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Position-dependent effect of non-magnetic impurities on superconducting properties of nanowires

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Abstract – Anderson’s theorem states that non-magnetic impurities do not change the bulk properties of conventional superconductors. However, as the dimensionality is reduced, the effect of impurities becomes more significant. Here we investigate superconducting nanowires with diameter comparable to the Fermi wavelength λ_F (which is less than the superconducting coherence length) by using a microscopic description based on the Bogoliubov-de Gennes method. We find that: 1) impurities strongly affect the superconducting properties, 2) the effect is impurity position dependent, and 3) it exhibits opposite behavior for resonant and off-resonant wire widths. We show that this is due to the interplay between the shape resonances of the order parameter and the subband energy spectrum induced by the lateral quantum confinement. These effects can be used to manipulate the Josephson current, filter electrons by subband and investigate the symmetries of the superconducting subband gaps.

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Introduction. – The effect of impurities on superconductivity has intrigued scientists for several decades. Adding impurities to a superconductor can not only provide a useful tool to investigate the superconducting state but can also be used to optimize the performance of certain devices. For example, impurities are used to distinguish between various symmetries of the superconducting state [1,2], to identify topological superconductors [3] or to pin vortices in order to enhance the superconducting critical current [4]. Strong disorder is often used to study the superconducting-insulator transitions and the localization of the Cooper pairs [5–10]. It is well known that magnetic impurities, which are pair breakers, suppress superconductivity. On the other hand, as Anderson’s theorem points out [11], for bulk conventional superconductors, small concentrations of non-magnetic impurities do not change the thermodynamic properties of the system, such as the superconducting critical temperature T_c , and that impurities have only local effects [1] on the superconducting order parameter (OP) and the density of states.

On the other hand, quasi-one-dimensional superconducting nanowires show different properties from the bulk and could have wide potential applications in the near future [12]. First, if, in some regions, the diameter of the cross-section of the wire is shorter than the

superconducting coherence length, ξ (also known as the healing length of the OP), superconductivity weakens there, thus affecting transport properties of the wires. Quantum phase slips, leading to the loss of phase coherence, are one of the main reasons for the appearance of normal regions giving rise to a finite resistance below T_c in nanowires [13–19]. Phase slip junctions can be fabricated in order to take advantage of this mechanism [20]. Normal regions can also be caused by interactions with photons and this can be used to build single-photon detectors [21,22]. Second, surface effects in nanoscale superconductors result in topological superconducting states [23]. Majorana fermions, which are their own anti-particles, were predicted as quasi-particles in such p-wave nanowires [24,25]. Third, quantum confinement results in quantum size effects [26–28], quantum size cascades [29], facilitates the appearance of new Andreev states [30] and gives rise to unconventional vortex states [31] induced by the wave-like inhomogeneous spatial distribution of the OP [27].

Up to now, the theoretical study of superconducting nanowires was limited to defect-free cases in the clean limit or to systems with weak links, which were treated in the one-dimensional limit. However, experiments such as Scanning Tunneling Microscopy (STM)

are nowadays able to measure the local density of states (LDOS) with atomic resolution [32–36] and consequently the finite width of nanowires can no longer be neglected. It is known that in low-dimensional superconductors phase fluctuations should play an important role [37–39]. The calculation presented here is done at zero temperature and at mean-field level, therefore it cannot describe fluctuations. Nevertheless, by calculating the modifications induced by the impurity on the Josephson current we are able to infer the phase robustness of the condensate, therefore indirectly provide information about the enhancement of fluctuations and the appearance of phase slips.

In this letter, we investigate the effect of a non-magnetic impurity on superconducting nanowires with diameter comparable to the Fermi wavelength, λ_F . The bulk coherence length at zero temperature, ξ_0 , is much larger than λ_F . For such systems, quantum confinement effects dominate and a description based on the microscopic Bogoliubov-de Gennes (BdG) equations is required. The impurity, which induces potential scattering on single electrons, not only affects local properties such as the OP and the LDOS, but also has global effects on the critical supercurrent. Quantum confinement leads to inhomogeneous superconductivity and therefore the effect of the impurity strongly depends on its transverse location.

The letter is organized as follows: First we briefly present our numerical method and the properties of the nanowires in the clean limit, then we show the effect of non-magnetic impurities on the profile of the order parameter and the local density of states. At the end we investigate the impurity effect on the Josephson critical current.

Theoretical approach. – We start from the well-known BdG equations:

$$[K_0 - E_F] u_n(\vec{r}) + \Delta(\vec{r}) v_n(\vec{r}) = E_n u_n(\vec{r}), \quad (1)$$

$$\Delta(\vec{r})^* u_n(\vec{r}) - [K_0^* - E_F] v_n(\vec{r}) = E_n v_n(\vec{r}), \quad (2)$$

where $K_0 = -(\hbar\nabla)^2/2m + U(\vec{r})$ is the kinetic energy with U being the potential barrier induced by the impurity and E_F the Fermi energy, $u_n(v_n)$ are electron(hole)-like quasi-particle eigen-wave functions, E_n are the quasi-particle eigen-energies. The impurity potential is modeled by a symmetrical Gaussian function, $U(\vec{r}) = U_0 \exp[-(\vec{r} - \vec{r}_0)^2/2\sigma^2]$ where U_0 is the amplitude, \vec{r}_0 is the location of the impurity and σ is the width of the Gaussian.

The pair potential is determined self-consistently from the eigen-wave functions and eigen-energies:

$$\Delta(\vec{r}) = g \sum_{E_n < E_c} u_n(\vec{r}) v_n^*(\vec{r}) [1 - 2f(E_n)], \quad (3)$$

where g is the coupling constant, E_c is the cutoff energy, and $f(E_n) = [1 + \exp(E_n/k_B T)]^{-1}$ is the Fermi distribution function, where T is the temperature. The local density of states is calculated as usual: $N(\vec{r}, E) = \sum_n [\delta(E_n - E) |u_n(\vec{r})|^2 + \delta(E_n + E) |v_n(\vec{r})|^2]$.

For simplicity, we consider a two-dimensional problem and introduce a long unit cell whose area is $S = L_x L_y$, where L_x is the length of the unit cell and L_y is the wire width. Periodic boundary conditions are set in the x -direction and L_x is set to be long enough such that physical properties are L_x independent. Due to quantum confinement in the transverse direction y , we set Dirichlet boundary condition at the surface (*i.e.* $u_n(\vec{r}) = v_n(\vec{r}) = 0$, $r \in \partial S$).

In order to solve more efficiently the self-consistent BdG equations (1)–(3), we expand $u_n(v_n)$ by using a two-step procedure. First, in order to get the eigen-states of the single-electron Schrödinger equation, $K_0 \phi_l = E_l \phi_l$, we Fourier expand ϕ_l :

$$\phi_l(x, y) = \sqrt{\frac{2}{L_x L_y}} \sum_{j>0, k} c_{j, k} \exp(ikx) \sin\left(\frac{\pi j y}{L_y}\right), \quad (4)$$

where $c_{j, k}$ are the coefficients of the expansion and wave vector $k = 2\pi m/L_x$, $m \in \mathbb{Z}$. Here we use a large number of basis functions in order to ensure the accuracy of the results. Next, we expand $u_n(v_n)$ in terms of $\phi_l(x, y)$. In this step, only states with energies $E_l < E_F + \varepsilon$ are included. In our calculation, ε is taken to be $30E_c$ and we find that any larger cutoff does not modify the results. We have checked our results, for a specific choice of parameters, against a more computationally intensive finite-difference method approach.

We choose to study NbSe₂ nanowires as an example because of the availability of high-quality nanowires with 2–25 nm in diameter [40,41]. Also, theoretical calculations are in good agreement with experiments, especially, for vortex lines [42–44]. In addition, the lower Fermi energy makes the calculations feasible. The parameters of bulk NbSe₂ are the following: $m = 2m_e$, $E_F = 40$ meV, $E_c = 3$ meV and coupling constant g is set so that the bulk gap $\Delta_0 = 1.2$ meV, which yields $T_c \approx 8.22$ K, $\xi_0 = 14.7$ nm and $k_F \xi_0 = 21.23$. In nanowires, the mean electron density n_e is kept to the value obtained when $L_x, L_y \rightarrow \infty$ by using an effective E_F , where $n_e = \frac{2}{S} \sum_n \int \{|u_n|^2 f(E_n) + |v_n|^2 [1 - f(E_n)]\}$. All the calculations are performed at zero temperature.

Numerical results. – We first show in fig. 1 important superconducting properties of clean nanowires, *i.e.* with $U \equiv 0$. The spatially averaged OP, $\bar{\Delta}$, shows quantum size oscillations as a function of the width, L_y , as seen from fig. 1(a). The resonant enhancements appear almost regularly with a period of half the Fermi wavelength, *i.e.* $\lambda_F/2$. They are due to the fact that the bottom of the relevant single-electron subbands passes through the Fermi surface, which results in a significant increase in the density of states, *i.e.* in the number of electrons which can form Cooper pairs. The different energy spectra for the resonance and off-resonance cases are the key to understand the behavior of the nanowires. For completeness, we show in fig. 1(b)–(h) more information for the resonance case,

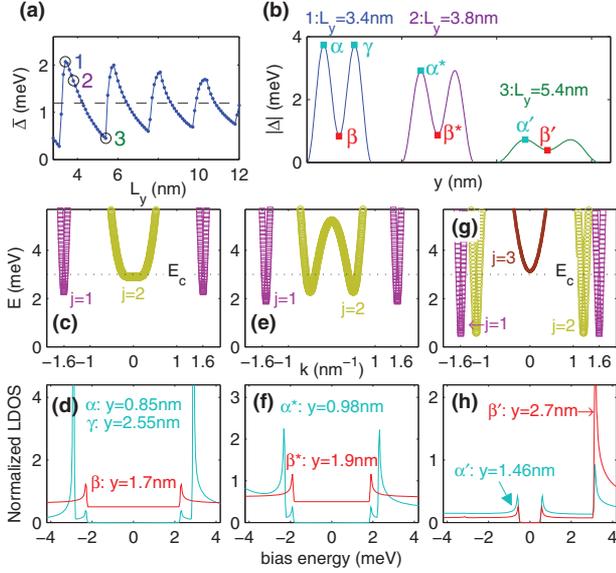


Fig. 1: (Color online) Properties of clean NbSe₂ nanowires. (a) Spatially averaged $\bar{\Delta}$ as a function of L_y . The open circles 1–3 indicate the resonance case ($L_y = 3.4$ nm), intermediate case ($L_y = 3.8$ nm) and off-resonance case ($L_y = 5.4$ nm), respectively. (b) OP $|\Delta(y)|$ for the three cases. The $\alpha\beta\gamma$ are defined as the positions where the OP has a local maximum/minimum for resonance, the $\alpha^*\beta^*$ are for intermediate and the $\alpha'\beta'$ are for off-resonance. The value of these positions are shown in the inset of the panels (d), (f) and (h), respectively. Panels (c) and (d) show energy spectrum and the corresponding LDOS at positions α , β and γ for resonance. Panels (e) and (f) show the same but for the intermediate case and positions α^* and β^* . Panels (g) and (h) show the same but for off-resonance and positions α' and β' . Note that in panels (d) and (f) the LDOS for position β and β^* are shifted for clarity.

with $L_y = 3.4$ nm, intermediate case, with $L_y = 3.8$ nm, and off-resonance case, with $L_y = 5.4$ nm [45]. The energy spectrum for resonance (see fig. 1(c)) shows two energy gaps: a smaller gap for subband $j = 1$ and a larger one for $j = 2$. Most quasi-particle states are just below the cutoff energy E_c for subband $j = 2$. This results in an enhancement of the OP, which shows two pronounced peaks and is strongly inhomogeneous in the y -direction (see fig. 1(b)). We consider the spatial positions $\alpha\beta\gamma$ and $\alpha'\beta'$ as given in fig. 1(d), (h) where the OP has either a maximum or a minimum. The corresponding LDOS at positions α and β are shown in fig. 1(d). We notice that there are two gaps at α and only one gap at β . The smaller sub-gap at α and the gap at β comes from the $j = 1$ subband. The main gap at α comes mostly from the $j = 2$ subband which is indicated by the ratio of the LDOS peaks at the main gap and at the sub-gap. In contrast, the off-resonance case shows the same energy gap for $j = 1$ and $j = 2$ (see fig. 1(g)) and the LDOS (see fig. 1(h)) is more conventional: only one superconducting gap and the amplitude of the LDOS is proportional to $|\Delta(y)|$, *i.e.* the LDOS at α' (local maximum) is larger than the one at β' (local minimum). Besides

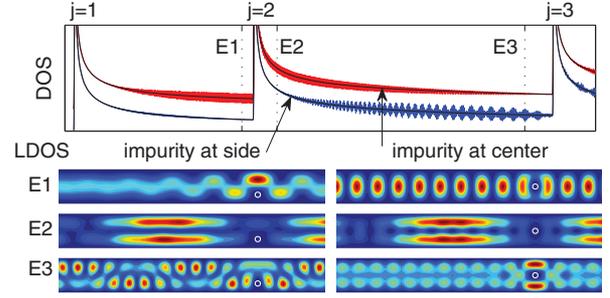


Fig. 2: (Color online) Effect of the impurities on the electronic structure when the nanowire is in normal state. Upper panel: DOS as a function of energy for an impurity at sided position (blue solid line) and at centered position (red solid line, shifted up for clarity), respectively. The black solid lines are for $U = 0$ as references. Lower panels: schematic corresponding LDOS(x, y) at energy $E1$, $E2$ and $E3$, respectively. The open circles indicate impurities' position.

the sub-gap shift seen in the energy spectrum, another important difference between the two cases is that for resonance there is always a large number of low-momentum quasi-particles (see fig. 1(c)) which are involved in pairing, whereas there are no quasi-particles at $k = 0$ in the off-resonance case (see fig. 1(e)). Note that subband $j = 3$ in off-resonance sits just outside of E_c and generates a large asymmetric peak in the LDOS (see fig. 1(f)). The intermediate case (see fig. 1(e) and (f)) mixes the characteristic from both resonance and off-resonance cases, where it has the intermediate gap difference between subbands $j = 1$ and $j = 2$ and the intermediate k -value for most quasi-particles states with subband $j = 2$.

Next, we consider an impurity in the nanowire. The impurity is strong enough to suppress completely the wave functions of the electronic states locally. Meanwhile, the spread of the impurity is smaller than the width of the nanowire. The effects of the impurity on the electronic structures of normal state are presented in fig. 2. The scattering due to the single impurity does not change the quasi-one-dimensional characteristic seen in the DOS. However, it results in additional small oscillations when compared with the clean case with $U = 0$. In addition, the oscillations show a different pattern for impurity at sided position and at centered position. It indicates the influence of the impurity depending on its position and the quantum number of the electronic state, *i.e.* j and k . Due to the sine-shaped transverse electronic wave functions, the impurity at center position affects the states with subband $j = 1$ more than states with subband $j = 2$. Thus, the DOS of the impurity at center position shows stronger oscillations than the one of the impurity at sided position between the peaks of $j = 1$ and $j = 2$. For the same reason, it shows opposite behavior in DOS between the peak of $j = 2$ and $j = 3$. Furthermore, the impurity leads to fast oscillations in the LDOS at energies $E1$ and $E3$ (see fig. 2 (lower panels)) because these states have a large wave number, *i.e.* k . In contrast,

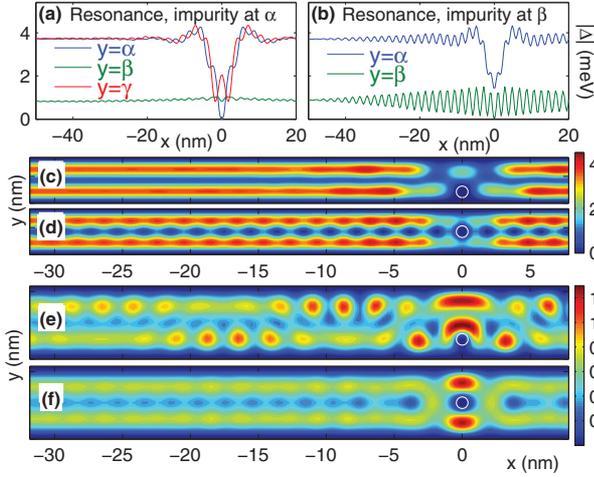


Fig. 3: (Color online) OP in the presence of an impurity. Panels (a) and (c) show $|\Delta(x)|$ at $y = \alpha, \beta, \gamma$ (defined in fig. 1) and contour plot of $|\Delta(x, y)|$ for an impurity sitting at α in resonance case, respectively. Panels (b) and (d) are the same as (a) and (c) but for the impurity sitting at the center β . Panels (e) and (f) show contour plot of $|\Delta(x, y)|$ for an impurity sitting at α' and β' in the off-resonance case, respectively. The white open circles indicate impurities' profile where $U = 0.1U_0$.

the impurity leads to oscillations with long wavelength in the LDOS at energy E_2 , due to the states with small k -value dominating near E_2 .

Now we move on to the superconducting state and consider an impurity at position $(0, \alpha)$ and $(0, \beta)$ for the resonance case and at $(0, \alpha')$ and $(0, \beta')$ when off-resonance. We set $U_0 = 20E_F$ and $\sigma = 0.02\text{ nm}$ so that the impurity strongly suppresses the local OP and the spread of the potential (full width at 1/10th of maximum) is 0.86 nm , which is shorter than the width of the nanowire. We show in fig. 3 the profile of the amplitude of the OP in the presence of the impurity. For the resonance (see figs. 3(c), (d)), the impurity suppresses the OP over the whole width which is more pronounced when in α than in β . Meanwhile, the asymmetrical impurity, at α , results in a local enhancement at position $(0, \gamma)$, as seen from fig. 3(a). For the impurity sitting in the center, β , the OP oscillates along the wire over a longer distance although the impurity sits at a local minima of the OP which intuitively should have a smaller effect. As seen from fig. 3(b), the OP oscillations extend to $x = \pm 50\text{ nm}$, which is much farther than the extent of the oscillations for the impurity at α . The reason is that the centered β impurity strongly affects the $j = 1$ subband quasi-particles due to the sine-shaped transverse wave function, leaving the $j = 2$ subband unaffected. Moreover, only high k quasi-particles in subband $j = 1$ play a role so that scattering on the impurity results in oscillations of the wave functions. On the other hand, the impurity at α affects mostly subband $j = 2$ but all states with $j = 2$ have low k so that the OP recovers fast and has longer wavelength oscillations. The local density of states in figs. 4(a)–(d) show evidence

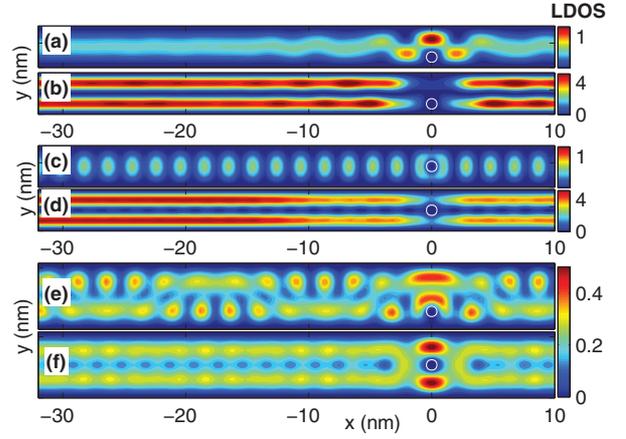


Fig. 4: (Color online) Contour plots of LDOS at the energies' (sub-)gap in the presence of an impurity. Panels (a)–(d) are for the resonance case with an impurity sitting at α at sub-gap (a) $E/\text{meV} = 2.32$ and gap (b) $E/\text{meV} = 2.93$ and with an impurity sitting at β at sub-gap (c) $E/\text{meV} = 2.36$ and gap (d) $E/\text{meV} = 2.93$. Panels (e) and (f) are for the off-resonance case with the impurity at α' and at β' at gap $E/\text{meV} = 0.68$ and 0.65 , respectively. The open circles indicate impurities' profile where $U = 0.1U_0$.

that supports this explanation. For the off-resonance case (see figs. 3(e), (f)), due to the combination of the $j = 1$ and $j = 2$ subbands which now have only high k quasi-particles, the impurity always induces strong oscillations in the OP. Note that the OP is affected more strongly when the impurity sits at a local maximum. The LDOS shown in figs. 4(e), (f) show the same patterns as the OP.

Finally, we study the effect of the impurity on the transport properties such as the Josephson current. In order to do so, we set a junction link of length $L_j = 30\text{ nm}$ at the center of the nanowire where Δ is obtained self-consistently. Outside the link, we fix the phase of the order parameter and impose a phase difference $\delta\theta$ between the two sides of the link, *i.e.* $\Delta(x < -15\text{ nm}) = |\Delta|e^{i0}$ and $\Delta(x > 15\text{ nm}) = |\Delta|e^{i\theta}$. Then, the supercurrent induced by the phase difference $\delta\theta$ can be calculated as follows:

$$\vec{J}(\vec{r}) = \frac{e\hbar}{2mi} \sum_{E_n < E_c} \left\{ f(E_n) u_n^*(\vec{r}) \nabla u_n(\vec{r}) + [(1 - f(E_n)) v_n(\vec{r}) \nabla v_n^*(\vec{r}) - \text{h.c.}] \right\}.$$

Please note that \vec{J} satisfies the continuity condition $\nabla \cdot \vec{J} = 0$ in the link due to the self-consistent Δ [46,47]. Outside the link, \vec{J} is discontinuous due to the fixed phase of the order parameter but these areas can be treated as current sources.

Figures 5(a) and (b) show the $J - \theta$ relation for resonant and off-resonant cases, respectively. For resonance, the current increases monotonically with the phase for the impurity at α but it shows a sine-shaped curve for the impurity at β . We find that the critical Josephson current is suppressed dramatically for the impurity at β

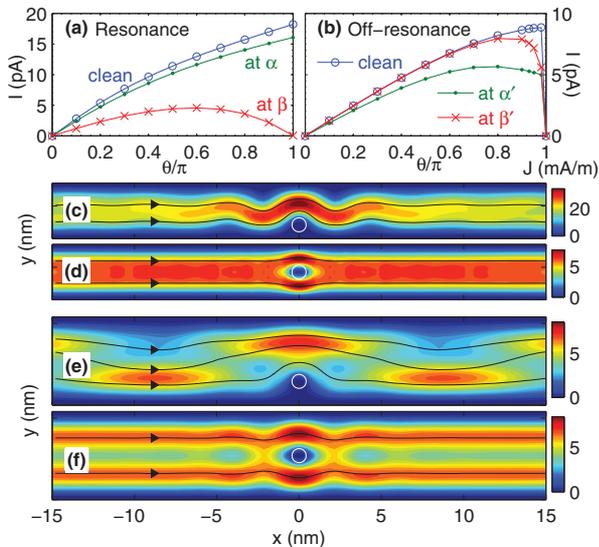


Fig. 5: (Color online) Effects of an impurity on Josephson current where the junction length is $L_j = 30$ nm. (a) Current-phase relation in the resonance case for clean limit, with impurity at α and at β . (b) Results in the off-resonance case for clean limit, impurity at α' and at β' . (c)–(f) The spatial distributions of current for an impurity at α , β for the resonance case and at α' , β' for the off-resonance case with phase differences where currents reach their critical Josephson currents. The color indicates the amplitude of the current and the streamlines indicate the direction of the current. The open circles indicate the impurity profile for which $U = 0.1U_0$.

while the impurity at position α has little effect. The explanation is that when the current is small, only the lowest quasi-particle states are involved. Moreover, almost all such states are from the $j = 1$ branch and as a result the current distribution $j(y) \propto \sin(\pi y/L_y)$ is as in the clean limit. This can be seen from fig. 5(d) for x far away from the impurity. Thus, the impurity blocking effect on the current for the impurity at the center β has a larger effect than the off-center position α . In contrast, for the off-resonance case, the current with the impurity at α' is more suppressed. The reason is the same but, here, the $j = 1$ and $j = 2$ branches contribute both to the current, and as a consequence the current distribution is $j(y) \propto |\sin(2\pi y/L_y)| + |\sin(\pi y/L_y)|$ and has a maximum at the α' position. This can also be seen from fig. 5(f) far away from the impurity. This position-dependent effect could be used to investigate the nature of the superconducting condensate, *e.g.* by using Scanning Gate Microscopy (SGM) in order to locally mimic the effect of the impurity and suppress the order parameter. By monitoring the change in the Josephson current, one can map out the symmetry of the order parameter and the distribution of the supercurrent along the y -direction.

Conclusions. – In conclusion, we studied the effect of non-magnetic impurities on narrow superconducting nanowires in the clean limit, in which quantum confinement plays an important role. By applying BdG

theory to the case of NbSe₂, we uncovered several regimes in which the impurity affects the superconducting properties of the nanowire in different ways. First, depending on whether the nanowire is in the resonant or off-resonant regime, the OP will show slow or fast oscillations away from the impurity, respectively. This is due to the different nature of the quasi-particles involved in the formation of the Cooper pairs, *i.e.* small or large momentum. Additionally, the impurity has a strong position-dependent effect on the Josephson critical current with opposite behavior in the resonant and off-resonance cases. In the resonant case an impurity at the center of the wire will strongly suppress the current while, for the off-resonance case, the current is slightly suppressed for an impurity sitting at an off-center location.

In experiments, the crystal structure of the material, the surface roughness of the specimen and the properties of the substrate will modify the Fermi level, the band structure, the electronic wave functions or the electron mean free path. All these factors could broaden the single-electron levels and modify the specific scattering patterns of the OP and electronic structures (LDOS). However, the superconducting shape resonances are robust, as shown in more realistic theoretical models [48]. In this case, quantum confinement dominates and the position dependence of the amplitude of the electronic wave functions and OP are robust. As a result, our conclusions about the position-dependent impurity effect (especially the effect on the Josephson current) will not be significantly altered, although specific details might change.

We believe that these effects could be used to investigate the nature of the superconducting condensate and the scattering of the various subbands on the impurity. Also in realistic nanowires, which contain impurities, one should see a strong impurity effect in the resonant case. Although the mean-field calculation presented here cannot describe fluctuations, by showing that the Josephson current can be strongly suppressed in the resonant case, one can infer that fluctuations will become more important. Our calculations could also provide a basis for a phenomenological toy model of a 1D disordered Josephson array with impurity position-dependent junction parameters.

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