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Andreev-Type States Induced by Quantum Confinement[¶]

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Abstract—The properties of a clean superconductor with nanoscale dimensions are governed by quantum confinement of the electrons. This results in a spatially inhomogeneous superconducting condensate and in the formation of new Andreev-type quasiparticle states. These states are mainly located beyond regions where the superconducting condensate is enhanced. A numerical self-consistent solution of the Bogoliubov–de Gennes equations for a cylindrical metallic nanowire shows that these new Andreev-type states decrease the ratio of the energy gap to the critical temperature.

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Recently, nanoscale superconducting specimens (nanowires and nanofilms) with a high degree of crystallinity have been fabricated [1–5]. The superconducting properties of such nearly clean nanosuperconductors are governed by quantum confinement (QC) of electrons. Since the classical papers by Gor'kov [6] and Bogoliubov [7], it is well-known that the superconducting order parameter $\Delta(\mathbf{r})$ can be seen as the wave function for the center-of-mass motion of the Cooper pairs. Hence, one can expect that in the presence of QC the order parameter varies with the position. Such variations of $\Delta(\mathbf{r})$ have recently been demonstrated for the case of cylindrical metallic nanowires [8–10] and for metallic nanofilms [11] by numerically solving the Bogoliubov–de Gennes equations. It was shown that spatial inhomogeneity in the spatial distribution of the order parameter is strongly enhanced when size/shape dependent superconducting resonances come into play [9–11]. These resonances were found [10] to be responsible for a width-dependent increase of the critical temperature T_c as recently observed in tin and aluminum nanowires [1, 12, 13].

As is well-known, spatial variations of the superconducting order parameter can give rise to the formation of Andreev states. Quasiparticles can "feel" a spatial variation of the superconducting condensate as a kind of potential barrier. This physical mechanism is the basis for Andreev quantization and will be referred to as the Andreev mechanism (AM) throughout this paper. Andreev states were investigated (i) for an isolated normal region of the intermediate state of a type-I superconductor [14] (or in a similar situation of superconducting-normal-superconducting (SNS) contacts [15]), and (ii) in the core of a single vortex for the case of the mixed state of a type-II-superconductor [16]. In both variants the superconducting condensate: $\Delta(\mathbf{r}) \longrightarrow \Delta_{\text{bulk}}$ when $|\mathbf{r}| \longrightarrow \infty$. The exterior of a nanoscale specimen is different due to QC. As follows from our numerical investigations of the Bogoliubov–de Gennes equations for a clean metallic cylindrical nanowire, in this case AM manifests itself through the formation of new Andreev-type states appearing due to spatial inhomogeneity of the superconducting condensate induced by QC. These Andreev-type states are mainly located beyond the regions where the order parameter is enhanced. We remark that such states cannot be localized in the regions where $|\Delta(\mathbf{r})|$ is significantly decreased because the characteristic length for spatial variations of the order parameter in the case of interest is about the Fermi wavelength λ_F ($\lambda_F \ll \xi$ with ξ the Ginzburg–Landau coherence length; typically, for metallic densities of electrons $\lambda_F \sim 1$ nm) in the case of interest. Our results strongly suggest that the lowest quasiparticle states in a clean nanosuperconductor are always such Andreev-like states induced by QC.

In order to give more details about the role and features of the new Andreev-type states, we investigate below the quasiparticle spectrum, critical temperature and superconducting order parameter in a clean cylindrical nanowire, using the numerical self-consistent solution of the Bogoliubov–de Gennes (BdG) equations [17]. In the absence of a magnetic field, $\Delta(\mathbf{r})$ can be chosen as a real quantity and the BdG equations [16] read:

$$E_i u_i(\mathbf{r}) = \left(-\frac{\hbar^2}{2m_e}\nabla^2 - \mu\right)u_i(\mathbf{r}) + \Delta(\mathbf{r})v_i(\mathbf{r}), \quad (1a)$$

$$E_i v_i(\mathbf{r}) = \Delta(\mathbf{r})u_i(\mathbf{r}) - \left(-\frac{\hbar^2}{2m_e}\nabla^2 - \mu\right)v_i(\mathbf{r}), \quad (1b)$$

[¶] The text was submitted by the authors in English.

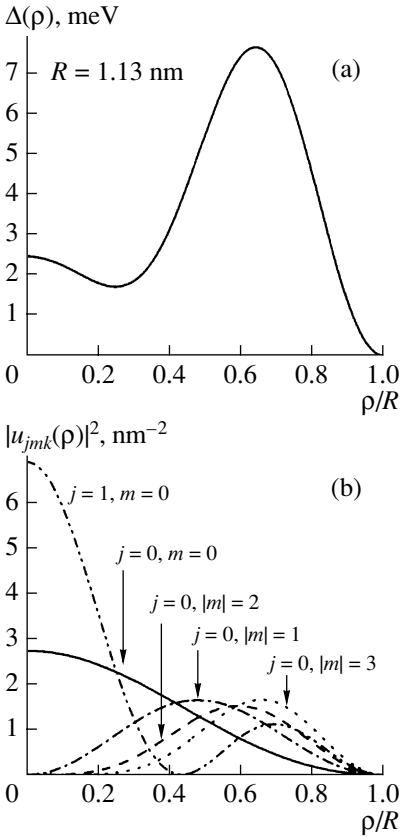

Fig. 1. The resonant point $R = 1.13$ nm: (a) the superconducting order parameter $\Delta(\rho)$ and (b) the square of the absolute value of the transverse particle-like wave function $u_{jmk}(\rho)$ for various quasiparticle branches (the lowest excitation is presented for any given quasiparticle branch).

with E_i the quasiparticle spectrum, μ the chemical potential (the Fermi level for nanowires) and m_e the electron band mass (it is set to the free electron mass below). Equations (1a) and (1b) should be solved in a self-consistent manner, using the supplemented self-consistency relation

$$\Delta(\mathbf{r}) = g\sum_i u_i(\mathbf{r})v_i^*(\mathbf{r})(1-2f_i) \qquad (2)$$

connecting $\Delta(\mathbf{r})$ with the particle-like and hole-like wave functions $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$. In Eq. (2) g is the coupling constant for the effective electron–electron attraction, and $f_i = f(E_i)$ stands for the Fermi function. Here the summation is over the eigenstates that have a positive quasiparticle energy E_i and the single-electron energy:

$$\xi_i = \int d^3r\left[u_i^*(\mathbf{r})\left(-\frac{\hbar^2}{2m_e}\nabla^2-\mu\right)u_i(\mathbf{r}) + v_i^*(\mathbf{r})\left(-\frac{\hbar^2}{2m_e}\nabla^2-\mu\right)v_i(\mathbf{r})\right], \qquad (3)$$

within the interval $[-\hbar\omega_D, +\hbar\omega_D]$ (see, for details, the textbook [16]). The chemical potential is related to the mean electron density n by

$$n = \frac{2}{V}\sum_i\int d^3r[|u_i(\mathbf{r})|^2 f_i + |v_i(\mathbf{r})|^2(1-f_i)], \qquad (4)$$

with $V = \pi R^2 L$ the system volume. In Eq. (4) the summation involves all the states with positive excitation energies E_i. Due to QC in the transverse directions we have to put $u_i(\mathbf{r})|_{\mathbf{r}\in S} = v_i(\mathbf{r})|_{\mathbf{r}\in S} = 0$ on the wire surface. In the longitudinal direction periodic boundary conditions are applied. For the cylindrical geometry we have $\Delta(\mathbf{r}) = \Delta(\rho)$, where ρ, φ, z are the cylindrical coordinates. So, it is seen from Eqs. (1a) and (1b) that

$$u_i(\mathbf{r}) = u_i(\rho)\frac{\exp(im\varphi)}{\sqrt{2\pi}}\frac{\exp(ikz)}{\sqrt{L}}, \quad v_i(\mathbf{r}) = v_i(\rho)\frac{\exp(im\varphi)}{\sqrt{2\pi}}\frac{\exp(ikz)}{\sqrt{L}}, \qquad (5)$$

where $i = \{j, m, k\}$ with j the quantum number associated with the transverse coordinate (the number of zeros of $u_i(\rho)$ and $v_i(\rho)$ for $\rho < R$), m the azimuthal quantum number, and k the wave vector of the quasi-free electron motion parallel to the nanowire.

The superconducting properties are dependent on the number of single-electron states (per unit volume and per spin projection) located in the Debye "window" $[-\hbar\omega_D, +\hbar\omega_D]$ [16]. This number changes with the nanowire width. The band of single-electron states in a clean metallic nanowire splits up in one-dimensional subbands. With increasing nanowire width, these subbands move down in energy. While the bottom of a subband passes through the Fermi surface, the number of single-electron states in the energy interval $[-\hbar\omega_D, +\hbar\omega_D]$ increases abruptly. This results in a series of width-dependent superconducting resonances [9, 10]. At a resonant point the order parameter is strongly enhanced as compared to its bulk value and has an extremely nonuniform spatial distribution. Fig. 1 shows the superconducting condensate $\Delta(\rho)$ (a) and quasiparticle spatial distribution $|u_{jmk}(\rho)|^2$ (b) calculated from Eqs. (1a) and (1b) at zero temperature $T = 0$ for aluminum cylindrical nanowire ($\hbar\omega_D = 32.31$ meV and $gN(0) = 0.18$ with $N(0)$ the bulk density of states [16]) for the resonant radius $R = 1.13$ nm. For these parameters the bulk condensate is $\Delta_{\text{bulk}} = 0.25$ meV ($T = 0$). The bulk Fermi level was set as $\mu_{\text{bulk}} = 0.9$ eV. This is the effective Fermi level that should be used together with the BdG equations treated in the parabolic band approximation (see, for details, Ref. 11). As seen from Fig. 1a, the superconducting order parameter is strongly enhanced with respect to the bulk one and exhibits profound spatial variations. There are eight relevant quasiparticle subbands contributing to the superconducting properties: with the quantum numbers $j = 0$, $m = 0$, $j = 1$, $m = 0$, $j = 0$, $|m| = 1$, $j = 0$, $|m| = 2$ and $j = 0$, $|m| = 3$ (the corresponding exci-

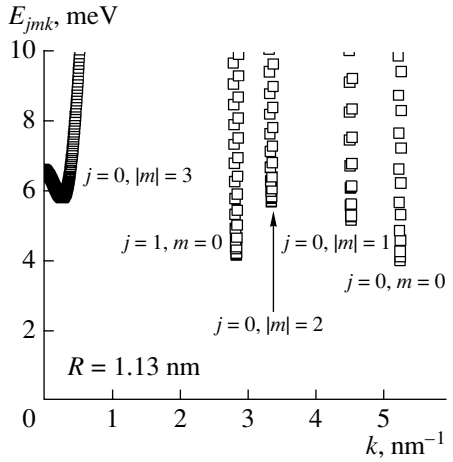

Fig. 2. The resonant point $R = 1.13$ nm: the excitations energies as functions of k for the relevant quasiparticle branches with $j = 0$, $m = 0$; $j = 1$, $m = 0$; $j = 0$, $|m| = 1$; $j = 0$, $|m| = 2$ and $j = 0$, $|m| = 3$.

tation energies E_{jmk} are given in Fig. 2). Note that only low-lying states of these subbands contribute to the superconducting quantities, while the others are excluded due to the criterion that the corresponding single-electron energies should belong to the interval $[-\hbar\omega_D, +\hbar\omega_D]$. The two branches with $j = 0$, $|m| = 3$ are specified by a high density of states and, so, have a dominant contribution to the superconducting characteristics, forming the profile of the enhancement of the order parameter at $\rho = 0.65R$. The bottoms of these single-electron subbands corresponding to these two quasiparticle branches are located in the Debye window. As seen from Fig. 1b, the profile for $|u_{jkm}(\rho)|^2$ at $j = 0$, $|m| = 3$ is indeed similar to the profile of the superconducting order parameter in the region of its enhancement. The other quasiparticle states with $j = 0$, $m = 0$, $j = 1$, $m = 0$, $j = 0$, $|m| = 1$ and $j = 0$, $|m| = 2$ contribute less to $\Delta(\rho)$. It is remarkable that these quasiparticle states try to "escape" the domain of enhanced order parameter (more or less successfully because QC is the dominating factor), which is a manifestation of AM. These quasiparticle branches are lower in energy and can be interpreted as new Andreev-type states induced by quantum confinement.

It is instructive to compare the results derived for the resonant point $R = 1.13$ nm with the data for $R = 1.23$ nm (at this point the resonance appearing at $R = 1.23$ nm has completely decayed). Figures 3 and 4 show $\Delta(\rho)$, $|u_{jkm}(\rho)|^2$ and E_{jmk} calculated for $R = 1.13$ nm. In this case we have the same relevant quasiparticle branches and a similar profile of $\Delta(\rho)$ as before for $R = 1.13$ nm but the spatially averaged order parameter is now only about 0.2 meV (close to the bulk value $\Delta_{\text{bulk}} = 0.25$ nm). Hence, we can expect a less important role of AM in this situation. As seen from Fig. 4, the difference in energy between the branches with $j = 0$, $|m| = 3$ and $j = 0$, $|m| = 1$ is not so significant as in Fig. 2.

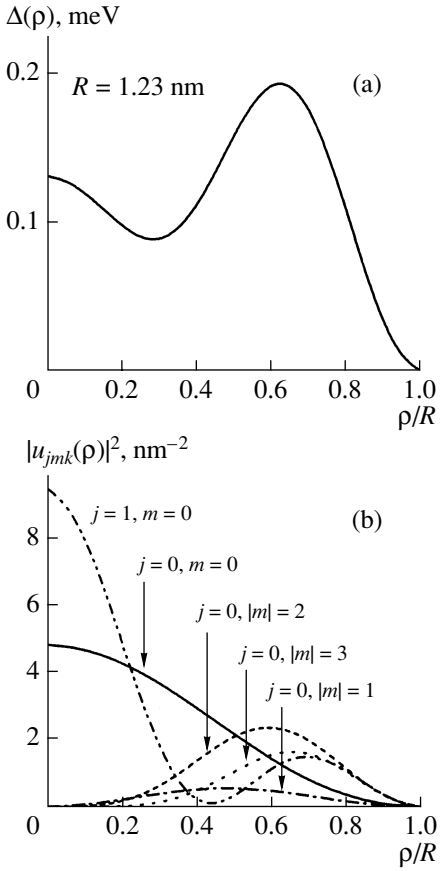

Fig. 3. Beyond the resonant regime: $R = 1.23$ nm: (a) the order parameter $\Delta(\rho)$ and (b) $|u_{jmk}(\rho)|^2$ for the relevant quasiparticle branches (k corresponds to the lowest state in a given branch).

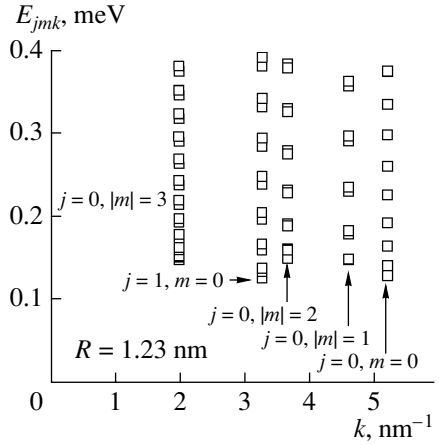

Fig. 4. Beyond the resonant regime: $R = 1.23$ nm: the quasiparticle energies versus k for $j = 0$, $m = 0$; $j = 1$, $m = 0$; $j = 0$, $|m| = 1$; $j = 0$, $|m| = 2$ and $j = 0$, $|m| = 3$.

An important consequence of AM is a change in the ratio $\Delta_E(T)/(k_B T_c)$, where $\Delta_E(T)$ is the temperature dependent energy gap in the quasiparticle spectrum, k_B is

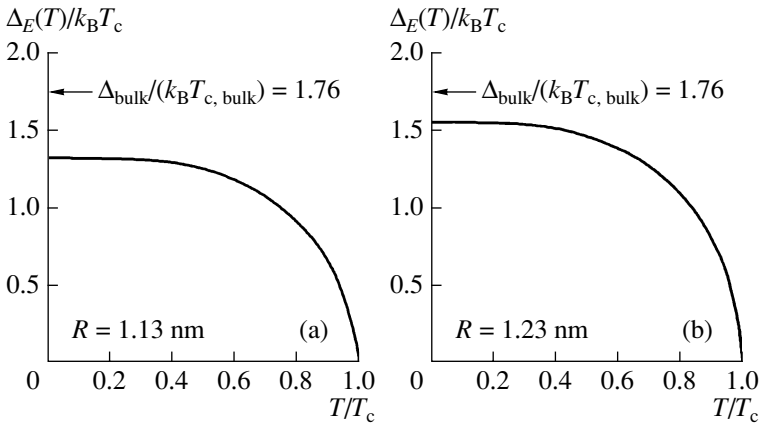

Fig. 5. The ratio $\Delta_E(T)/(k_BT_c)$ versus T/T_c at the resonant radius R = 1.13 nm (the left panel) and beyond the resonant regime at R = 1.23 nm (the right panel).

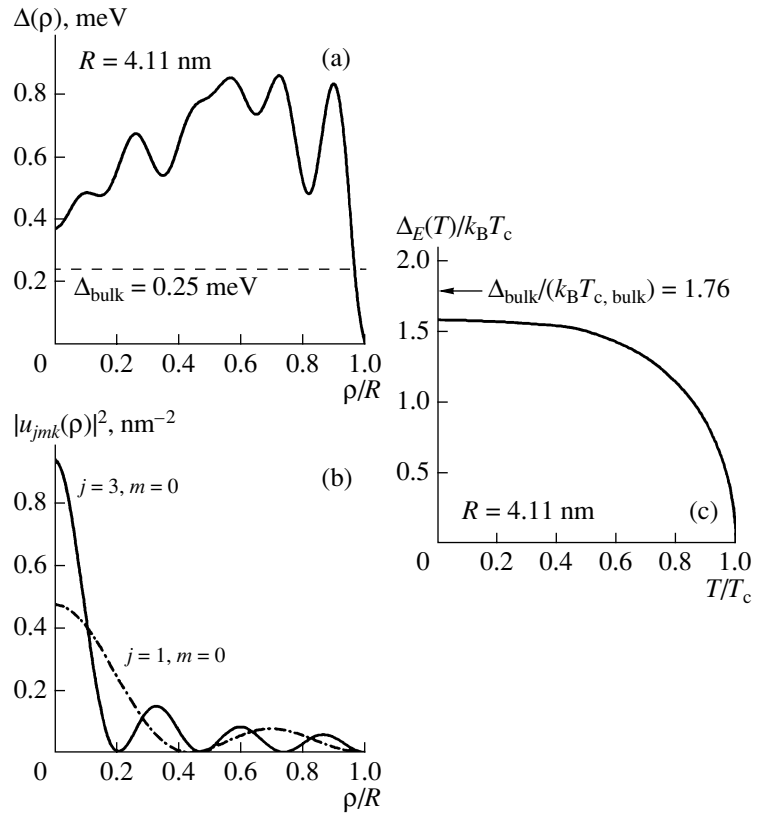

Fig. 6. The resonant point R = 4.11 nm: (a) the order parameter versus ρ/R, (b) $|u_{jmk}(\rho)|^2$ for the lowest (j = 3, m = 0) and next-to-lowest (j = 1, m = 0) quasiparticle branches, and (c) $\Delta_E(T)/(k_BT_c)$ versus T/T_c.

the Boltzmann constant and T_c is the critical temperature. Indeed, AM results in a decrease of the energy gap but has little effect on the critical temperature. In Fig. 5 the quantity $\Delta_E(T)/(k_BT_c)$ calculated for an aluminum cylindrical nanowire with R = 1.13 nm (the left panel) and R = 1.23 nm (the right panel) is plotted versus the relative temperature T/T_c. We remind the reader that in bulk $\Delta_{bulk}/(k_BT_{c,\,bulk}) = 1.76$ at $T = 0$ [16]. The numerical results for both R = 1.13 nm and R = 1.23 nm demonstrate deviations (about 10–20%) from the bulk regime. However, these deviations for the non-resonant R = 1.23 nm are less significant due to a smaller contribution from the AM.

So far we discussed the new Andreev-type states induced by QC in extremely narrow nanowires, to avoid discussion of an abnormal large number of quasiparticle species. At present, such nanowires are not experimentally attainable and, in addition, they are expected

to exhibit a finite resistance coming from thermal and, possibly, quantum fluctuations which should destroy superconductivity (see, for example, Ref. 12). For R = 4–8 nm, corresponding to the narrowest superconducting nanowires fabricated in recent experiments [1, 12], the resonances are much less profound as compared to $R \approx 1$ nm. However, they are still noticeable (see the right panel of Fig. 6), and the Andreev-type states are still of importance here. For example, $\Delta_E(T)/(k_B T_c)$ calculated at the resonant point $R = 4.11$ nm exhibits deviations (about 10%) from the bulk BCS behavior (the right panel of Fig. 6).

Concluding, quantum confinement is the major effect which governs the superconducting properties of a clean nanoscale metallic specimen and results in a nonuniform distribution of the order parameter. An order-parameter inhomogeneity in a clean nano-superconductor leads to the formation of new Andreev-like states. These new states are not localized. They try "to escape" the regions of enhanced order parameter and are mainly located beyond such regions. Appearance of such Andreev-like states results in a decrease of the energy gap in the quasiparticle spectrum and in deviations of the ratio of the energy gap to the critical temperature from the bulk regime. Numerical self-consistent solution of the Bogoliubov–de Gennes equations for a cylindrical nanowire has demonstrated that such decrease is significant for nanowires with width less than ~10 nm.

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