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Zero-energy Andreev surface bound states in the lattice model

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The conditions for zero-energy Andreev surface bound states to exist are found for the lattice model of d-wave superconductor with arbitrary surface orientation. Both nearest neighbors and next nearest neighbors models are considered. It is shown that the results are very sensitive to the surface orientation. In particular, for half-filled $(hl0)$-surface zero-energy Andreev surface states only appear under the condition that h and l are odd simultaneously.

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Significant feature of high temperature superconductors (HTS) are zero-energy Andreev surface bound states. The zero-energy states (ZES) form on surfaces of a d-wave superconductor with orientations different from the (100), due to the sign change of the order parameter. In high-temperature superconductors, such states manifest themselves as the zero-bias conductance peak in tunneling spectroscopy in the ab-plane [1 – 26], the anomalous temperature behavior of the Josephson critical current [27 – 30] and the upturn in the temperature dependence of the magnetic penetration depth [31 – 33]. At the same time the problem of ZES at the surface with arbitrary orientation is still not clear.

The conventional description of Andreev surface bound states, as well as the most of inhomogeneous superconducting problems, is based usually on the continuous quasiclassical approximation. From the this viewpoint the conditions for ZES to exist are quite simple. ZES are formed due changing of order parameter sign along the quasiclassical trajectory. There are no ZES for (100) (i.e. 0°) orientation, and there are ZES at all values $k_{||}$ for (110) (45°) orientation. For intermediate surface orientations the sign change does not take place for all incoming momentum directions, and the weight of the ZES decreases with deviation from 45°-orientation.

From the other side, the tight-binding BCS model is widely used for theoretical description of HTS. This model gives the same (as the continuous quasiclassical model) result for ZES at (100) and (110) orientations. However, for the intermediate surface orientations the question is very complicated. To the best of my knowledge only the simplest orientations (100), (110), (210) [21, 23, 34 – 37] have been studied. And even numerical calculation couldn't give the general answer for all surface orientations because of the lattice specific.

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In this paper the general analytical criterion for zero-energy Andreev surface bound states to exist at the surface of arbitrary orientation is presented. I consider two-dimensional tight-binding model on square lattice. The surface orientation is assumed to be arbitrary and characterized by the indexes $(hl0)$. Both nearest neighbors and next nearest neighbors models are considered. For simplicity I take the superconducting order parameter to be spatially constant. This approximation is reasonable for studying of low-energy quasiparticle states. The impenetrable surface is assumed to be smooth.

The Hamiltonian for a pure singlet superconductor in the tight-binding model can be written as:

$$\mathcal{H} = -\sum_{\mathbf{x},\mathbf{x}',\sigma} t(\mathbf{x},\mathbf{x}')c^\dagger_\sigma(\mathbf{x})c_\sigma(\mathbf{x}') + \\ +\sum_{\mathbf{x},\mathbf{x}'}\{\Delta(\mathbf{x},\mathbf{x}')c^\dagger_\uparrow(\mathbf{x})c^\dagger_\downarrow(\mathbf{x}') + \mathrm{h.c.}\}. \tag{1}$$

Here $t(\mathbf{x},\mathbf{x}) = \mu$ is the chemical potential; $t(\mathbf{x},\mathbf{x}\pm\mathbf{a}) = t(\mathbf{x},\mathbf{x}\pm\mathbf{b}) = t > 0$, $t(\mathbf{x},\mathbf{x}\pm\mathbf{a}\pm\mathbf{b}) = t' \le 0$ are the hopping elements; d-wave superconducting pairing is defined for nearest neighbors $\Delta(\mathbf{x},\mathbf{x}\pm\mathbf{a}) = -\Delta(\mathbf{x},\mathbf{x}\pm\mathbf{b}) = \Delta$. Here $\mathbf{x}$ – are the positions of lattice sites; $\mathbf{a}$, $\mathbf{b}$ – are the basic lattice vectors. Then the Bogoliubov-de Gennes equations take the form:

$$\sum_{\mathbf{x}'}\begin{bmatrix} -t(\mathbf{x},\mathbf{x}') & \Delta(\mathbf{x},\mathbf{x}') \\ \Delta^*(\mathbf{x},\mathbf{x}') & t(\mathbf{x},\mathbf{x}')\end{bmatrix}\begin{pmatrix} u(\mathbf{x}') \\ v(\mathbf{x}')\end{pmatrix} = E\begin{pmatrix} u(\mathbf{x}) \\ v(\mathbf{x})\end{pmatrix}. \tag{2}$$

We define new coordinates $(\hat{x}, \hat{y})$, rotated with respect to the crystal axes $(\hat{a}, \hat{b})$, where $\hat{x}$ is the direction normal to the surface and $\hat{y}$ is the direction along the surface. Superconductor is situated at $x > 0$. Lattice constant is taken to be unity, $a = 1$. The system is periodic along the y-direction with period $\sqrt{h^2 + l^2} \equiv d^{-1}$ and the crystal momentum component k_y of a quasiparticle is conserved. Instead of the usual square Brillouin zone (BZ) $k_a \in [-\pi,\pi]$, $k_b \in [-\pi,\pi]$ we now use the surface-adapted Brillouin zone (SABZ)[23, 36] given by $k_x \in [-\pi/d,\pi/d]$ and $k_y \in [-\pi d,\pi d]$. Here $d = 1/\sqrt{h^2+l^2}$ is the distance between the nearest chains (layers) aligned along the surfaces, i.e. all x-coordinates have discrete values with period d. The momenta in the two coordinate systems are simply related through rotation of an angle $\theta = \tan^{-1} h/l$.

Let us solve Eq.(2) for half-space $x>0$ and fixed k_y. General solution is constructed from all the solutions of uniform problem, which don't grow at $x\to+\infty$. Then the wave function for fixed k_y can be written as

$$\begin{pmatrix} u(x,k_y) \\ v(x,k_y)\end{pmatrix} = \sum_\alpha C_\alpha \begin{pmatrix} u_\alpha(k_y) \\ v_\alpha(k_y)\end{pmatrix} e^{ik_{x,\alpha}x}, \qquad (3)$$

here summation should be taken over all solutions $k_{x,\alpha}$ of equation

$$E^2 = \xi^2(k_x,k_y) + \Delta^2(k_x,k_y), \qquad (4)$$

with $\mathrm{Im}k_{x,\alpha}>0$. The boundary conditions are

$$\begin{pmatrix} u(-jd,k_y) \\ v(-jd,k_y)\end{pmatrix} = 0, \quad j=0,1,...,N-1, \qquad (5)$$

where $N=\max(h,l)$ for nearest neighbors model ($t\neq 0$, $t'=0$) or $N=h+l$ for next nearest neighbors model ($t,t'\neq 0$) [35]. The total number of solutions (4) with $\mathrm{Im}k_{x,\alpha}>0$ equals to $2N$. Some of them correspond to the intersections of line $k_y=$ const with Fermi-surface and have small imaginary part of $k_{x,\alpha}$, the others correspond to the point with $(\mathrm{Re}k_{x,\alpha},k_y)$ far from Fermi-surface. Therefore we obtain from (5) the system of $2N$ liner equations for constants C_α with E as a parameter. Then the equality of the determinant of the system to zero is the condition for existence of bound states with energy E:

$$\mathrm{Det}\begin{pmatrix} u_1 & ... & u_{2N} \\ v_1 & ... & v_{2N} \\ u_1 e^{ik_{x,1}d} & ... & u_{2N}e^{ik_{x,2N}d} \\ ... & & ... \\ v_1 e^{ik_{x,1}(N-1)d} & ... & v_{2N}e^{ik_{x,2N}(N-1)d}\end{pmatrix} = 0. \qquad (6)$$

We only consider now the possibility for dispersionless states with $E=0$ to exist in some region of k_y. Then all the solutions of (4) have the form $(u_\alpha(k_y),v_\alpha(k_y))^T = (1,-i\,\rho_\alpha)$ with $\rho_\alpha=\pm1$. From each point of intersection $k_y=$ const with Fermi-surface we obtain one solution with $\rho_\alpha = \mathrm{sgn}(v_{f,x}(k_{x,f},k_y)\Delta(k_{x,f},k_y))$ in quasiclassical approximation. And from each point far from Fermi-surface we obtain two solutions with close values of k_x and with opposite values of ρ_α.

Let n and m be numbers of solutions corresponding to $\rho_\alpha=\pm1$, respectively. Then we can obtain after some straightforward algebra that in the case of $n\neq m$ Eq.(6) is always true. For $n=m$ Eq.(6) can be reduced to

$$\prod_{\rho=-1,i<j}(k_{x,i}-k_{x,j}) \prod_{\rho=+1,i<j}(k_{x,i}-k_{x,j}) = 0. \qquad (7)$$

The wave vectors $k_{x,\alpha}$, corresponding to the same sign of ρ_α, can only coincide for a few values of k_y, for which different parts or Fermi-surface intersect with each other. Therefore we obtain the simple criterion for dispersionless zero-energy bound states to exist: $n\neq m$. Since the solutions, corresponding to the values of $\mathbf{k}$, which are situated far from Fermi-surface, always appear in pairs with opposite signs of ρ_α, we can safely take into account only solutions with $\mathbf{k}$ defined by the intersections of the line $k_y=$ const with Fermi-surface.

Let's apply this criterion to the model under consideration. In the quasiclassical approximation we need to obtain all intersections of the line $k_y=$ const with Fermi-surface in SABZ, and, then, calculate $\rho = $ $=$ sign $(v_{f,x}(\mathbf{k})\Delta(\mathbf{k}))$ for all these points. Let us consider all values of k_y simultaneously and find the positions of the edge of the regions where zero-energy surface states exist.

Due to the symmetry of the normal metal quasiparticle energy spectrum and the superconducting gap to the inversion: $\xi(\mathbf{k})=\xi(-\mathbf{k})$, $\Delta(\mathbf{k})=\Delta(-\mathbf{k})$, we need to consider only that points at Fermi-surface, where the sign of ρ changes. They are the points of the gap sign changing and the points of v_x sign changing.

It is easy to show that points of v_x sign changing can't modify the parameters n and m. These points are the tangent points of Fermi-surface and line $k_y=$ const. On the one side (along k_y-axis) from the point of v_x sign changing there are two solutions with opposite signs of ρ_α. On the other side from this point there are no real solutions, but there are two solutions, which have large imaginary part of k_x and opposite signs of ρ_α, too.

Thus let us consider only points of gap sign changing. We should take into account univocal correspondence the SABZ and the usual first BZ. Then there are only four points of gap sign changing in SABZ, just as in BZ: $(k_a^0,k_b^0) = (\pm\nu\pi,\pm\nu\pi)$ in crystal axes. Here parameter ν takes value π^{-1} arccos$(-\mu/4t)$ for the nearest neighbors model and

$$\nu = \pi^{-1}\arccos\left(\frac{-\mu}{2(t+\sqrt{t^2-t'\mu})}\right) \qquad (8)$$

for more general case of the next nearest neighbors model. Parameter ν is a relative coordinate of BZ point, where the gap sign changing takes place and correlated with the filling of the band. Maximal and minimal values of ν are 0 and 1. For the simplest case of half-filling ($\mu = 0$) we get $\nu = 1/2$. But ν is not strictly the filling of the band.

Now we need to obtain the coordinates k_y^0 of the gap sign changing points in SABZ. For $(hl0)$-orientation:

$$k_y^0 = -k_a^0 \frac{l}{\sqrt{h^2+l^2}} + k_b^0 \frac{h}{\sqrt{h^2+l^2}}, \qquad (9)$$

then for k_y^0-coordinates of four gap sign changing points

$$k_y^0 = (\pm h \pm l)\pi\nu d. \qquad (10)$$

Since k_y is a crystal momentum, one can move the k_y^0-coordinates of these points into the SABZ. Finally, we obtain the following regions of k_y where ZES exist:

$$|k_y^0| \in (k_{\min}, k_{\max}), \qquad (11)$$

where

$$k_{\min} = \min\{|F[(h-l)\pi\nu d]|, |F[(h+l)\pi\nu d]|\}. \qquad (12)$$

$$k_{\max} = \max\{|F[(h-l)\pi\nu d]|, |F[(h+l)\pi\nu d]|\}. \qquad (13)$$

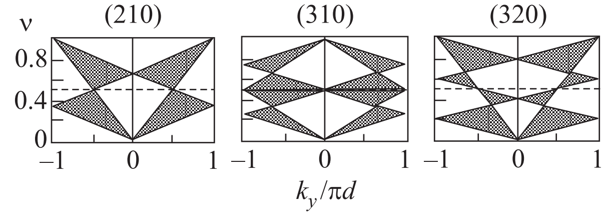
Here $F[...]$ is a function, which shifts argument to the permissible for SABZ value: $F[k_y] = (\{(1/2) + (k_y/2\pi d)\} - (1/2))\, 2\pi d$, $\{...\}$-is a fractional part of the argument. From Eq.(11) we can see that the region of k_y, where zero-energy bound states take place, always exists, except for the case of

$$k_{\min} = k_{\max}. \qquad (14)$$

It is easy to obtain from Eqs.(11)–(13) the regions of ZES existence for any cases under consideration. In Figure results for (210), (310), and (320) surfaces are shown. It is important to note, that regions with ZES and regions without them are separated by the lines of zero gap (for this values of k_y superconducting gap vanishes for one of the quasiparticle trajectories, forming the state).

For half-filled $(hl0)$-surface the result can be formulated in the general form: zero-energy Andreev surface states appear only for the case of odd h and l. Moreover, it is seen from (14) that for any surface orientation one can find set of values of ν, for which there are no zero energy states. From (14) we have $h + l$ values of ν (and the same number of band fillings):

$$\nu = i/l,\ j/h, \quad i = 1, ..., h-1, \ \ j = 1, ..., l-1. \qquad (15)$$



Grey – regions of ZES existence in (k_y, ν) plane. Black lines are the lines of zero gap. Dashed line corresponds to half-filling $\mu = 0$. Parameter $\nu = \pi^{-1}\arccos(-\mu/4t)$ for nearest neighbors model and $\nu = \pi^{-1}\arccos(-\mu/2(t + \sqrt{t^2 - t'\mu}))$ for next nearest neighbors model

The conditions for zero-energy Andreev surface bound state to exist are studied for the lattice model of d-wave superconductor. Arbitrary surface orientation is considered for nearest neighbors as well as for next nearest neighbors models. The result is very sensitive to the surface orientation, and doesn't change continuously under surface-to-crystal angle rotation. In particular, for half-filled $(hl0)$-surface zero-energy Andreev surface states only appear under the condition that h and l are odd simultaneously.

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