdominant is or id' component in high-T_c superconductors at finite fields. However, various inhomogeneities, such as surfaces, grain boundaries impurities, and vortices, have all been shown as sources of the locally time-reversal-symmetry-breaking states. In fact, a spontaneous split of the zero-bias conductance peak observed in the surface of $YBa_2Cu_8O_{7-\delta}$ was interpreted as a signal of spontaneous time-reversal-symmetry breaking implying the existence of an is or id_{xy} component localized near the surface.[27,28] The problem now is whether the global coherent $d+is$- or $d+id'$-wave state can be realized, as the overlap of the the local is and id' component generated around vortex cores increases with the magnetic field. Anyway, to study what new phenomena in the mixed state might associate with the time-reversal-symmetry-breaking $d+is$ and $d+id'$ states is always an interesting issue, at least for theoretical research.

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