Intrinsic reduction of Josephson critical current in short ballistic SNS weak links

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We present fully self-consistent calculations of the thermodynamic properties of three-dimensional clean SNS Josephson junctions, where S is an *s*-wave short-coherence-length superconductor and N is a clean normal metal. The junction is modeled on an infinite cubic lattice such that the transverse width of the S is the same as that of the N, and its thickness is tuned from the short to long limit. Intrinsic effects, such as a reduced order parameter near the SN boundary and finite gap to Fermi energy ratio, depress the critical Josephson current I_c, even in short junctions. Our analysis is of relevance to experiments on SNS junctions which find much smaller $I_c R_N$ products than expected from the standard (non-self-consistent and quasiclassical) predictions. We also find nonstandard current-phase relations, a counterintuitive spatial distribution of the self-consistently determined order parameter phase, and an unusual low-energy gap in the local density of states within the N region.

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Over the past decade, both experimental and theoretical interest in the superconductivity of inhomogeneous systems have been rekindled, thereby leading to a reexamination of even well-charted areas from the mesoscopic point of view.[1] For example, the Josephson effect in a superconductor–normal-metal–superconductor (SNS) weak link was known to be the result of the macroscopic condensate wave function leaking from the S into the N region. The induction of such superconducting correlations in the N, the so-called proximity effect, has been given a new real-space interpretation through the relative phase coherence of quasiparticles, correlated by Andreev reflection at the SN interface.[2] Moreover, the realization of the importance of tracking the phase coherence of single-particle wave functions in proximity-coupled metals of mesoscopic size has also unearthed new phenomena, such as quantization of the critical current in ballistic mesoscopic short SNS junctions at low enough temperature.[3,4] In short clean junctions, as $T \to 0$, the critical supercurrent $I_c = e\Delta/\hbar$ carried by a single conducting channel depends only on the superconducting energy gap Δ as the smallest energy scale $\Delta < E_{\mathrm{Th}} = \hbar v_F^N/L$ (in the long-junction limit $I_c \sim E_{\mathrm{Th}}$ is set[5] by the "ballistic" Thouless energy $E_{\mathrm{Th}} < \Delta$, which is a single-quasiparticle property determined by the Fermi velocity v_F^N in the N interlayer of length L). Thus, both mesoscopic and "classical" clean point-contact SNS junctions, with ballistic transport $l > L$ (l is the mean free path), are predicted to exhibit the same $I_c R_N = \pi\Delta/e$ product at $T = 0$. This has been known for quite some time as the Kulik-Omelyanchuk (KO) formula,[6] where R_N is the Sharvin point-contact resistance $R_N = h/2e^2 M$ of the ballistic N region containing M conducting channels.

Recent experimental activity[7] on highly transparent[8] ballistic short SNS junctions, where both I_c and R_N are independent of the junction length, reveals much lower values of $I_c R_N$ than the KO formula (similarly, the critical current steps found in an attempt[9] to observe discretized I_c are much smaller than the predicted $e\Delta/\hbar$). However, a proper interpretation of these results demands a clear understanding of the relationship between relevant energy and length scales. The criterion for the short-junction limit $\Delta < E_{\mathrm{Th}}$ introduces a "coherence length" of the junction $\xi_0 = \hbar v_F^N/\pi\Delta$; i.e., the maximum KO limit can be expected only for $L \ll \xi_0$. The relation between $k_B T$ and E_{Th} defines the high- ($k_B T > E_{\mathrm{Th}}$) versus low- ($k_B T < E_{\mathrm{Th}}$) temperature limits, which is equivalently expressed in terms of the junction thickness as $L > \xi_N$ versus $L < \xi_N$, respectively, with $\xi_N = \hbar v_F^N/2\pi k_B T$ being the normal-metal coherence length. The ξ_N sets the scale over which two quasiparticles in the N, correlated by Andreev reflection, retain their relative phase coherence (i.e., superconducting correlations imparted on the N region at finite temperature decay exponentially with ξ_N, while at zero temperature $\xi_N \to \infty$ and the condensate wave function decays inversely in the distance from the interface[10]). Therefore, the simple exponential decay of $I_c \sim \exp(-L/\xi_N)$ appears only in the high-temperature limit, while in the opposite low-temperature limit ξ_N ceases to be a relevant length scale and the decay is slower than exponential. The aforementioned experiments on clean SNS junctions[7] are conducted on Nb/InAs/Nb junctions which are tuned to lie in the regime where $\xi_S < L < \xi_0 \ll \xi_N$ ($\xi_S = \hbar v_F^S/\pi\Delta$ is the bulk superconductor coherence length). Thus, the large difference between ξ_S and ξ_0 means that there is a substantial Fermi velocity mismatch (typically an order of magnitude[7,9]), which must generate normal scattering at the SN interface in addition to Andreev reflection. This, together with other possible sources of scattering at the SN boundary, like imperfect interfaces[4,11,12] or charge accumulation layers[13] (typical of Nb/InAs contact), cannot be detected by only observing the independence of I_c and R_N on interelectrode separation (for intermediate[7] L). Nevertheless, this is frequently the criterion used in experiments[7] to ensure that the transport is ballistic. Therefore, the ideal maximum value for I_c could be achieved only for $\xi_S = \xi_0$ ($v_F^S = v_F^N$) and with a perfectly transparent interface, where the junction thickness satisfies $L \ll \xi_S$. Even in this case it is possible that the current in short junctions is smaller than expected due to a depressed value of the order parameter on the SN boundary when the transverse widths of the S and N regions are the same.[14] Such junctions cannot be treated by simplified approaches[3,4] assuming a step function for $\Delta(z)$ because the order parameter varies within the S due to the self-consistency.[14,15]

Here we undertake an idealized study of different *intrinsic* properties of three-dimensional SNS junctions which can be

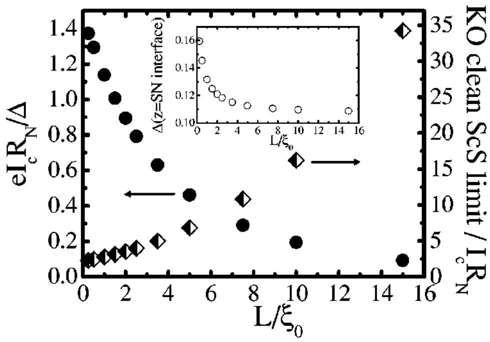

FIG. 1. Product of the critical current I_c and the normal-state resistance R_N as a function of the SNS junction thickness L. Both the S and N are at half-filling in the bulk. The value of I_cR_N is always below the product of the bulk critical current in the S leads and the Sharvin point-contact resistance, $I_c^{\mathrm{bulk}}R_{\mathrm{Sh}}=1.45\Delta/e$. The right axis measures the ratio of the Kulik-Omelyanchuk formula $I_cR_N=\pi\Delta/e$ for the clean superconducting point contact ($L\to0$) and I_cR_N of our junctions. The inset shows the decay of the order parameter at the SN interface for $I=0$, which reaches an asymptotic value of about one-half of the bulk Δ for $L\simeq 2\xi_S$ [$I_cR_N/\Delta(z=\mathrm{SN}$ interface) is virtually constant for $L<2\xi_S$].

detrimental to I_c, without invoking any sample-fabrication-dependent additional scattering at the SN interface. Two such effects are known: (i) the requirements of self-consistency, which becomes important for specific junction geometries delineated below, depresses the order parameter near the SN boundary and therefore the current in short junctions; (ii) a finite ratio Δ/μ (where μ is the Fermi energy measured from the bottom of the band) generates intrinsic normal scattering at the SN boundary (without the presence of impurities or barriers at the interface). For example, both effects can be of relevance in Josephson junctions based on newly discovered MgB_2 superconductors.[16] Therefore, even a clean junction (with ballistic transport above T_c) might not be in the ballistic limit[17] below the superconducting transition temperature T_c, unless the filling is tuned to the energy of the transmission resonances. Our principal result for the evolution of I_cR_N as a function of L is shown in Fig. 1. The I_cR_N drops by about an order of magnitude at $L\sim\xi_N$, thus showing how the characteristic voltage can be reduced dramatically in moderate length junctions, even in the low-temperature limit (to which our junctions belong). The reduction of I_c in our short junctions is determined by the depression of the order parameter in the S, as demonstrated by the inset in Fig. 1 where $\Delta(z)$ at the SN interface decreases asymptotically to a limiting value reached at $L\gtrsim 2\xi_S$ with $I_cR_N/\Delta(z=\mathrm{SN}$ interface) being nearly a constant for $L<2\xi_S$. For the junctions thicker than $2\xi_S$, the decay of the critical current $I_c\sim 1/L$ scales as[5] E_{Th}, while at nonzero temperatures and for long enough junctions $L>\xi_N$ it changes into a simple exponential decay. Thus, in the general case $\xi_S<\xi_N$, I_c can be independent of L only for $2\xi_S<L<\xi_0$, as observed in the experiments. However, such thickness-independent I_c can be substantially below $Me\Delta/\hbar$, as defined by the inevitable ($v_F^S\neq v_F^N$) interface scattering and/or reduced Δ, with its lowest value being set at $L\simeq 2\xi_S$ by the "inverse proximity effect" on the S side of a SN structure. We believe that ballistic behavior could be found in our junctions at even lower T, where $\xi_N\gg 2\xi_S$, but such calculations are technically more involved at present.

The SNS Josephson junction is modeled by a Hubbard Hamiltonian

$$H=-\sum_{ij\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i} U_i\left(c_{i\uparrow}^{\dagger}c_{i\uparrow}-\frac{1}{2}\right)\left(c_{i\downarrow}^{\dagger}c_{i\downarrow}-\frac{1}{2}\right), \qquad (1)$$

on a simple cubic lattice (with lattice constant a). Here $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) creates (destroys) an electron of spin σ at site i, and $t_{ij}=t$ (the energy unit) is the hopping integral between nearest-neighbor sites i and j. The SNS structure is comprised of stacked planes[18] where $U_i<0$ is the attractive interaction for sites within the superconducting planes (inside the N region $U_i=0$). In the Hartree-Fock approximation (HFA), this leads to a BCS mean-field superconductivity in the S leads, where for $U_i=-2$ and half-filling we get $\Delta=0.197t$ ($T_c=0.11t$) and $\xi_S=\hbar v_F^S/\pi\Delta\simeq 4a$. The lattice Hamiltonian (1) of the inhomogeneous SNS system is solved by computing a Nambu-Gor'kov matrix Green function. The off-diagonal block of this matrix is the anomalous average which quantifies the establishment of superconducting correlations in either the S [$\Delta(z)=|U(z)|F(z)$, where $F(z_i,z_i,\tau=0^+)$ is the pair-field amplitude] or the N region. For the local interaction treated in the HFA, computation of the Green function reduces to inverting an infinite block-tridiagonal Hamiltonian matrix in real space. The Green functions are thereby expressed through a matrix continued fraction (technical details are given elsewhere[18]). The final solution is fully self-consistent in the order parameter $|\Delta(z)|e^{i\phi(z)}$ inside the part of the junction comprised of the N region and the first 30 planes inside the superconducting leads on each side of the N interlayer. Our Hamiltonian formulation of the problem and its solution by this Green function technique are equivalent to solving a discretized version of the Bogoliubov–de Gennes[19] (BdG) equations formulated in terms of Green functions,[20] but in a fully self-consistent manner—by determining the off-diagonal pairing potential $\Delta(z)$ in the BdG Hamiltonian[15] after each iteration until convergence is achieved. The tight-binding description of the electronic states also allows us to include an arbitrary band structure or more complicated pairing symmetries. The calculation is performed at $T=0.09T_c$ where $\xi_N=40a$, which is a low-temperature limit for almost all of our junction thicknesses.

This technique is different from the quasiclassical use of a coarse-grained microscopic Gor'kov Green function[21] or non-self-consistent solutions of the BdG equations[3] which are applicable only for special geometries where the left and right S leads can be characterized by constant phases ϕ_L and ϕ_R, respectively. This neglects the phase gradient $(d\phi/dz)_{\mathrm{bulk}}$ inside the S, thereby violating current conservation. Such an assumption is justified when the critical current of the junction is limited by, e.g., a point-contact geometry, which requires a much smaller gradient than $1/\xi_S$ at the critical current density in the bulk, while the Josephson current is determined by the region within ξ_S from the junction.[3] Since we choose the S and N layers of the same transverse width, I_c/I_c^{bulk} can be close to 1 for thin junctions. In such cases, current flow affects appreciably the superconducting order parameter [i.e., $F(z)$ both inside and outside the N] and a self-consistent treatment becomes necessary (as is the general case of finding the critical current of a bulk superconductor[22,23]). Since for a clean SNS junction $R_N a^2 = [(2e^2/h)(k_F^2/4\pi)]^{-1} \approx 1.58 h a^2/2e^2$ is just the Sharvin point-contact resistance (i.e., inverse of the conductance, at half-filling, per unit area a^2 of our junction with infinite cross section), the absolute limit of the characteristic voltage, $I_c^{\rm bulk} R_{\rm N} = 1.45\Delta/e$, is set by the bulk critical current $I_c^{\rm bulk}$ of the S leads,[22] as shown in Fig. 1. In three-dimensional (3D) junctions $I_c^{\rm bulk} = 1.09 en\Delta/\hbar k_F$ (per unit area a^2, at half-filling) is slightly higher than the current density determined by the Landau depairing velocity $v_{\rm depair} = \Delta/\hbar k_F$, at which superfluid flow breaks the phase coherence of Cooper pairs,[22] because of the possibility of gapless superconductivity at superfluid velocities slightly exceeding[23] $v_{\rm depair}$. Although our $I_c R_N$ is always smaller than the ideal KO limit, it is still above the experimentally measured values[7] in the intermediate junction thicknesses, which are about 100 times smaller than the KO limit. This suggests that additional scattering confined to the interface region is indeed necessary to account for such small values.[11,13]

Since self-consistent calculations require a phase gradient inside the S (which we choose to be a boundary condition in the bulk of the superconductor), we must carefully define how to parametrize the Josephson current. There are two possibilities: either a global phase change across the N region[24] or the phase offset[14] which is related to the phase change by a nontrivial scale transformation. We use a global phase change which in a discrete model like Eq. (1) requires a convention. The thickness of the junction is defined to be the distance measured from the point z_L, in the middle of the last S plane on the left (at z_L^S) and the first adjacent N plane (at $z_L^N = z_L^S + 1$), to the middle point z_R between the last N and first S plane on the right. Since $\phi(z)$ is defined within the planes, we set $\phi(z_L) = [\phi(z_L^S) + \phi(z_L^N)]/2$ to be the phase at z_L and equivalently for $\phi(z_R)$. The phase change across the barrier is then given by

$$\phi = L\left(\frac{d\phi}{dz}\right)_{\rm bulk} + \delta\phi(z_R) - \delta\phi(z_L), \tag{2}$$

where $\delta\phi(z)$ is the "phase deviation" which develops self-consistently on top of the imposed linear background variation of the phase. The current versus phase change relation is plotted in Fig. 2. Non-self-consistent calculations predict that I_c occurs at $\phi_c = \pi$ for both[6] ScS and long SNS junctions (at $T=0$).[5] However, the self-consistent analysis leads to a sharp deviation from these notions,[14] which is most conspicuous in our SNS geometry with a single normal plane. In the long-junction limit (e.g., $L = 60a > \xi_N$) we find the usual $\phi_c \simeq \pi/2$. The non-negligible Δ/μ also leads to a lowering of ϕ_c [and a washing out of the discontinuities in $I(\phi)$ at $T=0$], but comparison with non-self-consistent calculations, which take such normal scattering into account,[17] shows that this is negligible compared to the impact of the self-consistency.

The macroscopic phase of the order parameter $\phi(z)$ varies monotonically (i.e., almost linearly) across the self-consistently modeled part of the junction. However, the plot of $\delta\phi(z)$, obtained after the linear background is subtracted from $\phi(z)$, reveals a peculiar spatial distribution which depends on the thickness of the junction (Fig. 3). In the short- and intermediate-junction limits, $\delta\phi(z)$ gives a negative contribution to $\phi(z)$, which turns into a positive one upon approaching I_c. For thick enough junctions (e.g., $L=20a$ in Fig. 3) a small bump as the remnant of this behavior persists at the SN boundary, but is completely washed out in the

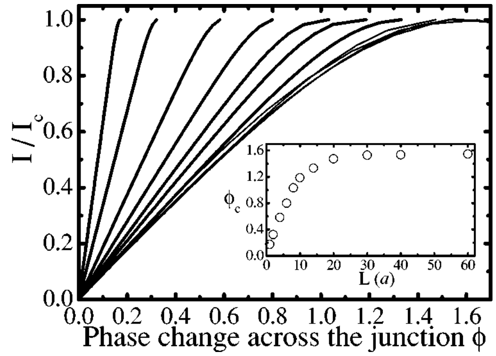

FIG. 2. Scaling of the current-phase relation $I(\phi)/I_c$ with the thickness of a clean SNS junction. Different curves correspond to, from left to right, $L=1,2,4,6,8,10,14,20,30,40,60$ (for $L \geqslant 30$ they start to overlap). Note that the phase change across the junction ϕ_c at the critical current $I_c = I(\phi_c)$ varies monotonically with the junction thickness, as shown in the inset, and is always far below π, which is the prediction of non-self-consistent calculations in both the short (Ref. 6) ($L \ll \xi_0$) and long (Ref. 5) ($L \gg \xi_0$) junction limits at $T \to 0$.

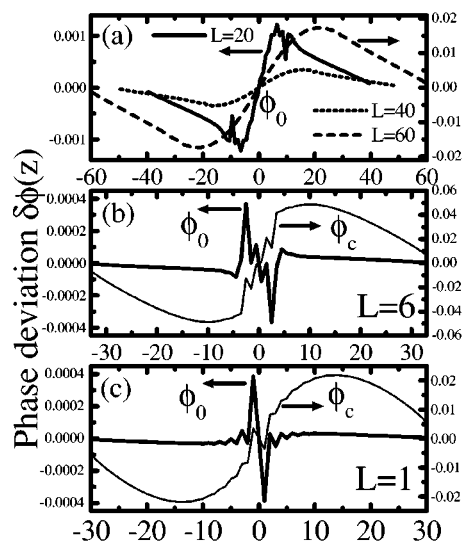

FIG. 3. Scaling of a spatial distribution of the phase deviation $\delta\phi(z)$ within the self-consistently modeled part of the clean SNS junction. The total phase change across the junction ϕ is the sum of the bulk phase gradient$\times L$ and the change in $\delta\phi(z)$ along the N interlayer, Eq. (2): ϕ_0 at small supercurrent and ϕ_c at the critical junction current I_c. At large enough junction thickness L [panel (a)] the shape of $\delta\phi(z)$ is just rescaled by the increase of the Josephson current, while for smaller L the shape changes abruptly upon approaching I_c [panels (b) and (c)].

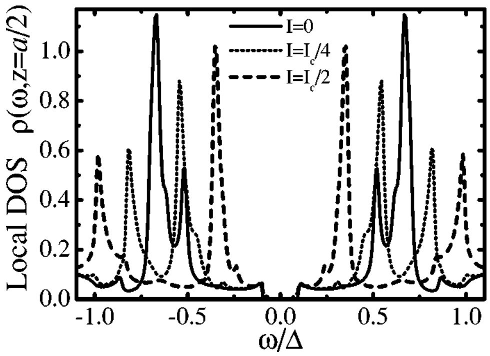

FIG. 4. Local density of states at the central plane of a clean 3D SNS junction (composed of ten normal planes, $L=10a$) for different supercurrent flows: $I=0$, $I=I_c/4$, and $I=I_c/2$. The peaks correspond to Andreev bound states (ABS's) confined within the N region at energies $E<\Delta$. For $I\neq 0$, the degeneracy of right- and left-moving electrons is lifted by a Doppler shift, giving rise to the Josephson dc current [or at least part of it (Refs. 5 and 20)]. The minigap around the Fermi energy $\omega=0$ in the N region appears to be a result of a finite $\Delta/\mu\approx 0.03$ generating normal scattering at the SN interfaces.

long-junction limit. Thus, $\delta\phi(z)$ forms a "phase antidipole" (i.e., its spatial distribution has positive and negative parts opposite to that of the phase dipole, introduced in Ref. 20), which is a self-consistent response to a supercurrent applied in the bulk. From the scaling features of the spatial distribution of $\delta\phi(z)$ we conclude that such counterintuitive phase pileup around the SN interface is generated by finite-Δ/μ effects.

Finally, we examine the local density of states (LDOS) $\rho(\omega,z_i)$ on the central plane of the $L=10a$ junction, as shown in Fig. 4. At zero Josephson current we find peaks in the LDOS, which are of finite width, corresponding to Andreev bound states[25] (ABS's). Moreover, instead of a nonzero LDOS all the way to the Fermi energy at $\omega=0$ (vanishing linearly as $\omega\to 0$), which stems from quasiparticles traveling almost parallel to the SN boundary, a minigap $E_g \sim\Delta^2/\mu$ is found which appears to be the consequence of finite Δ/μ induced scattering.[17] The quantized bound states are the result of an electron (with energy below Δ) being retroreflected into a hole at the SN interface, while a Cooper pair is injected into the superconductor and vice versa. The hole is in turn transformed into an electron on the opposite surface, so that in the semiclassical picture, a bound state forms corresponding to a closed quasiparticle trajectory (i.e., an infinite loop of Andreev reflections electron→hole →electron . . .). The time-reversed ABS's carry current in the opposite direction, and the two bound states are degenerate and decoupled (if there is no interface scattering). When the phase gradient is set within the S leads, a phase change appears across the junction (i.e., dc Josephson current), and the degenerate ABS's split due to the Doppler-shift. On the other hand, the minigap changes only slightly with increasing ϕ. The two Doppler-split peaks drift apart monotonically until a bulk phase gradient corresponding to $I_c/2$, when one of them reaches the BCS gap edge, while the other one approaches the minigap edge. The motion of the ABS's for larger current runs into numerical problems that are described in detail elsewhere.[26]

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