Suppression of the “quasiclassical” proximity gap in correlated-metal–superconductor structures

Branislav K. Nikolić,† J. K. Freericks,† and P. Miller*

†Department of Physics, Georgetown University, Washington, DC 20057-0995
*Department of Physics, Brandeis University, Waltham, MA 02454

We study the energy and spatial dependence of the local density of states in a superconductor–correlated-metal–superconductor Josephson junction, where the correlated metal is a non-Fermi liquid (described by the Falicov-Kimball model). Many-body correlations are treated with dynamical mean-field theory, extended to inhomogeneous systems. While quasiclassical theories predict a minigap in the spectrum of a disordered Fermi liquid which is proximity-coupled within a mesoscopic junction, we find that increasing electron correlations destroy any minigap that might be opened in the absence of many-body correlations.

PACS numbers: 71.27.+a, 74.50.+r

Fermi-liquid metals have excitation spectra that typically vary on energy scales of electron volts. Metals that become superconducting, have all low-energy electrons form pairs. Since it takes an energy equal to the superconducting gap Δ to break a pair of electrons and form an excitation, there is a low-energy gap (on the order of meV) in the single-particle density of states (DOS) [1]. The original states at the Fermi level are “pushed” to excitations near ±Δ, which yields a singularity in the DOS at zero temperature (and a large peak at finite T). When a superconductor (S) is connected to a normal metal (N) to form a SNS Josephson junction, the superconductivity leaks into the normal metal via the proximity effect [2], and a weak link is established between the two S through the N. What happens to the low-energy electrons in the N is quite interesting. An electron near the Fermi level of the N is localized within the N because there are no single-particle states at low energy for it to scatter into within the S. Instead, the electron is retroreflected into a hole in the N, and creates a superconducting pair in the S via a process called Andreev reflection [3]. This reflection occurs at the SN interface and the NS interface, creating Andreev bound states with well-defined energy levels. These states are doubly degenerate, one carrying supercurrent to the right and one to the left. The states are broadened to peaks in the DOS when one averages over all different perpendicular momenta. Thus, Andreev reflection mixes the electron and hole states in the same proportion that they are mixed to form Bogoliubov quasiparticles in the S, with weights determined by the self-consistency condition. Such partially superconducting properties of the proximity-coupled normal metal are responsible for Josephson effect, as well as other peculiar phenomena in inhomogeneous systems which have been drawing increased attention over the past decade due to advances in mesoscopic superconductivity [4].

Another aspect of the proximity effect is the modification of the DOS in both the S (“inverse proximity effect” [2]) and the N side of a SN boundary, which becomes most conspicuous in mesoscopic confined geometries [4]. For example, in a sufficiently long SNS junction at low enough temperature, the proximity of the superconductor induces a minigap in the local density of states (LDOS) inside N interlayer [5] that has chaotic classical dynamics [6–9,11]. The minigap is of the order of the Thouless energy $E_{\text{Th}} = \hbar/t_{\text{dwell}}$, where $t_{\text{dwell}}$ is the typical time spent by an electron during its diffusive motion [6–9,11] ($t_{\text{dwell}} \approx L^2/D$ for a $N$ strongly coupled to a $S$, where $D$ is the diffusion constant) or during its chaotic ballistic motion [7] through the N region of size $L$, before escaping into the superconductor (for integrable classical dynamics in the N, the LDOS is nonzero, but vanishes nearly linearly at the Fermi level [8]). These results were obtained using either quasiclassical approaches [6–9,11] or mean-field treatment by random matrix theory [10]. However, recent calculations [13], which include additional quantum effects through a supersymmetric non-linear σ-model (NLSM) [14], show that mesoscopic fluctuations cause an exponentially small smearing of the quasiclassical gap in a diffusive SNS junction (the DOS tails appearing below the quasi-classical gap edge are due to prelocalized states [14] which couple weakly to the $S$ leads). Using tunneling spectroscopy, the proximity affected LDOS can be measured as a function of the distance from the SN interface in both the normal metal [15] and superconductor [16].

While both quasiclassical and NLSM calculations rely on the picture of well-defined (noninteracting) quasiparticles, little attention has been paid to proximity effects in systems where the $N$ layers are dominated by strong many-body correlations (except in one dimension where anomalously enhanced DOS have been found in a Luttinger liquid coupled to a superconductor [16]). Here we explore the LDOS, in both the superconducting and correlated metal sides of a superconductor–correlated-metal–superconductor (SCmS) Josephson junction. The
Fig. 3. The minigap in the LDOS of the Cm remnant of the minigap would be the quasiclassical prediction, but seems to be just band center.

 Bulk DOS is flat in the plotted energy range around the non-Fermi liquid described by the FK model where the scattering in the open “quasiclassical” minigap in the DOS of the correlated metal, as shown in Fig. 1; this occurs due to the extensive broadening of the “Andreev bound states” by electron-electron interaction, within quasiclassics, only that specularly reflects), or $E_g = 3.12 E_{Th}$ in a diffusive SNS junction. The perturbative analysis of the electron-electron interaction, within quasiclassics, only generates a slightly smaller $E_g$. The NLSM calculations for a SNS junction, with $N$ being a disordered noninteracting electron system, find nonzero DOS at all $E < E_g$, but the tail of subgap states is small for good metals (except near $E_g$). Our results are complementary to these theories, showing how the minigap can disappear at a critical correlation strength, and are of special interest in understanding the limitations of a phenomenological application of standard proximity-effect theory to experiments dealing with unconventional inhomogeneous structures, such as high-$T_c$ Josephson junctions with underdoped cuprates (a strongly correlated electron system) playing the role of the “normal region”

The SCmS Josephson junction is modeled by a Hamiltonian

C_m region is a non-Fermi liquid modeled by a Falicov-Kimball (FK) Hamiltonian. We find that increasing electron correlations completely destroy any initially open “quasiclassical” minigap in the DOS of the correlated metal, as shown in Fig. 1; this occurs due to the extensive broadening of the “Andreev bound states” by the scattering in the Cm. The appearance of a nonzero LDOS inside the S region within a distance on the order of the superconducting coherence length $\xi_S$ is plotted in Fig. 2. Our analysis is fully self-consistent (i.e., we take into account the suppression of the superconducting order parameter inside the S leads) at zero Josephson current across the junction. The calculation includes all (many-body) quantum effects encompassed in the dynamical mean-field theory, which has only recently been generalized to treat inhomogeneous normal systems and Josephson junctions.

Thus, our principal result is substantially different from the standard lore of a proximity-induced “hard minigap” (i.e., no states inside an energy interval $E_g \sim E_{Th}$), which is supported by both quasiclassical calculations and the picture of bound states induced by Andreev reflection. Such qualitative considerations give an estimate for $E_g$, which comes close to the values of the quasiclassical minigap obtained from the solution of the Usadel equation: $E_g = 0.78 E_{Th}$ in the diffusive $N$ layer of an INS structure ($I$ is an insulator that specularly reflects), or $E_g = 3.12 E_{Th}$ in a diffusive SNS junction. The perturbative analysis of the electron-electron interaction, within quasiclassics, only generates a slightly smaller $E_g$. The NLSM calculations for a SNS junction, with $N$ being a disordered noninteracting electron system, find nonzero DOS at all $E < E_g$, but the tail of subgap states is small for good metals (except near $E_g$). Our results are complementary to these theories, showing how the minigap can disappear at a critical correlation strength, and are of special interest in understanding the limitations of a phenomenological application of standard proximity-effect theory to experiments dealing with unconventional inhomogeneous structures, such as high-$T_c$ Josephson junctions with underdoped cuprates (a strongly correlated electron system) playing the role of the “normal region”...
\[
H = -\sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U_i \left( c_{i\uparrow}^\dagger c_{i\uparrow} - \frac{1}{2} \right) \left( c_{i\downarrow}^\dagger c_{i\downarrow} - \frac{1}{2} \right)
+ \sum_{i\sigma} U_i^{FK} c_{i\sigma}^\dagger c_{i\sigma} \left( w_i - \frac{1}{2} \right),
\]

(1)
on an infinite set of stacked square lattice planes, whose connectivity is the same as a simple cubic lattice (with lattice constant \(a\)). Here \(c_{i\sigma}^\dagger\) \(c_{i\sigma}\) creates (destroys) an electron of spin \(\sigma\) at site \(i\), \(t_{ij} = t\) (the energy unit) is the hopping integral between nearest neighbor sites \(i\) and \(j\) (both within the planes and between planes), \(U_i < 0\) is the attractive Hubbard interaction for sites within the superconducting planes, \(U_i^{FK}\) is the FK interaction for planes within the \(Cm\) region, and \(w_i\) is a classical variable that equals 1 if an \(A\) ion occupies site \(i\) and is zero if a \(B\) ion occupies site \(i\). The chemical potential \(\mu\) is set equal to zero to yield half filling in the \(S\) and \(Cm\). The negative-\(U\) Hubbard term describes the real-space pairing of electrons due to a local instantaneous attractive interaction. This generates a superconducting order in the \(S\) leads which, when treated in the Hartree-Fock approximation, is equivalent to conventional BCS theory, except that here the DOS is non-constant and provides the energy cutoff.

The superconducting layers have \(U_i = -2\) and \(w_i = 0\) for all sites. Such a homogeneous bulk superconductor is characterized by the usual BCS parameters: the transition temperature \(T_c = 0.11t\), the zero-temperature order parameter \(\Delta = 0.198t\), and the coherence length \(\xi_S = \hbar v_F/(\pi \Delta) \approx 4a\). The \(Cm\) interlayer is described by a half-filled FK model in the symmetric limit of half filling for the “ions” \(\langle w_i \rangle = 0.5\). One can view the FK metal as a binary alloy of \(A\) and \(B\) ions at 50% concentration with \(U_i^{FK}\) being the difference in site energy between the \(A\) and \(B\) ionic sites. The many-body problem is solved by taking an annealed average that yields the coherent potential approximation. This is the simplest many-body problem which, nevertheless, mimics a metal-insulator transition (MIT) of the type seen in the repulsive Hubbard model (except the metallic phase is not a Fermi liquid here). In the bulk, the FK correlated metal undergoes a MIT at \(U_i^{FK} \approx 4.9t\) (which is close to half of the bandwidth \(6t\)). This is illustrated in Fig. 3 which shows the DOS in a bulk \(Cm\) as a function of \(U_i^{FK}\). The DOS is independent of temperature \([22]\). Since the system is not a Fermi liquid for nonzero \(U_i^{FK}\), the DOS first develops a pseudogap, and then is suppressed entirely to zero as the correlations increase, eventually driving the system into a correlated insulator. The opening of the gap is continuous. In order to focus only on the modification of the DOS induced by the proximity effect, we choose \(U_i^{FK} \leq 2\) for the strength of Coulomb interaction in the FK correlated metal, which ensures that the bulk DOS around the band center is essentially constant.

The problem of inhomogeneous superconductivity is solved by employing the Nambu-Gorkov matrix formulation for Green functions with a local self-energy \([20]\). We treat the problem self-consistently in the complex order parameter \(\Delta_i\) for the part of the junction comprised of the normal region (containing 5 or 10 planes) and 30 superconducting planes on each side of the \(Cm\) interlayer. Inside this “self-consistent-part” of the infinite \(SCmS\) junction, the superconducting gap \(\Delta_i\) heals to its bulk value since all signatures of the inverse proximity effect are gone on the length scale of few \(\xi_S\) away from the \(SCm\) interface. The calculation is performed at the temperature \(T = 0.09T_c\) where the BCS gap is fully developed. Details of our computational algorithm have been given elsewhere \([21]\). The final result is the self-consistent Green function which allows us to compute the (many-body) LDOS as a function of plane position \(z_i\) and frequency \(\omega\) from the real-axis analytic continuation, \(\rho(\omega, z_i) = -\text{Im } G(\omega + i\delta; z_i, z_i)/\pi\).

The strength of the superconductivity in the \(N\) interlayer is quantified by the nonzero pair amplitude \(F(z_i) = \Delta_i/|U_i|\) (a two-particle property) which decays exponentially, due to the absence of an attractive interaction, on the length scale \(\xi_N = \sqrt{\hbar D/2\pi k_B T}\) (or as a power law at zero temperature in a clean normal metal \([23]\)). This is the length scale over which two thermal electrons with energy \(\omega \approx \pi k_B T\) in the \(N\), correlated by Andreev reflection over the length scale \(L_\omega = \sqrt{\hbar D/2\omega}\), lose their relative phase coherence (which then determines the thermodynamic critical Josephson current \(I_e\)). However, single-particle properties (like the DOS) \([11,12]\), or kinetic quantities \([2]\), can be influenced on a much longer length scale (where Josephson coupling vanishes) \(L_\omega \gg \xi_N\) for low-energy electrons \(\omega \ll kT\), which is ultimately limited by the mesoscopic phase-breaking length \(L_\phi\) \([4]\). There-
fore, the anomalies in the DOS for low $\omega$ extend up to the energy dependent distances $\sim L_a [15]$ from the $SN$ interface (which is smeared upon approaching $L_a [13]$). In a “closed” geometry, where a finite-size $N$ is disconnected from any electron reservoirs [1], this leads to a position independent minigap edge at $E_g \sim E_{TH}$ for sufficiently long $E_{TH} \ll \Delta$ diffusive interlayer ($\ell \ll L$, where $\ell$ is the mean free path). Thus, both the quasiclassical and NLSM descriptions of the proximity effect rely on the essential concepts in disordered Fermi-liquid physics, such as $E_{TH}$ governing thermodynamic and quantum transport phenomena in mesoscopic systems. Since our $Cm$ layer is a non-Fermi liquid, these concepts are not directly transferable. Therefore, to compare our findings with standard notions, we proceed along a phenomenological route frequently (but unwarrantedly) employed in experiments on $SNS$ Josephson junctions with an unconventional $N$ interlayer [21]. Namely, we extract an effective diffusion constant from the Kubo conductivity of the FK model [21], using the Einstein relation $\sigma_{FK} = 2e^2N(0)/D$ and the DOS at half-filling $N(0)$ from Fig. 3, and then compute $E_{TH} = hD/L^2$. It is interesting to check if such an energy scale provides any heuristic guidance in interpreting our results at small $U_{FK}$ where the hard minigap is present in the $Cm$ spectrum. For example, in the largest $U_{FK} = 2.0$ sample, the resistivity of the FK correlated metal is $\rho_{FK} \approx 240 \mu\Omega cm$ (assuming $a = 3 \AA$). From here we get $D \approx 2ta^2/\hbar$ and $\xi_N \approx 5.6a$. This is surprisingly close to the true $\xi_N \approx 6.7a$ extracted from the decay of $I_c$ in the $SCmS$ junction as a function of the $Cm$ layer thickness [20] (the agreement improves for smaller $U_{FK}$). The quasiclassical analysis for a mesoscopic diffusive junction of the same resistivity and with thickness $L = 10a$ would give $E_{TH} \approx 0.1\Delta$ and $E_g \approx 0.32\Delta$. However, at $U_{FK} = 2.0$ no gap is found in the $Cm$ spectrum, while only a small dip (Fig. 1) in the LDOS persists as a remnant of the minigap opened for $U_{FK} \lesssim 1.0$. Moreover, the ratios of the minigap sizes $E^a_g/E^b_g$ in the $SCmS$ junctions with two different thicknesses $L_a = 5a$ and $L_b = 10a$ are: (i) $U_{FK} = 0.1 \Rightarrow E^a_g/E^b_g = 2.9$, (ii) $U_{FK} = 0.25 \Rightarrow E^a_g/E^b_g = 3.1$, (iii) $U_{FK} = 0.5 \Rightarrow E^a_g/E^b_g = 4.4$, is a function of $U_{FK}$. These are different from the expected results of $E^a_g/E^b_g = (L_b/L_a)^2 = 4$ or $E^a_g/E^b_g = L_b/L_a = 2$, which would follow from $E_g \sim E_{TH}$ analogy with the quasiclassical description of the proximity effect in a diffusive Fermi-liquid metal of the same resistivity [11], or a clean but chaotic interlayer [3], respectively.

The last two pieces of information needed to characterize proximity-induced effects in correlated metals are: (1) the LDOS is position dependent, while $E_g$ is spatially constant (which is the same as the quasiclassical phenomenology [11]), and does not change upon lowering the temperature below our reference $T/T_c = 0.091$ for Fig. 1; (2) the minigap is open for small enough $U_{FK}$, where Andreev bound states also clearly coexist with it, as shown by the peaks below $\Delta$ in the $U_{FK} = 0.1$ case in Fig. 4. In fact, we find the largest minigap in the limit $U_{FK} \rightarrow 0$ (corresponding to a clean $SNS$ junction), which is generated by the normal reflection at the $SN$ interface due to a non-negligible $\Delta/\mu \approx 0.03$ determining the amplitude of the scattering [20] ($\mu$ is the Fermi energy measured from the bottom of the band). It appears that increasing of electron correlations by increasing $U_{FK}$ then just leads to a monotonic vanishing of any initially open minigap in the noninteracting case $E_g(U_{FK} = 0)$ depends on $U_i$, as illustrated in the inset of Fig. 1, and is outside of the quasiclassical approximation [24], but belongs to the realm of “noninteracting quasiparticle” physics. This should be contrasted with the quasiclassical minigap as a function of quenched disorder [17]: the minigap forms for arbitrarily small concentration of impurities, increases with $1/\ell$ to a maximum value when $\ell \sim L$, and then decreases in the diffusive limit as $E_{TH} \sim v_F \ell$. On the superconducting side of our $SCmS$ junction we find that position dependent LDOS is nonzero in the energy range $2\Delta$ (Fig. 3), and decays to zero on the length scale of a few $\xi_S$ from the $SCm$ boundary [4].

Acknowledgments: Support from ONR grant number N00014-99-1-0328 is gratefully acknowledged. Computer calculations were partially supported by HPC time from the Arctic Region Supercomputer Center.

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