Density of States below the Thouless Gap in a Mesoscopic SNS Junction

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Quasiclassical theory predicts an existence of a sharp energy gap $E_g \sim \hbar D/L^2$ in the excitation spectrum of a long diffusive superconductor–normal metal–superconductor (SNS) junction. We show that mesoscopic fluctuations remove the sharp edge of the spectrum, leading to a nonzero density of states (DOS) for all energies. Physically, this effect originates from the quasilocalized states in the normal metal. Technically, we use an extension of Efetov's supermatrix σ model for mixed NS systems. A nonzero DOS at energies $E < E_g$ is provided by the instanton solution with broken supersymmetry.

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When a small piece of a normal (N) metal is placed in contact with a superconductor (S), paired electrons enter the N region, changing its excitation spectrum. How drastic are these changes? Recent studies [1–5] demonstrate that the answer depends crucially on the type of dynamics in the N region: In the case of *integrable* classical dynamics, the density of states (DOS) of excitations is suppressed at low energies and vanishes nearly linearly at the Fermi level. Contrary, in N systems with *chaotic* dynamics, coupling to a superconductor produces a gap in the DOS of the order of $\hbar/\tau_c$, where τ_c is the typical time needed to establish contact with the superconductor.

To illustrate this statement, consider a generic example of a chaotic NS system: an SNS junction made of a disordered conductor of size L connected to the S terminals. When the N metal is diffusive, with the mean free path $l \ll L$, and sufficiently long, with the Thouless energy $E_{\rm Th} = \hbar D/L^2 \ll \Delta$ (here $D = v_F l/3$ is the diffusion constant, and Δ is the superconductive gap in the terminals), then τ_c is given by the diffusion time across the N region, $\tau_c \sim \hbar/E_{\rm Th}$. Thus, the energy gap $E_g \sim E_{\rm Th}$ develops in the DOS [3,4].

However, all the results mentioned above are based either on the quasiclassical theory of superconductivity and proximity effect [6–8] or on the mean-field treatment of the random-matrix theory (RMT). Although usually this is a good approximation, it is interesting to check whether some effects, which are beyond quasiclassics, may lead to qualitative changes in the above picture.

In this Letter we show that, indeed, mesoscopic fluctuations smear the hard gap in the quasiparticle spectrum of dirty SNS junctions, producing a tail of the subgap states with energies $E < E_g$. These low-lying states are due to the existence of quasilocalized states [9,10] in the N part of the junction which are weakly coupled to the S terminals, thereby having a larger τ_c. The magnitude of this mesoscopic effect is controlled by the dimensionless normal-state conductance $G \equiv h/e^2R_n$ of the junction, and is small (except for the vicinity of E_g) at $G \gg 1$. A related problem was considered recently in Ref. [11], where a hypothesis of universality and some nontrivial results from the RMT [12] were used to find an exponentially small DOS below the mean-field gap in the N dot weakly connected to a superconductor. We will show that their conjecture holds for sufficiently narrow junctions at E close to E_g. Technically, our approach is completely different from Ref. [11] as we employ the fully microscopic supermatrix σ-model method [13] for mixed NS systems [14]. We find a nontrivial instanton solution to the saddle-point equations of the supermatrix σ model responsible for the nonzero DOS at energies $E < E_g$. The same instanton approach was used recently by Lamacraft and Simons [15] for the study of subgap states in a superconductor with magnetic impurities. Their instanton is pretty similar to that of ours, leading to the same energy scaling for the subgap DOS in the limit $E \to E_g$.

We consider an SNS junction with the N region being a rectangular bar of size $L \times L_y \times L_z$, coupled to the S terminals by the ideal contacts situated at $x = \pm L/2$. We neglect superconductivity suppression in the bulk terminals, provided that they are sufficiently large, and assume zero superconductive phase difference between them. The dimensionless conductance of the N region, $G(L, L_y, L_z) = 4\pi\nu D L_y L_z/L$, where ν is the normal-metal DOS per a single projection of spin.

Our results can be summarized as follows. The behavior of the subgap DOS $\langle\rho(E)\rangle$ depends on the relation between L_y, L_z, and the effective transverse length $L_\perp(E)$, scaling as $L_\perp(E \to E_g) \sim L(1 - E/E_g)^{-1/4}$ and $L_\perp(E \ll E_g) \sim L$. *In the vicinity of the quasiclassical gap,* at $E \to E_g$, we find an intermediate asymptotic behavior $\ln\langle\rho(E)\rangle \sim -\mathcal{G}(E)(1 - E/E_g)^{3/2} \propto -(1 - E/E_g)^{(6-d)/4}$, where $\mathcal{G}(E) = G[L, \min\{L_y, L_\perp(E)\}, \min\{L_z, L_\perp(E)\}]$, and d is the effective transverse dimensionality of the junction: $d = 0$ for narrow junctions with $L_y, L_z \ll L_\perp(E)$, $d = 1$ for wider junctions with $L_y \gg L_\perp(E) \gg L_z$, and $d = 2$ for films with $L_y, L_z \gg L_\perp(E)$. *In the low-energy limit,* $E \ll E_g$, the behavior of the DOS is log normal in 0D: $\ln\langle\rho(E)\rangle \sim -G\ln^2(E_g/E)$, and is a power law in 1D: $\ln\langle\rho(E)\rangle \propto -G\ln(E_g/E)$. These results are similar to those for the distribution of relaxation times in 1D and 2D diffusive conductors [9], although with an important difference: the basic energy scale in our case is given by E_g, whereas in Ref. [9] it was the level spacing $\delta = 1/\nu V$.

As a warm-up, we recall the standard quasiclassical approach [3,4] to diffusive SNS junctions based on the Usadel equation [8] for the quasiclassical retarded Green function $\hat{G}^R(\mathbf{r}, E)$. For the latter we will assume the angular parametrization, $\hat{G}^R = \tau_z \cos\theta + \tau_x \sin\theta \cos\varphi + \tau_y \sin\theta \sin\varphi$, where τ_i are the Pauli matrices in the Nambu space. In the absence of the phase difference between the S terminals, one can set $\varphi \equiv 0$, and the Usadel equation acquires the form (hereafter $\hbar = 1$):

$$D\nabla^2\theta + 2iE\sin\theta = 0, \qquad \theta(x = \pm L/2) = \pi/2. \tag{1}$$

The local density of states is given by $\rho_{\rm local}(\mathbf{r}, E) = 2\nu \,\mathrm{Re}\cos\theta(\mathbf{r})$. The substitution $\theta(x) = \pi/2 + i\psi(x)$ leads to the real equation for the function $\psi(x)$ with $\psi(\pm L/2) = 0$. It can be easily integrated yielding the relation between E and the magnitude of $\psi(x)$ at $x = 0$:

$$\sqrt{\frac{E}{E_{\rm Th}}} = \int_0^{\psi(0)} \frac{d\psi}{\sqrt{\sinh\psi(0) - \sinh\psi}}. \tag{2}$$

Equation (2) has real solutions for $\psi(0)$ only for $E \le E_g = cE_{\rm Th}$, with $c = 3.12$. At $E > E_g$, $\psi(0)$ becomes complex resulting in the square-root singularity [3] in the DOS [here and below we provide results for the DOS integrated over the whole N region, $\langle\rho(E)\rangle = \int d\mathbf{r}\,\langle\rho_{\rm local}(\mathbf{r}, E)\rangle$]:

$$\langle\rho(E)\rangle_{\rm quasicl.} = 3.72\delta^{-1}\sqrt{E/E_g - 1}. \tag{3}$$

Below the mean-field gap, at $E < E_g$, Eq. (2) has two real solutions, $\psi_1(0)$ and $\psi_2(0) > \psi_1(0)$, merging at $E = E_g$. They determine the corresponding solutions $\theta_{1,2}(x) = \pi/2 + i\psi_{1,2}(x)$ to Eq. (1). Having real $\psi(x)$, both of them do not contribute to the DOS at $E < E_g$. Usually the solution $\psi_1(x)$ is chosen by the continuity argument, as it obeys the natural condition $\lim_{E\to 0}\psi_1(x, E) = 0$, while $\psi_2(x, E)$ diverges in the limit of vanishing E. We will see however that it is this second solution which is responsible for the finite DOS below the quasiclassical gap.

In order to extend the quasiclassical solution and take into account mesoscopic fluctuations, we will use the nonlinear supermatrix σ model similar to that derived in [14]. The starting point is representation of $\hat{G}^R$ in terms of the functional integral:

$$\hat{G}^R(\mathbf{r}, \mathbf{r}', E) = -i\int \phi_{\rm F}(\mathbf{r})\phi_{\rm F}^+(\mathbf{r}')e^{-S[\phi]}D\phi^*D\phi,$$
$$S[\phi] = \int d\mathbf{r}\,\phi^+(\mathbf{r})(E + i0 - \hat{\mathcal{H}})\phi(\mathbf{r}). \tag{4}$$

In this expression ϕ is the 4-component superfield consisting of commuting (complex; $\phi_{\rm B}$) and anticommuting (Grassmann; $\phi_{\rm F}$) parts. The Hamiltonian $\hat{\mathcal{H}}$ is a matrix in the Nambu-Gor'kov (N) space:

$$\hat{\mathcal{H}} = \tau_z\left[\frac{\hat{\mathbf{p}}^2}{2m} - E_F + U(\mathbf{r})\right] + \Delta(\mathbf{r})\tau_x, \tag{5}$$

where $\Delta(\mathbf{r}) = \Delta\theta(|x| - L/2)$, and $U(\mathbf{r})$ is the random potential. In the absence of magnetic field, one has to double the field space in order to account for the time-reversal symmetry, introducing the "time-reversal" (TR) space according to $\Phi = (\phi, i\tau_y\phi^*)^T/\sqrt{2}$. This definition coincides with the one used in [16]; it differs from the notations of [13,14] by the factor $i\tau_y$ in the ϕ^* sector. Pauli matrices operating in the TR space are denoted by σ_i.

After this definition the derivation of the σ model is straightforward [13,14,16]. One has to carry out (i) averaging over the random potential with the correlator $\langle U(\mathbf{r})U(\mathbf{r}')\rangle = \delta(\mathbf{r} - \mathbf{r}')/2\pi\nu\tau$; (ii) Hubbard-Stratonovich transformation introducing an 8×8 matrix Q acting in the product of FB (Fermi-Bose), N, and TR spaces; (iii) expansion to the leading terms in ∇Q, E, and Δ. The result is

$$\langle\rho_{\rm local}(\mathbf{r}, E)\rangle = \frac{\nu}{4}\,\mathrm{Re}\int DQ\,\mathrm{str}\{k\Lambda Q(\mathbf{r})\}e^{-S[Q]}, \tag{6}$$

$$S[Q] = \frac{\pi\nu}{8}\int d\mathbf{r}\,\mathrm{str}[D(\nabla Q)^2 + 4iQ(i\tau_x\Delta + \Lambda E)]. \tag{7}$$

Here $\Lambda = \sigma_z\tau_z$, the matrix $Q = U^{-1}\Lambda U$ with the proper set [14] of matrices U is subject to the condition $Q = CQ^TC^T$, where $C = -\tau_x\sigma_z[(1 + k)\sigma_x + (1 - k)i\sigma_y]/2$, and $k = \mathrm{diag}(1, -1)_{\rm FB}$. The manifold of Q matrices is parametrized by eight ordinary and eight Grassmann variables.

The next step is to find the saddle-point solutions to the action (7). We start from the simplest case when Q does not contain Grassmann variables. Among eight commuting variables entering Q, only four are nonzero at the saddle points. Below we retain only these four variables in the parametrization of the Q matrix, which then splits into the Fermi-Fermi (FF) and Bose-Bose (BB) sectors:

$$Q_{\rm FF} = \sigma_z\tau_z\cos\theta_{\rm F} + \tau_x\sin\theta_{\rm F}, \tag{8a}$$

$$Q_{\rm BB} = [\sigma_z\cos k_{\rm B} + \tau_z\sin k_{\rm B}(\sigma_x\cos\chi_{\rm B} + \sigma_y\sin\chi_{\rm B})] \times [\tau_z\cos\theta_{\rm B} + \sigma_z\tau_x\sin\theta_{\rm B}]. \tag{8b}$$

The variables $\theta_{\rm F,B}$ coincide (at the supersymmetric saddle point) with the standard Usadel angle θ.

Minimization of the action for a uniform superconductor at $E \ll \Delta$ gives $Q_S = \tau_x$, i.e., $\theta_{\rm F,B} = \pi/2$ and $k_{\rm B} = 0$, that provides the boundary conditions for Q in the N region. In the absence of the phase difference between the S terminals, the angle $\chi_{\rm B}$ = const at the saddle point in the N part of the structure. Introducing new variables $\alpha_{\rm B} = \theta_{\rm B} + k_{\rm B}$ and $\beta_{\rm B} = \theta_{\rm B} - k_{\rm B}$ in the BB sector, one obtains for the saddle-point action

$$S[\theta_{\rm F}, \alpha_{\rm B}, \beta_{\rm B}] = 2S_0[\theta_{\rm F}] - S_0[\alpha_{\rm B}] - S_0[\beta_{\rm B}], \tag{9}$$

$$S_0[\theta] = \frac{\pi\nu}{4} \int d\mathbf{r}\,[D(\nabla\theta)^2 + 4iE\cos\theta]. \qquad (10)$$

Varying with respect to θ, one recovers Eq. (1) as the saddle-point equation for the action (10).

The Usadel equation (1) possesses, apart from the x-dependent solutions discussed above, solutions which depend on the transverse (y,z) coordinates. The role of the transverse dimensions will be discussed later, while now we will consider the 0D case, relevant for sufficiently narrow junctions with $L_x, L_y \ll L_\perp(E)$. Then, according to the previous analysis, the Usadel equation has two solutions, $\theta_1(x)$ and $\theta_2(x)$. Therefore, the full action (9) has in total eight different saddle-point solutions: $(\theta_F, \alpha_B, \beta_B) = (\theta_i, \theta_j, \theta_k)$, with $i, j, k = 1,2$, that will be referred to as (i,j,k). However, only four of them with $\theta_F = \theta_1$ can be reached by a proper deformation of the integration contour.

The simplest is the *supersymmetric* saddle point (1,1,1). In this case, Gaussian integrations over commuting and anticommuting variables near it cancel each other, and the contribution to $\langle\rho(E)\rangle$ reduces to the form (3) with the vanishing DOS below E_g. Thus, the saddle-point approximation for the σ model (7) restricted to the supersymmetric saddle point is equivalent [14] to the quasiclassical treatment based on the Usadel equation (1).

To get a nonzero DOS below E_g it is necessary to take saddle points with *broken supersymmetry* into account. [Note that the global supersymmetry of the action is preserved by the Grassmann zero mode; cf. the term $\zeta\xi$ in Eq. (11).] Such a solution with the lowest action is (1,1,2) [actually, a whole degenerate family of the saddle points, and, in particular, (1,2,1), can be obtained from it by rotation on the angle $\chi_B \in [0, 2\pi)$]. The key point is that Gaussian fluctuations near this saddle point have a negative eigenvalue which leads to an additional imaginary unity in the preexponent and, consequently, to the nonzero DOS. This contribution is suppressed by the factor $e^{-\Delta S}$, where $\Delta S = S_0[\theta_1] - S_0[\theta_2] > 0$. Finally, the saddle point (1,2,2) has the action $2\Delta S$ and its contribution can be disregarded at $\Delta S \gg 1$. Thus, the subgap DOS can be estimated with exponential accuracy as $\langle\rho(E)\rangle \sim \delta^{-1} e^{-\Delta S(E)}$. Below we will calculate $\langle\rho(E)\rangle$ in the limiting cases $E \to E_g$ and $E \ll E_g$.

Now we turn to actual calculations at energies E close to E_g. It is possible to find the one-instanton contribution to the DOS in the energy range $G^{-2/3} \ll 1 - E/E_g \ll 1$ *including the preexponential factor*. An important observation to be used below is that the solutions $\theta_1(x)$ and $\theta_2(x)$ merge at E_g. Let us start with the supersymmetric saddle point (1,1,1) and look at fluctuations around it. Almost all of them are hard (with a mass of the order of E_g or larger) and can be neglected. There are only eight (corresponding to four commuting and four anticommuting variables) soft modes whose mass vanishes at $E = E_g$. Half of them transform the saddle point (1,1,1) to the instanton (1,2,1), and the other half transform it to the instanton (1,2,2). Below we will consider the case when $\Delta S \gg 1$ that allows one to disregard the contribution of the instanton (1,2,2) and to take Gaussian integrals over the corresponding soft fluctuations. As a result, in order to calculate the DOS in this limit it is sufficient to retain only two commuting (q and χ_B) and two Grassmann (ζ and ξ) variables parametrizing the relevant soft degrees of freedom in the matrix $Q = e^{-W^c/2} e^{-W^a/2} \Lambda e^{W^a/2} e^{W^c/2}$. Here the matrix W^a contains anticommuting variables: $W^a_{FB} = [if_0(x)/4][(\zeta + \xi)(i\tau_y + \tau_z\sigma_x) + (\zeta - \xi)(i\tau_y\sigma_z + \tau_z i\sigma_y)]$, $W^a_{BF} = \tau_x\sigma_x(W^a_{FB})^T\tau_x i\sigma_y$, while in the absence of W^a, Q reduces to the form (8) with $\theta_F = \beta_B = \theta_1(x)$, $\alpha_B = \theta_1(x) + iqf_0(x)$. The function $f_0(x)$ is the normalized difference $\delta\psi(x) = \psi_2(x) - \psi_1(x)$ at E_g: $f_0(x) = \lim_{E\to E_g} \delta\psi(x)/\|\delta\psi(x)\|$, where $\|F(x)\|^2 \equiv (1/L)\int_{-L/2}^{L/2} F^2(x)\,dx$. Evaluating the action, integrating over the cyclic angle χ_B, and performing the x integration, one obtains

$$S = \tilde{G}\left[\sqrt{\tilde{\varepsilon}}\,q^2 - \frac{q^3}{3} + \zeta\xi(2\sqrt{\tilde{\varepsilon}} - q)\right], \qquad (11)$$

$$\tilde{G} = \frac{\pi c_2 E_g}{2\delta} = \frac{cc_2}{8}G, \qquad \tilde{\varepsilon} = \frac{2c_1}{c_2}\varepsilon, \qquad \varepsilon = \frac{E_g - E}{E_g}, \qquad (12)$$

where $c_n = \int_{-L/2}^{L/2} \cosh\psi_0(x) f_0^{2n-1}(x)\,dx/L$, and $\psi_0(x) = \psi_{1,2}(x, E_g)$; $c_1 = 1.15$, and $c_2 = 0.88$. The action (11) has two saddle points: $q = 0$ and $q = 2\sqrt{\tilde{\varepsilon}}$ which correspond to the instantons (1,1,1) and (1,2,1), respectively. The invariant measure near the instanton (1,2,1) is given by $DQ = 4\sqrt{\tilde{\varepsilon}}\,dq\,d\zeta\,d\xi$. Substituting $\int \mathrm{str}(k\Lambda Q)\,dV = 2ic_1 V(4\sqrt{\tilde{\varepsilon}} - q)$ into Eq. (6) and integrating by the saddle-point method near $q = 2\sqrt{\tilde{\varepsilon}}$ we arrive at the one-instanton contribution to the DOS:

$$\langle\rho(E \to E_g)\rangle_{0D} = \frac{c_1}{\delta}\sqrt{\frac{\pi}{8\tilde{G}\sqrt{\tilde{\varepsilon}}}}\,\exp\left(-\frac{4}{3}\tilde{G}\tilde{\varepsilon}^{3/2}\right), \qquad (13)$$

where tilded quantities are defined in Eq. (12). This result is valid provided that $\varepsilon \gg G^{-2/3}$ when the contribution of the instanton (1,2,2) can be neglected.

The 0D result (13) can be generalized for a normal dot of an arbitrary shape coupled to a superconductor (cf. [1,11]), provided that the numbers c, c_n are defined with the use of the exact solutions $\theta_{1,2}(\mathbf{r})$ of the Usadel equation in a given geometry: $c_n = (1/V)\int \cosh\psi_0(\mathbf{r}) f_0^{2n-1}(\mathbf{r})\,d\mathbf{r}$. It is worth mentioning that the energy scaling of the result (13) coincides with the RMT conjecture of Ref. [11] by Vavilov *et al.*, who considered a quantum dot connected to a superconducting terminal through a perfectly transparent ($\Gamma = 1$) interface. The fact that a similar result is obtained for a system with very different, diffusive, dynamics is an indication that the energy scaling of the DOS tail always has the RMT form once the mean-field DOS has a well-defined square-root edge $\langle\rho(E)\rangle \sim \sqrt{E - E_g}$, regardless of the geometry and type of dynamics of the normal part of the system. The RMT conjecture of Ref. [11] was proved in a very recent preprint [17]. The limit of an opaque ($\Gamma \ll 1$) NS interface can be treated by the present approach, provided that the action (7) is supplied with the appropriate boundary term [13].

Turning to the limit of small energies, $E \ll E_g$, one obtains $\psi_1(x) \approx 0$ and $\psi_2(x) \approx A(1 - 2|x|/L)$, where, according to Eq. (2), $A \approx \ln(E_g/E)$ (cf. Ref. [9]). Thus, the action of the instanton (1,1,2) becomes $\Delta S(E) \approx -S_0[\theta_2] = \pi E_{\text{Th}} A^2/\delta$, and the result for the DOS reads

$$\langle \rho(E \ll E_g) \rangle_{0D} \sim \frac{1}{\delta} \exp\left(-\frac{G}{4} \ln^2 \frac{E_g}{E}\right). \qquad (14)$$

Equation (14) is derived in the range $\delta \ll E \ll E_g$. It may not be applicable at the scale of the level spacing, $E \sim \delta$, where the contribution of the soft fluctuations of the symmetry class CI [14] may become important.

Now let us consider the role of the saddle-point solutions which depend on the transverse coordinates y, z. At $E \to E_g$, one has to retain only soft modes associated with the instanton (1,1,2). As a result, the action (11) acquires a gradient term:

$$S = \tilde{G} \int \frac{dy}{L} \frac{dz}{L} \left(\frac{L^2}{2cc_2} (\nabla_\perp q)^2 + \sqrt{\tilde{\varepsilon}}\, q^2 - \frac{q^3}{3} \right), \qquad (15)$$

where the Grassmann variables are discarded as we are not interested in the preexponent. Comparing the first and the second term in Eq. (15), one extracts the characteristic transverse scale $L_\perp(E) = L(cc_2/2)^{-1/2} \tilde{\varepsilon}^{-1/4} \sim L\varepsilon^{-1/4}$, which determines the effective dimensionality of the system. If L_y or L_z is shorter than $L_\perp(E)$, then it costs too much energy to have gradients in that direction, and the corresponding dimension "freezes out." The 0D case considered above referred to the limit $L_y, L_z \ll L_\perp(E)$. Otherwise, an instanton will appear in the transverse direction to minimize the total action. In the 1D case [$L_y \gg L_\perp(E) \gg L_z$], the action (15) achieves its stationary point at $q(y) = 3\sqrt{\tilde{\varepsilon}} \cosh^{-2}(y/L_\perp)$, leading to

$$\langle \rho(E \to E_g) \rangle_{1D} \sim \frac{1}{\delta} \exp\left(-\frac{12\pi}{5} \sqrt{2cc_2}\, \nu D L_z \tilde{\varepsilon}^{5/4}\right). \qquad (16)$$

Analogously, in the 2D case [$L_y, L_z \gg L_\perp(E)$], the quasiparticle DOS tail has the form

$$\langle \rho(E \to E_g) \rangle_{2D} \sim \delta^{-1} \exp(-48.7 \nu D L \tilde{\varepsilon}). \qquad (17)$$

The length $L_\perp(E)$ diverges at E_g, indicating that any junction becomes effectively 0D close to the quasiclassical gap. However, different parts of the DOS tail may exhibit different exponents, from 1 to 3/2.

The value of $L_\perp(E)$ is getting shorter as E decreases, and becomes of the order of L at $E \ll E_g$. Then the solution of the 1D problem can be found following Ref. [9] where similar calculations were done in the problem of prelocalized states in a 2D disordered metal. The function $\psi_2(x, y)$ has a sharp peak at the center of the instanton and with the logarithmic accuracy is given by $\psi_2(x, y) = -4 \ln(2\sqrt{x^2 + y^2}/L)$. The result for the DOS then reads

$$\langle \rho(E \ll E_g) \rangle_{1D} \sim \delta^{-1} (E/E_g)^{4\pi^2 \nu D L_z}. \qquad (18)$$

To conclude, we have shown that mesoscopic fluctuations smear the quasiclassical gap in the DOS of a diffusive SNS junction. The tail of the DOS is due to the states anomalously localized in the N part of the junction and weakly coupled to the S terminals.

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