Shape resonances in the superconducting order parameter of ultrathin nanowires

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We study the shape resonance effect associated with the confined transverse superconducting modes of a cylindrical nanowire in the clean limit. Results of numerical investigations of the Bogoliubov-de Gennes equations show significant deviations of the energy gap parameter from its bulk value with a profound effect on the transition temperature. The most striking is that the size of the resonances is found to be by about order of magnitude larger than in ultrathin metallic films with the same width.

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Modern rapid miniaturization of electronic circuits requires good understanding of basic mechanisms responsible for the electronic properties of nanoscale structures. The most important point about these structures is that the quantum-confinement effects play the corner-stone role in this case. One can even say in general that recent success in nanofabrication technique has resulted in great interest in various artificial physical systems with unusual phenomena driven by the quantum confinement (quantum dots, nanoscale semiconductors, nanosuperconductors, etc.). The quantum-confined superconductivity is here of special interest due to the macroscopic quantum character: any effect on electron wave functions manifests itself directly in the superconducting order parameter.

An obvious consequence of the confinement in a nanoscale superconducting structure is nonuniform spatial distribution of the superconducting condensate because, as it is known since the classical papers by Gor’kov [1] and Bogoliubov [2], the superconducting order parameter can be interpreted as the wave function of the center-of-mass motion of a Cooper pair. It is also known that the Cooper-pair wave function involves important in-medium terms [3]. In the presence of the electron confinement these terms can result in shape resonances in the energy gap parameter, another confinement effect first found and investigated in the paper by Blatt and Thompson [4] for ultrathin metallic films. A shape resonance in the dependence of the energy-gap parameter on the specimen dimensions can occur any time when an electron subband appearing due to the size quantization passes through the Fermi surface [4]. Strong indications for such behaviour are found not only in ultrathin films but also in nanoparticles (see, for example, Refs. [5] and [6]) and superfluid nuclei [7, 8] (as it had been predicted by Blatt and Thompson). Recently a new technique of electrodeposition into extended nanopores has been developed [9], which makes it possible to produce single-crystal nanowires of high quality. Thus, the shape resonances in the nanowire superconducting order parameter can be investigated in the clean limit, with a direct link to the microscopic (BSC) theory. In particular, it is of importance to explore the situation where the QPS (quantum phase slips) regime [9, 10, 11, 12] is expected to generate a new low-temperature metallic phase with proliferating quantum phase slips of the superconducting order parameter (for radii less than 5 nm) [13]. The point is that when calculating the QPS energy barrier [13] in ultrathin nanowires, one assumes the superconducting order parameter being uniform in the transverse direction but with the phase slips in the longitudinal one [13]. The absolute value of the order parameter is set to be equal to the bulk one. However, at a resonant point the superconducting condensate shows significant spatial variations in the transverse direction, and its mean absolute value can be much larger than that of the bulk material. Note that the quantum confinement can influence the superconducting state by two channels. The first is due to change in electron wave functions (this is a main reason for the shape resonance effect). Whereas the second is connected with the confined phonons. The both channels were examined for ultrathin metallic films [14], which makes it possible to expect that confinement modifications of the phonon modes can produce quantitative corrections if the nanowire width is less than or about 2 nm. In the present work the first channel is under consideration, while the phonons are taken to be the same as in the bulk material. Thus, below we investigate the shape resonance effect associated with the confined transverse superconducting modes of an ultrathin nanowire in the clean limit.

To explore the superconducting order parameter varying with position, one should use the Bogoliubov-de Gennes (BdG) equations [15]. We are interested in numerical solutions of BdG equations taken in the absence of magnetic field for a superconducting cylinder with the radius $R$ and length $L$. In all the calculations $L$ remains the same and equal to 2000 nm while $R$ is varied from 1 nm to 10 nm. In the absence of magnetic field the superconducting order parameter $\Delta(r)$ can be chosen as a real quantity (phase effects are beyond the scope of our consideration) and the
FIG. 1: The relative gap of the quasiparticle spectrum $\Delta_R/\Delta_{\text{bulk}}$ (panels (a1) and (b1)) and relative chemical potential $\mu_R/\mu_{\text{bulk}}$ (panels (a2) and (b2)) versus the nanowire radius $R$: the panels (a1) and (a2) represent the data calculated for $n_e = 3.878$ nm$^{-3}$ (the bulk chemical potential $\mu_{\text{bulk}} = 900$ meV); the panel (b1) and (b2) are the data for $n_e = 20$ nm$^{-3}$ ($\mu_{\text{bulk}} = 2687$ meV). Squares are the results of numerical investigations of the BdG equations, the solid line is the spline interpolation.

BdG equations have the form

$$E_n u_n(r) = \left(-\frac{\hbar^2}{2m^*} \nabla^2 - \mu \right) u_n(r) + \Delta(r) v_n(r),$$

(1)

$$E_n v_n(r) = \Delta(r) u_n(r) - \left(-\frac{\hbar^2}{2m^*} \nabla^2 - \mu \right) v_n(r),$$

(2)

where $E_n$ stands for the quasiparticle spectrum, $\mu$ is the chemical potential and $m^*$ denotes the electron band mass. The single electron wave functions $u_n$ and $v_n$ make a contribution to the order parameter via the self-consistency relation

$$\Delta(r) = g \sum_n u_n(r) v_n^*(r) (1 - 2f(E_n)),$$

(3)

where $g$ is the coupling constant and $f(x)$ is the Fermi function $f(x) = 1/(\exp(\beta x) + 1)$, $\beta = 1/(k_B T)$ with $T$ the temperature and $k_B$ the Boltzmann constant. Summation in Eq. (3) is taken over the eigenstates with the kinetic energy (including the chemical potential) within the window $[-\hbar \omega_D, \hbar \omega_D]$, and $\omega_D$ is the Debye frequency. The chemical potential is fixed by

$$n_e = 2 \sum_n \left[ |u_n(r)|^2 f(E_n) + |v_n(r)|^2 (1 - f(E_n)) \right]$$

(4)
Then, a matrix form convenient for the numerical iteration procedure typical for a self-consistent mean-field treatment.

The resonance size is now by order of magnitude larger than in ultrathin films of the same width (see the results for cylindrical nanowire in agreement with the results for ultrathin films and nanoparticles. But what is surprising is that due to the electron confinement in the transverse directions we should put

\[ n = (j, m, k) \]

with \( n_e \) the total electron density. Introducing the cylindrical coordinates \( \rho, \varphi, z \), we can write \( \Delta(r) = \Delta(\rho) \) as the periodical boundary conditions are implied in the longitudinal (\( z \)) direction. In this case we get

\[
u_{jm}(r) = \bar{u}_{jm}(\rho) e^{im\varphi} e^{ikz}, \quad v_{jm}(r) = \bar{v}_{jm}(\rho) e^{im\varphi} e^{ikz}, \quad (5)
\]

where \( n = (j, m, k) \) with \( j \) the quantum number associated with \( \rho \)-coordinate, \( m \) the azimuthal quantum number and \( k \) the wave vector in \( z \)-direction. Substituting Eq. (5) into Eqs. (1) and (2), we recast the BdG equations in terms of \( \bar{u} \) and \( \bar{v} \):

\[
E_{jm} \bar{u}_{jm}(\rho) = \left[ -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) - \frac{m^2}{\rho^2} - k^2 \right] \bar{u}_{jm}(\rho) + \Delta(\rho)\bar{v}_{jm}(\rho),
\]

\[
E_{jm} \bar{v}_{jm}(\rho) = \Delta(\rho)\bar{u}_{jm}(\rho) - \left[ -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) - \frac{m^2}{\rho^2} - k^2 \right] \bar{v}_{jm}(\rho).
\]

Due to the electron confinement in the transverse directions we should put

\[
\bar{u}_{jm}(R) = \bar{v}_{jm}(R) = 0.
\]

Then, \( \bar{u} \)– and \( \bar{v} \)–functions are expanded in terms of the Bessel functions, and Eqs. (6) and (7) can be converted into a matrix form convenient for the numerical iteration procedure typical for a self-consistent mean-field treatment.

Numerical investigation of Eqs. (6) and (7) reveals the resonance structure of the energy gap parameter of a cylindrical nanowire in agreement with the results for ultrathin films and nanoparticles. But what is surprising is that the resonance size is now by order of magnitude larger than in ultrathin films of the same width (see the results for ultrathin metallic films with the width 10 nm (1) and R = 5.75 nm (2) for the Al parametric set; (b), the resonance point R = 9.642 nm for the Sn parameters.

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**FIG. 2:** The superconducting order parameter \( \Delta(\rho) \) versus \( \rho \) at \( n_e = 3.878 \, \text{nm}^{-3} \) and \( T = 0 \): (a), the resonance points \( R = 5.06 \, \text{nm} \) (1) and \( R = 5.75 \, \text{nm} \) (2) for the Al parametric set; (b), the resonance point \( R = 9.642 \, \text{nm} \) for the Sn parameters.
but depends on the width. For example, for the resonances at $R = 0.86 \text{ nm}$ and $R = 1.12 \text{ nm}$ (the panel (a1) of Fig[1]) we have found $\Delta R/(k_B T_{c,R}) \approx 1.28$. Hence, to get an idea about $T_{c,R}/T_c$ for $0.8 \text{ nm} \leq R \leq 1.8 \text{ nm}$ at $n_0 = 3.878 \text{ nm}^{-3}$, one can simply multiply the data of Fig[1] (a1) by a factor of about 1.375. Situation with panel (b1) of Fig[1] is very similar. Here this factor is close to 1.66. Shape resonances in the dependence of the quasiparticle spectrum gap on the wire width are accompanied by strong increase and significant spatial variations of the order parameter $\Delta(\rho)$. Even for $R > 5 \text{ nm}$ the resonance effect is still considerable, and the superconducting order parameter differs significantly from the bulk value (see two examples of resonances in Fig[2] (a)). In agreement with calculations for $R > 10 \text{ nm}$[17], we observe strong oscillations of the order parameter with the frequency roughly proportional to $k_F$. These oscillations are washed out at large radii about 100 nm (see the results of Ref. [17]).

As it is shown, $T_{c,R}$ sharply rises at a resonant point (more than by order of magnitude) and drops down to a value about $T_c$ between resonances. This makes it possible to expect that the effect will survive for fluctuating width in a smoothed variant depending on the scenario of fluctuations. Here it is necessary to mention the increase of the superconducting temperature by a factor of 1.1 for a single-crystal Sn nanowire with $R = 10 \text{ nm}$[4]. Numerical investigation of Eqs. (6) and (7) for the Sn parameters ($gN(0) = 0.25$ and $\hbar \omega_D/k_B = 195 \text{ K}$, see Ref. [10]) indeed shows the presence of resonances with $\Delta R/\Delta_{\text{bulk}} \approx 1.1$ near the point $R = 10 \text{ nm}$. One of them is situated at $R = 9.642 \text{ nm}$, where $\Delta R/\Delta_{\text{bulk}} = 1.13$. The superconducting order parameter at this resonant point has still significant spatial variations in the transverse direction and goes well above the bulk value (see Fig[2] (b)). It is worth noting that when exploring the BdG equations for nanowires with $R > 10 \text{ nm}$, the authors of Ref. [17] have found 10% – 20% deviations of the averaged order parameter from the bulk limit even with radius fluctuations taken into account.

In summary we investigated influence of the confinement on the transverse superconducting modes in a cylindrical nanowire at $R < 10 \text{ nm}$ in the clean limit. Numerical investigations of the BdG equations revealed a sequence of significant shape resonances in the dependence of the energy gap parameter on the nanowire width. The resonant deviations of $\Delta R$ from the bulk value are by about order of magnitude larger than the shape resonances in the energy gap parameter of ultrathin metallic films of the same width. This makes it possible to expect that some smoothed but still profound effect will remain even in the presence of fluctuations of the wire radius (much less significant resonances in the superconducting order parameter survive for a nanowire with the average radius $R \approx 10 \text{ nm}$ for the variations $\delta R < 0.5 \text{ nm}$[17]).

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