Lattice model for the broken-time-reversal-symmetry pairing state near a surface of *d*-wave superconductors

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(Received 13 August 1998; revised manuscript received 25 September 1998)

Based on an extended Hubbard model, the spatial variation of the order parameter is calculated self-consistently near the surface of *d*-wave superconductors. It is shown a $d+is$ order parameter can be induced near a {110} surface, leading to splitting of the zero-energy peak in the surface local density of states and the generation of a spontaneous surface supercurrent. This splitting can be diminished by the increase of orthorhombicity, on-site repulsive interaction, or temperature. Our results give a microscopic explanation for the surface broken-time-reversal-symmetry pairing state.
[S0163-1829(99)04705-0]

After many years of experimental and theoretical study,[1] a commonly shared point of view is that the pairing state of high-temperature superconductors is predominantly of *d*-wave symmetry. For such a pairing state, the energy gap can have a sign change along some nodal lines of an essentially cylindrical Fermi surface. As one of the direct consequences, Hu[2] has shown that midgap states with energy arbitrarily close to the Fermi surface can be formed near the {110} surface of a $d_{x_a^2-x_b^2}$-wave superconductor, where *a* and *b* are the crystalline axes. Midgap states do not exist on any surface of *s*-wave superconductors and on a {100} surface of $d_{x_a^2-x_b^2}$-wave superconductors. One of the most intriguing features of high-temperature superconductors, the zero-bias conductance peak (ZBCP) observed when tunneling into the *ab*-oriented thin films[3–5] can be explained quite well in terms of the midgap states induced at surfaces.[6,7] More recently, Covington *et al.*[8] reported the splitting of the ZBCP observed for copper/insulator/Y-Ba-Cu-O in-plane tunnel junctions at low temperatures in zero magnetic field. It is believed that this zero-field splitting is caused by the energy shift of the Andreev bound states in a broken-time-reversal-symmetry (BTRS) state.[9,10] Several previous works[11,12] predicted that a subdominant *s*-wave order parameter, which has a relative phase $\pi/2$ with respect to the dominant *d*-wave order parameter, could appear near the surface. However, within these continuum theories, an attractive subdominant *s*-channel interactions should be explicitly introduced for the realization of the surface BTRS $d+is$ state, even though this *s*-wave pairing interaction normally cannot compete with the *d*-wave pairing interaction in the bulk.[13] In addition, it is unclear to what extent the continuum approach that was used for *s*-wave superconductors is valid for treating *d*-wave superconductors with short coherence length. This situation presents a strong impetus for further study of the surface electronic states in *d*-wave superconductors.

In this paper, by introducing the supercell concept and using the exact diagonalization technique, we study the electronic states at the surface of a *d*-wave superconductor defined on a two-dimensional square lattice within an extended Hubbard model. The order parameter is self-consistently determined. We find that at low temperatures an (extended) *s*-wave component of the order parameter, which is $\pi/2$ out of phase with the suppressed *d*-wave component, is induced near a {110} surface. As a result, the local density of states (LDOS) near the surface is split at zero energy, which directly corresponds to the splitting of the ZBCP. This splitting is decreased with increased temperature and finally disappears at a critical temperature much lower than the bulk transition temperature. In addition, we also find that at a fixed low temperature, the zero-energy splitting in the LDOS can be reduced by the orthorhombicity and the increase of on-site repulsive interaction.

To model decoupled copper-oxygen layers in high-T_c superconductors, we consider the single-band extended Hubbard Hamiltonian on a two-dimensional square lattice

$$H=-\sum_{\langle \mathbf{ij}\rangle\sigma} t_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma}+\sum_{\mathbf{i}\sigma} U_{\mathbf{i}} n_{\mathbf{i}\sigma}-\mu\sum_{\mathbf{i}\sigma} n_{\mathbf{i}\sigma} - V_0\sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}-\frac{V_1}{2}\sum_{\langle \mathbf{ij}\rangle\sigma\sigma'} n_{\mathbf{i}\sigma} n_{\mathbf{j}\sigma'}. \tag{1}$$

Here **i** and **j** are site indices and the angle bracket implies that the hopping and interactions are only considered up to nearest-neighbor sites, $n_{\mathbf{i}\sigma}=c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma}$ is the electron number operator on site **i**, and μ is the chemical potential. To model the orthorhombicity effect, the hopping integral $t_{\mathbf{ij}}$ are taken to be direction-dependent and are respectively t_x, t_y along the crystalline *a* and *b* axes. $t_x=t_y$ corresponds to the tetragonal structure. The depletion of the carrier density at the surface is simulated by a single-layer impurity scattering potential: $U_{\mathbf{i}}$

$=U_0\Sigma_{\mathbf{i}'\in I}\delta_{\mathbf{i}',\mathbf{i}}$ with the summation over the set of impurity sites. The amplitude of the single-site potential is sufficiently strong so that the tunneling of carriers between both sides of the single layer is negligible. The quantities V_0, and V_1 are on-site and nearest-neighbor interaction strength, respectively. Positive values of V_0 and V_1 mean attractive interactions and negative values mean repulsive interactions. When $V_0<0$ and $V_1>0$, the d-wave pairing state is favorable. The extended Hubbard model has been previously used to study the single vortex structure,[14,15] electronic states on a twin boundary,[16,17] the effects of disorder[18,19] and single impurity scattering,[20] and the effect of surface roughness.[21] However, the existence of BTRS pairing state at the surface within this model has not been explored.[22]

To study the electronic states near the surface, we introduce the supercells. For the {110} surface, the size of each supercell is $N_x\sqrt{2}a\times N_y\sqrt{2}a$, where a is the lattice constant. The system Hamiltonian is invariant under a supercell translation. We then define the supercell Bloch states labeled by a wave vector $\mathbf{k}$ and a site index $\mathbf{i}$ within the supercell. Within the mean-field approximation, the diagonalization of Eq. (1) can be transformed to find the solutions to the lattice Bogoliubov–de Gennes (BdG) equations[23]

$$\sum_{\mathbf{j}}\begin{pmatrix} H_{\mathbf{ij}}(\mathbf{k}) & \Delta_{\mathbf{ij}} \\ \Delta_{\mathbf{ij}}^{\dagger} & -H_{\mathbf{ij}}(\mathbf{k})\end{pmatrix}\begin{pmatrix} u_{\mathbf{j}}^{n,\mathbf{k}} \\ v_{\mathbf{j}}^{n,\mathbf{k}}\end{pmatrix}=E_{n,\mathbf{k}}\begin{pmatrix} u_{\mathbf{i}}^{n,\mathbf{k}} \\ v_{\mathbf{i}}^{n,\mathbf{k}}\end{pmatrix}. \tag{2}$$

Here $u_{\mathbf{i}}^{n,\mathbf{k}}$ and $v_{\mathbf{i}}^{n,\mathbf{k}}$ are the Bogoliubov amplitudes corresponding to the eigenvalue $E_{n,\mathbf{k}}$,

$$H_{\mathbf{ij}}(\mathbf{k})=-t_{\mathbf{ij}}e^{i\mathbf{k}\cdot\boldsymbol{\delta}a/\sqrt{2}}\delta_{\mathbf{i}+\boldsymbol{\delta},\mathbf{j}}+(U_{\mathbf{i}}-\mu)\delta_{\mathbf{ij}}, \tag{3}$$

$$\Delta_{\mathbf{ij}}=\Delta_0(\mathbf{i})\delta_{\mathbf{ij}}+\Delta_{\boldsymbol{\delta}}(\mathbf{i})\delta_{\mathbf{i}+\boldsymbol{\delta},\mathbf{j}}, \tag{4}$$

where $\boldsymbol{\delta}=\pm\hat{\mathbf{x}}\pm\hat{\mathbf{y}}$ are the unit vectors, and $k_{x,y}=2\pi n_{x,y}/\sqrt{2}M_{x,y}N_{x,y}$ with $n_{x,y}=0,1,2,...,M_{x,y}-1$. The integers $M_{x,y}$ label the supercell. The energy gaps for on-site and nearest-neighbor pairing are determined self-consistently

$$\Delta_0(\mathbf{i})=\frac{V_0}{M}\sum_{n,\mathbf{k}}u_{\mathbf{i}}^{n,\mathbf{k}}v_{\mathbf{i}}^{n,\mathbf{k}*}\tanh(E_{n,\mathbf{k}}/2k_BT), \tag{5}$$

$$\Delta_{\boldsymbol{\delta}}(\mathbf{i})=\frac{V_1}{2M}\sum_{n,\mathbf{k}}[u_{\mathbf{i}}^{n,\mathbf{k}}v_{\mathbf{i}+\boldsymbol{\delta}}^{n,\mathbf{k}*}e^{-i\mathbf{k}\cdot\boldsymbol{\delta}a}+u_{\mathbf{i}+\boldsymbol{\delta}}^{n,\mathbf{k}}v_{\mathbf{i}}^{n,\mathbf{k}*}e^{i\mathbf{k}\cdot\boldsymbol{\delta}a}]\tanh(E_{n,\mathbf{k}}/2k_BT), \tag{6}$$

where k_B is the Boltzmann constant, $M=M_x\times M_y$ is the number of supercells. This technique has several merits: (i) the desired resolution to resolve the resonance in energy can be obtained; (ii) the band structure effect can be taken into account; (iii) it can be easily implemented to study more general situations.

We solve the BdG equations self-consistently by starting with an initial gap function. After exactly diagonalizing Eq. (2), the obtained Bogoliubov amplitudes are substituted into Eqs. (5) and (6) to compute a new gap function. We then use it as input to repeat the above process until the relative error in the gap function between successive iterations is less than the desired accuracy. Throughout our work, we use $V_1=2.5t_x$, $\mu=-t_x$, and $U_0=100t_x$. This set of parameter values give the $\Delta_d=0.266t_x$ and $T_c=0.418t_x$ for the bulk tetragonal structure and the corresponding coherence $\xi=\hbar v_F/\pi\Delta_d\approx 4a$.

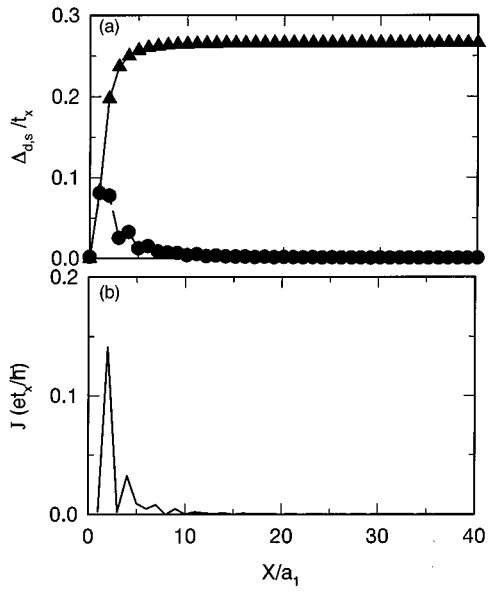

FIG. 1. The spatial variation of the amplitudes of order parameter (a) and the spontaneous current (b) away from the {110} surface of a tetragonal superconductor. The distance is measured in units of $a_1=a/\sqrt{2}$. The solid line (with filled triangle) corresponds to the d-wave component and the dashed line (with filled circle) to the s-wave component. The parameters $k_BT=0.02t_x$ and $V_0=0$.

Since a quasiparticle reflected from the {110} surface will see an order parameter, which has a different sign from that experienced before its reflection, the pair breaking effect at this surface is most pronounced. In Fig. 1(a), we plot the spatial variation of the amplitudes of d- and s-wave order parameters defined as[14]

$$\Delta_d(\mathbf{i})=\frac{1}{4}[\Delta_{\hat{x}}(\mathbf{i})+\Delta_{-\hat{x}}(\mathbf{i})-\Delta_{\hat{y}}(\mathbf{i})-\Delta_{-\hat{y}}(\mathbf{i})], \tag{7a}$$

$$\Delta_s(\mathbf{i})=\frac{1}{4}[\Delta_{\hat{x}}(\mathbf{i})+\Delta_{-\hat{x}}(\mathbf{i})+\Delta_{\hat{y}}(\mathbf{i})+\Delta_{-\hat{y}}(\mathbf{i})], \tag{7b}$$

for the {110} surface of a tetragonal d-wave superconductor at $T=0.02t_x$ and $V_0=0$. The spatial variation of the average current which given by

$$J_{\mathbf{ij}}=-\frac{2iet}{M\hbar}\sum_{n,\mathbf{k}}\{[f(E_n)u_{\mathbf{i}}^{n,\mathbf{k}*}u_{\mathbf{i}+\boldsymbol{\delta}}^{n,\mathbf{k}}e^{-i\mathbf{k}\cdot\boldsymbol{\delta}a/\sqrt{2}}+[1-f(E_n)]v_{\mathbf{i}}^{n}v_{\mathbf{i}+\boldsymbol{\delta}}^{n,\mathbf{k}*}e^{i\mathbf{k}\cdot\boldsymbol{\delta}a/\sqrt{2}}]-\text{c.c.}\} \tag{8}$$

is plotted in Fig. 1(b), where the Fermi distribution function $f(E)=[\exp(E/k_BT)+1]^{-1}$. Our numerical results show that the d-wave component of order parameter comes from the real part of the bond order parameter, while the extended s-wave component from the imaginary part. Therefore, it is demonstrated unambiguously that the relative phase between s- and d-wave components is $\pi/2$. The d-wave order parameter is suppressed near the surface and increases monotonically to the bulk value at a coherence length scale ξ. The induced s-wave component near the surface oscillates at an

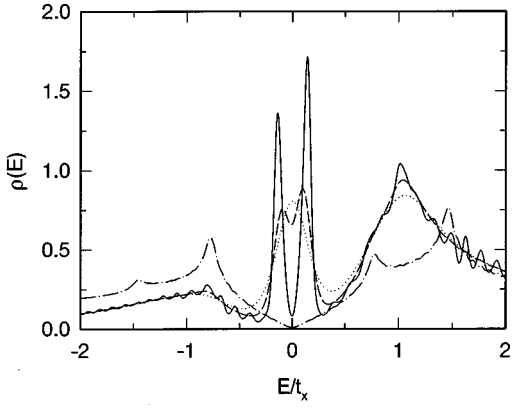

FIG. 2. The local density of states as a function of energy at a distance $a/\sqrt{2}$ from the {110} surface of a tetragonal superconductor at temperature $k_BT=0.02t_x$ (solid line), $0.05t_x$ (dashed line), and $0.1t_x$ (dotted line). For comparison, the bulk density of states (dotted-dashed line) at $k_BT=0.02t_x$ is also displayed. The parameter $V_0=0$.

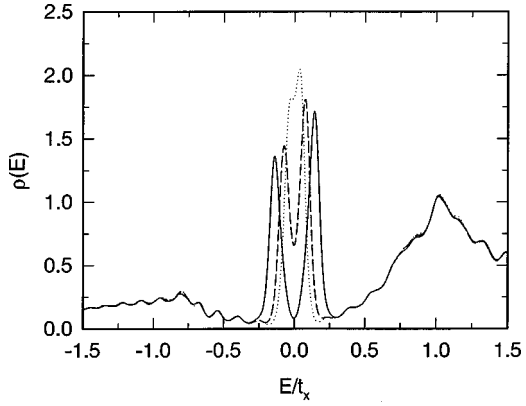

FIG. 3. The local density of states as a function of energy at a distance $a/\sqrt{2}$ from the {110} surface of a tetragonal superconductor at $k_BT=0.02t_x$ with the on-site repulsion $V_0=0$ (solid line), $-1.5t_x$ (dashed line), and $-3t_x$ (dotted line).

atomic scale and vanishes into the bulk region at a distance ξ. Correspondingly, the current flowing along the surface is limited to the surface region.

Once the BdG equations (2) are solved self-consistently, we can calculate the thermally broadened local density of states (LDOS)

$$\rho_{\mathbf{i}}(E)=-\frac{2}{M}\sum_{n,\mathbf{k}}\left[|u_{\mathbf{i}}^{n,\mathbf{k}}|^2 f'(E_{n,\mathbf{k}}-E)+|v_{\mathbf{i}}^{n,\mathbf{k}}|^2 f'(E_{n,\mathbf{k}}+E)\right], \tag{9}$$

where the prefactor 2 comes from the twofold spin degeneracy and $f'(E)$ is the derivative of $f(E)$. $\rho_{\mathbf{i}}(E)$ is proportional to the local differential tunneling conductance which is measured in a scanning-tunneling microscope (STM) experiment.[24] In Fig. 2 we plot the LDOS as a function of energy at a distance $a/\sqrt{2}$ from the {110} surface of a tetragonal superconductor for various temperatures. For comparison, we have also displayed the density of states for the bulk system, where a gaplike feature with $\Delta_{\max}\approx 0.78t_x$ is exhibited. From the figure, the splitting of LDOS at zero energy can be seen clearly. Calculations without surface pair breaking, do not allow one to describe the splitting of the zero-energy peak in the LDOS. The asymmetry line shape in $\rho(E)$ with respect to zero energy reflects the lack of particle-hole symmetry as the chemical potential μ deviates from zero. When the temperature is increased, the splitting diminishes and finally a single zero-energy peak evolves at a critical temperature T_s, which is estimated to be 16% of T_c. We find that the *s*-wave component becomes vanishingly small at T_s, which gives a direct signature of BTRS surface pairing state. The estimated T_s is a little larger than the experimentally observed value 10%.[8] However, as will be shown below, this T_s can be decreased by the presence of orthorhombicity and by increasing the on-site repulsion. Figure 3 shows the LDOS as a function of energy at a distance $a/\sqrt{2}$ from the {110} surface of a tetragonal superconductor for various values of on-site repulsive interaction at $T=0.02t_x$. Clearly, the increase of on-site repulsive interaction reduces splitting of the zero-energy peak. In particular, splitting of the zero-energy peak can even be destroyed by a stronger on-site repulsive interaction. Thus the splitting of the ZBCP is not always observable in a high-temperature superconductor, which depends on the strength of the microscopic interaction. The spin-singlet interaction within the extended Hubbard model with on-site repulsion ($-V_0>0$ in our definition) and nearest-neighbor ($-V_1<0$) attraction in the real space can be Fourier transformed into the momentum space as $V(\mathbf{k},\mathbf{k}')=-V_0-V_1(\cos k_x a+\cos k_y a)(\cos k_x' a+\cos k_y' a)-V_1(\cos k_x a-\cos k_y a)(\cos k_x' a-\cos k_y' a)$, in which the first two terms correspond to the *s*-channel interaction and the third term to the *d*-channel interaction. Thus the on-site repulsion and nearest-neighbor attraction compete with each other in determining the *s*-channel interaction. As a result, the increase of on-site repulsive interaction is unfavorable to the *s*-channel pairing, which leads to the reduction of the induced *s*-wave component near the surface. The lattice model discussed here gives a possible origin for the induction of subdominant *s*-wave order parameter near the surface and provides a natural explanation for the observed splitting of the ZBCP in high-temperature superconductors.

We have also studied the orthorhombicity effect on the splitting of the zero-energy peak. As shown in Fig. 4, the splitting of the zero-energy peak is reduced by the presence

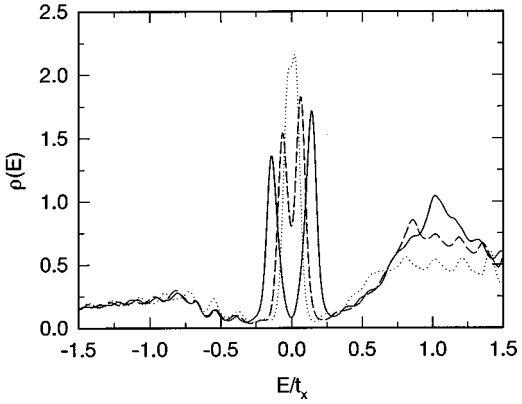

FIG. 4. The local density of states as a function of energy at a distance $a/\sqrt{2}$ from the {110} surface of an orthorhombic superconductor with $t_y/t_x=1$ (solid line), 1.2 (dashed line), and 1.5 (dotted line). The parameters $k_BT=0.02t_x$ and $V_0=0$.

of orthorhombicity (represented by the ratio t_y/t_x in our work). When the orthorhombicity is very strong, the splitting will disappear. This result verifies a previous prediction of the local BTRS state based on Ginzburg-Landau (GL) theory.[11] The GL free energy density for a homogeneous orthorhombic *d*-wave superconductor is given by

$$\mathcal{F}_s = \sum_{i=d,s} [\alpha_i|\Delta_i|^2 + \beta_i|\Delta_i|^4] + \gamma_1|\Delta_s|^2|\Delta_d|^2 + \gamma_2(\Delta_s^{*2}\Delta_d^2 + \Delta_s^2\Delta_d^{*2}) + \gamma_3(\Delta_s^*\Delta_d + \Delta_s\Delta_d^*), \tag{10}$$

where all coefficients (except α_i) are assumed to be positive. The γ_2 term favors $\pi/2$ relative phase between the *s*- and *d*-wave components. The orthorhombicity effect is represented by the γ_3 term, which favors the relative phase 0 or π. Within this GL formulation, to ensure a pure *d*-wave state in a bulk tetragonal superconductor, it is required that the effective second order coefficient of Δ_s is positive, i.e., $\tilde{\alpha}_s(T) = \alpha_s + (\gamma_1 - 2\gamma_2)|\Delta_d|^2 > 0$, for all temperatures, where $|\Delta_d| = [-\alpha_d/\beta_d]^{1/2}$. At the {110} surface, the *s*-wave component could be induced due to the suppression of *d*-wave component. However, the presence of the orthorhombicity discourages the $\pi/2$ relative phase, which leads to the decrease of splitting of the zero-energy peak. This result predicts that the BTRS state may be easier to measure for tetragonal samples like $Tl_2Ba_2CuO_{6+\delta}$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$. So far, the BTRS state has not been observed in these materials, which may be due to a relative large on-site interaction.

Note that there is no sign change of a *d*-wave order parameter for a {100} surface, we do not see the induction of an *s*-wave component near the surface of a tetragonal superconductor and the splitting of ZBCP is not exhibited.

This work was supported by the Texas Center for Superconductivity at the University of Houston and by the Robert A. Welch Foundation, and by the ARP-ATP program of the State of Texas.

[1] D. J. van Harlingen, Rev. Mod. Phys. **67**, 515 (1995).
[2] C. R. Hu, Phys. Rev. Lett. **72**, 1526 (1994); J. Yang and C. R. Hu, Phys. Rev. B **50**, 16 766 (1994).
[3] J. Geerk, X. X. Xi, and G. Linker, Z. Phys. B **73**, 329 (1988).
[4] J. Lesueur, L. H. Greene, W. L. Feldmann, and A. Inam, Physica C **191**, 325 (1992).
[5] M. Covington, R. Scheuerer, K. Bloom, and L. H. Greene, Appl. Phys. Lett. **68**, 1717 (1996).
[6] Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. **74**, 3451 (1995); S. Kashiwaya Y. Tanaka, M. Koyanagi, H. Takashima, and K. Kajimura, Phys. Rev. B **51**, 1350 (1995).
[7] J. H. Xu, J. H. Miller, and C. S. Ting, Phys. Rev. B **53**, 3604 (1996).
[8] M. Covington, M. Aprili, E. Faraoaru, L. H. Greere, F. Xu, J. Zhu, and C. A. Moleir, Phys. Rev. Lett. **79**, 277 (1997).
[9] M. Fogelström, D. Rainer, and J. A. Sauls, Phys. Rev. Lett. **79**, 281 (1997).
[10] Jian-Xin Zhu and C. S. Ting, Phys. Rev. B **57**, 3038 (1998).
[11] M. Sigrist, D. B. Bailey, and R. B. Laughlin, Phys. Rev. Lett. **74**, 3249 (1995).
[12] M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn. **65**, 2194 (1996).
[13] Jian-Xin Zhu, W. Kim, and C. S. Ting, Phys. Rev. B **57**, 13 410 (1998).
[14] P. I. Soininen, C. Kallin, and A. J. Berlinsky, Phys. Rev. B **50**, 13 883 (1994).
[15] Y. Wang and A. H. MacDonald, Phys. Rev. B **52**, R3836 (1995).
[16] D. L. Feder, A. Beardsall, A. J. Berlinsky, and C. Kallin, Phys. Rev. B **56**, R5751 (1997).
[17] M. E. Zhitomirsky and M. B. Walker, Phys. Rev. Lett. **79**, 1734 (1997).
[18] T. Xiang and J. M. Wheatly, Phys. Rev. B **51**, 11 721 (1995).
[19] M. Franz, C. Kallin, and A. J. Berlinsky, Phys. Rev. B **54**, R6897 (1996).
[20] M. E. Flatté and J. M. Byers, Phys. Rev. Lett. **80**, 4546 (1998).
[21] Y. Tanuma Y. Tanaka, M. Yamashiro, and S. Kashiwaya, Phys. Rev. B **57**, 7997 (1998).
[22] The study of the surface problem within the *t*-*J* model was more recently presented by Y. Tanuma, Y. Tanaka, M. Ogata, and S. Kashiwaya, J. Phys. Soc. Jpn. **67**, 1118 (1998), and by K. Kuboki and M. Sigrist, cond-mat/9803032 (unpublished).
[23] P. G. de Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966).
[24] M. Tinkham, *Introduction to Superconductivity* (McGraw-Hill, New York, 1975).