

Density of states in d -wave superconductors of finite size

Ya. V. Fominov^{1,*} and A. A. Golubov^{2,†}

¹*L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia*

²*Faculty of Science and Technology, University of Twente, 7500 AE Enschede, The Netherlands*

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We consider the effect of the finite size in the ab plane on the surface density of states (DOS) in clean d -wave superconductors. We demonstrate that the angle-resolved DOS consists of energy bands that are formed similarly to the Kronig-Penney model. In contrast to the gapless DOS on a surface of a bulk sample, finiteness of the superconductor in one dimension provides the energy gap for all directions of quasiparticle motion except for $\theta=45^\circ$ (θ is the angle between the trajectory and the surface normal). As a result, the angle-averaged DOS behaves linearly at low energies. At the same time, the transport DOS can still have a gap. In the special case of $\alpha=0^\circ$ (α is the angle between the a axis of the crystal and the surface normal), the spectrum is gapped for all trajectories θ ; the angle-averaged DOS is also gapped. For $\alpha=45^\circ$, the spectrum is gapless for all θ ; the angle-averaged DOS is then large at low energies.

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A characteristic property of the d -wave superconductivity is the gapless spectrum of quasiparticles. The pair potential is anisotropic, and the gap vanishes along the nodal directions. Another source of low-energy quasiparticles is the surface, which leads to forming the midgap states (MGS)¹ due to the change of the sign of the pair potential along a trajectory upon reflection.

The d -wave superconductors can be employed in novel types of logic elements, qubits;^{2,3} there is experimental progress in this direction.^{4,5} However, the low-energy quasiparticles introduce decoherence in d -wave qubits.^{6,7} At the same time, the authors of Ref. 2 mention the possibility to suppress the low-energy quasiparticles due to the finite size of the d -wave banks.

In this paper, we systematically study the influence of the finite size of a d -wave superconductor on the low-energy density of states at the surface for all crystalline orientations and both types of low-energy states. There is only a limited number of results related to particular aspects of this issue. The angle-averaged surface density of states (DOS) was numerically studied by Nagato and Nagai for 45° -oriented superconductors.⁸ There are also results on the DOS in clean SN systems (where S is a conventional s -wave superconductor and N is a normal metal), which are relevant to the nodal directions of finite-size d -wave superconductors due to similarity of the pair potential profile along quasiparticle trajectories in the two systems. The works by van Gelder⁹ and Gallagher¹⁰ are the most relevant in this respect. In Ref. 11, Shelankov and Ozana suggested a method to treat multiple-interface superconducting systems and, as an application, numerically considered the DOS in a finite-size bilayer. Their results are relevant for the 45° trajectory in the d -wave system. Finally, we mention an analytical result of Ref. 12, where Fauchère *et al.* considered an SN system with repulsive interaction between the electrons in the N layer. In our language, their result refers to the splitting of the MGS.

We consider the system shown in Fig. 1(a). The profile of the pair potential along a quasiparticle trajectory depicted in Fig. 1(b), is not self-consistent, while the self-consistent pair potential is suppressed near the surfaces. However, the width

of the regions where this happens has the characteristic scale of the coherence length $\xi = v_F / 2\pi T_c$ (v_F is the Fermi velocity and T_c is the superconducting critical temperature). We assume $L \gg \xi$, then the piecewise constant Δ is a good approximation.

Technically, we solve the Eilenberger equations¹³ along the trajectory, determining the normal Green function g and the anomalous Green functions f and \bar{f} . Since the Green functions along the trajectory are continuous upon specular reflection at the surfaces of the d -wave superconductor, they obey the same condition in the effective one-dimensional problem described by Fig. 1(b): g , f , and \bar{f} must be continuous at the edges of the intervals of constant Δ . In addition, the Green functions are $2d$ periodic.

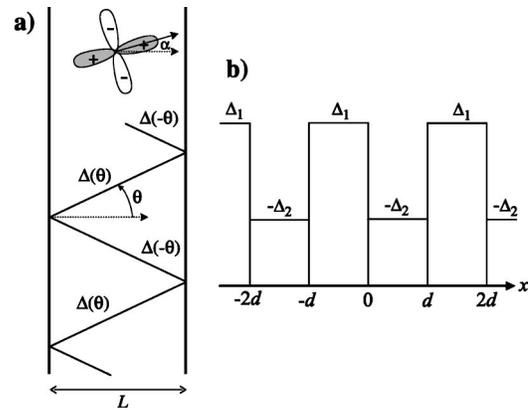


FIG. 1. (a) $d_{x^2-y^2}$ -wave superconductor of finite width L in the ab plane (quasi-two-dimensional strip). The orientation of the crystalline a axis with respect to the surface normal is denoted by α , then the angular dependence of the pair potential is $\Delta(\theta) = \Delta_0 \cos(2\theta - 2\alpha)$. We assume $0^\circ \leq \alpha \leq 45^\circ$ —this interval covers all physically different situations. (b) The pair potential along the trajectory described by the angle θ changes periodically between $\Delta_1 = \Delta(\theta)$ and $-\Delta_2 = \Delta(-\theta)$ on the surfaces of the superconductor; $d = L / \cos \theta$. The signs are chosen in such a way that the midgap states exist at $\Delta_1, \Delta_2 > 0$. For definiteness, we choose $\Delta_1 \geq \Delta_2$.

The DOS (normalized by its normal-metal value) is determined by the real part of the normal Green function $\nu = \text{Re } g$. The DOS is symmetric, $\nu(E) = \nu(-E)$. Straightforwardly solving the Eilenberger equations, we find the DOS at the interface between the intervals of constant Δ (this corresponds to the surface DOS in the d -wave superconductor):

$$\nu(x=0) = \text{Re} \frac{E \left[\sqrt{\Delta_1^2 - E^2} \tanh\left(\frac{k_2 d}{2}\right) + \sqrt{\Delta_2^2 - E^2} \tanh\left(\frac{k_1 d}{2}\right) \right]}{\sqrt{\left(\frac{\sqrt{\Delta_1^2 - E^2} \sqrt{\Delta_2^2 - E^2}}{\cosh(k_1 d/2) \cosh(k_2 d/2)} \right)^2 - \left[(E^2 + \Delta_1 \Delta_2) \tanh\left(\frac{k_1 d}{2}\right) \tanh\left(\frac{k_2 d}{2}\right) - \sqrt{\Delta_1^2 - E^2} \sqrt{\Delta_2^2 - E^2} \right]^2}}, \quad (1)$$

where $k_{1(2)} = 2\sqrt{\Delta_{1(2)}^2 - E^2}/v_F$.

A similar formula was obtained by Gallagher;¹⁰ at the same time, our results are different since his formula refers to the center of the strip in the d -wave problem, while we study the surface DOS. The zero-energy DOS can be found immediately. If $\Delta_1 \neq \Delta_2$, then Eq. (1) yields $\nu(E=0)=0$. If $\Delta_1 = \Delta_2$ ($\equiv \Delta$), then we obtain $\nu(E=0) = \cosh(\Delta d/v_F)$.

In Eq. (1), we did not assume $\Delta d/v_F \gg 1$, however, the piecewise constant pair potential [Fig. 1(b)] is a good approximation only under this condition.

Below we analyze Eq. (1) at low energies, $E \ll \Delta$, in the following relevant cases. (a) $\Delta_2 = 0$ (nodal directions), (b) $\Delta_1 \neq \Delta_2$, and (c) $\Delta_1 = \Delta_2$ (the latter two cases correspond to the presence of the MGS in the infinite system).

(1) *Effect of finite size on the nodal quasiparticles.* A nodal direction corresponds to $\Delta_2 = 0$. For brevity, we shall denote Δ_1 by Δ . In the bulk, the DOS along a nodal direction is normal metallic, $\nu_\infty = 1$.

The finite-size problem was considered previously (although in a different context) by van Gelder⁹ and Gallagher.¹⁰ They numerically demonstrated that in this superconducting version of the Kronig-Penney model,¹⁴ the quasiparticle spectrum consists of energy bands with square-root singularities at the band edges. Below we present analytical results for this problem.

Taking into account that $\Delta d/v_F \gg 1$ and $E \ll \Delta$, we obtain from Eq. (1) that there is a sequence of bands and the center of the lowest band is

$$E_0 = \frac{\pi v_F}{2d} \left(1 - \frac{v_F}{\Delta d} \right) \approx \frac{\pi v_F}{2d}. \quad (2)$$

In the vicinity of E_0 , the DOS can be written as

$$\nu = \frac{2\Delta_1 \Delta_2}{\Delta_1 + \Delta_2} \text{Re} \frac{E}{\sqrt{- \left[E^2 - \left(\frac{2\Delta_1 \Delta_2}{\Delta_1 + \Delta_2} \right)^2 (e_2 - e_1)^2 \right] \left[E^2 - \left(\frac{2\Delta_1 \Delta_2}{\Delta_1 + \Delta_2} \right)^2 (e_2 + e_1)^2 \right]}}, \quad (5)$$

where $e_{1(2)} = \exp(-\Delta_{1(2)} d/v_F)$.

$$\nu = \text{Re} \frac{v_F/d}{\sqrt{\left[2 \frac{v_F}{d} \exp\left(-\frac{\Delta d}{v_F}\right) \right]^2 - [E - E_0]^2}}, \quad (3)$$

hence the width of the band is

$$\delta E = 4 \frac{v_F}{d} \exp\left(-\frac{\Delta d}{v_F}\right) \quad (4)$$

and the DOS has square-root singularities at the edges of the band.

The physical mechanisms behind the above results are quite transparent. Instead of the normal-metallic situation that takes place for the nodal directions in the bulk, in the finite system we obtain the profile of the pair potential corresponding to the SN superlattice [Fig. 1(b) with $\Delta_2 = 0$]. Then the energy spectrum in each normal layer consists of the Andreev levels¹⁵ which are smeared into the bands due to periodicity of the system. The energy of the lowest Andreev level corresponds to the center of the band, see Eq. (2), while smearing is due to tunneling across the barrier of height Δ and width d , and thus contains the tunneling exponential, see Eq. (4).

(2) *Effect of finite size on the midgap states.* In the infinite system ($L, d \rightarrow \infty$), the midgap states arise if the pair potential changes its sign upon reflection from the surface.¹ According to our definitions (Fig. 1), this happens at $\Delta_1, \Delta_2 > 0$. The MGS are localized near the surfaces and have exactly zero energy; the corresponding DOS is $\nu_\infty = 2\pi \Delta_1 \Delta_2 (\Delta_1 + \Delta_2)^{-1} \delta(E)$. Below we consider the effect of finite d on this result; the results for the cases of differing and coinciding Δ_1 and Δ_2 will be qualitatively different.

In the general case, Δ_1 and Δ_2 are nonzero and different. Employing $\Delta_1 d/v_F, \Delta_2 d/v_F \gg 1$, and $E \ll \Delta_1, \Delta_2$, and expanding Eq. (1), we obtain

This yields two bands, symmetric around $E=0$. The center and the width of the positive-energy band are

$$E_0 = \frac{2\Delta_1\Delta_2}{\Delta_1 + \Delta_2} \exp\left(-\frac{\Delta_2 d}{v_F}\right), \quad (6)$$

$$\delta E = \frac{4\Delta_1\Delta_2}{\Delta_1 + \Delta_2} \exp\left(-\frac{\Delta_1 d}{v_F}\right). \quad (7)$$

At the edges, the DOS has square-root singularities.

The position of the center of the band in the limit $\Delta_1 \gg \Delta_2$ was calculated in Ref. 12 (although in a different context), while only discrete energy levels were discussed and the width of the band was not studied. Physically, the obtained results can be explained as follows. In the infinite system $d \rightarrow \infty$, the zero-energy levels are localized near the interfaces between Δ_1 and $-\Delta_2$. The first effect of finite d is to split the levels at the two neighboring interfaces due to tunneling across the Δ_2 barrier (the lowest barrier). This splitting is symmetric with respect to $E=0$. Physically, it is similar to the level splitting in the double-well potential. The second effect of finite d is to smear each of the split levels due to periodicity of the system (similarly to the Kronig-Penney model¹⁴); the smearing is due to tunneling across the Δ_1 barriers. As a result, the center and the width of the band (6) and (7) are determined by the tunneling exponentials containing Δ_2 and Δ_1 , respectively. Since $\Delta_2 < \Delta_1$, the splitting of the zero-energy level is larger than its smearing, hence a gap in the spectrum arises.

Now we consider the case $\Delta_1 = \Delta_2$ ($\equiv \Delta$). Then

$$\nu = \frac{\Delta}{\sqrt{E_b^2 - E^2}}, \quad E_b = 2\Delta \exp\left(-\frac{\Delta d}{v_F}\right). \quad (8)$$

Thus the MGS is smeared into the band of width $2E_b$ around zero. At the edges of the band, the DOS has square-root singularities.

This result means that the two bands (positive and negative) that existed at $\Delta_1 > \Delta_2$, touch each other at $E=0$ and merge into a single band, while the singularities at $E=0$ transform into the minimum. The equivalent result about the band centered at $E=0$ was numerically obtained in Ref. 11 (although in a different context).

The physical explanation of these results is the same as in the previous case $\Delta_1 > \Delta_2$. The only difference is that in the case of equal barriers $\Delta_1 = \Delta_2$, the splitting of the zero-energy level is exactly the same as its smearing, hence no gap in the spectrum appears.

The results for the angle-resolved DOS are illustrated in Fig. 2, which is a result of self-consistent numerical calculations. Our numerical method is similar to the one employed in Ref. 16.

The energy gap for the lowest band along the nodal direction ($\theta=25^\circ$) (Ref. 17) is larger than for the MGS directions ($\theta=30^\circ, 35^\circ, 40^\circ$, and 45°); this agrees with the analytical results according to which the gap for the nodal direction does not contain an exponentially small factor [see Eq. (2)]. The energy bands for the MGS directions are gapped if θ

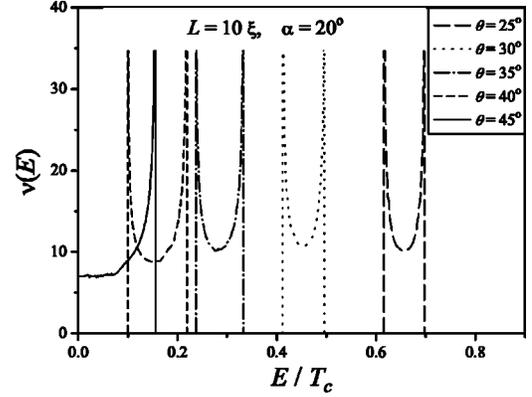


FIG. 2. The low-energy DOS for several trajectories θ .

$\neq 45^\circ$, which corresponds to the case $\Delta_1 \neq \Delta_2$. The $\theta=45^\circ$ direction corresponds to the case $\Delta_1 = \Delta_2$; the energy band is then gapless.

(3) *Angle-averaged DOS.* Let us consider the behavior of the angle-averaged surface DOS at $E \rightarrow 0$. The only contribution to the DOS arises from the vicinity of the angles at which $\Delta_1 = \Delta_2$; these are the $\theta = \pm 45^\circ$ angles (at any orientation α).

Denoting $\vartheta = \theta - \pi/4$, we simplify Eq. (5) at small ϑ and find that the angles contributing to the angle-averaged DOS at energy E , lie in the interval $-\vartheta_b < \vartheta < \vartheta_b$, where

$$\vartheta_b = \frac{E}{\frac{2\Delta\Delta'd}{v_F} \exp\left(-\frac{\Delta d}{v_F}\right)}, \quad (9)$$

and $\Delta = \Delta_0 \sin 2\alpha$, $\Delta' = 2\Delta_0 \cos 2\alpha$. We assume that $\Delta' \vartheta d/v_F \ll 1$; this condition for all ϑ up to ϑ_b is equivalent to $E \ll E_b$, where $E_b = 2\Delta \exp(-\Delta d/v_F)$ is the upper edge of the band. The angle-averaged DOS is

$$\nu_{\text{av}} = \frac{2}{\pi} \int_{-\vartheta_b}^{\vartheta_b} \nu(\vartheta) d\vartheta = \frac{E}{\frac{2\Delta\Delta'd}{v_F} \exp\left(-\frac{2\Delta d}{v_F}\right)}. \quad (10)$$

The DOS is zero at zero energy, and behaves linearly at small E . Thus the averaged surface DOS remains gapless but is strongly suppressed compared to that in the bulk d -wave superconductor.

The gapless structure of the angle-averaged DOS (10) is due to integrating in the vicinity of $\theta = \pm 45^\circ$, where the gap in the angle-resolved DOS vanishes. At the same time, the DOS probed by transport methods is

$$\nu_{\text{tr}} \sim \int \nu(\theta) D(\theta) d\theta, \quad (11)$$

and differs from Eq. (10) by the weighting factor $D(\theta)$, the angle-dependent transparency of the tunneling interface. When the tunneling interface has finite thickness, the function $D(\theta)$ is exponentially suppressed at not too small θ , then the contribution of the $\theta = \pm 45^\circ$ trajectories can be signifi-

cantly suppressed [since $\nu_{tr} \sim D(45^\circ)\nu_{av}$]. In this case, we can expect that the transport DOS ν_{tr} will be gapped despite the angular averaging. The directional selectivity of tunneling is most pronounced in the scanning tunneling spectroscopy experiments, where the effective tunneling cone around the surface normal can be as narrow as $\delta\theta \sim 20^\circ$.¹⁸

The result (10) does not refer to the cases $\alpha=0^\circ$ and $\alpha=45^\circ$; these cases are special. At $\alpha=0^\circ$, the MGS do not appear, and the low-energy DOS is entirely due to the nodal directions, the spectrum along which acquires a gap due to the finite size. The angular averaging preserves the gap, approximately given by Eq. (2).

At $\alpha=45^\circ$, the condition $\Delta_1=\Delta_2$ (which implies the gapless spectrum) is satisfied not only at $\theta=\pm 45^\circ$ but at any θ . Then angular averaging does not introduce new qualitative features (compared to the angle-resolved result), and the DOS at small energies is large. Comparing with the bulk case, we can say that the zero-energy peak in the DOS is smeared but not split. This agrees with the self-consistent numerical calculation of Nagato and Nagai.⁸

The above results refer to the surface DOS. However, the averaged DOS is linear at low energies also inside the strip, although the slope is different from Eq. (10), because the MGS contributing to this result decay into the bulk of the sample. For example, in the middle of the strip the angle-averaged DOS differs from Eq. (10) by an additional factor $2 \exp(-\Delta d/v_F)$. This result is again valid at $E \ll E_g$; this interval shrinks in the limit of large d , where the DOS is mainly determined by the standard nodal contribution at larger E .

Conclusions. Due to the finite size of the superconductor, the spectrum of nodal quasiparticles acquires an energy gap. The midgap states acquire the angle-dependent gap that vanishes for the $\theta=45^\circ$ trajectory; this result is valid unless the crystal is 0° or 45° oriented ($\alpha \neq 0^\circ$ or 45°). At $\alpha=0^\circ$, the MGS are absent, and the spectrum is gapped for all trajectories θ . On the opposite, at $\alpha=45^\circ$, the spectrum is gapless for all θ . In all the cases, the angle-resolved DOS consists of energy bands.

At $\alpha=0^\circ$ the angle-averaged DOS has a gap, while at $\alpha=45^\circ$ the angle-averaged DOS is finite at low energies. At $\alpha \neq 0^\circ$ or 45° , the angle-averaged surface DOS is strongly suppressed due to finite size, while remains gapless and behaves linearly at small energies. The low-energy contribution comes from the trajectories with $\theta \approx 45^\circ$, hence we can expect that the energy gap survives upon angular averaging if one measures the *transport* DOS in the case when the 45° -angle contribution is suppressed by the transparency of the tunneling barrier.

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*Electronic address: fominov@landau.ac.ru

[†]Electronic address: a.golubov@tnw.utwente.nl

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¹⁷At $\alpha=20^\circ$, one of the nodal directions in the bulk is $\theta=-25^\circ$. In the strip geometry, we call the $\theta=25^\circ$ direction nodal because the corresponding trajectory includes the nodal $\theta=-25^\circ$ segments [see Fig. 1(a)].

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