Minisubbands in electron excitation spectra of layered short-coherence-length superconductors

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Quasiparticle excitation spectra of short-coherence-length layered superconductors ($\widetilde{S}$) are considered assuming a periodic alternation of the superconducting order parameter $\Delta(x)$ versus the lateral coordinate x in the c direction. The found self-consistent solution suggests that the electron-hole Andreev scattering in such a periodic $\Delta(x)$ causes the appearance of minisubbands in the electron spectrum of $\widetilde{S}$, in a ''clean'' limit manifested as periodic spikes in the density of electron states at energies $E_n=(2n+1)\Delta_0$ (Δ_0 is the energy gap amplitude; n is a natural number). [S0163-1829(96)06445-4]

I. INTRODUCTION

For many years layered superconductors have been a subject of visible attention. Initial examples of inhomogeneous superconducting state have been addressed to an intermediate state of type-I superconductors (SC's), where the existence of isolated normal regions changes the transport and thermodynamic properties of the system substantially.[1,2] The first superconducting/normal (S/N) multilayers Nb/Cu having dissimilar structure were prepared by Schuller.[3] The investigation of artificial layered structures, composed by classic superconductors, has been made in numerous experimental papers,[4–7] while initial theoretical models have been proposed in other papers.[8–13]

Nevertheless, an enhanced interest in properties of layered SC's was caused by metal oxides with a microscopic layered crystal structure.[14] In these compounds, below the critical temperature T_c superconductivity is maintained mainly by Cu-O layers[15] separated from each other by normal or dielectric interlayer regions. The value of the coherence length $\xi_\perp$ here can be very small,[16] i.e., in the c direction it can be comparable even to the lattice constant $c_\perp$ (see also, e.g., Ref. 15). Hence, one can expect that the periodic layered crystal structure may cause a periodic alternation of the SC order parameter $\Delta(x)$ (x is the coordinate in the c direction) as well. Thus, this kind of SC system can be naturally connected with the structure of metal oxides itself, but should be exhibited only below T_c.

Despite important distinctions between the metal oxides and layered SC's, it is reasonable to compare both these systems. Preliminary theoretical models[8,9,12] considered the classic layered SC as a periodic one-dimensional $\ldots S\text{-}N\text{-}S\text{-}N\text{-}S\ldots$ infinite system (S is an ordinary long-coherence-length SC; N is a normal metal), in the so-called quasiclassical approximation operating with a small parameter $c_\perp/\xi_{\rm cl}\ll 1$ ($\xi_{\rm cl}$ is the coherence length of a classic superconductor). Within the approach of Refs. 8 and 12, the order parameter $\Delta(x)$ was assumed to be dependent periodically on the coordinate x, to be constant $\Delta(x)=\Delta_0$ inside the S regions while $\Delta(x)=0$ in the N regions. According to Refs. 8 and 12, the scattering of the electron-hole excitations in the rectangular periodic gap potential $\Delta(x)$ leads to the appearance of bands in the electron spectrum, which may be observed as features in the tunneling I-V curves.[17,18] In analogy to the bound states, taking place for the vortex core,[19–21] these bands with energy $E>\Delta_0$ were treated[9] as scattering states.[19,20] Initial tunneling experiments made on granular and ''dirty'' metal oxide samples indicated weak anomalies in the electron density of states,[17,18] which were interpreted in the paper[12] in terms of the Kronig model.[8] However, the model[8,12] contained some contradictory assumptions e.g., sharp alternation of $\Delta(x)$ cannot be correctly considered within used in papers[8,12] that on quasiclassical (or Andreev[22]) approximations. Actually, as is known,[23] this WKBJ-type approximation neglects the terms $\propto\xi_\perp$, which in fact are not as small for sharp interfaces. Although the WKBJ-type anzatz[9,20] allows the peculiarities of the $\Delta(x)$ variation to be neglected [because only a spatially integrated form of $\Delta(x)$ in this quasiclassical anzatz is important[9]] the situation with the short coherence-length SC is different. Really, in irregular metal oxide samples used in works,[17,18] the ratio $c_\perp/\xi_\perp\sim 1$ and $\lambda_{\rm DB}\approx c_\perp$ ($\lambda_{\rm DB}$ is the electron de Broglie wave length). This means that the quasiclassical solution[24–28] itself could be dubious for the last mentioned case, while the problem should be handled self-consistently, for the details of the electron spectrum dependent on the $\Delta(x)$ shape. A different approach was implemented in works[11,29] to calculate the electron spectrum of a multilayered metal oxide within the tunneling Hamiltonian formalism. In Ref. 29, the electron spectrum was determined for a system with only one primitive cell. It was assumed, that the cell consists of distinct layers (including superconducting layers with different values of the energy gap as well as normal layers), which interact via an interlayer tunneling. Although the mentioned model[29] predicts a finite number of anomalies in the electron density of states due to the interlayer exchange, the effect of periodicity was ignored. Thus, it is tempting to examine a periodic and more simple structure, but avoiding any quasiclassical restrictions.[8,9,12,22–28,30,31]

The mentioned issue of inhomogeneous state in the metal oxides suggests a question about the value of the coherence length $\xi_\perp$. For a BCS ''clean'' superconductor $\xi_\perp^{\rm BCS}\simeq\hbar v_F/\pi\Delta$ (v_F is the Fermi velocity) or equally $k_F\xi_\perp^{\rm BCS}\simeq(2/\pi)(E_F/\Delta)$ where E_F is the Fermi energy. For the metal oxides typically[15,32] one has $E_F/\Delta\approx 30-50$, thus $k_F\xi_\perp^{\rm BCS}\approx 20-30$ (k_F is the value of the Fermi wave vector),

which itself is much larger than $k_F\xi_\perp \sim 1$, which had been estimated independently from many $H_{c2}(T)$ measurements.[15,32] A probable reason why $\xi_\perp$ is much smaller than $\xi_\perp^{\rm BCS}$ seems to consist in the fact that the last mentioned $H_{c2}(T)$ data were related to dirty irregular samples characterized by a very short electron mean free path l_i. This reduction in accordance with Ref. 2 is estimated as $\xi_\perp = \sqrt{l_i \xi_\perp^{\rm BCS}}$. Therefore, to solve the problem of the actual value of $\xi_\perp^{\rm BCS}$, one must pay a special attention to experiments on clean regular single crystals of the metal oxides available recently,[33] which may correspond to the ''clean'' $\xi_\perp^{\rm BCS} \gg \xi_\perp$ as well. Because of the high value of T_c, the magnitude of $\xi_\perp^{\rm BCS}$ can be much smaller than that in classic SC's. It means that any inhomogeneities of samples cause a spatial alternation of the SC order parameter on the scale of $\xi_\perp^{\rm BCS}$. Since the inhomogeneities are present even in clean samples (e.g., the sample's surface or interfaces, or different kinds of irregularities), the issue is quite general to refer to many particular situations. From a theoretical point of view, of course, it is highly desirable to establish a clear distinguished feature of such a inhomogeneous state suggested.

In this paper, we would like to consider layered periodic SC systems with only two layers in the period, within a model, extended beyond the quasiclassical approximation in a clean limit. The problem is solved using a self-consistent approach, and we show that the SC state can be inhomogeneous with the order parameter alternating on the scale of clean BCS coherence length $\xi_\perp^{\rm BCS}$. We find that the electron movement becomes well quantized, and that the electron-hole interference is signatured by the sharp minisubband structure in the quasiparticle excitation spectrum, taking place due to the Andreev reflection effect in the periodic $\Delta(x)$. In Sec. II, we formulate a general approach as well as the basic equations which are confined to examine the spectrum of a layered short-coherence-length superconductor. Then, for illustration, we analyze two simplest but non-self-consistent limiting cases: an ordinary rectangular approximation for $\Delta(x)$ and a harmonic approximation for the gap potential as well. The models allows us to distinguish the main features of the inhomogeneous SC state, as well as the origin of anomalies in the electron spectrum. Finally, in Sec. III, we obtain general solution of the problem, calculating the excitation spectrum and the spatial variation of $\Delta(x)$ self-consistently. We find that the inhomogeneous state in certain conditions may be pronounced in the electron density of states, causing sharp singularities which can be observable in tunneling spectroscopy experiments on clean single crystals.

II. PERIODIC LAYERED SUPERCONDUCTORS

A. Basic equations

The model which applied in this paper to describe layered periodic SC systems is based on an assumption that the amplitude of the superconducting order parameter $\Delta(x)$ is homogeneous within each ab plane, while is periodically alternated versus the lateral coordinate x in the c direction. The electron spectrum of the layered superconducting system is calculated here from a self-consistent solution of the Bogolubov equation[2]

$$\hat{1}E\begin{pmatrix} u_{p\uparrow} \\ v_{p\downarrow} \end{pmatrix} = \hat{H}^{(0)}\begin{pmatrix} u_{p\uparrow} \\ v_{p\downarrow} \end{pmatrix}, \tag{1}$$

$$\hat{H}^{(0)} = \hat{\tau}_3\left(-\frac{\hbar^2\nabla_x^2}{2m_\perp^*} + \xi_p^\parallel - \mu + V_{\rm reg}(x) \right) + \hat{\tau}_1\phi(E,x) + \hat{1}\Sigma_1(E,x), \tag{2}$$

where $\xi_p^\parallel = p_\parallel^2/2m_\parallel^*$ is the excitation kinetic energy within ab plane, $m_\parallel^*$ and $m_\perp^*$ are the electron effective masses in the ab planes and in the lateral c direction, respectively, μ is the electron chemical potential, τ_1 and τ_3 are the Pauli matrices, E is the energy variable, $u_{p\uparrow}$ is the wave function of an electron with the momentum $\mathbf{p}$ and the spin ''up'' while $v_{p\downarrow}$ is the wave function of a hole with the spin ''down,'' and $\Sigma_1(E,x) = [1 - Z_{\rm dyn}(E,x)]E$; $Z_{\rm dyn}(E,x)$ is a renormalization function[34] which describes a dynamic renormalization of the electron mass due to many-body effects which we discuss later. In the total Hamiltonian $\hat{H} = \hat{H}^{(0)} + \hat{H}^{\rm int}$, the diagonal part $\hat{H}^{(0)}$ [see, i.e., Eq. (2)] describes the electron spectrum in the regular interlayer potential $V_{\rm reg}(x)$ and for periodic order parameter $\phi(E,x)$. The interaction part $\hat{H}^{\rm int}$ includes scattering effects, i.e., (i) scattering with phonons, electron-electron scattering, etc., and (ii) contribution from ''incoherent'' interlayer motion, which can be caused by thermally excited oscillations in the interstitial regions. The contribution to the elastic scattering comes from electron-impurity collisions, as well as it can be due to irregularities $V_{\rm rd}$ in the interlayer potential $V(x) = V_{\rm reg}(x) + V_{\rm rd}(x)$. Here we consider small deviations $|V_{\rm rd}/V_{\rm reg}| \ll 1$ corresponding to the clean limit $\tau_{\rm el}\Delta \gg 1$, $\tau_{\rm el}^{-1} \approx 2\pi c_i N(0) \langle |V_{rd}(x)|^2 \rangle_{\rm sample}$, c_i is the effective ''impurity'' concentration; $N(0)$ is the electron density of states at the Fermi level, and $\langle \cdots \rangle_{\rm sample}$ is the averaging over the sample. A similar treatment can be applied to the inelastic contribution[35] as well, which itself depends also on the temperature.

Of course, speaking generally, the problem must be treated self-consistently.[9] This means that $\Delta(x) = \phi(E,x)/Z(E,x)$ [$Z(E,x)$ is the total renormalization function] entering Eq. (2) has to be determined from an equation on the energy gap which itself is found from minimum of the total SC free energy $\mathcal{F}_s \leqslant \mathcal{F}_s^{(0)} + \langle \hat{H}^{\rm int} \rangle_0$ ($\mathcal{F}_s^{(0)}$ is the part of the free energy corresponding to $\hat{H}_0$; $\langle \cdots \rangle_0 = {\rm Tr}\{(\cdots)\exp(-\hat{H}_0/kT)\}/{\rm Tr}\{\exp(-\hat{H}_0/kT)\}$). The explicit form of $\hat{H}_0$ depends on a pairing mechanism and it takes into account many-body effects.

Within the ''scattering time'' approximation for Z one writes

$$Z(E,x) = 1 + Z_{\rm dyn}(\mathbf{p},E,x) + \frac{i}{2\tau_{\rm el}} \left\langle \frac{1}{\sqrt{E^2 - \Delta^2(\mathbf{p},E,x)}} \right\rangle_p + \delta Z_\epsilon, \tag{3}$$

where $\langle \cdots \rangle_p$ means the averaging over angles of $\mathbf{p}$; the last two terms in Eq. (3) originate from $\hat{H}^{\rm int}$, namely, from elastic and inelastic scattering, respectively. A similar contribution

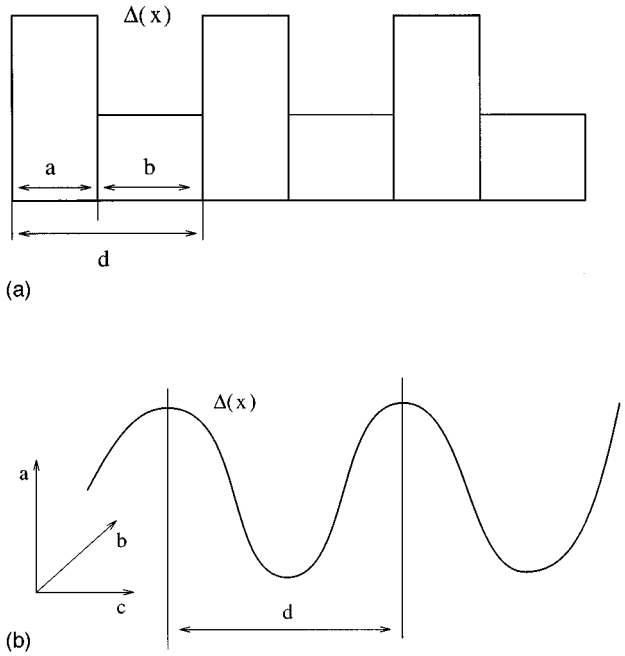

FIG. 1. Simplified sketches for the (a) rectangular and (b) harmonic geometries of $\Delta(x)$.

from s-wave scattering to ϕ takes place only for conventional SC's while for d-wave $\widetilde{S}$ it is canceled due to averaging over the angles.

As a preamble, we begin with the analysis of two different simple setups, namely, rectangular and harmonic approximations for $\Delta(x)$. Then, we perform a self-consistent solution of the problem. For illustrative purposes we begin with the traditional geometries sketched in Fig. 1. While in the short-coherence-length SC one may have $\xi_\perp \sim c_\perp$, the electron de Broglie wavelength there can be comparable in value with both $\xi_\perp$ and $c_\perp$. Then, the terms which are $\propto \delta k_{e\text{-}h} = k_e - k_h \simeq 2\pi\Delta/\hbar v_F$ become negligible no longer in comparison with other terms, which are $\propto k_F$ (k_F is the Fermi wave vector, respectively). Therefore, here we must avoid to apply the quasiclassical approximation,[22] which implements the small parameter $c_\perp/\xi_\perp \ll 1$ (or $\lambda_{\mathrm{DB}}/\xi_\perp \gg 1$).

B. Rectangular approximation for layered SC structures

Employing a simple rectangular geometry[8,9,12] sketched in Fig. 1(a), we begin with superconducting periodic structure having two different superconducting layers in the period $\ldots S'\text{-}S\text{-}S'\text{-}S \ldots$. Similar setups, i.e., $\ldots S\text{-}N\text{-}S\text{-}N \ldots$, were considered in Refs. 8 and 9, but they did not address the $\ldots S\text{-}S'\text{-}S\text{-}S'\text{-}S\text{-}S' \ldots$ case. Besides, the authors of Refs. 8 and 9 used quasiclassical approximation, which we would like to avoid here. For simplicity we assume the gap potential to be

$$\Delta(x) = \begin{cases} \Delta_a & \text{if } nd < x < a + nd, \\ \Delta_b & \text{otherwise.} \end{cases} \tag{4}$$

Thus, in the unit cell of a sublattice having period d one layer is assumed to be of the width a while the width of another is $b = d - a$. In Eq. (1), we set also $V(x) \equiv$ const as well as $\Sigma_1(E,x) \equiv 0$, and implement the continuity and periodicity conditions[8]

$$\hat{\psi}(x+a+b) = \lambda\hat{\psi}(x), \quad |\lambda| = 1,$$
$$\hat{\psi}(b) = \lambda\hat{\psi}(-a), \quad \nabla_x\hat{\psi}(b) = \lambda\nabla_x\hat{\psi}(-a). \tag{5}$$

The above equations (5) are reduced to a secular equation $\det = 0$ for the eigenvalues [det is the determinant of the linear system which follows from Eqs. (5)], if one assumes a harmonic solution with constant coefficients. Then at $\Delta_b = 0$, the task with $\Delta(x)$ in the form (4) can be solved even analytically.[8,9,12] However, at $\Delta_b \neq 0$ the analytical solution[8,9,12] is available no longer, even in this simplest case. Therefore, one has to implement a numerical solution of the mentioned secular equation. We calculate the eigenvalues of the excitation energy $E_p^{(j)}$ for the branch j versus the electron momentum $\mathbf{p}$ ($\mathbf{p} = \{\mathbf{p}_\parallel, p_\perp\}$; $p_\perp$ is the component of the electron momentum in the lateral c direction), which are obtained from the secular equation $\det = 0$. Since the gap alternates only in the c direction, the resulting electron spectrum is highly anisotropic. The electron density of states is expressed as

$$N(E) = \sum_{j,p} \left| \frac{\partial \mathbf{p}}{\partial E_p^{(j)}} \right|_{E_p^{(j)} = E}. \tag{6}$$

Since the roots $E_p^{(j)}$ of $\det = 0$ are defined not everywhere—namely, there are regions of forbidden energy[8]—the density of states $N(E)$ exhibits these subbands. In a special case the subbands can be quite narrow and can manifest themselves as singular anomalies in the electron density of states $N(E)$. In tunneling experiments, these anomalies are observed in the current-voltage I-V characteristics. Therefore, making a correspondence to the experiments, we plot the curves for the tunnel differential resistivity in Fig. 2:

$$R_{dA}(U) = \left(\frac{dI(U)}{dU} \right)^{-1}, \tag{7}$$

where the tunnel current is

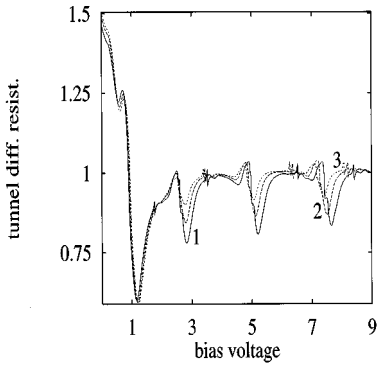

FIG. 2. Normalized differential resistivity $R_{dA}(U)/R_N$ of the tunnel junction M-I-$\widetilde{S}$ plotted versus the bias voltage U for different ratio of ξ/d.

$$I(U)=\frac{1}{eR_N}\int dE N_M(E) N_{\tilde{S}}(E-eU)[n_{E-eU}-n_E], \quad (8)$$

R_N is the normal state resistivity, n_E is the quasiparticle distribution function, E is the energy variable, U is the bias voltage, $N_M(E)$ is the density of states of injector M, and $N_{\tilde{S}}(E)$ is the normalized density of states of the layered SC. Different curves of the normalized characteristic $R_{dA}(U)/R_N$ in Fig. 2 are related to various thickness of layer a, while the other parameters are $\Delta_a=1+i0.01$, $\Delta_b=0.8+i0.01$, the imaginary parts of Δ_a and Δ_b were introduced to handle singularities in integrals over the energy variable, $T/\Delta_a=0.2$, $d=2$, $\xi_\perp=1.33$, and $k_{F\perp}=1.1$ is the Fermi wave vector. The energy-dimensional parameters, for convenience, are expressed here in units of the energy gap Δ_a, while the spatial characteristics (as well as reciprocal to them) in units of the lattice half-period $d/2$. Curve 1 in Fig. 2 is attributed to $a=0.27$, curve 2 to $a=0.19$, and curve 3 to $a=0.13$, respectively. One can see that for the selected parameters there are pronounced features occurring in the differential resistivity $R_{dA}(U)$ at certain values of the reduced bias voltage eU/Δ_a. These features are somewhat similar to those obtained in WKBJ-type calculations,[8,12,25] but in the present nonquasiclassical approach they are essentially sharper. At given parameters, the features correspond to $U\approx\Delta_a, 3\Delta_a, 5\Delta_a$, and $7\Delta_a$, having a complex structure combined by maxima and minima, and can be attributed to the scattering states. The features at $U<\Delta_a$ are related to the bound states. Thus, one can conclude that the made non-self-consistent calculations predict a series of singularities in the electron density of states $N(E)$ as well as in the differential tunnel resistance $R_{dA}(U)$. These singularities are related to the quantization of the electron movement in the periodic gap potential $\Delta(x)$. The origin of the mentioned features is similar to the origin of the bands predicted in Refs. 8,9 and 12 for the layered SC in the quasiclassical limit. The singularities are quite narrow, because of a small difference in values between Δ_a and Δ_b, but are more pronounced in the limit of the short coherence length. Their amplitude is fairly sensitive to the contribution of inelastic scattering at low energies. Besides, for the non-self-consistent rectangular approximation of $\Delta(x)$, the spikelike structure takes place for $\xi_\perp\approx k_F^{-1}$.

One must add, however, that the simple description of tunneling experiments in terms of the density of electron states (6) is not always possible. In particular, the formula (8) is not valid, if tunneling processes occur with a selection over the electron momentum $\mathbf{p}$ (see, e.g., Ref. 36), because the electron spectrum in the sample electrode $\tilde{S}$ is highly anisotropic. In such a case of the M-I-$\tilde{S}$ junction, the tunneling matrix element (which itself is determined by the properties of the barrier I) is $T_{pp'}=T(\cos\gamma)$, where γ is the angle between the electron momentum and the perpendicular to the barrier I. For the used here ordinary approximation [see Eq. (8)] $T(\cos\gamma)=T=$const while in the opposite case of ideal selection $T(\cos\gamma)=\delta(1-\cos\gamma)$. Nevertheless, the case $T(\cos\gamma)\neq$const requires a special experimental setup and will be considered elsewhere.

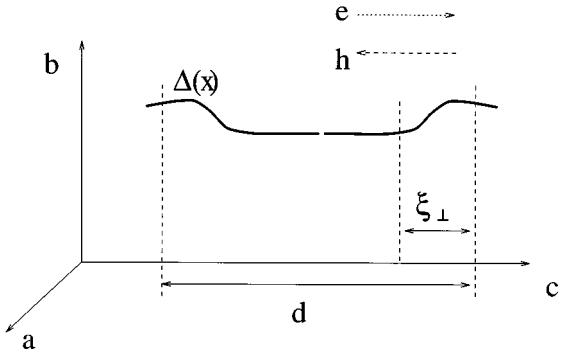

FIG. 3. Two scales of $\Delta(x)$ behavior—the coherence length $\xi_\perp$ and the c-axis lattice constant $c_\perp$.

C. Harmonic spatial variations of the order parameter

While for the used rectangular shape of $\Delta(x)$ the Fourier series contains many components, one may attribute the complex structure of the electron density of states in the vicinity of subbands rather to the artifact of approximation itself than to a real observable phenomenon. Besides, in high-quality samples of the layered metal oxide single crystal,[33] $\Delta(x)$ may be rather ''smooth'' alternating on a ''clean'' coherence length scale $\xi_\perp^{\mathrm{BCS}}$. Therefore, it is tempting to consider another limiting simplest case [see Fig. 1(a)], which corresponds to the modeling $\Delta(x)$ as

$$\Delta(x)=\Delta_0+\Delta_1\cos Gx, \quad (9)$$

where $\Delta_1\ll\Delta_0$, $G=\pi/d$ is the reciprocal sublattice vector of the gap potential, and d is the period of alternation of the gap potential along c axes. It implies that $\Delta(x)$ is homogeneous in the ab directions within each Cu-O layer, while its value can be reduced inside the interlayer regions. Of course, speaking more generally, one has at least two scales for the $\Delta(x)$ behavior in the c direction (see Fig. 3). One scale, e.g., can be determined by the period $d=c_\perp$ of the layered structure, while another scale is linked to the value of the coherence length $\xi_\perp$. Nevertheless, to get a simple analytical solution of Eq. (1) which could be useful here for an illustrative reason, we assume that $d=\xi_\perp$, that the gap potential given by Eq. (9), and that the electric potential $V(x)\simeq 0$. Another point is related to many-body effects, recently discussed with respect to the metal oxide SC's (see, for instance, Ref. 15). The strong electron-electron correlations taking place in the Cu-O planes may lead to a retardation effect, causing particularly a dynamic renormalization of the electron mass $m_\perp^*$. This is described by the function $Z(E,x)$, entering the Eq. (1). For convenience, however, when calculating the electron density of states, this dynamic renormalization can be taken into account by introducing an effective dependence of $m_\perp^*$ on the absolute value of electron momentum $p=|\mathbf{p}|$. In Fig. 4, we illustrate the aforesaid by the dispersion curve E_p, which is modified due to dynamic renormalization of the electron mass versus p/p_F (this is shown in the inset to the same Fig. 4 as well; p_F is the Fermi electron momentum). The flatness of $E_p(p/p_F)$ can be quite essential at $|p-p_F|/p_F\ll 1$. This effective dependence of $m_\perp^{\mathrm{dyn}}$ on the electron momentum one can model by

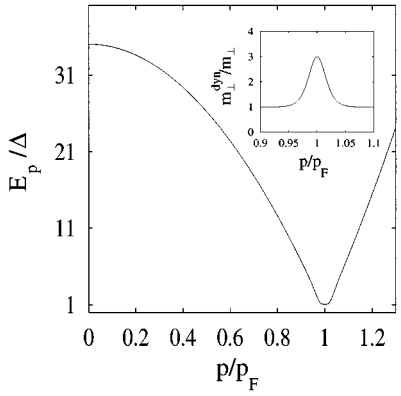

FIG. 4. Dynamic renormalization of the effective electron mass $m_{\perp}^{\mathrm{dyn}}$ due to the many-body effects.

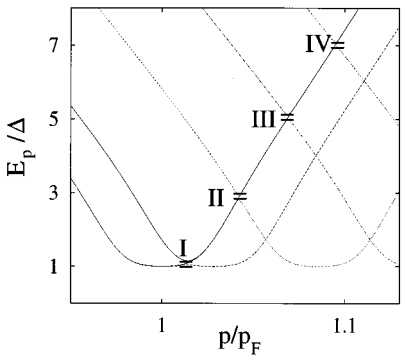

FIG. 5. Minisubband structure $E(\mathbf{p}/\mathbf{p_F})/E_F$ for the layered superconductor with the spatially modulated energy gap calculated in the two-wave approximation.

$$\frac{m_{\perp}^{\mathrm{dyn}}}{m_{\perp}^{*}}=1+\frac{A_m}{\cosh[B_m(|p|/p_F-1)]}, \tag{10}$$

where A_m and B_m are parameters to be determined from independent experiments or band structure calculations.[32] A simple analytical solution of Eq. (1) is available in a two-wave approximation. This approximation[37] suggests that the main contribution to the condition of resonance near the zone boundary comes from only two waves with $g=0$ and $g=G$. Within this approximation, the trial wave function can be written as

$$\hat{\psi}(x)=\begin{pmatrix} a_p e^{ip_{\perp}x}+a_{p-G}e^{i(p_{\perp}-G)x} \\ b_p e^{ip_{\perp}x}+b_{p-G}e^{i(p_{\perp}-G)x} \end{pmatrix}. \tag{11}$$

In fact, we act here in analogy to a classic band structure theory for normal conductors (see, e.g., Ref. 37), and arrive again at a secular equation on eigenvalues in the form

$$0=\det\equiv\begin{vmatrix} -\xi_p+E & 0 & -\Delta_0 & -\Delta_1 \\ 0 & -\xi_{p-G}+E & -\Delta_1 & -\Delta_0 \\ -\Delta_0 & -\Delta_1 & \xi_p+E & 0 \\ -\Delta_1 & -\Delta_0 & 0 & \xi_{p-G}+E \end{vmatrix}, \tag{12}$$

where G in Eq. (11) runs the allowed values $G_m=2m\pi/L$, $m=\overline{0,\ldots,N}$, L is the sample's size in the c direction, N is the number of primitive cells, $\xi_p=\xi_p^{\parallel}+p_{\perp}^2/2m_{\perp}^{*}$ and $\xi_{p-G}=\xi_p^{\parallel}+(p_{\perp}-G)^2/2m_{\perp}^{*}$. The eigenvalues of the quasiparticle excitation energy $E_p^{(j)}$ then have four branches $j=\overline{1,\ldots,4}$. They are found in a simple analytical form as

$$E_p^{(1,2,3,4)}=\pm\sqrt{\xi_p^2+\xi_{p-G}^2+2\Delta_1^2+2\Delta_0^2\pm\sqrt{(\xi_p^2-\xi_{p-G}^2)^2+4\Delta_1^2[(\xi_p-\xi_{p-G})^2+4\Delta_0^2]}}/\sqrt{2}, \tag{13}$$

where ξ_p is the kinetic energy of electron with momentum $\mathbf{p}$. The excitation energy curves E_p for this case are plotted versus p/p_F in Fig. 5 for $\Delta_0=1$, $\Delta_1=0.05$, $A_m=2$, $B_m=50$, and $d=110/k_F$ and for the value of Fermi energy $E_F=\hbar^2k_F^2/2m_{\perp}^{*}=35$. The all-energy quantities are expressed in units of the energy gap amplitude Δ_0. The allowed values of the quasiparticle wave vector G_m in the first Brillouin zone are restricted by $G_0=\pi/d$, for this is the boundary of the zone. We assumed here that the period of $\Delta(x)$ is $d=\hbar v_F/\Delta_0$, and corresponds to the alternation of the gap potential on the scale of the BCS coherence length in the ''clean limit'' $\xi_{\perp}^{\mathrm{BCS}}=1/q_{\perp}=\hbar v_F/\pi\Delta_0$ (where $q_{\perp}=G_0$ is the wave vector of sublattice). Also we took into account, that the second as well as the next Brillouin zones are formed already with alternation of the electron-to-hole momentum in the Andreev reflection processes $\sim\pi(2n+1)\Delta_0/v_F$, which requires an additional alternation of the momentum $\delta p\sim 2\pi\Delta_0/v_F$, for each extra Cooper pair created. The ''even'' subbands are not formed, because this is in contradiction to the momentum and charge conservation in the Andreev reflection processes. One can see that at higher excitation energies $(2n+1)\Delta_0$ corresponding to Andreev reflection for the first $(n=0)$ and the next $(n>0)$ Brillouin zones, except the common gap $|\Delta_0\pm\Delta_1|$ (which splits itself in two branches), there are smaller gaps $2\Delta_1$.

Another issue, which has widely been discussed recently in respect to the metal oxides (see, i.e., Ref. 38), is related to the d-wave pairing symmetry. This anisotropic pairing concept suggests that the energy gap $\Delta(\theta,\phi,x)$ is dependent already on angles of the electron momentum $\mathbf{p}$, and that it has nodes at certain points and along lines on the Fermi surface, as well as petals with different phase. This kind of unconventional symmetry is quite important in special cases, when the electron tunneling occurs between the petals of gap with a shifted phase, or in a tunnel junction, where the selection over the electron momentum in the tunneling processes[39] takes place. In present paper we examine the density of electron states of a regular ''clean'' single crystal,

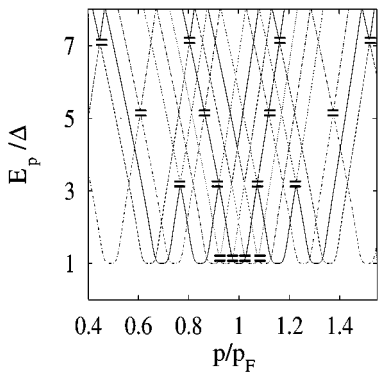

FIG. 6. Electron spectrum computed in the five-wave approximation. One can see minisubbands due to spatial modulation of the order parameter $\Delta(x)$.

for which a disorientation of petals of the order parameter in the neighbor layers is not essential. For the mentioned quantity, the effect of the d-wave pairing is thus reduced only to the energy gap anisotropy $\Delta(\theta,\phi,x)$. The generalization of the above solution for the case of anisotropic pairing is clear. One solves the equation $\det=0$, already taking into account the symmetry of $\Delta(\theta,\phi,x)$. Then, $E_p^{(j)}(\theta,\phi)$ are used for further computation of the electron tunneling density of states:

$$N(E)=\sum_{j,p}\ \mathrm{Im}\{\mathrm{Tr}\hat{G}^R(\mathbf{p},E)\}, \tag{14}$$

where the summation is performed over the branch index j and the electron momentum $\mathbf{p}$, and where $\hat{G}_p^R(\mathbf{p},E)$ is the total retarded Green function.[34] To include the effect of elastic and inelastic scattering one uses the equation[34] $[\hat{G}^R(\mathbf{p},E)]^{-1}=[\hat{G}_0^R(\mathbf{p},E)]^{-1}-\hat{\Sigma}_p^R(E)$; $\hat{G}_0^R(\mathbf{p},E)$ is calculated with $\hat{H}_0$ while $\hat{\Sigma}_p^R(E)$ is the self-energy corresponding to $\hat{H}^{\mathrm{int}}$. In the scattering approximation, the expression for $\hat{\Sigma}_p^R(E)$ coincides with the well-known formula for the electron-impurity self-energy,[34] in which the electron-impurity-scattering time is replaced by τ_{el}. As a good approximation then one can use

$$N(E)=\frac{1}{\pi}\sum_{j,p}\ \mathrm{Im}\left\{\frac{\Gamma_\epsilon(E)}{[E-E_p^{(j)}(\theta,\phi)]^2+\Gamma_\epsilon^2(E)}\right\}, \tag{15}$$

where $\Gamma_\epsilon=(2\tau_{\mathrm{el}})^{-1}+[2\tau_\epsilon(E)]^{-1}$.

III. SELF-CONSISTENT SOLUTION

The above-considered examples demonstrate the role of periodicity of the gap potential in formation of the quasiparticle excitation spectrum E_p. Nevertheless, the modeling of $\Delta(x)$ by any given form may serve for illustrative purposes only. Since we solve the problem beyond the quasiclassical approximation, it is necessary to know precisely the spatial alternation $\Delta(x)$, which determines details of the electron spectrum, because the integrated form[9] $\int\Delta(x)dx$ is not sufficient in this case. A more adequate description can be achieved by a self-consistent solution of equations (1) and a self-consistency equation. Nevertheless, a straightforward task of obtaining a complete self-consistency may be difficult even in simplest cases, although visible progress can be made by minimizing the free energy functional[20,30]

$$\mathcal{F}_s=-2kT\sum_n\ \ln\left\{2\cosh\left(\frac{E_n}{2kT}\right)\right\}+\int_{\mathrm{sample}}dx\,\frac{|\Delta(x)|^2}{\Upsilon(x)} \tag{16}$$

over variable parameters, entering $\Delta(x)$. In the above formula, written for the clean limit, E_n is an eigenvalue of the Bogolubov equation, and $n=\{\mathbf{p},j\}$. Thus, we find a fair approximation to a self-consistent solution in the following way. At the beginning, we set some guessing coefficients Δ_g in the energy gap potential

$$\Delta(\theta,\phi,x)=\sum_{m=0}^{M}\ \Delta_m(\theta,\phi)\cos\left(\frac{2\pi}{d}mx\right), \tag{17}$$

where M is a finite number, and θ and ϕ are the angles of the electron momentum for the anisotropic gap. The value of period d is chosen as a guessing parameter too. Since here we pay attention to the inhomogeneous state, we set the value of $d=\hbar v_F/\Delta_0$, which is consistent with alternation of $\Delta(x)$ on the natural scale of the BCS coherence length $\xi_\perp=\hbar v_F/\pi\Delta_0$ in a clean limit. Of course, the setting $d=\xi_\perp$ as a maximal period omits possible bound states, which may occur at $E<\Delta_{(0)}^{\max}$ ($\Delta_{(0)}^{\max}$ is the amplitude of the gap at $\theta=0$ for $d_{x^2-y^2}$ pairing symmetry) due to slow alternation of $\Delta(x)$. While we are restricted by computation facilities here, we consider only scattering states. The last scale $\sim\xi_\perp$ is much larger than the lattice constant $c_\perp$. It allows us to replace the electric potential $V(x)$ (which itself alternates on the small scale $c_\perp$) by its averaged value $\overline{V(x)}^D=0$, in some region by size $D\simeq\xi_\perp$. Similar remarks could also be applied in respect to the form of the pairing potential $\Upsilon(x)$, which basically depends on a pairing mechanism. Actually, the pairing is concentrated within the Cu-O planes, while it vanishes in the interplane regions. However, since we are interested here in the scale $D\gg c_\perp$, we can replace $\Upsilon(x)$ by its averaged value $\Upsilon_A=\overline{\Upsilon(x)}^D$. In order to examine the properties of the inhomogeneous state (apart from its particular origin), we introduce a deviation of the attractive BCS potential $\delta\Upsilon(x)=\Upsilon_1\cos(x/\xi_\perp^{\mathrm{BCS}})$ from its regular form $\Upsilon(x)$ which is smooth on the scale of $\xi_\perp^{\mathrm{BCS}}$. Then we substitute Eq. (17) together with a trial wave function

$$\hat{\psi}_p(x)=\sum_q\ \begin{pmatrix}a_{p-q}\\ b_{p-q}\end{pmatrix}e^{i(p-q)x} \tag{18}$$

to the Bogolubov equation (1) to get a secular equation on the coefficients a_p and b_p, at the given coefficients Δ_m. From this secular equation, we find the eigenvalues $E_p^{(j)}$ of excitation energy to be used for the calculation of free energy (16) which itself has to be minimized in respect to the coefficients Δ_m. The expression (16) must already contain the deviation $\delta\Upsilon(x)$ in the aforementioned explicit form. The advantage of this procedure (see, e.g., Refs. 20 and 30), is that it is not necessary to know the eigenvectors a_p and b_p, because the eigenvalues $E_p^{(j)}$ are fairly sufficient to compute Eq. (16). Despite the number M being finite, the above

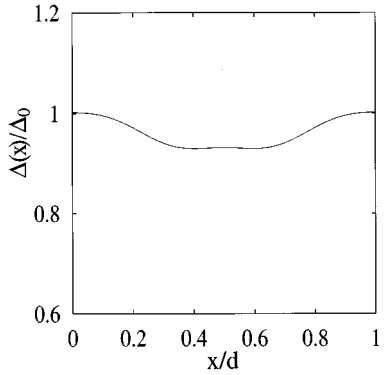

FIG. 7. Equilibrium spatial alternation of $\Delta(x)$ related to a minimum of the free energy $\mathcal{F}_s$.

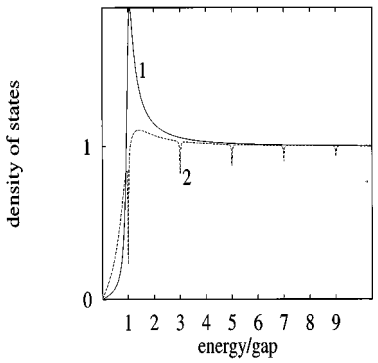

FIG. 8. The BCS density of states (curve 1) and the electron density of states for the layered system with spatially oscillating gap potential (curve 2).

procedure affords one to obtain a good approximation for a self-consistent solution of the problem in a clean limit.

For calculations, we implement the linear combination (18) for the functions $u_{p\uparrow}$ and $v_{p\downarrow}$ consisting of five plane waves. The determinant has the size 10×10; thus the eigenvalues $E_p^{(j)}(\theta,\phi)$ are computed numerically, for some guessing initial values of Δ_m. Then, these $E_p^{(j)}$ are substituted into Eq. (16) to calculate the free energy $\mathcal{F}_s$. Varying the coefficients Δ_m which play the role of parameters in Eq. (16), one finds a set of these parameters corresponding to a minimum of $\mathcal{F}_s$. The electron spectrum for the anisotropic pairing case additionally depends on the angles of the electron momentum $\mathbf{p}$ due to dependence of $\Delta(\mathbf{p})$. At $\theta=0$ for $d_{x^2-y^2}$ pairing symmetry $\Delta(\theta,\phi)$ achieves its maximal value $\Delta_{\max}(x)$. In Fig. 6, we plot the electron spectrum versus p/p_F corresponding to such a minimum found for the following parameters. The Fermi energy is $E_F=\hbar^2k_F^2/2m_\perp=35$, $\lambda_c=N(0)\Upsilon_A=0.9$ is the BCS constant, $\lambda_1=N(0)\Upsilon_1=0.1$, $d=61.4/k_F$, and $\Delta(\theta,\phi)=\Delta_0^{\max}$. For the conventional symmetry $\Delta(\theta,\phi)\equiv\Delta$. All the energy quantities are expressed in units of the energy gap amplitude $\Delta_0^{\max}$, which is determined from the ''normalization'' condition $\Sigma_{k=0}^{3}|\Delta_k|^2/|\Delta_{\max}|^2=1$. The dynamic renormalization factor for the effective mass is taken in a model form (10), with the same parameters as for Fig. 4. One can see that in this approximation the electron spectrum exhibits a subband structure. In Fig. 7, we plot the self-consistent $\Delta_{\max}(x)$ profile, which originates from the Andreev scattering as well. The spatial variation of $\Delta_{\max}(x)$ in Fig. 7 is related to a minimum of the free energy $\mathcal{F}_s$ which is found as a result of the self-consistent computation. This kind of equilibrium solution corresponds to the following values of the computed coefficients: $\Delta_0=0.96$, $\Delta_1=0.04$, $\Delta_2=0.006$, and $\Delta_3=-0.004$. An introduction of elastic and inelastic scattering in the system corresponds to $\hat{H}^{\rm int}\neq0$. It causes an addition to $\mathcal{F}_s$ determined by eq. (16) which modifies both the energy gap function and the excitation spectrum. In the s-wave case, nonmagnetic impurities do not affect the SC electron spectrum (due to the Anderson's theorem[34]). To take the impurity scattering into account in the d-wave case, however, one can modify the expression for the free energy (16) in a simple way. It is done in accordance with formula (3), if one replaces the energy eigenvalues, E_n entering the Eq. (16) by

$$E_n'=E_n+\left\langle\left\langle\frac{E_n'}{2\tau_{\rm el}\sqrt{E_n'^2-\Delta^2(\mathbf{k},x)}}\right\rangle_k\right\rangle_{\rm sample}. \quad (19)$$

In Fig. 8, we show the normalized BCS density of states (curve 1) and an example of the tunneling electron density of states for the clean layered system with spatially inhomogeneous gap potential (curve 2), which exhibits sharp spikes at the energies $E_n\simeq(2n+1)\Delta_0$. We computed $N(E)$ for a small concentration of nonmagnetic impurities (incoherent contribution), $\tau_{\rm el}^{-1}=0.1$. The pairing symmetry for harmonics Δ_m is $d_{x^2-y^2}$. One can see that the amplitude of the spikes is lowered as energy increases, while the BCS-like gap edge peak at $E\simeq\Delta_0$ (curve 1) is less pronounced for the system with the periodic gap (curve 2). The decreasing of the amplitude of spikes here is due to the energy dependence of the inelastic (or incoherent) contribution to the Cooper pairing. The inelastic contribution we modeled as $\tau_\epsilon^{-1}\approx\kappa(E/\Delta)^\alpha$ [for the curve 2, we used the parameters $\kappa=0.1$, $\alpha=0.3$]. The width of spikes is $\simeq2\Delta_1$. Detailed calculations show that for the case of the d-wave symmetry when $\tau_{\rm el}^{-1}$ and κ are increased, the spikes are washed out. For conventional symmetry of the harmonics Δ_m, the spikes are affected only by inelastic part of collisions. An analogy to the classic band theory[37] affords the following interpretation. The first singularity at $E_1\simeq\Delta_0$ corresponds to the lowest minisubband due to the Andreev reflection of incident electron with the energy $\approx\Delta_0$ which is coupled to an electron in the valence zone with energy $\approx-\Delta_0$. This reflection creates a hole with energy $\approx\Delta_0$ as well as a Cooper pair with the gain of energy $2\Delta_0$. The standing wave occurs inside the wells formed by a minimum of the gap potential due to an electron-hole interference, with alternation of the momentum in this process to be $\delta p\simeq2\pi\Delta_0/v_F$. The higher minisubbands $E_n\simeq(2n+1)\Delta_0$ (the alternation of the electron-to-hole momentum is already $\delta p_n\simeq2\pi\Delta_0 n/v_F$) physically correspond to the creation of more than one Cooper pair in the Andreev reflection process. For instance, at $n=1$, the electron (or a hole) having the excitation energy $E^{(a)}\simeq\Delta_0$ should be coupled with an electron (or a hole) having the energy $E^{(b)}\simeq-3\Delta_0$, creating two Cooper pairs in addition to the hole (or to electron). At $n=2$, the energy

$E^{(a)}$ remains the same, while $E^{(b)} \simeq -5\Delta_0$, and three additional Cooper pairs are created, etc.

IV. CONCLUSIONS

The above self-consistent calculations conducted beyond the quasiclassical approximation show an important role of an inhomogeneous state in the ''clean'' short-coherence-length SC at low temperatures $T \ll \Delta$. This state corresponds to a minimum of free energy, and is established with the order parameter alternating in the c direction on the scale of coherence length $\xi_\perp$. The electron spectrum then is formed by the Andreev scattering processes, occurring in such a periodic gap potential. We find that this kind of scattering leads to the formation of pronounced minisubbands in the quasiparticle excitation spectrum at energies $E_n = (2n+1)\Delta_0$, which serve as a signature of inhomogeneous state and can be observable in tunneling spectroscopy experiments.

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