

Lifshitz Tail in the Density of States of a Superconductor with Magnetic Impurities

A. V. Balatsky* and S. A. Trugman

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 9 May 1997)

We argue that *any* superconductor with magnetic impurities is gapless due to a Lifshitz tail in the density of states extending to zero energy. At low energy the density of states $\nu(E \rightarrow 0)$ remains finite. We show that fluctuations in the impurity distribution produce regions of suppressed superconductivity, which are responsible for the low energy density of states. [S0031-9007(97)04452-9]

PACS numbers: 74.62.Dh, 71.55.-i

The role of impurities in superconductors is a rich subject, going back to the pioneering papers by Abrikosov and Gor'kov [1] and by Anderson [2]. However, the majority of work has been concentrated so far on the "mean-field" treatment of the impurity problem in superconductors. Here we will address the role of the fluctuations of the distribution of magnetic impurities in an *s*-wave superconductor.

It has been experimentally known for some time that the density of states (DOS) in a superconductor with magnetic impurities is far greater at low energies than one would expect from Abrikosov-Gor'kov theory [3]. Using the suppression of the critical temperature to infer the pair breaking parameter, one typically arrives at a substantially lower DOS at $E \ll \Delta_0$ than is observed. (Δ_0 is the superconducting gap in the spectrum.) We suggest here that the *observed deviations from the Abrikosov-Gor'kov theory at small E are caused by fluctuations in the impurity distribution and the Lifshitz tail in the DOS of an impure superconductor.*

We observe that for any, no matter how small, concentration n of magnetic impurities in a superconductor there are fluctuations in the distribution of impurities across the sample. There are finite regions of high impurity concentration, where the superconducting state is suppressed due to scattering. These large regions of essentially normal metal produce low lying, $E \ll \Delta_0$ single particle states in the averaged density of states of the superconductor. It is clear that any unique singularity in the DOS, if one occurs, should be at $E = 0$ due to the particle-hole symmetry of the superconducting state, which we assume here and which is preserved even with magnetic impurities. We find that at low energy $E \ll \Delta_0$ the DOS is

$$\nu(E) \propto (1/\Delta_{L_0}) \exp(-\text{const} \times L_0^d), \quad (1)$$

where $\nu(E)$ is scaled with the normal state DOS, d is the dimensionality of space, Δ_{L_0} is the mean level spacing in the fluctuation region of the size of length $L_0 = (\xi_0 l)^{1/2}$, where $\xi_0 = \pi v_f / \Delta_0$ is the $T = 0$ superconducting coherence length, and l is the mean free path. The constant in the exponent will be given below. The tail in the DOS of a superconductor is similar to the tail in the DOS of a semiconductor, the so-called Lifshitz tail [4].

For any particular model of impurity scattering (e.g., Born versus unitary scattering), we assume that there exists a critical concentration n_c at which a thermodynamic superconducting sample will become normal due to the pairbreaking effect of impurities. The specific value of n_c obviously depends on the model. For the case of the Born scattering limit of magnetic impurities, within the Abrikosov-Gor'kov theory, $n_c = O(1)\Delta_0 N_0 / [J^2 N_0^2 S(S+1)]$, where N_0 is the normal metal DOS, J is the magnetic exchange between conduction electrons and the impurity, and S is the magnitude of the impurity spin [1]. This specific value is not important for our subsequent considerations. We will use n_c as a model-dependent input to our final answer. All concentrations are given in terms of the dimensionless concentration per unit cell of linear size a .

Here we will consider the case of arbitrary impurity exchange strength. It is known that magnetic impurities induce intragap states [5]. The energy of these states for large S is approximately $\omega_0 = \Delta_0 [1 - J^2 N_0^2 S(S+1)] / [1 + J^2 N_0^2 S(S+1)]$. These impurity states have a wave function $\Psi(r) \sim \exp(-r/\xi_{\omega_0})$ of size $\xi_{\omega_0} = \xi_0 [1 - (\omega_0/\Delta_0)^2]^{-1/2} \geq \xi_0$, where ξ_0 is the zero temperature superconducting coherence length. For subsequent consideration we assume that $n_c (\xi_0/a)^d \gg 1$, generally true for realistic systems, so that intragap states are strongly overlapping in the region where the impurity concentration is n_c . Impurity states form an impurity band, centered around ω_0 [5]. Fluctuations in the distribution of impurities lead to tails in this impurity band, which extend to zero energy.

Consider a fluctuation in the impurity distribution such that inside a region $V(L) = L^d$ [6], the local concentration of impurities is n_c (averaged over distances much greater than ξ_{ω_0} but smaller than L), as shown in Fig. 1. We assume that $L \gg l \geq \xi_{\omega_0}$, where l is the mean free path at the critical impurity concentration n_c .

The low energy single particle spectrum in the fluctuation region will be normal, since the local concentration is n_c . The proximity coupling to the superconducting reservoir at the boundary cannot open up a gap at large distances $\sim L \gg \xi_0$ due to pair breaking scattering. We ignore the region of size ξ_0 from the boundary where the

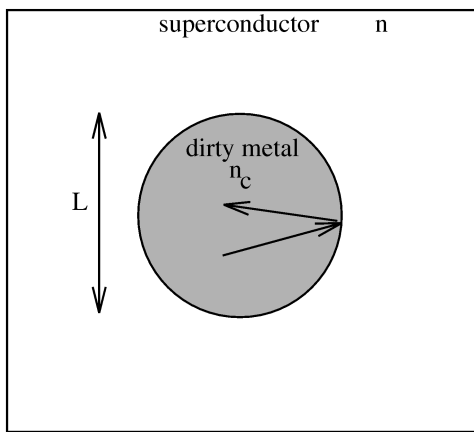


FIG. 1. Fluctuation region of size L , with concentration of impurities n_c inside the superconductor, is shown schematically. The equilibrium concentration is $n < n_c$. The fluctuation region has a metallic spectrum. Andreev reflection modifies the spectrum of quasiparticles [7]. In any local probe of the DOS, e.g., an STM, one would find that the I - V characteristics have a gap in the outer region, but are gapless if measured at any point inside the fluctuation region. The average DOS of a superconductor as $E \rightarrow 0$ hence will be the sample average of the DOS of the fluctuation regions.

gap is decaying. The single particle spectrum inside $V(L)$ will be equivalent to the spectrum of a normal metallic region with magnetic impurities in tunneling contact with a bulk superconductor.

To verify that the spectrum of the fluctuation region is indeed gapless we have numerically calculated the spectrum of a random superconductor in the mean-field approximation. Specifically, we considered the 1D BCS superconductor with the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_i \Delta_i^* c_{i,\uparrow} c_{i,\downarrow} + \text{H.c.} \\ + J \sum_{i \in V(L), \alpha, \beta} \vec{S}_i \cdot c_{i,\alpha}^\dagger \vec{\sigma}_{\alpha,\beta} c_{i,\beta}, \quad (2)$$

where i labels the sites of 1D chain, $V(L)$ are the impurity sites, t is the nearest-neighbor electron hopping, Δ_i is the pairing amplitude on the site i , J is the exchange coupling between the conduction electron and impurity spin, and \vec{S}_i is a *random* classical Heisenberg impurity spin on the site i . The last term in Eq. (2) describes the impurity scattering effects of the fluctuation region, which we assume to be in the middle of the superconducting region.

We consider a superconducting system of 40 sites with impurity spins present at a high concentration x on 10 of these sites. This approximation was chosen to mimic the high impurity density fluctuation region, which is responsible for the low energy DOS. For classical spins, the coupling J and impurity spin magnitude enter into the answer in the combination JS , hence the specific values of each of them separately does not matter. We have calculated the spectrum of quasiparticles in the mean-field

approximation, ignoring the self-consistency condition for the gap [8]. The DOS for this model is shown in Fig. 2.

Since $\Delta = 0$ in the impurity region, there are intragap states even for $JS = 0$. (There is only one such state for the parameters of Fig. 2.) We find that the intragap state evolves into an impurity band, and gradually fills the entire gap as the concentration or the coupling constant JS increases. This evolution of the impurity band is similar to the evolution of the band in doped semiconductors. The calculation confirms all the basic features one might expect: the appearance of impurity states inside the gap region, the growth of the impurity band, and finally the filling of states at low energies with nonzero $\nu(0)$.

A similar calculation is shown in Fig. 3, but with the mean-field superconducting gap $\Delta = 0.5$ everywhere, including the impurity region. In this case, there are no intragap states for $JS = 0$. For small JS , intragap states first appear at ω_0 , which is just below the energy Δ of the uniform gap. As JS increases, the gap gradually fills in. A larger value of JS is required to completely close the gap than in Fig. 2, because the density must spread down from Δ rather than from the intragap levels that already exist in Fig. 2 at $JS = 0$.

To illustrate the importance of the clustering of impurities for the DOS at low energies, we have numerically calculated the spectrum for a random distribution of impurities, and compared it to the case where the impurity distribution is constrained to be uniform; i.e., the Lifshitz tail is artificially suppressed (see Fig. 4). This approach is more accurate than the Abrikosov-Gor'kov calculation, where only the averaged scattering rate was considered. The first calculation in Fig. 4 allows for any distribution of impurities across the sample with the appropriate statistical weight, including clusters of high density. Comparison of these results clearly shows that the moment we

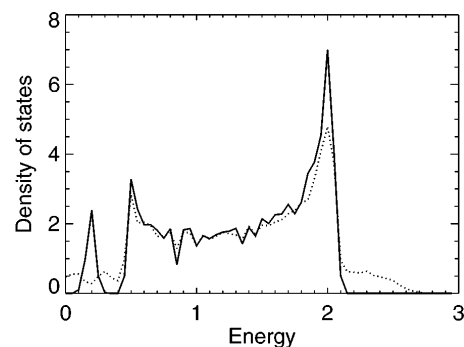


FIG. 2. The density of states is plotted for a 1D BCS superconductor with 40 sites. There is an impurity region of 10 sites, in which the superconducting gap Δ is taken to be zero. Classical Heisenberg impurity spins with random orientation occupy the impurity region with concentration $x = 0.5$. The solid line is for coupling $JS = 0.1$, and the dotted line is $JS = 1.0$. Other parameters are $t = 1$ and $\Delta = 0.5$. The DOS is averaged over 1500 realizations. The fine-scale roughness in the middle of the band is due to finite size effects.

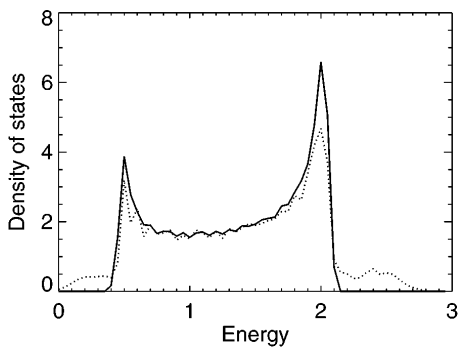


FIG. 3. Same as Fig. 2, but with the superconducting gap $\Delta = 0.5$ throughout the sample, including the impurity region.

allow high density clusters to appear, the DOS at low energies is dramatically increased due to Lifshitz tails.

A similar problem for a metallic grain in the presence of time reversal violating fields (e.g., impurity spins) in contact with a superconductor was considered by Altland and Zirnbauer [9]. At energies small compared to the Thouless energy $E_T = D/L^2$, one can ignore the spatially inhomogeneous solutions of the nonlinear- σ model. In this limit the spectrum of the grain is given by random matrix theory. The single particle DOS in Ref. [9] is $\nu_L(E) = 1/\Delta_L(1 + \frac{\sin(2\pi E/\Delta_L)}{2\pi E/\Delta_L})$, which goes to constant as $E \rightarrow 0$. Here Δ_L (not to be confused with the gap Δ_0) is the mean level spacing of the grain of linear size L , and $\nu_L(E)$ is averaged over all realizations of the random spectrum for grains of size L . We are interested in $E \ll \omega_0$, where the constraint $E \ll E_T$ is not important since $E_T/\omega_0 \sim (\Delta_0/\omega_0)(\xi_0 l/L^2)$ and this ratio is small except in the limit $\omega_0 \rightarrow 0$, where special care should be

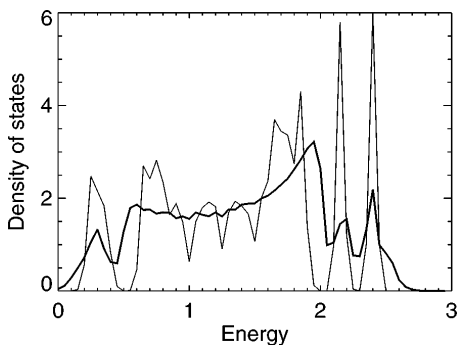


FIG. 4. The density of states is calculated numerically for a homogeneous superconductor with 40 sites, $\Delta = 0.5$ throughout the sample, and randomly oriented Heisenberg magnetic impurities with coupling $JS = 1.0$. The heavy line is the DOS for magnetic impurities that occupy each site with probability 0.2, averaged over 4000 realizations. The light line is the DOS for the same impurity concentration, but with all density fluctuations suppressed; a magnetic impurity is placed on every fifth site. When the spontaneous statistical fluctuations in the local density (Lifshitz tails) are suppressed, the density of states at zero energy vanishes.

taken. We will not address this limit here. We believe that the result $\nu(E) \sim \text{const}$ will still hold.

If we make the assumption that the spectrum of the fluctuation region in Fig. 1 is equivalent to the spectrum of a normal metal grain, it is easy to estimate the average DOS $\nu(E)$ from the distribution $P_L(n_c; n)$ in the size of the fluctuation regions,

$$\nu(E) \sim \int dV(L) P_L(n_c; n) \nu_L(E). \quad (3)$$

We now consider the probability distribution for a normal region of volume $V(L)$ with linear size $L \gg \xi_0$ to occur. This question is equivalent to finding the probability $P_L(n_c; n)$ of a fluctuation region of diameter L , taken to be spherical in d dimensions, with a concentration of impurities in this region equal to or greater than n_c , while the average concentration is n . This probability can be easily evaluated, following, for example, the arguments of Refs. [4,10]. We find

$$\ln[P_L(n_c; n)] = \delta\sigma = -V(L)\phi(n_c; n) \\ \phi(n_c; n) \approx n_c \ln(n_c/n) - n_c + n, \quad (4)$$

where $\delta\sigma$ is the change in entropy due to a fluctuation with homogeneous concentration n_c in the region $V(L)$, and $\phi(n_c; n)$ is the entropy density for the discussed fluctuation, which is model dependent. Equation (4) applies for small n and n_c [11]. Strictly speaking, Eq. (4) gives the probability of a fluctuation with a concentration equal to n_c . In principle one should integrate this probability over the range $n \geq n_c$ to obtain the total probability that the normal region $V(L)$ will occur. Taking into account this effect will only change the coefficient in $\phi(n_c; n)$ and the prefactor in Eq. (1).

The ratio of the mean level spacing to the superconducting gap is given by $\Delta_L/\Delta_0 = \kappa(n_c, J, N_0)L^{-d}$, where $\kappa(n_c, J, N_0)$ is a model-dependent dimensionless function of n_c, J, N_0 [12]. With the aid of Eq. (4) and using Δ_L we find

$$\nu(E) = \int_{V(L_0)} dV(L) P_L(n_c; n) \nu_L(E) \\ \sim \Delta_{L_0}^{-1} \exp[-L_0^d \phi(n_c; n)]. \quad (5)$$

This is our main result. In writing Eq. (5) the lower limit of the volume integration was taken at $L = L_0 = (\xi_0 l)^{1/2}$, when $E_T \sim \Delta_0$, because at smaller distances the gap acquires a nonzero mean value due to strong coupling to the bulk superconductor.

The fact that $\nu(E)$ is nonzero at arbitrarily small energy implies that a superconductor with magnetic impurities is always gapless. This does not, however, mean that the system is not superconducting. A dc current can flow through the system (around the impurity regions) with no dissipation, i.e., there is a condensate. The dissipation is nonzero for essentially any ac current due to dissipation in the normal metal regions.

A few comments are in order here. (i) It should be noted that there is a qualitative difference between the DOS in the tails for a superconductor as compared to a semiconductor. In the case of a high impurity concentration region of size L in a semiconductor, the energy has a quadratic dispersion $E - E_0 = \pi^2/2mL^2$, where E_0 is the lowest energy of the crystal composed of only the impurity atoms. This results in a $\nu(E) \propto \exp[-\text{const}/(E - E_0)^{d/2}]$ for the Lifshitz tail in a semiconductor. The difference comes from the fact that in a semiconductor tails are formed near the bottom of the band, whereas in our case the destruction of the superconducting gap leads to disordered normal regions. (ii) The suppression of superconductivity occurs at quite a low concentration $n_c \sim 1\%$. This allows for substantial fluctuations of the impurity distribution inside $V(L)$. However, it is clear that the most important configuration responsible for the low lying states is the one with a nearly homogeneous distribution with local concentration close to n_c . Any fluctuations with local $n(r) \leq n_c$ are ineffective for $\nu(E \rightarrow 0)$. We expect any improvement of the above consideration will lead to corrections to $\phi(n_c; n)$. (iii) We have ignored the possible interactions between impurity spins. This does not have to be the case in real systems, where in order to suppress superconductivity one has to have many impurities in regions of the size of the coherence length: $n_c(\xi_0/a)^d \gg 1$. Interactions between spins in this situation may be important, as was pointed out by Larkin *et al.* [13]. (iv) Similar considerations should apply to any system with a spontaneously induced gap due to interactions, i.e., charge density wave and spin density wave systems and to unconventional, e.g., d -wave, superconductors.

The present work is related to that of Larkin and Ovchinnikov [14]. They considered the DOS fluctuations for a disordered superconductor due to fluctuations of the gap $\Delta_0(\mathbf{r})$, and also found that the DOS is finite at small energies due to this process. We have considered here a different mechanism for generating a nonzero DOS.

We benefited from discussions with Markku Salkola at an early stage of this work. We are grateful to B. L. Altshuler, A. F. Andreev, A. R. Bishop, A. I. Larkin, D. J. Scalapino, and M. Zirnbauer for useful discussions. We are grateful to G. Aeppli for bringing Refs. [3] to our attention. Part of this work was done at ITP, Santa Barbara. This work has been supported by the Department of Energy and by NSF Grant No. PHY94-07194 at ITP.

*Also at Landau Institute for Theoretical Physics, Moscow, Russia.

- [1] A. A. Abrikosov and L. P. Gor'kov, *Sov. Phys. JETP* **12**, 1243 (1961).
- [2] P. W. Anderson, *Phys. Rev. Lett.* **3**, 325 (1959); T. Tsuneto, *Prog. Theor. Phys.* **28**, 857 (1962); D. Markowitz and L. P. Kadanoff, *Phys. Rev.* **131**, 563 (1963).
- [3] See, for example, M. A. Wolf and F. Reif, *Phys. Rev.* **137**, A557 (1965); A. S. Edelstein, *Phys. Rev. Lett.* **19**, 1184 (1967); S. D. Bader *et al.*, *Solid State Commun.* **16**, 1263 (1975).
- [4] I. M. Lifshitz, *Sov. Phys. Usp.* **7**, 549 (1965); [*Usp. Fiz. Nauk* **83**, 617 (1964)].
- [5] L. Yu, *Phys. Sinica* **21**, 75 (1965); H. Shiba, *Prog. Theor. Phys.* **40**, 435 (1968); A. I. Rusinov, *Sov. Phys. JETP Lett.* **9**, 85 (1969).
- [6] We ignore constants in the relation between $V(L)$ and L as the answer will be given up to an unknown constant.
- [7] This particle-hole admixture will enter in terms of "coherence factors," determining the effective charge of the excitation and related to the coefficients in Eq. (1). This effect is only one of the sources of uncertainty in this coefficient and will not be addressed in detail here.
- [8] For the spectrum of a region of size $L \gg \xi_0$, the self-consistent solution will presumably modify the gap only in a small region of size ξ_0 near the surface. The statistical properties of the spectrum of the fluctuation region will not be affected by self-consistent modifications of the gap function.
- [9] A. Altland and M. Zirnbauer, cond-mat/9602137.
- [10] B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer-Verlag, Berlin, 1984), Chap. 12.3, p. 277.
- [11] Recall that for superconducting metals it takes only a few percent of magnetic impurities to suppress superconductivity completely, e.g., superconducting La with 1% Gd becomes a normal metal.
- [12] The specific dependence of Δ_L in, e.g., the unitary versus the Born scattering limit on n_c and JS is determined by the particular model. A few features, however, remain universal regardless of the strength of the impurity scattering and concentration. The total number of impurity generated states inside the region $V(L)$ is $N(L) = n_c V(L)$. The bandwidth of the impurity band at small concentrations is $W \propto n_c^{1/2}$, and one finds qualitatively $\Delta_L = W/N(L) \propto L^{-d}$ with all the model-dependent coefficients being assembled in $\kappa(n_c, J, N_0)$.
- [13] A. I. Larkin, V. I. Melnikov, and D. E. Khmel'nitskii, *Zh. Eksp. Teor. Fiz.* **60**, 846 (1971) [*Sov. Phys. JETP* **33**, 458 (1971)].
- [14] A. I. Larkin and Y. N. Ovchinnikov, *Zh. Eksp. Teor. Fiz.* **61**, 2147 (1971) [*Sov. Phys. JETP* **34**, 1144 (1972)].