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Andreev bound states for cake shape superconducting–normal systems

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Abstract

The energy spectrum of cake shape normal–superconducting systems is calculated by solving the Bogoliubov–de Gennes equation. We take into account the mismatch in the effective masses and Fermi energies of the normal and superconducting regions as well as the potential barrier at the interface. In the case of a perfect interface and without mismatch, the energy levels are treated by semi-classics. Analytical expressions for the density of states and its integral, the step function, are derived and compared with that obtained from exact numerics. We find a very good agreement between the two calculations. It is shown that the spectrum possesses an energy gap and the density of states is singular at the edge of the gap. The effect of the mismatch and the potential barrier on the gap is also investigated.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

At the interface of the mesoscopic hybrid normal–superconducting (NS) junctions the underlying physics is controlled by the coherent evolution of electrons into holes due to the mechanism called Andreev reflection [1]. The growing interest in studying the role of the phase coherent Andreev reflection is motivated by the recent technological progress in manufacturing almost ballistic semiconductors of mesoscopic size coupled to a superconductor (for overview of the recent progress in this field see e.g. [2–5]). A ballistic normal dot weakly coupled to a superconductor is commonly called an Andreev billiard. The excitation spectrum (Andreev states) of such NS systems can be calculated from the Bogoliubov–de Gennes equation (BdG) [6]. A film of normal metal in contact with a semi-infinite superconductor was considered by de Gennes and Saint-James [7], and can be regarded as the first such Andreev billiard. The bound states of Andreev billiards have been extensively studied over the past

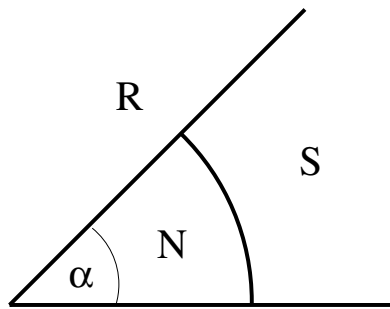


Figure 1. A cake shape Andreev billiard formed from a cake shape of normal dot (N) in contact with a superconductor (S).

ten years [8–16, 18–20]. The excitation spectrum was studied for SNS junctions [21–25], too. The energy levels of the strong magnetic field were investigated for a semi-infinite N region in contact with a semi-infinite S region [26] and ring-shaped Andreev billiards [27]. The Andreev bound states for superconducting–ferromagnetic systems have also been studied (see, e.g., [28] and references therein).

An important physical quantity for Andreev billiards is the density of states (DOS). For a perfect NS interface (in the absence of a tunnel barrier at the NS interface, and mismatch in the Fermi energies and effective masses between the N and S regions) a semi-classical Bohr–Sommerfeld approximation of the DOS was derived for excitation energies close to the Fermi energy [9, 10, 13–15]. It was shown that the DOS can be related to the purely geometry-dependent path length distribution $P(s)$ which is the classical probability that an electron entering the N region at the NS interface returns to the interface after a path length s . In recent works [19, 20, 28] an improved semi-classical Bohr–Sommerfeld approximation of the DOS has been presented, in which the energy-dependent phase shift for Andreev reflections is properly taken into account. It has been shown that the exact quantum mechanical calculations for different Andreev billiards with a perfect NS interface gives good agreement with the semi-classical predictions for all energies below the bulk superconducting gap (not only at energies close to the Fermi energy). For an NS system possessing a finite cut-off in $P(s)$, a gap appears in the energy spectrum which can be as large as half of the bulk superconducting gap [19]. Based on the semi-classical expression of the DOS, a simple formula for this gap was also derived for such Andreev billiards.

In this paper our aim is twofold. First, we propose a new class of Andreev billiards which can also exhibit a gap owing to the finite cut-off in $P(s)$. Second, we study how the gap is suppressed for realistic NS systems in which the NS interface is imperfect. To this end we consider a ‘cake shape Andreev billiard’ shown in figure 1 in which the boundaries of the N and S regions are formed by two radii at an angle α and the NS interface is an arc between them.

Recently Adagideli *et al* [16] investigated the Andreev billiards formed from an arbitrary shape of normal region surrounded by superconductors. Their theoretical predictions have been tested numerically in the case of circular shape of normal region. Similarly, the circular case has been studied by Stone [17]. This NS system is very similar to our cake shape Andreev billiards for $\alpha = 2\pi$. The only difference is that in our case there is an infinite potential barrier along a radius.

The text is organized as follows. In section 2 a quantization condition (secular equation) is derived from the BdG equation for the general case of imperfect NS interface. In section 3

the density of states is derived from semiclassics for the case of perfect NS interface. Our numerical results for the gaps in case of imperfect NS interface are presented in sections 4 and 5. Finally, the conclusions are given in section 6.

2. Exact quantum calculation

In this section we derive a secular equation for the energy levels of cake shape Andreev billiards shown in figure 1, in the general case of imperfect NS interface. The BdG equation for the NS systems can be written as

$$\begin{pmatrix} H_0 & \Delta(\mathbf{r}) \\ \Delta(\mathbf{r})^* & -H_0 \end{pmatrix} \Psi = E\Psi, \quad (1)$$

where $H_0 = \mathbf{p}^2/2m_{\text{eff}} + V(\mathbf{r}) - \mu$ is the single-particle Hamiltonian, $\mu = E_F^{(N)}, E_F^{(S)}$ are the Fermi energies, $m_{\text{eff}} = m_N, m_S$ are the effective masses in the N/S regions, Ψ is a two-component wavefunction, and E is the quasi-particle energy measured from the Fermi energy $E_F^{(N)}$. The tunnel barrier $V(\mathbf{r})$ at the NS interface in polar coordinates (r, φ) is modelled in a usual way by $V(r, \varphi) = U_0\delta(r - R)$. We also adopt the usual step-function model [29] for the pair potential and take $\Delta(\mathbf{r}) = \Delta\Theta(r - R)$. An infinite potential is assumed at the straight segments of the boundary of the NS system, i.e., the Dirichlet boundary conditions are applied for the wavefunction Ψ . In this work we are interested in the discrete energy levels, i.e., it is assumed that $0 < E < \Delta$.

It is easy to see that the Hamiltonian is separable in polar coordinates. The φ dependence of wavefunction Ψ is identical in the N and S regions. After separating the φ dependence of Ψ the BdG equation reduces to two Bessel equations [30] for the radial dependence of the two components of Ψ . Thus, one can show that the ansatz for the wavefunctions in the N region can be written as

$$\Psi_m^{(N)}(r, \varphi) = \begin{pmatrix} a_+ J_{\nu_m}(k_+ r) \\ a_- J_{\nu_m}(k_- r) \end{pmatrix} \sin(\nu_m \varphi), \quad (2)$$

while in the S region the wavefunction has the form

$$\Psi_m^{(S)}(r, \varphi) = \left[c_+ \begin{pmatrix} \gamma_+ \\ 1 \end{pmatrix} H_{\nu_m}^{(1)}(q_+ r) + c_- \begin{pmatrix} \gamma_- \\ 1 \end{pmatrix} H_{\nu_m}^{(2)}(q_- r) \right] \sin(\nu_m \varphi), \quad (3)$$

where $\nu_m = \frac{m\pi}{\alpha}$ ($m = 1, 2, \dots$), $J_{\nu_m}(x)$ and $H_{\nu_m}^{(1,2)}(x)$ are the Bessel and the Hankel functions [30], and

$$k_{\pm} = k_F^{(N)} \sqrt{1 \pm \frac{E}{E_F^{(N)}}}, \quad (4)$$

$$q_{\pm} = k_F^{(S)} \sqrt{1 \pm i \frac{\sqrt{\Delta^2 - E^2}}{E_F^{(S)}}}, \quad (5)$$

$$\gamma_{\pm} = e^{\pm i \arccos(E/\Delta)}. \quad (6)$$

Here \pm refer to the electron/hole-like quasi-particle excitation and the Fermi wavenumbers in the N/S regions are given by $k_F^{(N)} = \sqrt{2m_N E_F^{(N)}/\hbar^2}$ and $k_F^{(S)} = \sqrt{2m_S E_F^{(S)}/\hbar^2}$. The eigenfunctions of the energy levels are labelled by a fixed integer number m . In the N region only the Bessel function can be used for the radial wavefunction since the Neumann function is singular at the origin. The wavefunction Ψ in the S region must tend to zero as $r \rightarrow \infty$. This condition can be satisfied by choosing the appropriate Hankel function for the electronic and

hole-like component of Ψ in the following way. It is known [30] that for large r the Hankel functions $H_{\nu_m}^{(1)}(q_+r) \sim \sqrt{2/(q_+r)}e^{iq_+r}$. Since q_+ has a positive imaginary part one finds that $H_{\nu_m}^{(1)}(q_+r) \rightarrow 0$ for $r \rightarrow \infty$. Similarly, $H_{\nu_m}^{(2)}(q_-r) \rightarrow 0$ for $r \rightarrow \infty$.

The φ -dependent part of the wavefunctions in the N and S regions ensures that they satisfy the Dirichlet boundary conditions at the straight segments of the Andreev billiard. At the NS interface the matching conditions [31, 18] should be applied. The four coefficients a_{\pm} , c_{\pm} in equations (2) and (3) are determined from the matching conditions:

$$\Psi_m^{(N)}|_{r=R} = \Psi_m^{(S)}|_{r=R}, \quad (7)$$

$$\frac{d}{dr} \left[\Psi_m^{(N)} - \frac{m_N}{m_S} \Psi_m^{(S)} \right] \Big|_{r=R} = -\frac{2m_N}{\hbar^2} U_0 \Psi_m^{(S)} \Big|_{r=R}. \quad (8)$$

Substituting the ansatz given by equations (2) and (3) into (8) one finds the following secular equation for the eigenvalues E of the NS system for fixed mode index m :

$$\text{Im}\{\gamma_+ D_m^{(+)}(E) D_m^{(-)}(E)\} = 0, \quad (9)$$

where $\text{Im}\{\cdot\}$ stands for the imaginary part and the two by two determinants $D_m^{(\pm)}(E)$ are given by

$$D_m^{(+)}(E) = \begin{vmatrix} D_{11}^{(+)} & D_{12}^{(+)} \\ D_{21}^{(+)} & D_{22}^{(+)} \end{vmatrix}, \quad (10)$$

$$D_m^{(-)}(E) = [D_m^{(+)}(-E)]^*, \quad (11)$$

with matrix elements

$$D_{11}^{(+)} = J_{\nu_m}(k_+R), \quad (12)$$

$$D_{12}^{(+)} = H_{\nu_m}^{(1)}(q_+R), \quad (13)$$

$$D_{21}^{(+)} = k_+ J'_{\nu_m}(k_+R), \quad (14)$$

$$D_{22}^{(+)} = -2k_F^{(N)} Z H_{\nu_m}^{(1)}(q_+R) + \frac{m_N}{m_S} q_+ H_{\nu_m}^{(1)'}(q_+R), \quad (15)$$

and $Z = U_0 k_F^{(N)} / (2E_F^{(N)})$ is the normalized barrier strength used by Blonder *et al* [29]. The primes denote the derivatives of the Bessel and Hankel functions with respect to their arguments. For a given quantum number m the energy levels of cake shape Andreev billiards for an imperfect interface are the solutions of the secular equation given by equation (9). This equation is exact in the sense that the usual Andreev approximation is not used. In the Andreev approximation it is assumed that $\Delta/E_F^{(S)} \ll 1$ and quasiparticles whose incident/reflected directions are approximately perpendicular to the NS interface [5].

3. Perfect NS interface

In the case of a perfect NS interface, the semi-classical expression for the DOS can be derived from the secular equation (9). We assume that there is no mismatch or tunnel barrier at the NS interface ($m_N = m_S$, $E_F^{(N)} = E_F^{(S)}$ and $Z = 0$). For simplicity, we shall omit the superscript N and S in the wavenumbers and the Fermi energies.

In the Andreev approximation ($\Delta/E_F \ll 1$) we take $k_+ \approx q_+$ in places where they are multiplied by the Bessel or Hankel functions in $D_m^{(+)}(E)$ given by equation (10) but in the arguments of the Bessel and Hankel functions we keep them different. To approximate $D_m^{(+)}(E)$ the Debye asymptotic expansion [30] of the Bessel functions will be used for $|\nu_m| < k_+R - \sqrt[3]{k_+R}$. For Hankel functions of a complex argument z the principal asymptotic

forms [30] $H_v^{(1)}(z) \approx \sqrt{2/(\pi z)} e^{i(z - \frac{1}{2}v\pi - \frac{\pi}{4})}$ for $|z| \rightarrow \infty$ will be applied. After some algebra, the quantization condition (9) can be simplified as

$$\frac{\vartheta(k_+R, v_m) - \vartheta(k_-R, v_m) - \arccos \frac{E}{\Delta}}{\pi} = n, \quad (16)$$

where

$$\vartheta(x, v) = \sqrt{x^2 - v^2} - |v| \arccos \frac{|v|}{x}, \quad (17)$$

and n is a non-negative integer. This is the Bohr–Sommerfeld quantization condition for cake shape Andreev billiards. The function $\vartheta(k_{\pm}R, v_m)$ is proportional to the radial action of the electron/hole-like quasiparticles [32]. For a given m and n the solution of (16) gives the E_{mn} energy level in the Bohr–Sommerfeld approximation.

We now introduce the so-called step function $N(E)$ which is the number of energy levels below the energy E . This is indeed the integrated DOS $\varrho(E)$ of the Andreev billiards:

$$N(E) = \int_{-\infty}^E \varrho(E') dE' = \sum_{mn} \Theta(E - E_{mn}), \quad (18)$$

where $\Theta(x)$ is the Heaviside function. To calculate the step function in the Bohr–Sommerfeld approximation, equation (16) is Taylor expanded in terms of the small quantity E/E_F . Keeping the leading terms one finds

$$\frac{E}{E_F} \sqrt{(k_F R)^2 - v_m^2} = n\pi + \arccos \frac{E}{\Delta}. \quad (19)$$

Substituting the solutions E_{mn} of this equation into (18) gives the step function $N_{BS}(E)$ in the Bohr–Sommerfeld approximation. Applying the Poisson summation formula [33, 32] in the sum over m of $N(E)$ and keeping only the non-oscillating term we find

$$N_{BS}(E) = \sum_{n=0}^{\infty} \int_{-\frac{1}{2}}^{M+\frac{1}{2}} \Theta(E - E_{mn}) dm = \sum_{n=0}^{\infty} m^*(E, n), \quad (20)$$

where $m^*(E, n)$ is the solution of equation (19) for m at a given E and n , and $M = \frac{\alpha}{\pi} k_F R$ is the largest m for which the argument of the square root in the left-hand side of (19) is still positive.

After some simple algebra we obtain the final form of the step function in the Bohr–Sommerfeld approximation:

$$N_{BS}(E) = M \sum_{n=0}^{\infty} \{1 - F[s_n(E)]\}, \quad (21)$$

where

$$F(s) = \int_0^s P(s') ds', \quad (22)$$

$$P(s) = \frac{1}{(2R)^2} \frac{s}{\sqrt{1 - (s/2R)^2}} \Theta(2R - s), \quad (23)$$

$$s_n(E) = \frac{n\pi + \arccos \frac{E}{\Delta}}{E/\Delta} \pi \xi_c, \quad (24)$$

$M = \frac{\alpha}{\pi} k_F R$ and $\xi_c = \hbar v_F / (\pi \Delta) = 2E_F / (\pi k_F \Delta)$ is the coherence length. It can be shown that $P(s)$ is the classical probability that an electron entering the billiard at the NS interface returns to the interface after a path length s . One can see that $P(s)$ depends only on the radius R of the

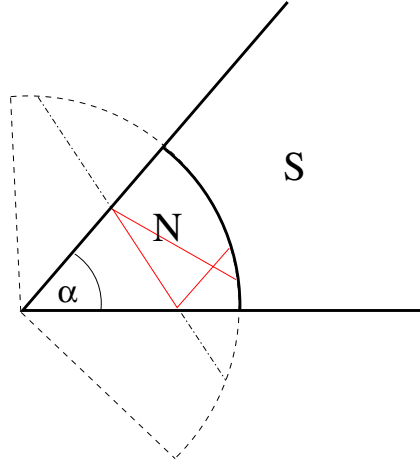


Figure 2. Unfolded trajectory in the cake shape Andreev billiard.

N region and is independent of the angle α . This feature can be understood from a classical point of view. The unfolded trajectory of the particle starting and ending at the NS interface shown in figure 2 is always a chord of a circle of radius R , thus its length is independent of the angle α . The path length distribution $P(s)$ is normalized to one, i.e., $\int_0^\infty P(s) ds = 1$. The integrated path length distribution is $F(s) = (1 - \sqrt{1 - (s/2R)^2})\Theta(2R - s)$.

The DOS $\varrho_{\text{BS}}(E) = dN_{\text{BS}}(E)/dE$ in the Bohr–Sommerfeld approximation can be easily obtained from (21) and reads as

$$\varrho_{\text{BS}}(E) = M \int_0^\infty ds P(s) \left[\frac{s}{\hbar v_F} + \frac{1}{\sqrt{\Delta^2 - E^2}} \right] \sum_{n=0}^\infty \delta \left(\frac{sE}{\hbar v_F} - \left(n\pi + \arccos \frac{E}{\Delta} \right) \right), \quad (25)$$

where v_F is the Fermi velocity. Note that expressions (21) and (25) for the step function and the DOS in the semi-classical approximation are the same as that presented in [19, 20] for general shapes of Andreev billiards. Our formula for the DOS, valid for all energy $E < \Delta$, can be regarded as an extension of that derived by Melsen *et al* [9, 10], Lodder and Nazarov [13], Schomerus and Beenakker [14], and Ihra *et al* [15] in the limit $E \ll \Delta$. In these works, the energy-dependent phase shift $-\arccos(E/\Delta)$, due to Andreev reflections, was approximated by $\pi/2$, while in our result this phase shift is fully incorporated.

In figure 3 the numerically calculated exact step function $N(E)$ obtained by solving equation (9) together with its semi-classical approximation $N_{\text{BS}}(E)$ from equation (21) as functions of the energy E below the bulk gap Δ are shown for angles $\alpha = \pi, \pi/2, \pi/3$. One can see that the agreement between the two results is excellent for all energy $E < \Delta$. To see the difference between the two calculations, the inset shows an enlarged part of the main frame.

The step functions shown in figure 3 have cusps at some energies. This implies that the DOS has peaks at these energy values. Since the semi-classical approximation of the exact step function is very good, one can derive an expression for the positions of these peaks starting from (21). It is clear from (23) that $P(s)$ is singular at $s = 2R$. This implies that the DOS will be singular at those energies when $s_n(E) = 2R$. Using (24) and the approximation $\arccos(E/\Delta) \approx \pi/2 - E/\Delta$ the positions of these singularities in the DOS are given by

$$\frac{E_n^{(\text{sing})}}{\Delta} = \frac{(n + 1/2)\pi}{1 + 2R/(\pi \xi_c)} \quad (26)$$

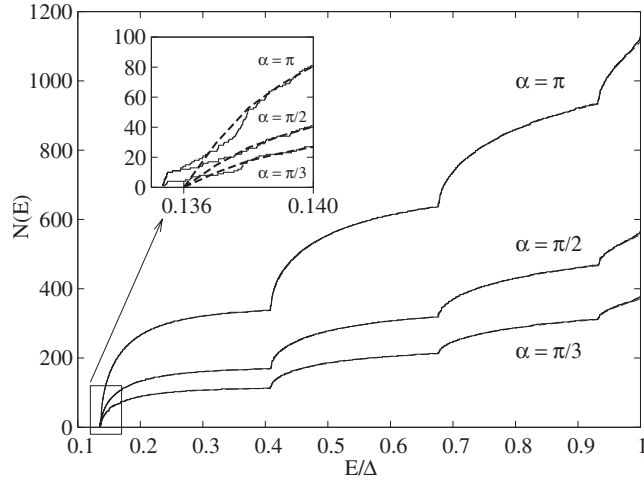


Figure 3. The exact step function $N(E)$ (solid curves) from equation (9) and its semi-classical approximation $N_{BS}(E)$ (dashed curves) given by equation (21) for the cake shape Andreev billiards of angles $\alpha = \pi, \pi/2, \pi/3$ as functions of E/Δ . The inset shows an enlarged part of the main frame. The parameters are $k_F R = 350$ and $\Delta/E_F = 0.03$. With these data $\xi_c/R = 0.06$. The numerically obtained exact gap from equation (9) is $E_{\text{gap}}/\Delta = 0.1355$, while its semi-classical value from equation (27) is $E_{\text{gap}}/\Delta = 0.1366$.

valid for all integral n for which $E_n^{(\text{sing})} < \Delta$. It is worth mentioning that the positions of the singularities are *independent* of the angle α of the cake shape Andreev billiards.

Figure 3 also shows that in the energy spectrum of the system there is a quite large gap. This gap always exists for cake shape Andreev billiards. To derive a formula for the value of the gap one can also start from the semi-classical approximation. It is obvious that $P(s)$ possesses an upper cut-off, i.e., $P(s) = 0$ if $s > s_{\text{max}} = 2R$. Thus, from equation (24) it follows that the energy spectrum has a lower bound. An approximate value of this energy can be obtained by setting $n = 0$ in (26) since the position of the singularity and the upper cut-off of $P(s)$ is identical for cake shape Andreev billiards. The lowest energy level (the gap of the spectrum) in the semi-classical approximation becomes

$$\frac{E_{\text{gap}}}{\Delta} = \frac{\pi/2}{1 + 2R/(\pi\xi_c)}. \quad (27)$$

For $\xi_c \ll R$ the gap is $E_{\text{gap}}/\Delta \approx \pi^2\xi_c/(4R)$. It is clear that the value of the gap is also *independent* of the angle α of the cake shape Andreev billiards. From figure 2 one can see that the length of the longest possible chord is $2R$. Therefore, the cut-off of the path length distribution $P(s)$ is always $2R$ and obviously independent of α .

It is easy to express the gap E_{gap} in units of the mean level spacing δ_N of the isolated normal region. It is well known that $\delta_N = 2\pi\hbar^2/(m_N A)$, where $A = \frac{1}{2}R^2\alpha$ is the area of the normal region [32]. Then, from (27) one finds

$$\frac{E_{\text{gap}}}{\delta_N} = \frac{\alpha k_F R}{16} \quad (28)$$

for $\xi_c \ll R$. In a macroscopic sample $k_F R \sim R/\lambda_F \gg 1$, where λ_F is the de Broglie wavelength. Thus, the gap in the cake shape Andreev billiards can be a large value on the energy scale of the mean level spacing.

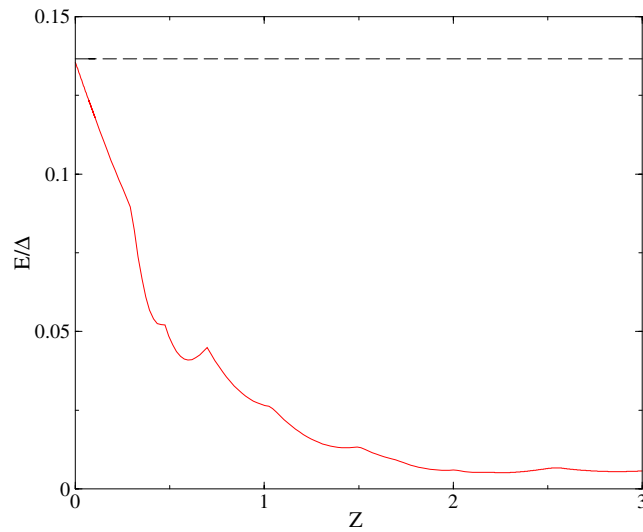


Figure 4. Numerically calculated energy gap (in units of Δ) as a function of Z . For $Z = 0$ the semi-classical result from (27) is indicated by the dashed curve. The parameters are the same as in figure 3, and $r_k = 1$ and $r_v = 1$.

4. NS interface with potential barrier

In this section we investigate the dependence of the gap on the potential barrier at the NS interface. Here we assume that the effective masses and the Fermi energies between the normal and the superconducting regions are the same. Following Mortensen *et al* [34] the mismatch of the N and S regions is characterized by the ratio of the Fermi wavenumbers and the Fermi velocities of the two regions $r_k = k_F^{(N)}/k_F^{(S)}$ and $r_v = v_F^{(N)}/v_F^{(S)}$. It is easy to show that the ratio of the effective masses and the Fermi energies appearing in the secular equation (9) can be expressed by the parameters r_k and r_v in the following way: $m_S/m_N = r_v/r_k$ and $E_F^{(N)}/E_F^{(S)} = r_k r_v$. The energy levels of the systems are calculated by solving the secular equation (9) for different Z , and for $r_k = 1$ and $r_v = 1$. The result is shown in figure 4. It is seen from the figure that the gap is decreased with increasing potential barrier. This is owing to the fact that the probability of the normal reflection is increased and the condition for perfect Andreev reflection is suppressed.

5. NS interface in the case of mismatch

We now present our numerical results for the gap when there is a mismatch in the effective masses and the Fermi energies of the N and S regions. The numerical solution of the secular equation (9) gives the energy levels of the system. The lowest level can be associated with the gap. In figure 5 the gap is plotted as a function of r_k and r_v . The surface plot shows that the suppression of the gap is very sensitive to the parameter r_v but practically independent of r_k .

6. Conclusions

We calculated the Andreev bound states of cake shape Andreev billiards by solving the Bogoliubov–de Gennes equation. Matching the wavefunctions in the normal and

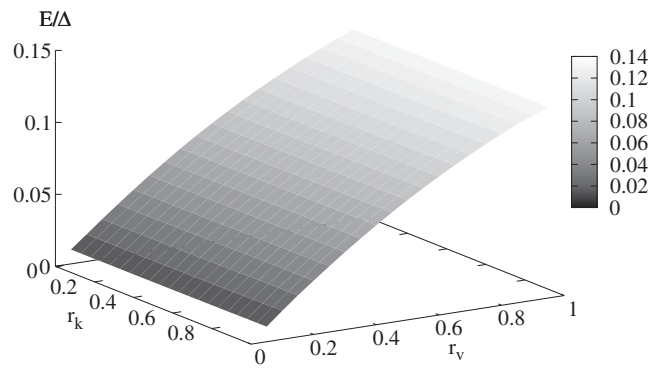


Figure 5. Numerically calculated energy gap (in units of Δ) as a function of r_k and r_v . The parameters are $\alpha = \pi$, $k_F^{(N)}R = 350$, $\Delta/E_F^{(N)} = 0.03$ and $Z = 0$.

superconducting regions we obtained a secular equation for the energy levels of the system. In the exact calculation the different effective masses and Fermi energies of the two regions, and the potential barrier at the NS interface, are taken into account. For a perfect interface we derived a semi-classical expression for the step function and the DOS of the energy spectrum. These quantities are expressed by the classical return probability $P(s)$ of the particles. It was found that the cake shape Andreev billiards always possessed a gap. An analytical expression was derived for the value of the gap for perfect interface. We also showed that the DOS has singularities at some energies given by a simple formula. Since the cut-off of $P(s)$ is the same as that at which $P(s)$ is singular, we found that at the edge of the gap the DOS is singular. Similarly, the gap is independent of the angle α of the cake shape Andreev billiard. We think that these facts can be exploited experimentally to measure the value of the gap. The Andreev bound states determine the tunnelling conductance of the NS systems. Thus, the measured conductance (proportional to the DOS) should be changed abruptly at the edge of the gap. A cake shape Andreev billiard with $\alpha = \pi$ can be made by cutting a semi-circle region from a semi-infinite bulk superconductor and replacing that by a normal region.

We also investigated that how the imperfect NS interface and mismatch in the material parameters of the normal and superconducting regions can affect the value of the gap. We found that the gap decreases with increasing potential barrier at the NS interface. We also calculated the value of the gap as a function of the ratio r_k of the Fermi wavenumbers and the ratio r_v of the Fermi velocities of the normal and superconducting regions. In [34] it has been shown that r_k determines the ratio of the sines of the incident and outgoing angles of a particle at the NS interface. This implies, and this is indeed supported by our numerical results, that the value of the gap is very weakly dependent on the parameter r_k . However, our numerics show a strong dependence of the gap on the parameter r_v : increasing the mismatch in the Fermi velocities decreases the value of the gap.

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