Tail States in a Superconductor with Magnetic Impurities

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A field theoretic approach is developed to investigate the profile and spectrum of sub-gap states in a superconductor subject to a weak magnetic impurity potential. Such states are found to be associated with inhomogeneous supersymmetry broken instanton configurations of the action.

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While spectral properties of an s-wave superconductor are largely unaffected by weak non-magnetic impurities [1], the pair-breaking effect of magnetic impurities leads to the destruction of superconductivity. Remarkably, the suppression of the quasi-particle energy gap is more rapid than that of the superconducting order parameter, admitting the existence of a narrow 'gapless' superconducting phase [2]. According to the conventional (mean-field) theory due to Abrikosov and Gor'kov (AG), a gap is maintained up to a critical concentration of magnetic impurities. Yet, being unprotected by the Anderson theorem, it is clear that the gap structure predicted by the mean-field theory is untenable and will be destroyed by rare configurations of the random impurity potential. Indeed, since the pioneering work of AG, several authors [3–8] have explored the nature of the 'sub-gap' states. The aim of this work is to investigate quantitatively the spectrum and profile of sub-gap states in weakly disordered superconductors.

In the earliest works [3–5], attention was focussed on the the influence of strong impurities. In the unitarity limit, it was shown that a single magnetic impurity leads to the local suppression of the order parameter and creates a bound sub-gap quasi-particle state. For a finite impurity concentration, these intra-gap states broaden into a band. This mechanism contrasts with the AG theory [2] for *weak* magnetic impurities which predicts a gradual suppression of the quasi-particle energy gap. Defining $\zeta \equiv 1/\tau_s|\Delta|$, where $|\Delta|$ represents the self-consistent order parameter, and τ_s denotes the Born scattering time due to magnetic impurities, one finds $E_{\rm gap}(\tau_s) = |\Delta|(1-\zeta^{2/3})^{3/2}$, showing an onset of the gapless region when $\zeta = 1$ (note $\hbar = 1$ throughout). However, even for weak disorder, optimal fluctuations of the random potential generate sub-gap states. Extending the arguments of Balatsky and Trugman [7], a fluctuation of the random potential which leads to an effective scattering rate $1/\tau_s'$ in excess of $1/\tau_s$ over a range in excess of the coherence length, $\xi = (D/|\Delta|)^{1/2}$, induces quasi-particle states down to energies $E_{\rm gap}(\tau_s')$. These sub-gap states are localised, bound to the region or 'droplet' where the scattering rate is large, and coupled through the proximity effect to the rest of the environment.

The situation bares comparison with band tail states in semi-conductors. Here rare or optimal configurations of the random impurity potential generate bound states, known as Lifshitz tail states [9], which extend well below the band edge. However, the correspondence is, to some extent, superficial: band tail states in semi-conductors are typically associated with smoothly varying, nodeless wavefunctions. By contrast, the tail states below the superconducting gap involve the superposition of states around the Fermi level. As such, one expects these states to be rapidly oscillating on the scale of the Fermi wavelength, but modulated by an envelope which is localised on the scale of the coherence length. This difference is not incidental. Firstly, unlike the semi-conductor, one expects the spectrum of the tails states within the superconducting gap to be 'universal', independent of the nature of the weak impurity distribution, but dependent only on the scattering time τ_s. Secondly, as we will see, one can not expect a straightforward extension of existing theories [9–11] of the Lifshitz tails to describe the profile of tail states in the superconductor.

The aim of this letter is two-fold: firstly we will propose a general field theoretic scheme which accommodates the AG theory as a mean-field, and whose fluctuations determine phase coherence effects in the gapless system. Secondly, we will relate the appearance of tail states to inhomogeneous supersymmetry breaking instanton configurations of the action.

To keep our discussion simple, we will take the quenched distribution of magnetic impurities to be 'classical' and non-interacting throughout. For practical purposes, this entails the consideration of structures where both the Kondo temperature [6] and, more significantly, the RKKY induced spin glass temperature [12] is smaller than the relevant energy scales of the superconductor. The remaining energy scales are arranged in the quasi-classical and dirty limits: $\epsilon_F \gg 1/\tau \gg (|\Delta|, 1/\tau_s)$ where $1/\tau$ represents the scattering rate associated with non-magnetic impurities. The random system we consider is specified by the Gor'kov Hamiltonian

$$\hat{H} = \left(\frac{\hat{\mathbf{p}}^2}{2m} - \epsilon_F + V(\mathbf{r})\right)\sigma_3^{\rm PH} + |\Delta|\sigma_2^{\rm PH} + J\mathbf{S}\cdot\sigma^{\rm SP} \quad (1)$$

where Pauli matrices $\{\sigma_i^{\rm PH}\}$ and $\{\sigma_i^{\rm SP}\}$ operate on particle/hole and spin indices respectively. Here $\mathbf{S}(\mathbf{r})$ and $V(\mathbf{r})$ represent Gaussian δ-correlated magnetic and non-magnetic impurity potentials with zero mean and variance $\langle JS_\alpha(\mathbf{r})JS_\beta(\mathbf{r}')\rangle_S = (6\pi\nu\tau_s)^{-1}\delta^d(\mathbf{r}-\mathbf{r}')\delta_{\alpha\beta}$ and $\langle V(\mathbf{r})V(\mathbf{r}')\rangle_V = (2\pi\nu\tau)^{-1}\delta^d(\mathbf{r}-\mathbf{r}')$ respectively, and ν represents the average density of states (DoS).

Phase coherence properties of the Hamiltonian (1) rely on its invariance under symmetry transformations. The magnetic impurity potential breaks both time-reversal and spin rotation symmetry leaving only charge conjugation symmetry,

$$\hat{H} = -\sigma_2^{\rm PH} \otimes \sigma_2^{\rm SP} \hat{H}^T \sigma_2^{\rm SP} \otimes \sigma_2^{\rm PH}. \quad (2)$$

When applied to the corresponding Gor'kov Green function, $\hat{G}_+(\epsilon) = -\sigma_2^{\rm PH} \otimes \sigma_2^{\rm SP} \hat{G}_-^T(-\epsilon)\sigma_2^{\rm SP} \otimes \sigma_2^{\rm PH}$, the same transformation converts an advanced function into a retarded function implying single-particle interference effects as $\epsilon \to 0$ [13]. To investigate their influence on spectral (and transport) properties of the microscopic Hamiltonian it is convenient to cast the problem in the form of a functional field integral. Following a standard route [14], the Gor'kov Green function can obtained from the generating function

$$\mathcal{Z}[0] = \int D(\bar{\Psi}, \Psi) \exp\left[i \int d\mathbf{r} \bar{\Psi}(\hat{H} - \epsilon\sigma_3^{\rm CC})\Psi\right],$$

where Ψ represent 16-component superfields with indices referencing the particle/hole (PH), spin (SP), charge-conjugation (CC), and boson/fermion (BF) spaces, and the Pauli matrices $\{\sigma_i^{\rm CC}\}$ act in the CC space. The elements of the superfields Ψ are not independent and exhibit the symmetry relation $\Psi = -\sigma_2^{\rm PH} \otimes \sigma_2^{\rm SP} \gamma \bar{\Psi}^T$ with $\gamma = {\rm diag}(i\sigma_2^{\rm CC}, -\sigma_1^{\rm CC})_{\rm BF}$.

As with normal disordered conductors [14], when subject to an ensemble average over the random impurity distribution, the functional integral over the Ψ fields can be traded for an integral involving matrix fields Q weighted by a non-linear σ-model action. Physically, the fields Q, which vary slowly on the scale of the mean-free path ℓ, describe the soft modes of density relaxation. When perturbed by the superconducting order parameter, the extension of the field integral approach is straightforward [15,16]. Taking into account the magnetic impurity potential, the local single-particle DoS can be expressed as $\langle \nu(\mathbf{r};\epsilon)\rangle_{V,S} = \nu \langle {\rm tr}(\sigma_3^{\rm PH} \otimes \sigma_3^{\rm CC}\, Q(\mathbf{r}))\rangle_Q/16$, where $\langle \cdots \rangle_Q = \int_{Q^2=\mathbb{1}} DQ\, (\cdots) e^{-S[Q]}$ with

$$S[Q] = -\frac{\pi\nu}{8} \int d\mathbf{r}\, {\rm str}\left[D(\partial Q)^2 - 4\left(i\epsilon\sigma_3^{\rm CC} \otimes \sigma_3^{\rm PH} - |\Delta|\sigma_1^{\rm PH}\right) Q - \frac{1}{3\tau_s}(\sigma_3^{\rm PH} \otimes \sigma^{\rm SP} Q)^2\right]. \quad (3)$$

Here $D = v_F^2\tau/d$ represents the classical diffusion constant associated with the non-magnetic impurities. The supermatrix fields are subject to the auxiliary symmetry condition: $Q = \sigma_1^{\rm PH} \otimes \sigma_2^{\rm SP} \gamma Q^T \gamma^{-1} \sigma_2^{\rm SP} \otimes \sigma_1^{\rm PH}$. Although the soft mode action is stabilised by the large parameter $\epsilon_F\tau \gg 1$, the majority of field fluctuations of the action are rendered massive: both the order parameter and the magnetic impurity potential lower the symmetry of the low-energy theory. To assimilate the effect of these terms, and to establish contact with the AG theory, it is necessary to explore the saddle-point equation.

Varying the action with respect to fluctuations of Q, subject to the non-linear constraint, one obtains the saddle-point or mean-field equation,

$$D\partial\,(Q\partial Q) + [Q, i\epsilon\sigma_3^{\rm CC} \otimes \sigma_3^{\rm PH} - |\Delta|\sigma_1^{\rm PH}] + \frac{1}{6\tau_s}\,[Q, \sigma_3^{\rm PH} \otimes \sigma^{\rm SP} Q \sigma_3^{\rm PH} \otimes \sigma^{\rm SP}] = 0\,.$$

With the ansatz: $Q_{\rm MF} = \sigma_3^{\rm CC} \otimes \sigma_3^{\rm PH} \cosh\hat{\theta} + i\sigma_1^{\rm PH} \sinh\hat{\theta}$, where $\hat{\theta} = {\rm diag}(\theta_1, i\theta)_{\rm BF}$, the saddle-point equation decouples into boson and fermion sectors and takes the form

$$\partial_{\mathbf{r}/\xi}^2 \hat{\theta} + 2i\left(\cosh\hat{\theta} - \frac{\epsilon}{|\Delta|}\sinh\hat{\theta}\right) - \zeta\sinh(2\hat{\theta}) = 0\,, \quad (4)$$

a result reminiscent of the Usadel equation of quasi-classical superconductivity [17]. This is no coincidence: when subject to an inhomogeneous order parameter, the same effective action (3) describes the proximity effect in a hybrid normal/superconducting compound [16]. In the present context, when combined with the self-consistent equation for the order parameter [18], the homogeneous form of Eq. (4) coincides with the mean-field equations obtained by AG [2,19].

The AG solution is not unique: for $\epsilon \to 0$, the saddle-point equation admits an entire manifold of homogeneous solutions parameterised by the transformations $Q = TQ_{\rm MF}T^{-1}$ where $T = \mathbb{1}_{\rm PH} \otimes \mathbb{1}_{\rm SP} \otimes t$ and $t = \gamma(t^{-1})^T\gamma^{-1}$: soft fluctuations of the fields, which are controlled by a non-linear σ-model defined on the manifold $T \in {\rm OSp}(2|2)/{\rm GL}(1|1)$ (symmetry class D in the classification of Ref. [20]), control the low-energy, long-range properties of the gapless system giving rise to unusual localisation and spectral properties. (For a comprehensive discussion of the physics of the gapless phase, we refer to Refs. [13,21–25].)

This completes the formal description of the bulk superconducting phase. The mean-field solution of the AG equation defines the global phase structure of the bulk states. Soft fluctuations around the AG mean-field describe phase coherence effects due to quantum interference. However, within the present scheme it is not yet clear how to accommodate sub-gap states in the gapped phase of the AG theory. To identify such states, it is necessary to return to the saddle-point equation (4) and seek spatially *inhomogeneous* solutions. We will see that such configurations necessarily break supersymmetry.

To keep our discussion simple, let us focus on a quasi one-dimensional geometry. The generalisation to higher dimensions follows straightforwardly. To stay firmly within the diffusive regime, we require the system size L to be much smaller than the localisation length of the normal system $\xi_{\rm loc.} \simeq \nu L_{\rm w} D$, where $L_{\rm w}$ denotes the cross-section. Furthermore, we focus on the interval near to the gapless region (i.e. $\zeta \lesssim 1$), where self-consistency of the order parameter can be safely neglected. To define the inhomogeneous field configurations it is convenient to deal not with the saddle-point equation (4) itself, but its first integral, $(\partial_{x/\xi}\hat{\theta})^2 + V(\hat{\theta}) = $ const., where

$$V(\hat{\theta}) \equiv 4i \left(\sinh\hat{\theta} - \frac{\epsilon}{|\Delta|}\cosh\hat{\theta} \right) - \zeta \cosh(2\hat{\theta}) \ ,$$

represents the effective complex 'potential'. Let us denote by $\theta_{\rm AG}$ the values of θ_1 and $i\theta$ at the conventional AG saddle-point. From the mean-field DoS, $\nu(\epsilon) = \nu \ {\rm Re}\cosh\theta_{\rm AG}$, it is evident that for $\epsilon < E_{\rm gap}$, Im $\theta_{\rm AG} = \pi/2$. The corresponding value of Re $\theta_{\rm AG}$ depends sensitively on the energy, with Re $\theta_{\rm AG} = 0$ for $\epsilon = 0$. Taking into account the condition that the solution should coincide with $\theta_{\rm AG}$ at infinity, one can identify a "bounce" solution parameterised by $\theta_1 = i\pi/2 + \phi$, with ϕ real, involving the *real* potential $V_{\rm R}(\phi) \equiv V(i\pi/2 + \phi)$ with endpoint ϕ' such that $V_{\rm R}(\phi') = V_{\rm R}(\phi_{\rm AG})$.

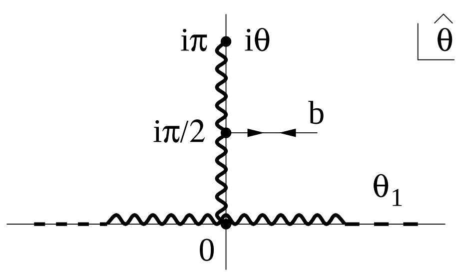

FIG. 1. Integration contours for boson-boson and fermion-fermion fields in the complex $\hat{\theta}$ plane. The bounce solution for $\epsilon = 0$ (labelled as 'b') is shown schematically.

Now integration over the angles $\hat{\theta}$ is constrained to certain contours [14]. Is the bounce solution accessible to both? As usual, the contour of integration over the boson-boson field θ_1 includes the entire real axis, while for the fermion-fermion field $i\theta$ runs along the imaginary axis from 0 to $i\pi$. With a smooth deformation of the integration contours, the AG saddle-point is accessible to both the angles $\hat{\theta}$ [16]. By contrast, the bounce solution *and* the AG solution can be reached simultaneously by a smooth deformation of the integration contour *only* for the boson-boson field θ_1 (see Fig. 1). The bounce is associated with a *spontaneous breaking of supersymmetry* at the level of the saddle point.

Having identified the saddle-point field configuration, we now turn to the role of fluctuations. Here we sketch the important aspects of the expansion, referring to Ref. [25] for a detailed analysis. Field fluctuations can be separated into "radial" and "angular" contributions. The former involve fluctuations of the diagonal elements $\hat{\theta}$, while the latter describe rotations including those Grassmann transformations which mix the BF sector. Both classes of fluctuations play a crucial role.

As usual, associated with radial fluctuations around the bounce, there exists a zero mode and a negative energy mode due to translational invariance of the solution. The latter, which necessitates a $\pi/2$ rotation of the corresponding integration contour to follow the line of steepest descent (c.f. Ref. [26]), has two effects: firstly it ensures that the non-perturbative contributions to the local DoS are non-vanishing, and secondly, that they are positive. Turning to the angular fluctuations, the spontaneous breaking of supersymmetry is accompanied by the appearance of a Grassmann zero mode separated by a gap from higher excitations. The zero mode ensures that the supersymmetry breaking saddle-point respects the normalisation condition $\langle \mathcal{Z}[0]\rangle_{V,S} = 1$, and that the local DoS is non-vanishing only in the vicinity of the bounce.

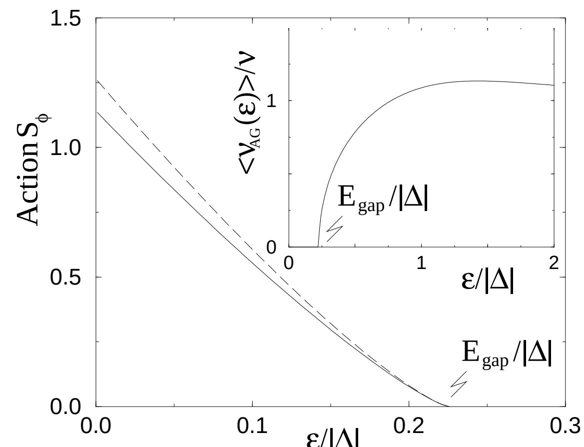

FIG. 2. Action S_ϕ for $\zeta = 0.5$ obtained numerically (solid curve) together with the expansion in $E_{\rm gap} - \epsilon$ (dotted curve) as determined by Eq. (6). Note that the action vanishes as $\epsilon \to E_{\rm gap}$. The AG solution for the DoS is shown inset.

Taking into account Gaussian fluctuations and zero modes, one obtains the non-perturbative, one instanton contribution to the sub-gap DoS:

$$\frac{\langle \nu(\epsilon)\rangle_{V,S}}{\nu} \sim \ (-i|K|) \int dx \ i(\sinh\phi(x) - \sinh\phi_{\rm AG})|\varphi_0(x)|^2 \times \sqrt{\frac{LS_\phi}{\xi}} \ \exp\left[-4\pi\nu L_{\rm w}\sqrt{D|\Delta|}S_\phi \right] \ , \qquad (5)$$

where $S_\phi \equiv \int_{\phi_{\rm AG}}^{\phi'} d\phi \sqrt{V_{\rm R}(\phi_{\rm AG}) - V_{\rm R}(\phi)}$. Here, the factor $\sqrt{LS_\phi/\xi}$ represents the Jacobian associated with the introduction of the collective coordinate [26], $-i|K|$ is the overall factor from the non-zero modes, and $\varphi_0(x)$ represents the normalised eigenfunction associated with the Grassmann zero mode [25]. Fig. 2 shows the action S_ϕ for a typical value of ζ. These results show that, for arbitrarily small but finite impurity concentrations, the DoS remains *finite* even at $\epsilon = 0$. For energies ϵ just below $E_{\rm gap}$, an analytical solution can be obtained for the bounce in arbitrary dimension. Generally, one finds the exponent $4\pi g(\xi/L)^{d-2}S_\phi$ where

$$S_\phi = a_d\, \zeta^{-2/3}(1-\zeta^{2/3})^{-(2+d)/8}\left(\frac{E_{\rm gap}-\epsilon}{|\Delta|}\right)^{(6-d)/4}. \quad (6)$$

Here $g = \nu D L^{d-2}$ denotes the bare conductance, and a_d is a numerical constant ($a_1 = 8\ \sqrt[4]{24}/5$). Furthermore, the optimal solution extends over a length scale $\xi((E_{\rm gap}-\epsilon)/|\Delta|)^{-1/4}$, set by the coherence length (as expected), and diverges as $\epsilon \to E_{\rm gap}$ (c.f. Ref. [27]).

To conclude, let us make some remarks. Firstly, the procedure outlined above has a number of close relatives in the literature. As well as the investigation of tail states in semi-conductors [11], a supersymmetric field theory was developed by Affleck [28] (see also Refs. [29]) to investigate tail states in the lowest Landau level. There it was shown that tail states correspond to supersymmetry broken configurations of the Ψ-*field action* (c.f. Ref. [11]). It is also interesting to compare the present scheme with the study of 'anomalously localised states' [30] (see also, Ref. [31]). There one finds that long-time current relaxation in a disordered wire is also associated with spontaneous breaking of supersymmetry. Finally, we note that the Lifshitz argument has been applied on the level of the Usadel equation in the study of gap fluctuations due to inhomogeneities of the BCS interaction [27].

Although we have focussed on the question of tail states in the superconducting gap, the general scheme is more widely applicable. For example, in the present system, the transition to bulk superconductivity will be preempted by the nucleation of superconducting islands or droplets within the metallic/insulating phase (c.f. Ref. [32]). Similarly, the Stoner transition to a bulk itinerant ferromagnet in a disordered system will be mediated by the formation of a droplet phase in which islands become ferromagnetic [33]. In both cases, we expect these 'droplet phases' to be associated with inhomogeneous (replica) symmetry broken saddle-point field configurations of the corresponding low-energy action.

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[1] P. W. Anderson, J. Phys. Chem. Sol. **11**, 26 (1959).
[2] A. A. Abrikosov and L. P. Gor'kov, Sov. Phys. JETP **12**, 1243 (1961).
[3] Lu Yu, Physica Sinica **21**, 75 (1965)
[4] H. Shiba, Prog. Theo. Phys. **40**, 435 (1968).
[5] A. I. Rusinov, JETP Lett. **9**, 85 (1969).
[6] K. Maki, Phys. Rev. **153**, 428 (1967).
[7] A. V. Balatsky and S. A. Trugman, Phys. Rev. Lett. **79**, 3767 (1997).
[8] I. S. Beloborodov, B. N. Narozhny and I. L. Aleiner, cond-mat/9912216
[9] I. M. Lifshitz, Sov. Phys. Usp. **7**, 549 (1965).
[10] B. I. Halperin and M. Lax, Phys. Rev. **148**, 722 (1966); J. Zittartz and J. S. Langer, Phys. Rev. **148**, 741 (1966).
[11] J. Cardy, J. Phys. C **11**, L321 (1978).
[12] A. I. Larkin, V. I. Melnikov and D. E. Khmel'nitskii, Sov. Phys. JETP **33**, 458 (1971).
[13] A. Altland and M. R. Zirnbauer, Phys. Rev. Lett. **76**, 3420 (1996); Phys. Rev. B **55**, 1142 (1997).
[14] K. B. Efetov, *Supersymmetry in Disorder and Chaos* Cambridge University Press, 1997.
[15] R. Oppermann, Nucl. Phys. B **280**, 753 (1987); V. E. Kravtsov and R. Oppermann, Phys. Rev. B **43**, 10865 (1991).
[16] A. Altland, B. D. Simons and J. P. D. Taras-Semchuk, JETP Lett. **67**, 22 (1998); Adv. in Phys. **49**, 321 (2000).
[17] K. D. Usadel, Phys. Rev. B **4**, 99 (1971).
[18] When cast as an *interacting* theory (using, e.g., the replica method), a variation of the action with respect to Δ obtains the self-consistent equation $|\Delta| = (\pi g_\Delta/\beta\delta)\sum_{\epsilon_n}\sin\theta(\epsilon_n)$, where the sum runs over fermionic Matsubara frequencies ϵ_n, g_Δ denotes the pairing interaction constant, and $\beta = 1/k_B T$ [25].
[19] For a random matrix Hamiltonian of rank N, corrections to the homogeneous AG equation from massless fluctuations enter at $O(N^{-1})$ implying that the density of tail states vanishes in the limit $N\to\infty$. We note that this conclusion contradicts the findings of Ref. [8].
[20] M. R. Zirnbauer, J. Math. Phys. **37**, 4986 (1996).
[21] R. Bundschuh *et al.*, Phys. Rev. B **59**, 4382 (1999).
[22] T. Senthil and M. P. A. Fisher, Phys. Rev. B **61**, 9690 (2000).
[23] N. Read and D. Green, Phys. Rev. B **61**, 10267 (2000).
[24] M. Bocquet, D. Serban and M. R. Zirnbauer, Nucl. Phys. B **578**, 628 (2000).
[25] A. Lamacraft and B. D. Simons, unpublished
[26] See, e.g., S. Coleman, in *Aspects of Symmetry* (CUP) (1985).
[27] A. I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP **34**, 1144 (1972).
[28] I. Affleck, J. Phys. C **17**, 2323 (1984).
[29] K. Benedict, Nucl. Phys. B **280**, 549 (1987); K. B. Efetov and V. G. Marikhin, Phys. Rev. B **40**, 12126 (1989); O. Viehweger and K. B. Efetov, Phys. Rev. B **44**, 1168 (1991).
[30] B. A. Muzykantskii and D. E. Khmel'nitskii, Phys. Rev. B **51**, 5840 (1995).
[31] V. I. Fal'ko and K. B. Efetov, Europhys. Lett. **32**, 627 (1995); A. D. Mirlin, Phys. Rev. B **53**, 1186 (1996).
[32] L. B. Ioffe and A. I. Larkin, Sov. Phys. JETP **54**, 378 (1981).
[33] A. Andreev and A. Kamenev, Phys. Rev. B. **58**, 5149 (1998); B. N. Narozhny, I. L. Aleiner and A. I. Larkin, preprint cond-mat/0005267