Local density of states for the corner geometry interface of *d*-wave superconductors within the extended Hubbard model

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The spatial variations of the order parameter and the local density of states on the corner of *s*-wave or $d_{x^2-y^2}$-wave superconductors, as well as in superconductor–insulator–normal metal interfaces, are calculated self-consistently by exact diagonalization of the Bogoliubov–de Gennes Hamiltonian within the two-dimensional extended Hubbard model. Due to the suppression of the dominant *d*-wave order parameter, the extended *s*-wave order parameter is induced near the surface, which alternates its sign for the topmost sites at adjacent edges of the lattice and decays to zero in the bulk. The presence of surface roughness results in the appearance of a zero-bias conduction peak near the corner surface which is lacking from the predictions of the quasiclassical theory.

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I. INTRODUCTION

The determination of the order parameter symmetry has become one of the main aspects in the research on high-temperature superconductors.[1,2] Tunneling conductance experiments report the existence of a zero-bias conduction peak (ZBCP).[3–7] The origin of the experimental ZBCP is explained in the context of zero-energy states (ZES's) formed near the [110] surfaces of *d*-wave superconductors.[8] These ZES's do not appear for *s*-wave superconductors or near the [100] surface of *d*-wave superconductors and are one of the features that characterize the *d*-wave superconductors.

The quasiclassical theory of superconductivity has been used to calculate the tunneling conductance in interfaces of unconventional superconductors with normal metals or ferromagnets.[9–11] In the quasiclassical approximation the quasiparticles move in classical trajectories with internal degrees of freedom which are the spin and particle-hole degrees of freedom. The orientation dependence of the spectra as well as the *V* line shape of the conductance curve are explained by the formation of bound states close to the interface due to the sign change of the pair potential that the transmitted quasiparticles experience.

Moreover, the concept of a phase shift by π of the order parameter in orthogonal directions in *k* space, which is equivalent to the sign change of the Josephson critical current, can be observed in corner junctions of anisotropic superconductors with conventional *s*-wave superconductors as a dip of the Fraunhofer pattern at zero magnetic field.[2,12] It is an indication of *d*-wave symmetry of the order parameter. The spontaneous flux modulation with surface orientation in such junctions has been calculated and can be used to distinguish the subdominant components *s* or d_{xy} that are induced at regions where the *d*-wave order parameter is suppressed.

The Bogoliubov–de Gennes (BdG) equations have been solved in the continuum limit for the case of a single *d*-wave vortex[13,14] and around an impurity.[15] The BdG equations within the extended Hubbard model in a two-dimensional lattice have been used to study single-vortex structure,[16,17] time reversal symmetry breaking across twin boundaries[18] or near surfaces,[19] the effect of disorder,[20] and the effect of surface roughness.[21] In this paper the BdG equations are solved in a two-dimensional square lattice within the context of an extended Hubbard model. The spatial variation of the order parameter and the local density of states (LDOS), which in the limit of a low-transparency barrier converges to the tunneling conductance, are calculated for various types of surfaces and interfaces, e.g., a corner surface, the interface of a *d*-wave or *s*-wave superconductor along the [110] direction with normal metals. The evolution of the local density of states is studied as a function of the distance from the surface. Also a comparison with the quasiclassical theory and the experimental data is made.

It is seen that the extended *s*-wave order parameter is induced due to the suppression of the dominant *d*-wave order parameter which alternates its sign for the topmost sites at adjacent edges of the lattice and decays to zero in the bulk. The LDOS is symmetric when $\mu=0$ and it becomes asymmetric when μ deviates from zero due to the breakdown of the electron-hole symmetry. We also investigate the effect of the surface roughness near the corner. In general surface roughness which in real samples is of atomic length scale modifies the properties of the quasiparticles since the coherence length of the cuprates is much smaller than the conventional *s*-wave superconductors. Our model treats the quasiparticle properties on the atomic length scale and goes beyond the quasiclassical approximation. The presence of surface roughness results in the appearance of the ZBCP near the corner surface which is not predicted by the quasiclassical theory.

The article is organized as follows. In Sec. II we develop the model and discuss the formalism. In Sec. III we present the results for the corner of superconductor. In Sec. IV we present the *s*-wave superconductor–insulator–normal metal (*s*-*i*-*n*) and *d*-wave superconductor–insulator–normal metal (*d*-*i*-*n*) interfaces. In Sec. V the effect of the surface roughness is considered. In Sec. VI a connection with the experiment is made. Finally, summary and discussions are presented in the last section.

II. BdG EQUATIONS WITHIN THE HUBBARD MODEL

The Hamiltonian for the extended Hubbard model on a two-dimensional square lattice is

$$H=-t\sum_{\langle i,j\rangle\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+\mu\sum_{i\sigma} n_{i\sigma}+\sum_{i\sigma} \mu_i^I n_{i\sigma}+V_0\sum_i n_{i\uparrow}n_{i\downarrow} + \frac{V_1}{2}\sum_{\langle ij\rangle\sigma\sigma'} n_{i\sigma}n_{j\sigma'}, \quad (1)$$

where i,j are sites indices and the angular brackets indicate that the hopping is only to nearest neighbors; $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ is the electron number operator in site i, μ is the chemical potential, and V_0, V_1 are on-site and nearest-neighbor interaction strengths. Negative values of V_0 and V_1 mean attractive interaction and positive values mean repulsive interaction. When $V_1<0$ the pairing interaction gives rise to d-wave superconductivity in a restricted parameter regime.[17] To simulate the effect of the depletion of the carrier density at the surface or impurities the site-dependent impurity potential $\mu^I(r_i)$ is set to a sufficiently large value at the surface sites. This prohibits the electron tunneling over these sites. Within the mean-field approximation Eq. (1) is reduced to the BdG equations[22]

$$\begin{pmatrix} \hat{\xi} & \hat{\Delta} \\ \hat{\Delta}* & -\hat{\xi} \end{pmatrix}\begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix}=\epsilon_n\begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix}, \quad (2)$$

such that

$$\hat{\xi}u_n(r_i)=-t\sum_{\hat{\delta}} u_n(r_i+\hat{\delta})+[\mu^I(r_i)+\mu]u_n(r_i), \quad (3)$$

$$\hat{\Delta}u_n(r_i)=\Delta_0(r_i)u_n(r_i)+\sum_{\hat{\delta}} \Delta_{\delta}(r_i)u_n(r_i+\hat{\delta}), \quad (4)$$

where the gap functions are defined by

$$\Delta_0(r_i)\equiv V_0\langle c_{\uparrow}(r_i)c_{\downarrow}(r_i)\rangle, \quad (5)$$

$$\Delta_{\delta}(r_i)\equiv V_1\langle c_{\uparrow}(r_i+\hat{\delta})c_{\downarrow}(r_i)\rangle, \quad (6)$$

where $\hat{\delta}=\hat{x},-\hat{x},\hat{y},-\hat{y}$. Equation (2) is subject to the self-consistency requirements

$$\Delta_0(r_i)=V_0\sum_n u_n(r_i)v_n^*(r_i)\tanh\left(\frac{\beta\epsilon_n}{2}\right), \quad (7)$$

$$\Delta_{\delta}(r_i)=\frac{V_1}{2}\sum_n [u_n(r_i+\hat{\delta})v_n^*(r_i) + u_n(r_i)v_n^*(r_i+\hat{\delta})]\tanh\left(\frac{\beta\epsilon_n}{2}\right). \quad (8)$$

We start with the approximate initial conditions for the gap functions (7) and (8). After exact diagonalization of Eq. (2) we obtain the $u(r_i)$ and $v(r_i)$ and the eigenenergies ϵ_n. The quasiparticle amplitudes are then inserted into Eqs. (7) and (8) and new gap functions $\Delta_0(r_i)$ and $\Delta_{\delta}(r_i)$ are evaluated. We reinsert these quantities into Eqs. (3) and (4), and we proceed in the same way until we achieve selfconsistency, i.e., when the norm of the difference of $\Delta_0(r_i)$ and $\Delta_{\delta}(r_i)$ from their previous values is less than the desired accuracy. We then compute the d-wave and the extended s-wave gap functions given by the expressions[16]

$$\Delta_d(r_i)=\frac{1}{4}[\Delta_{\hat{x}}(r_i)+\Delta_{-\hat{x}}(r_i)-\Delta_{\hat{y}}(r_i)-\Delta_{-\hat{y}}(r_i)], \quad (9)$$

$$\Delta_s^{ext}(r_i)=\frac{1}{4}[\Delta_{\hat{x}}(r_i)+\Delta_{-\hat{x}}(r_i)+\Delta_{\hat{y}}(r_i)+\Delta_{-\hat{y}}(r_i)]. \quad (10)$$

The number density at the ith site is given by

$$n_i=n_{i\uparrow}+n_{i\downarrow}=\sum_n \{|u_n(r_i)|^2 f(\epsilon_n)+|v_n(r_i)|^2[1-f(\epsilon_n)]\}, \quad (11)$$

and the LDOS at the ith site is given by

$$\rho_i(E)=-2\sum_n [|u_n(r_i)|^2 f'(E-\epsilon_n)+|v_n(r_i)|^2 f'(E+\epsilon_n)], \quad (12)$$

where the factor of 2 comes from the twofold spin degeneracy and f' is the derivative of the Fermi function,

$$f(\epsilon)=\frac{1}{\exp(\epsilon/k_BT)+1}. \quad (13)$$

III. CORNER OF SUPERCONDUCTOR

In this section the results for the order parameter and the LDOS close to the corner surface of a two-dimensional square lattice are presented for different order parameter symmetries, i.e., s-wave and d-wave symmetries. The different symmetries are introduced by varying the strength of the local and nonlocal pairing interaction constants V_0 and V_1. We consider a two-dimensional system of 30×30 sites and we suppose fixed boundary conditions by setting the impurity potential $\mu^I=100t$ at the surface. The parameters $V_0=0.0$ and $V_1=-2.5t$ are such that d-wave superconductivity is stable. The d-wave order parameter Δ_d is enhanced near the surface from its bulk value and goes to zero at the surface atoms because the hopping to these sites is suppressed due to the impurity barrier (see Fig. 1). The induced extended s-wave order parameter Δ_s^{ext}, seen in Fig. 2(a) oscillates near the surface at an atomic scale and vanishes in the bulk region at a distance of few lattice sites. It reverses its sign on either side of the lattice edge and it is exactly zero in the diagonal direction. Next to the corner we see an enhancement from the edge value. It appears to have a d-wave-like structure just at the corner of the square lattice. This behavior is also seen near impurities[20] and across twin boundaries[18] using BdG equations within the extended Hubbard model in a two-dimensional orthorhombic lattice. The explanation is the sign change of the d-wave order parameter across the [110] direction close to the corner. To understand the effect of the

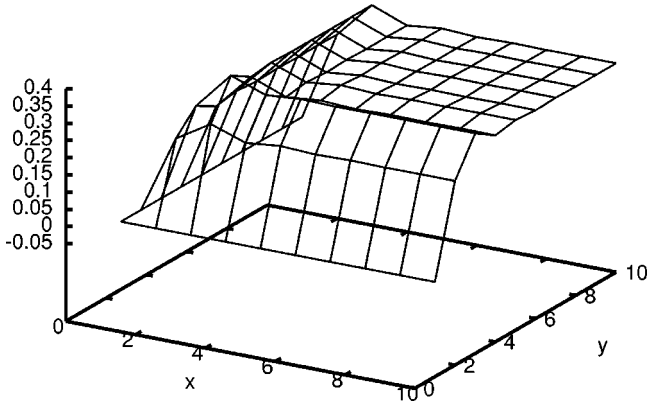

FIG. 1. Spatial dependence of the *d*-wave order parameter close to the corner of a two-dimensional square lattice, for chemical potential $\mu=0$. The temperature is $k_BT=0.1t$.

Fermi surface line shape and also the depletion of the charge density for high-T_c superconductors we consider also the case where μ deviates from zero. The Δ_s^{ext}, seen in Fig. 2(b) for $\mu=t$, is more enhanced for larger values of the chemical potential. In summary the *d*-wave and the induced extended *s*-wave order parameter show atomic size oscillations that do not appear in the quasiclassical approximation.

The local density of states plotted in Fig. 3(a) for $\mu=0$ is symmetric with respect to $E=0$ due to electron-hole symmetry. The LDOS is site dependent and shows a complicated gap structure. Also no ZBCP has been observed, in agreement with the results of the quasiclassical theory.[9] As we move to the interior of the lattice the LDOS converges to the bulk density of states in a two-dimensional square lattice. For $\mu=t$ the LDOS becomes asymmetric as seen in Fig. 3(b). This feature reflects the breakdown of the electron hole symmetry. However, no ZBCP is formed. The LDOS close the the [100] lattice surface [see Fig. 4(a)] has the *V*-like line shape due to the presence of line nodes of the pair potential on the Fermi surface, is symmetric with respect to $E=0$ due to the electron-hole symmetry, and has the minimum at $E=0$. These features are compatible with the *d*-wave symmetry of the order parameter. The symmetric form of the LDOS line shape is lost when the chemical potential deviates from zero, as seen in Fig. 4(b) for $\mu=t$.

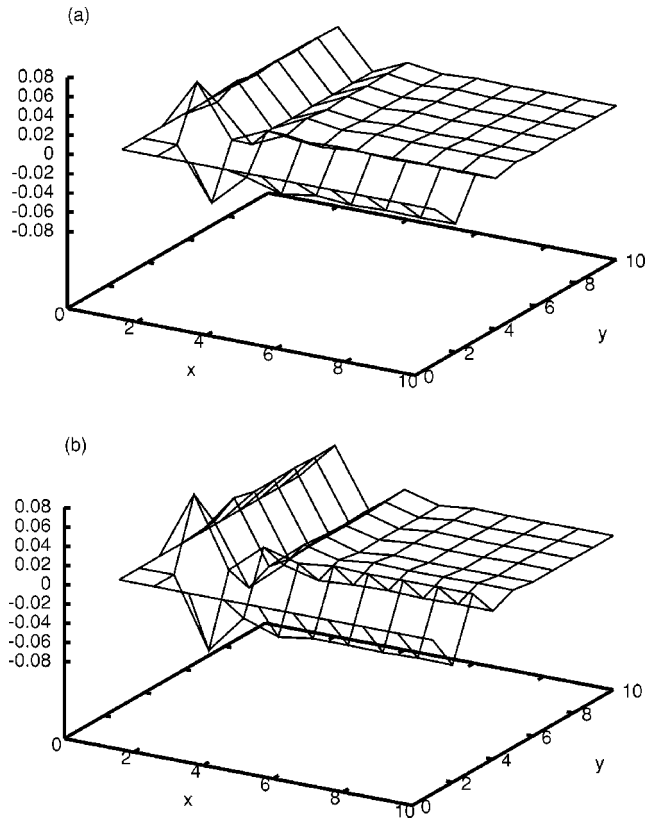

FIG. 2. Spatial dependence of the extended *s*-wave Δ_s^{ext} order parameter close to the corner of a two dimensional square lattice. (a) $\mu=0$, (b) $\mu=t$.

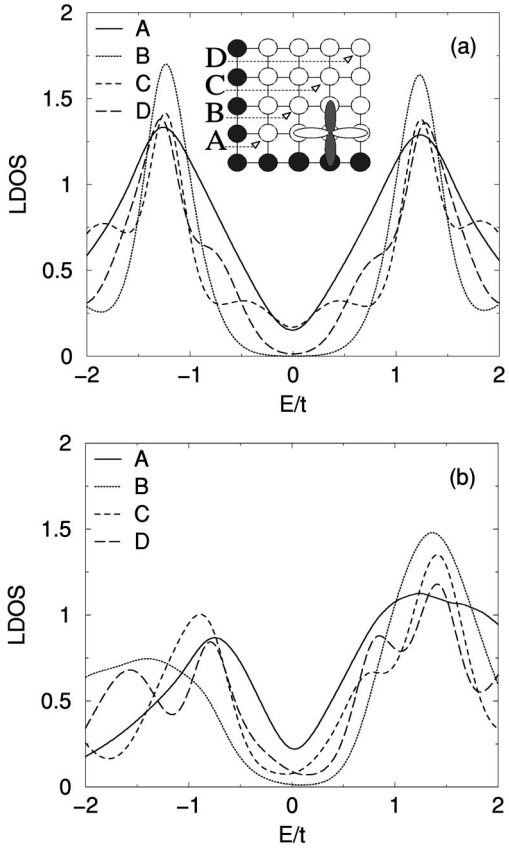

FIG. 3. The local density of states at sites A,B,C,D along the diagonal of the two-dimensional square lattice shown in the inset. (a) $\mu=0$, (b) $\mu=t$. The chemical potential is set to $\mu^I=100t$ at the shaded surface sites.

To understand the effect of the different symmetry we study the *s*-wave order parameter by setting the local pairing interaction to the value $V_0=-2.5t$ and the nonlocal interaction to the value $V_1=0$. The *s*-wave order parameter evolves nonmonotonically to the bulk value as seen in Fig. 5. For $\mu=t$ the order parameter shows small amplitude oscillations relative to the bulk value. The LDOS close to the corner [see Fig. 6(a)] for $\mu=0$ shows gap structure with *U*-like line shape due to the absence of nodes of the pair potential on the Fermi surface. Furthermore, the LDOS is insensitive to the orientation of the surface and is site independent. The LDOS

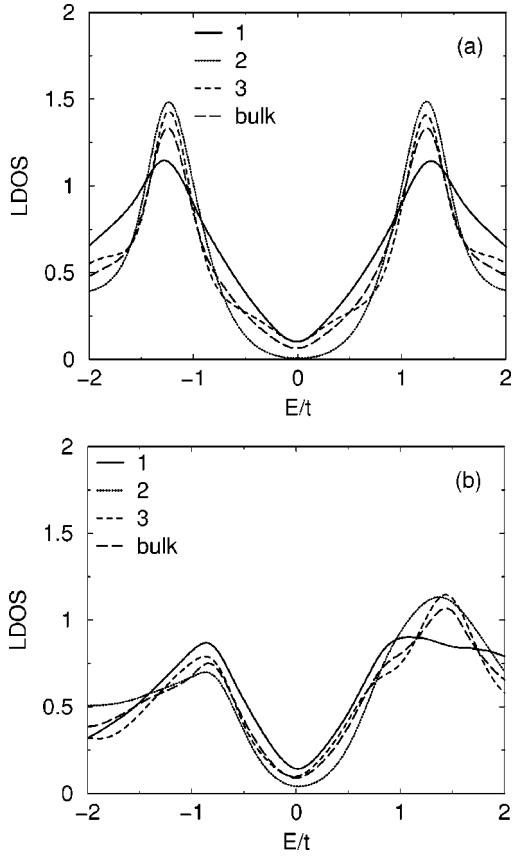

FIG. 4. The local density of states at the sites of distance $x=1,2,3$ form the [100] surface of the two-dimensional square lattice and the bulk density of states. (a) $\mu=0$, (b) $\mu=t$.

near the [100] surface is similar as seen in Fig. 6(b). The LDOS line shape for the *s*-wave case is different to what we see for the *d*-wave case. However, the nonmonotonous increase with atomic size oscillations of the order parameter occurs both in the *s*-wave and *d*-wave corner geometry interfaces since the reflected quasiparticles do not experience any sign change of the pair potential.

The absence of ZBCP's in the LDOS is in agreement with the results of the quasiclassical theory both for *s*-wave and

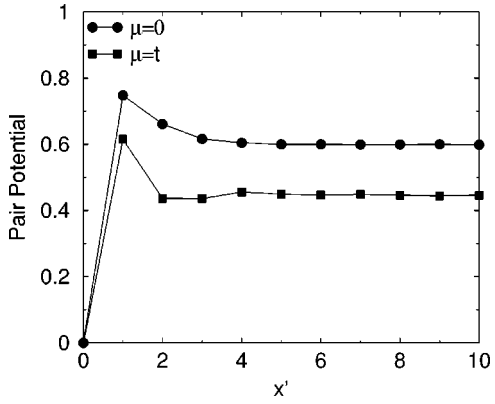

FIG. 5. Spatial dependence of the *s*-wave order parameter along the diagonal of the lattice (x'), for two different values of the chemical potential $\mu=0,\mu=t$.

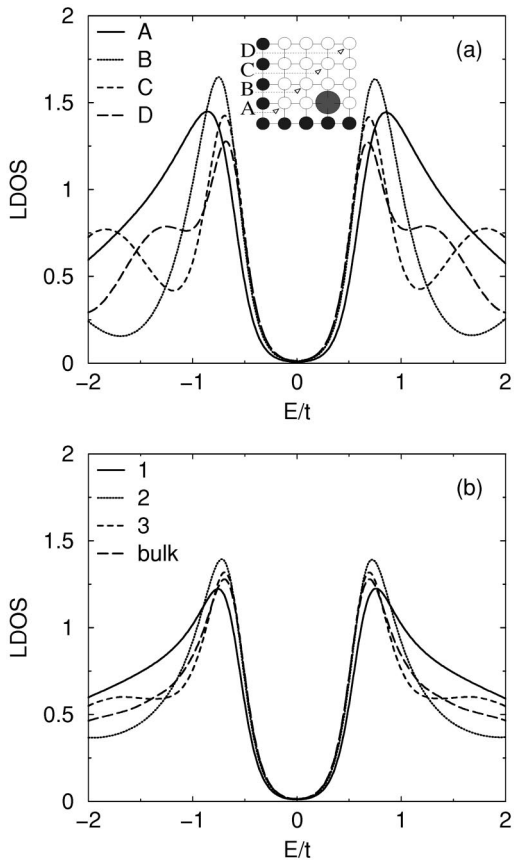

FIG. 6. (a) The local density of states at sites A,B,C,D along the diagonal of the two-dimensional square lattice shown in the inset. The pairing symmetry is *s*, $\mu=0$. The chemical potential is set to $\mu^I=100t$ at the shaded surface sites. (b) The local density of states at sites of distance $x=1,2,3$ from the [100] surface of the two-dimensional square lattice and the bulk density of states. The pairing symmetry is *s* and $\mu=0$.

d-wave corner geometry interfaces. The condition for the formation of ZBCP's is the change of sign of the quasiparticles in the scattering from the surface of the superconductor. In *s*-wave superconductors this sign change does not occur at surfaces or interfaces due to the isotropy of the pair potential. In anisotropic superconductors this sign change is possible for certain orientation of the surface. However, for the corner surface, at the direction where the lobes of the *d*-wave order parameter are at right angles to the surface, a typical trajectory of a quasiparticle would consist of two subsequent reflections from the lattices edges, in none of which does a sign change of the order parameter occur. Therefore the quasiparticle does not feel the sign change of the order parameter and no ZBCP is formed. For a corner where the lobes are not exactly at right angles to the surface the condition for the formation of Andreev bound states at the surface can occur and also the ZBCP.

IV. *s-i-n*, *d-i-n* INTERFACES ALONG THE [110] DIRECTION

We now discuss the effect of the orientation of the interface on the order parameter and the local density of states for

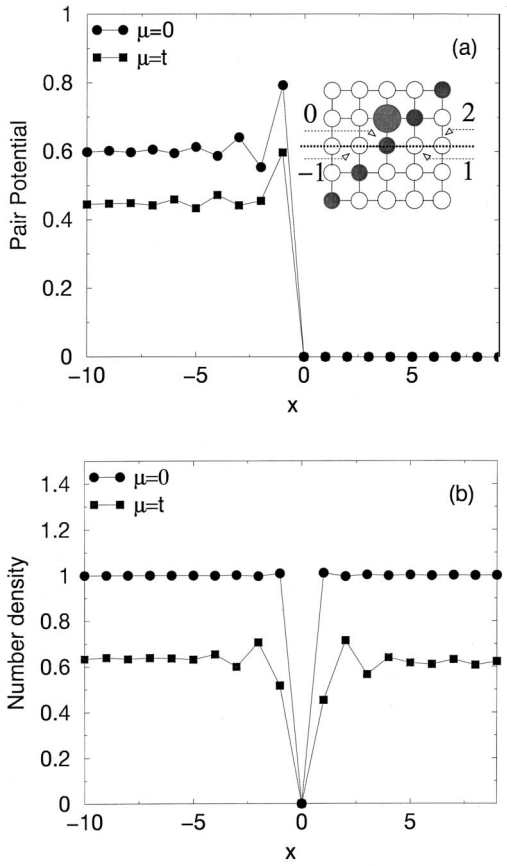

FIG. 7. (a) The magnitude of the *s*-wave component Δ_s of the superconducting order parameter as a function of *x*, for the *s*-*i*-*n* interface along the [110] direction shown in the inset, for $\mu=0,t$. The spatial distribution of impurities is indicated by solid circles, and also the labeling of the sites along the *x* directions is shown. The order parameter is calculated along the thick dashed line in the direction *x* shown in the inset. (b) The number density n_i as a function of *x* shown in (a), for a *s*-*i*-*n* interface for $\mu=0, t$.

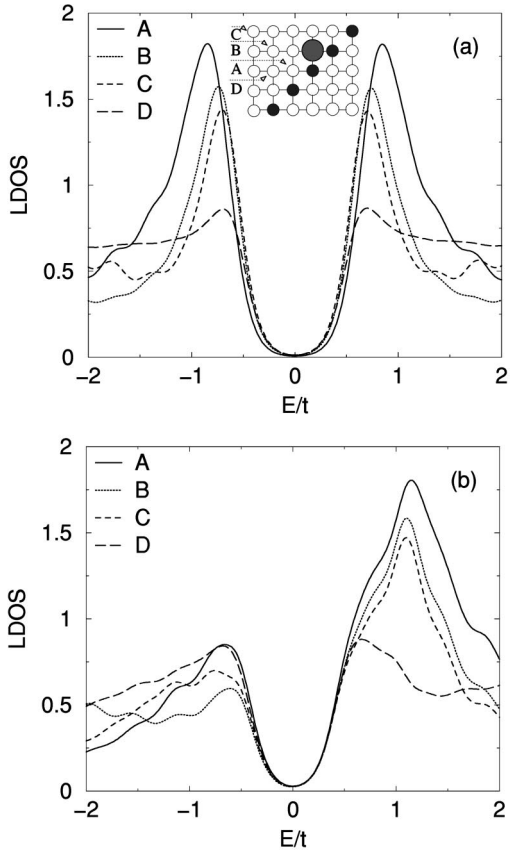

FIG. 8. (a) LDOS at the sites A,B,C,D for the *s*-*i*-*n* interface shown in the inset, for $\mu=0$. The spatial distribution of impurities is indicated by solid circles. (b) The same as in (a) but for $\mu=t$.

different symmetries. For [110] interface the reflected quasiparticles for *d*-wave superconductors are subject to the sign change of the order parameter. This affects both the order parameter and the LDOS. The interface is modeled by a line of sites along the diagonal of the lattice, y' direction, where the chemical potential is set to a value in accordance with the strength of the barrier we want to model. The value of the interaction strength in each part of the interface determines the particular system that we are considering.

To understand the effect of the symmetry of the pair potential we consider first the *s*-*i*-*n* interface shown in the inset of Fig. 7(a). The local interaction in the region where $x'<0$ (x' is the direction perpendicular to the interface) is $V_0=-2.5t$, and the strength of the barrier is $\mu^{110}=100t$. The *s*-wave order parameter Δ_s presented in Fig. 7(a) is suppressed near the interface and increases nonmonotonically to the bulk value at a few lattice sites. The enhancement at the topmost sites close to the interface is similar to the spatial variation of the *d*-wave order parameter close to the [100] surface seen in Fig. 1 since in both cases the reflected quasiparticles do not feel any sign change of the pair potential. The bulk order parameter is suppressed when μ deviates from 0 and also the spatial oscillations close to the interface are of reduced amplitude as seen in Fig. 7(a). To demonstrate the charge density depletion near the interface and also the sensitivity of the charge density on the μ, we present in Fig. 7(b) the number density n_i for the electrons for two different values of the chemical potential, i.e., $\mu=0$ and $\mu=t$. For $\mu=0$ the number density is unity (one electron per site) in the bulk and decays to zero at the interface. However, for finite μ the number density is reduced.

The LDOS seen in Fig. 8(a) is symmetric for $\mu=0$ and shows the gap structure with *U*-like line shape. Comparing to case of the [100] interface we see that the LDOS is insensitive to the direction of the interface. For finite $\mu=t$ seen in Fig. 8(b) the LDOS keeps its *U*-like line shape. However, it becomes asymmetric due to the breakdown of the electron-hole symmetry.

To understand the effect of the different symmetry and also the orientation of the interface we consider then the *d*-*i*-*n* interface, shown in the inset of Fig. 9, where $V_1=-2.5t$ and $\mu^{110}=100t$. We present in Fig. 9 the spatial variation of the *d*-wave component Δ_d and the extended *s*-wave component Δ_s^{ext} of the order parameter. It is seen that for $\mu=0$, Δ_s^{ext} is not modified by the presence of the interface. In contrast Δ_d drops to zero at the interface and increases monotonically into a few lattice sites to the bulk

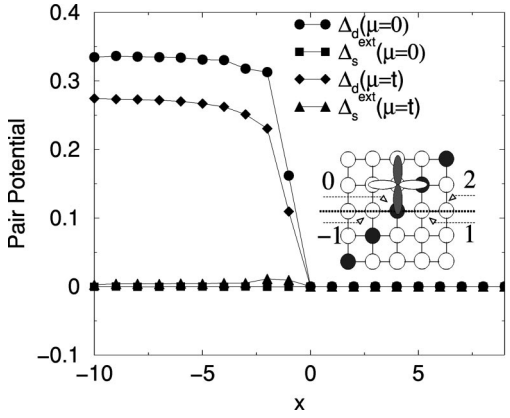

FIG. 9. The magnitude of the Δ_d and Δ_s^{ext} as a function of x, for the d-i-n interface shown in the inset, for $\mu=0,t$. The spatial distribution of impurities is indicated by solid circles, and also the labeling of the sites along the x directions is shown. The order parameter is calculated along the thick dashed line in the direction x shown in the inset.

value. For $\mu=t$ the Δ_d is much more suppressed close to the interface while the induced Δ_s^{ext}-wave component is more enhanced. This monotonic increase is consistent with the quasiclassical results. The reflected quasiparticles from the [110] oriented interface are subject to the sign change of the

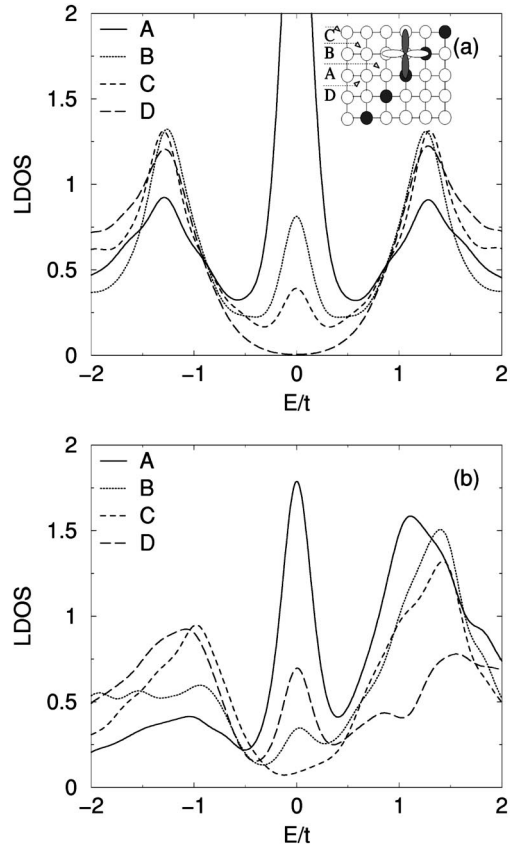

FIG. 10. (a) LDOS at sites A,B,C,D for the d-i-n interface shown in the inset, for $\mu=0$. The spatial distribution of impurities is indicated by solid circles. (b) The same as in (a) but for $\mu=t$.

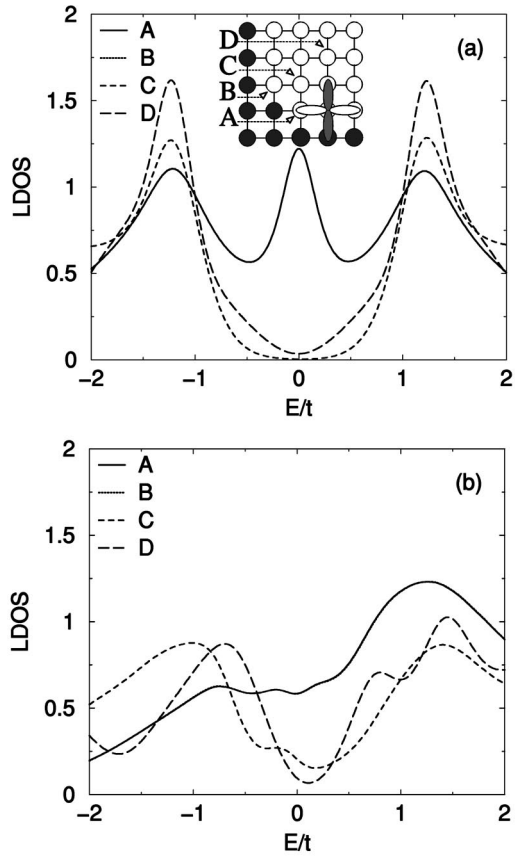

FIG. 11. (a) The local density of states at the specified sites A,B,C,D for the corner surface, with a 1×1 step structure shown in the inset, for $\mu=0$. The chemical potential is set to $\mu^I=100t$ at the shaded surface sites. (b) The same as in (a) but for $\mu=t$. Due to the symmetry of the structure, the LDOS is identical for sites A and B.

order parameter. This makes the interface pair breaking and results into a monotonic variation in the d-wave order parameter near the surface. This is different to the s-i-n case and also to the [100] surface of the d-wave superconductor seen in Fig. 1 where this increase is nonmonotonous since the reflected quasiparticles do not feel any sign change of the pair potential. In the latter case the interface is not pair breaking. However, the spatial oscillations of the order parameter at atomic scale are completely neglected in the quasiclassical approximation. The number density is similar to the case of the s-i-n interface.

The main difference between the two symmetries appears in the LDOS as we can see in Fig. 10(a), for $\mu=0$. As expected the LDOS line shape is symmetric since $\mu=0$. The ZBCP is formed and its height decreases exponentially as we move to the interior of the lattice along the direction perpendicular to the interface. However, at site D no ZBCP is formed. The disappearance of the ZBCP at D denotes that the ZES's wave functions have a spatial variation close to the interface with nodes at specific sites. In this case the site D corresponds to a node and therefore the ZBCP disappears. The ZBCP is explained in the context of zero-energy states[8] formed near the [110] surfaces of d-wave superconductors

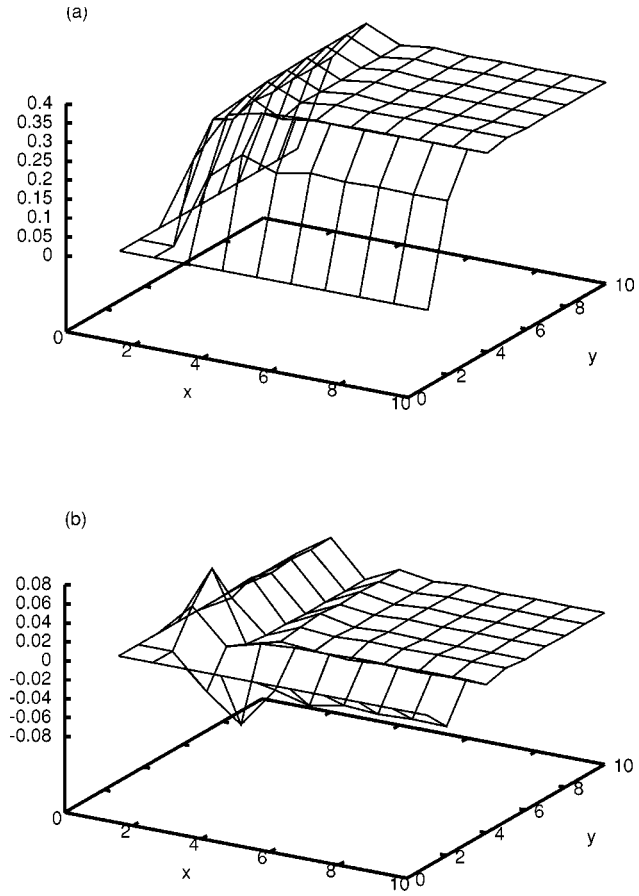

FIG. 12. Spatial dependence of the (a) *d*-wave and (b) the extended *s*-wave order parameter for the specified geometry of Fig. 11(a).

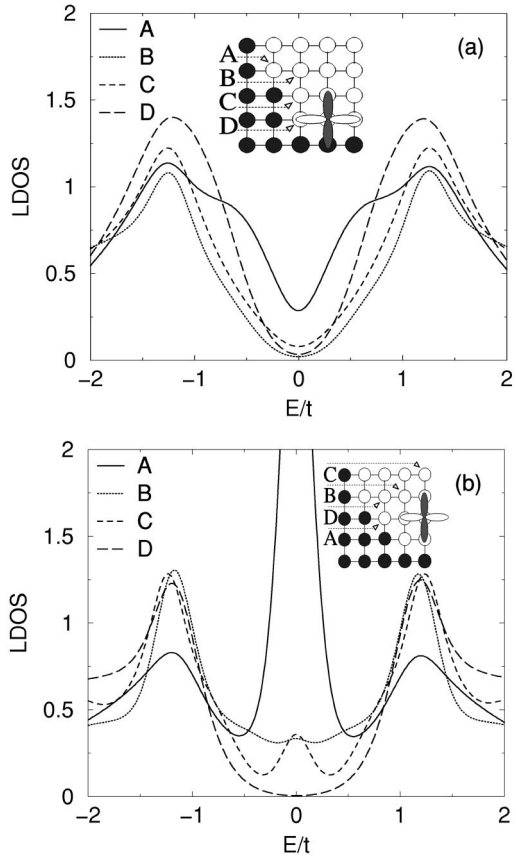

FIG. 13. (a) The local density of states at the specified sites A,B,C,D for the corner surface, with a 1×2 step structure shown in the inset for $\mu=0$. The chemical potential is set to $\mu^I=100t$ at the shaded surface sites. (b) The local density of states at the specified sites A,B,C,D for the corner surface, with a [110] structure shown in the inset for $\mu=0$. The chemical potential is set to $\mu^I=100t$ at the shaded surface sites.

due to the sign change that the quasiparticles experience in different directions in k space. However, the absence of ZBCP's for the [110] at specific sites is not predicted by the quasiclassical theory. For finite $\mu=t$ seen in Fig. 10(b) the LDOS keeps its *V*-like line shape. However, it becomes asymmetric due to the breakdown of the electron-hole symmetry. Also the ZBCP is reduced. We conclude that the *d*-wave order parameter as well as the local density of states is influenced by the orientation of the interface.

V. RESULT FOR THE SURFACE ROUGHNESS

In the following we describe the effect of the surface roughness near the corner of the lattice for *d*-wave superconductors. The quasiparticle properties near the corner are expected to be influenced by the atomic size roughness, since the coherence length of the *d*-wave superconductors is small nearly at atomic size. For the case of one step structure, for $\mu=0$, shown in the inset of Fig. 11(a) the LDOS shows ZBCP's at points A,B but not in C as presented in Fig. 11(a). Moreover, the ZBCP is suppressed compared to the case of flat [110] surface seen in Fig. 10. The quasiclassical theory predicts that for that direction the ZBCP is maximum[9] since the one step structure corresponds to the $a=\pi/4$ (where a is the orientation of the surface). The suppression of the ZBCP and also the disappearance of ZBCP from specific sites are explained by the spatial variation of the ZES's. It is seen that the wave functions of the ZES's form standing waves that decay in the bulk. The sites A and B, which show ZBCP's, correspond to an antinode while for the rest of the lattice sites the amplitude of the ZES's is zero. For finite μ the ZBCP disappears from sites A and B due to the destructive interference of the ZES's as shown in Fig. 11(b). In addition the overall line shape of the conductance curve is asymmetric due to the breaking of the electron-hole symmetry. In Fig. 12 the spatial variation of the *d*-wave and extended *s*-wave order parameter is plotted for $\mu=0$ at sites close to the lattice corner. It is seen that the *d*-wave order parameter is suppressed at the impurity site while the extended *s*-wave order parameter is not much influenced.

For the 1×2 step structure shown in the inset of Fig. 13(a) the LDOS, presented in Fig. 13(a) for $\mu=0$, at points A,B,C,D shows no ZBCP. The quasiclassical theory predicts a ZBCP since this geometry corresponds to a surface tilted from $a=0$ or $a=\pi/2$. The absence of ZBCP's is explained by the destructive interference of the standing waves and also by the asymmetricity of the structure. For $\mu=t$ some

tiny conductance peak recovers.

The ZBCP at the topmost sites recovers for the geometry shown in the inset of Fig. 13(b) for sites A,C, for $\mu=0$ as presented in Fig. 13(b). However, unlike the flat [110] surface no ZBCP is formed in site B due to the destructive interference of the standing waves. Moreover, when finite chemical potential is introduced the spatial distribution of the ZES's is disturbed and for example the ZBCP appears even for sites, e.g., D, where normally for $\mu=0$ is absent.

VI. EXPERIMENTAL RELEVANCE

In this section a comparison is made with available experimental data on corner Josephson junctions and also on the tunneling effect in high-T_c superconductors. Recent phase-sensitive measurements on corner junctions showed a minimum in the critical current versus the magnetic field and provided a strong evidence for the $d_{x^2-y^2}$-wave symmetry.[2,12] However, as demonstrated in this paper the effect of the surface roughness at atomic scale near the corner strongly modifies the quasiparticle properties near the corner. This may lead to a deviation from the sinusoidal Josephson current phase relation and may influence also the critical currents and the spontaneous magnetic flux.

As regarding the tunneling experiments, the existence of ZBCP's has been so far investigated for various surface orientations using *s-i-n* thin-film or single-crystal tunnel junctions, or point-contact measurements or a scanning tunneling microscope (STM) on a single-crystal surface.[3–7] For the [110] surface, almost all groups reported ZBCP's, while for [100] surfaces ZBCP's have also been found. The quasiclassical theory as well as the calculations presented in this paper predict that the ZBCP is maximum for the [110] surface and is absent for the [100] surface. However, it has been shown that the introduction of surface roughness in the above theoretical approaches results in the appearance of a ZBCP even for the [100] surfaces.[21,23] Furthermore we reproduced several anomalous features that have been observed in tunneling experiments and cannot be explained within the quasiclassical theory. These include the absence of ZBCP's at specific sites close to the [110] surface,[24] asymmetric structures due to the depletion of the chemical potential close to the surface, multiple dips and large dips inside the gap, and residual values of the conductance at the zero-bias level.

VII. CONCLUSIONS

We calculated the LDOS and the order parameter of a two-dimensional lattice of *d*-wave superconductor within the extended Hubbard model, self-consistently. The dominant order parameter decays monotonically for the [110] interface and *d*-wave order parameter symmetry, while nonmonotonically for the [100] interface, *d*-wave or *s*-wave order parameter symmetry. The induced extended *s*-wave order parameter, that decays to zero in the bulk, changes sign at the topmost sites at either side of the lattice similarly to the case near impurities and twin boundaries. The LDOS is symmetric when $\mu=0$ and it becomes asymmetric when μ deviates from zero. The presence of surface roughness at the corner strongly modifies the quasiparticle properties near the corner. The ZBCP which is absent for perfect corner, consistent with the quasiclassical theory, appears when the roughness at atomic size is introduced due to the oscillatory form of the bound states. The last result is not predicted in the quasiclassical approximation. The sensitivity of the properties on the atomic scale roughness has to be taken into account for the correct interpretation of the experiments on corner Josephson junctions.

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