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Tail states in disordered superconductors with magnetic impurities: the unitarity limit

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Abstract

When subject to a weak magnetic impurity distribution, the order parameter and quasi-particle energy gap of a weakly disordered bulk *s*-wave superconductor are suppressed. In the Born scattering limit, recent investigations have shown that ‘optimal fluctuations’ of the random impurity potential can lead to the nucleation of ‘domains’ of localized states within the gap region predicted by the conventional Abrikosov–Gor’kov mean-field theory, rendering the superconducting system gapless at any finite impurity concentration. By implementing a field theoretic scheme tailored to the weakly disordered system, the aim of the present paper is to extend this analysis to the consideration of magnetic impurities in the unitarity scattering limit. This investigation reveals that the qualitative behaviour is maintained while the density of states exhibits a rich structure.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

In the absence of Coulomb interaction effects, the spectral and transport properties of a bulk singlet *s*-wave superconductor are largely insensitive to the presence of a weak non-magnetic impurity potential. This effect, which is ascribed to the Anderson theorem [1], limits the influence of long-range phase coherence phenomena to situations in which low-energy quasi-particles persist: notably, the physics of hybrid SN-compounds, and those which exhibit unconventional (e.g. *d*-wave) symmetry. However, another method of inducing low-energy quasi-particle states in the disordered superconducting environment is to impose an external time-reversal symmetry breaking perturbation which has a pair-breaking effect on the condensate.

Considering mechanisms of time-reversal symmetry breaking, it is possible to conceive of at least two distinct physical situations. The first is the imposition of a homogeneous

magnetic field: the diamagnetic properties of the superconductor limit considerations either to a vortex phase of a type II superconductor, or to superconductors whose lateral dimension is smaller than the penetration depth. In each case, field lines are able to penetrate the sample. A second method of breaking the intrinsic time-reversal symmetry of the system is to impose a magnetic impurity distribution. With both mechanisms, the perturbation acts with opposite sign on the two members of the Cooper pair. In the first case, the paramagnetic term in the single particle Hamiltonian reverses sign under $\mathbf{p} \rightarrow -\mathbf{p}$. In the second case, the spin of the magnetic impurity acts on different spin components with different sign. Building on the existing literature, the aim of this paper is to explore the quasi-particle properties of a weakly disordered superconductor subject to a magnetic impurity distribution with unitarity limit scattering.

1.1. Background: Abrikosov–Gor’kov theory

In the earliest work in this area, attention was focussed on the influence of a weak magnetic impurity distribution in which the influence of disorder could be treated in the Born approximation. In a seminal work by Abrikosov and Gor’kov [2], it was shown that the pair-breaking potential brings about only a gradual suppression of the superconducting order parameter. More surprisingly, according to the self-consistent mean-field theory, the energy gap in the quasi-particle density of states (DoS) is suppressed more rapidly than the order parameter, admitting a region in the phase diagram where the superconductor exhibits a ‘gapless’ phase. More precisely, defining the dimensionless control parameter,

$$\zeta = \frac{1}{\tau_s |\Delta|}$$

where $|\Delta|$ represents the self-consistent bulk order parameter, and $1/\tau_s$ denotes the Born scattering rate due to the magnetic impurities, the Abrikosov–Gor’kov mean-field theory shows the energy gap to vary as $\epsilon_g = |\Delta|(1 - \zeta^{2/3})^{3/2}$, showing an onset of the gapless region when $\zeta = 1$. Soon after its introduction, it was realized that the general Abrikosov–Gor’kov scheme applies equally to other mechanisms of pair-breaking (such as that imposed by a uniform magnetic field in a thin film or by a supercurrent)—requiring only a reinterpretation of the dimensionless parameter ζ (see, e.g. [3]).

In later works [4–8], various authors explored the influence of isolated magnetic impurities. In particular, in the unitarity limit, it was shown that a single *classical* magnetic impurity of spin S leads to the local suppression of the order parameter [7, 8] and nucleates a bound sub-gap quasi-particle state at energy [5]

$$\frac{\epsilon_B}{|\Delta|} = \frac{|1 - \alpha|}{1 + \alpha}$$

where, defining the density of states $\nu = 1/(L^d \delta)$ of a normal conductor, with δ being the single-particle level spacing, $\alpha = (\pi \nu J L^d |S|)^2$ represents the dimensionless scattering amplitude associated with the magnetic impurity.

For a finite impurity concentration, the sub-gap states weakly overlap, hybridize, and broaden into a band [5] centred on energy ϵ_B . Here, as in the Abrikosov–Gor’kov theory, the mean-field theory again predicts a gradual suppression of the quasi-classical energy gap ϵ_g , with the superconductor entering the gapless phase when $\zeta = \zeta_0 \equiv (1 - \alpha)^2$. Increasing the magnetic impurity concentration α , two qualitatively different situations can be realized: in the first case, when ζ reaches the value ζ_1 , the impurity band can merge with the continuum of bulk states before the system enters the gapless phase ($\zeta_1 < \zeta_0$), while in the second case ($\zeta_0 < \zeta_1$), the opposite situation pertains (see figure 1).

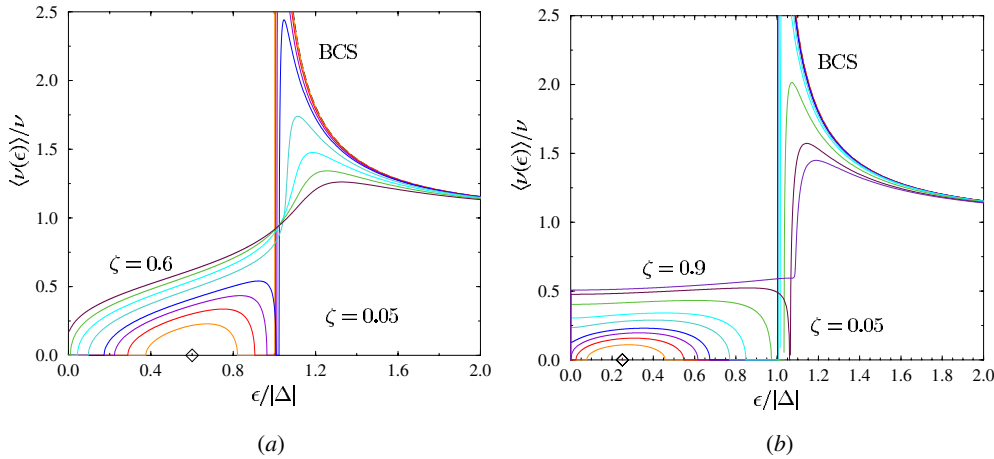


Figure 1. Quasi-particle density of states of a disordered superconductor with magnetic impurities drawn from a Poissonian distribution: (a) $\alpha = 0.25$ ($\zeta_1 < \zeta_0$), the value of ζ is increased from $\zeta = 0.05$ to $\zeta = 0.6$. The localized excited state for the one impurity problem is located at $\epsilon_B/|\Delta| = 0.6$. (b) $\alpha = 0.6$ ($\zeta_0 < \zeta_1$), the value of ζ is increased from $\zeta = 0.05$ to $\zeta = 0.9$. The localized excited state for the one impurity problem is located at $\epsilon_B/|\Delta| = 0.25$.

1.2. Beyond mean-field theory

Despite the success of the Abrikosov–Gor’kov mean-field theory and its extension to the unitarity limit scattering, two questions present themselves:

- Firstly, the existence of phase coherent low-energy quasi-particle states in the gapless phase renders the spectral and (thermal) transport properties of the superconductor susceptible to the influence of long-range quantum interference effects.
- Secondly, according to the mean-field description, a hard energy gap is maintained up to a critical concentration of magnetic impurities³. Yet, being unprotected by the Anderson theorem, it would seem that the gap structure predicted by the mean-field theory is untenable and may be destroyed by ‘optimal fluctuations’ of the random impurity potential.

In recent years, both issues have come under scrutiny. In particular, it has been shown that the long-range, low-energy spectral and transport properties of a weakly disordered superconductor can be classified according to their fundamental symmetries [9]. In the quasi-classical limit $\epsilon_F \tau \gg 1$, where $1/\tau$ represents the scattering rate of the non-magnetic impurity distribution, the spectral and transport properties of the weakly disordered system can be presented in the framework of a statistical field theory of non-linear σ -model type (for a review see, e.g., [10]). Within this approach, the conventional Abrikosov–Gor’kov mean-field theory is identified as the set of (homogeneous) saddle-point equations. Mesoscopic fluctuations due to quantum interference effects in the particle/hole channel are recorded in the soft field fluctuations around the homogeneous mean-field solution.

In the present case, such investigations reveal that mechanisms of quantum interference lead to the delocalization of the quasi-particle states even in low dimension [11–14]. This behaviour provides a striking contrast with that of other superconducting (and normal metallic)

³ In the Born scattering limit at $T = 0$, the critical concentration of magnetic impurities at which the energy gap goes to zero is $2e^{-\pi/4} \simeq 0.91$ times the critical concentration at which superconductivity is destroyed. In the unitarity limit, the critical value is decreased to $2[(1 - \alpha)/(1 + \alpha)]^2 e^{-\pi/4} \frac{(1-\alpha)^2}{1+\alpha}$.

systems where the mechanism of quantum interference has a tendency to bring about localization of the quasi-particle states. At the same time, the same general theoretical framework provides a means to explore the integrity of the gapped phase in the superconducting system. Earlier considerations of the ballistic system (i.e. with no non-magnetic impurities) by Balatsky and Trugman [15] had already indicated that ‘optimal fluctuations’ of the magnetic impurity potential could nucleate localized states below the predicted mean-field gap edge. In the framework of the statistical field theory, a general mechanism was subsequently elucidated [16] which showed that optimal fluctuations of even a non-magnetic impurity potential in the symmetry broken system are responsible for the spontaneous nucleation of domains or droplets, creating an entire band of localized states which fill the gap region: the gap edge predicted by mean-field becomes a quasi-particle mobility edge separating regions of localized from delocalized quasi-particle states.

The tail states predicted by the quantum field theory differ substantially in character from the bound states induced by an isolated magnetic impurity. The former derive from mesoscopic fluctuations of the electron and hole wavefunctions of the normal system: specifically, in regions where the phase sensitivity is anomalously high, the pair-breaking effect of magnetic impurities (or an external magnetic field) is enhanced over that predicted by the mean-field. Here, quasi-particle states localize over length scales comparable to the superconducting coherence length, $\xi = (D/|\Delta|)^{1/2}$, where $D = v_F^2 \tau / d$ represents the classical diffusion constant.

As well as presenting a concise review of the field theory of the disordered superconducting system with magnetic impurities, the aim of the present paper is to explore the integrity of the sub-gap state picture when in the presence of unitarity limit scattering. More precisely, at the level of mean-field, we have seen that, over a wide region of the phase diagram, the latter induces a delocalized band of bulk states centred on the bound state energy ϵ_B . In this case, do optimal fluctuations of the random potential lead to the nucleation of localized states in the vicinity of the narrow band?

The paper is organized as follows. In section 2 we refine the field theory of the weakly disordered superconducting system to incorporate the presence of magnetic impurities. Here we will take the magnetic impurities to be drawn from a random Poisson distribution allowing a continuous interpolation from the unitarity scattering limit to the Born scattering limit. Having obtained the low-energy effective field theory, in section 2.6 we will explore the homogeneous mean-field solution obtained from the saddle-point of the effective action. In this case, we correctly recover the phenomenology of [5] and identify the limit in which the Born scattering Abrikosov–Gor’kov theory [2] is obtained. By exploring instanton field configurations of the action, in section 3 we explore the integrity of the mean-field density of states. In particular, we will show that the gap edges predicted by the mean-field theory become mobility edges separating regions of bulk delocalized states from localized ‘droplet’ states generated by optimal configurations of the random impurity potential. A brief discussion of these results is contained within the concluding section.

2. Field theory of the superconducting system

Previous investigations have shown that, in the quasi-classical limit, the properties of the weakly disordered superconducting system can be expressed in the framework of a statistical field theory of non-linear σ -model type. In the present case, one must consider simply how to tailor this analysis to the consideration of the unitarity scattering limit of the magnetic impurity system. Since the general theoretical framework has been reviewed in a number of

publications [17, 11] and discussed for the magnetic impurity system in particular [16], we will keep our discussion concise focusing primarily on the idiosyncrasies of the present theory.

2.1. The model

In the mean-field BCS approximation, a bulk s-wave disordered superconductor in the presence of magnetic impurities is specified by the Gor'kov Hamiltonian

$$\hat{H}_G = \begin{pmatrix} \hat{H} & |\Delta|\sigma_2^{\text{SP}} \\ |\Delta|\sigma_2^{\text{SP}} & -\hat{H}^\top \end{pmatrix}_{\text{PH}}$$

where the index PH refers to the particle/hole space, and Pauli matrices σ^{SP} operate in the spin space. Here

$$\hat{H} = \hat{\zeta}_{\hat{p}} + V(\mathbf{r}) + J\mathbf{S}(\mathbf{r}) \cdot \boldsymbol{\sigma}^{\text{SP}}.$$

denotes the single particle Hamiltonian, with $\hat{\zeta}_{\hat{p}} = \hat{p}^2/2m - \epsilon_F$, ϵ_F is the Fermi energy, and $|\Delta|$ is the spatially homogeneous order parameter determined from the self-consistency condition, $\Delta = -L^d g_\Delta \langle \psi_\downarrow \psi_\uparrow \rangle$. In addition to a non-magnetic impurity potential, $V(\mathbf{r})$, drawn at random from a Gaussian white-noise impurity distribution with zero mean and variance,

$$\langle V(\mathbf{r}_1)V(\mathbf{r}_2) \rangle_V = \frac{1}{2\pi\nu\tau} \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

the system is subjected to a *classical* quenched Poisson distributed magnetic impurity potential:

$$\mathbf{S}(\mathbf{r}) = L^d \sum_i \delta^d(\mathbf{r} - \mathbf{r}_i) \mathbf{S}_i$$

i.e. where the points \mathbf{r}_i are drawn from a random Poissonian distribution. Here, for simplicity, we will suppose that the spins corresponding to different magnetic impurities are statistically independent, and that the distribution over the orientation is uniform, while the magnitude, S is fixed: i.e. $P(\{\mathbf{S}_i\}) = \prod_i \delta(S_i^2 - S^2)$.

Before proceeding, we should comment on the limitations of the present scheme. In the unitarity limit, one would expect spin 1/2 quantum magnetic impurities to be fully Kondo screened by the itinerant electron system. Our classical model is therefore limited either to situations in which the magnitude of the spin is sufficiently large that the moment cannot be fully compensated or, more realistically, to systems where the mutual RKKY interaction of the magnetic impurities leads to a spin glass ordering of the moments.

2.2. Generating functional

To formulate a field theory of the non-interacting superconducting system, we will follow the standard scheme [17, 11] and begin with the generating functional for the single quasi-particle Green function:

$$\mathcal{Z}[j] = \int D(\psi^\dagger, \psi) \exp \left\{ i \int d\mathbf{r} [\psi^\dagger (\epsilon_+ - \hat{H}_G) \psi + \psi^\dagger j + j^\dagger \psi] \right\}.$$

Here $\epsilon_+ = \epsilon + i0$, while $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$ represent two independent eight component supervector fields with PH, SP and boson/fermion (BF) internal indices. By incorporating an equal number of fermionic and bosonic components, the normalization $\mathcal{Z}[0] = 1$ is automatically imposed. In the following, it is convenient to implement a gauge transformation $\psi \mapsto U\psi$, where $U = E_{11}^{\text{PH}} - E_{22}^{\text{PH}} \otimes i\sigma_2^{\text{SP}}$ and $E_{11}^{\text{PH}} = \text{diag}(1, 0)_{\text{PH}}$, $E_{22}^{\text{PH}} = \text{diag}(0, 1)_{\text{PH}}$, whereupon, the Gor'kov Hamiltonian takes the simpler form

$$\hat{H}_G = [\hat{\zeta}_{\hat{p}} + V(\mathbf{r})]\sigma_3^{\text{PH}} + |\Delta|\sigma_2^{\text{PH}} + J\mathbf{S}(\mathbf{r}) \cdot \boldsymbol{\sigma}^{\text{SP}}.$$

As mentioned above, to determine the influence of quantum interference effects on the disordered superconducting system, it is useful to first classify the microscopic Hamiltonian according to its fundamental symmetries. In the absence of magnetic impurities the Gor'kov Hamiltonian exhibits both time-reversal symmetry and the particle/hole symmetry

$$\hat{H}_G = -\sigma_2^{\text{PH}} \otimes \sigma_2^{\text{SP}} \hat{H}_G^{\text{T}} \sigma_2^{\text{SP}} \otimes \sigma_2^{\text{PH}}. \quad (1)$$

In the presence of magnetic impurities the time-reversal is broken, while the particle/hole symmetry is conserved. Applied to the corresponding Gor'kov Green function, $\hat{G}_G^{R,A}(\epsilon) = (\epsilon_{\pm} - \hat{H}_G)^{-1}$, the particle/hole transformation (1) converts an advanced function into a retarded one:

$$\hat{G}_G^{R,A}(\epsilon) = -\sigma_2^{\text{PH}} \otimes \sigma_2^{\text{SP}} [\hat{G}_G^{A,R}(-\epsilon)]^{\text{T}} \sigma_2^{\text{SP}} \otimes \sigma_2^{\text{PH}}.$$

As usual [18, 11], to accommodate quantum interference effects in the particle/hole channel, it is convenient to affect a further space doubling $\psi^{\dagger} \hat{G}_G^R(\epsilon) \psi = \bar{\Psi} \hat{G}_G^R(\epsilon \sigma_3^{\text{CC}}) \Psi$, where, in the charge conjugation space, the vector fields take the form⁴:

$$\Psi = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi \\ \sigma_2^{\text{PH}} \otimes \sigma_2^{\text{SP}} \psi^{\dagger \text{T}} \end{pmatrix}_{\text{CC}} \quad \bar{\Psi} = \frac{1}{\sqrt{2}} (\psi^{\dagger} \quad -\psi^{\text{T}} \sigma_2^{\text{SP}} \otimes \sigma_2^{\text{PH}})_{\text{CC}}.$$

This completes the formulation of the generating functional for the single particle properties of the Gor'kov Hamiltonian. The theory is specified in terms of 16-component supervector fields Ψ and $\bar{\Psi}$ with the following symmetry relations:

$$\Psi = -\sigma_2^{\text{PH}} \otimes \sigma_2^{\text{SP}} \gamma \bar{\Psi}^{\text{T}} \quad \bar{\Psi} = \Psi^{\text{T}} \sigma_2^{\text{PH}} \otimes \sigma_2^{\text{SP}} \gamma^{\text{T}}$$

with $\gamma = i\sigma_2^{\text{CC}} E_{11}^{\text{BF}} - \sigma_1^{\text{CC}} E_{22}^{\text{BF}}$. As before, $E_{11}^{\text{BF}} = \text{diag}(1, 0)_{\text{BF}}$ and $E_{22}^{\text{BF}} = \text{diag}(0, 1)_{\text{BF}}$ represent projection operators on the boson/fermion space.

2.3. (Non-magnetic) impurity averaging

An ensemble average of the generating functional over the non-magnetic impurity distribution V induces a quartic interaction of the fields which can be decoupled by means of a Hubbard-Stratonovich transformation with the introduction of 16×16 supermatrix fields $Q(\mathbf{r})$

$$\left\langle \int \exp \left[-i \int d\mathbf{r} \bar{\Psi} V \sigma_3^{\text{PH}} \Psi \right] \right\rangle_V = \int DQ \exp \left[\int d\mathbf{r} \left(\frac{\pi v}{8\tau} \text{str} Q^2 - \frac{1}{2\tau} \bar{\Psi} Q \sigma_3^{\text{PH}} \Psi \right) \right].$$

The symmetry properties of Q are inherited from the dyadic product $\sigma_3^{\text{PH}} \Psi(\mathbf{r}) \otimes \bar{\Psi}(\mathbf{r})$ and impose the condition

$$Q = \sigma_1^{\text{PH}} \otimes \sigma_2^{\text{SP}} \gamma Q^{\text{T}} \gamma^{\text{T}} \sigma_2^{\text{SP}} \otimes \sigma_1^{\text{PH}}. \quad (2)$$

In principle we could immediately subject the generating functional to a further average over the Poisson distributed magnetic impurity potential. However, such an approach proves to be unprofitable. Since the typical separation of magnetic impurities, $\ell_s = v_F \tau_s$, is greatly in excess of the mean-free path associated with the non-magnetic impurities, $\ell = v_F \tau$, it is more sensible to postpone the second ensemble average until the quasi-classical theory has

⁴ The transposition operation for the supervectors ψ and ψ^{\dagger} and the supermatrix F is chosen according to the convention

$$\psi^{\text{T}} = (\phi \quad \chi)_{\text{BF}} \quad \psi^{\dagger \text{T}} = \begin{pmatrix} \phi^* \\ -\chi^* \end{pmatrix}_{\text{BF}} \quad F^{\text{T}} = \begin{pmatrix} a & \rho \\ -\sigma & b \end{pmatrix}_{\text{BF}}.$$

been developed. Therefore, at this stage, let us proceed by integrating out the superfields after which the generating functional assumes the form

$$\langle \mathcal{Z}[0] \rangle_V = \int DQ \exp \left\{ \frac{\pi\nu}{8\tau} \int d\mathbf{r} \operatorname{str} Q^2(\mathbf{r}) - \frac{1}{2} \int d\mathbf{r} \operatorname{str} \langle \mathbf{r} | \ln \hat{\mathcal{G}}^{-1} | \mathbf{r} \rangle \right\} \quad (3)$$

where $\hat{\mathcal{G}}$ represents the supermatrix Green function,

$$\hat{\mathcal{G}}^{-1} = \hat{\mathcal{G}}_0^{-1} + \epsilon \sigma_3^{\text{CC}} - |\Delta| \sigma_2^{\text{PH}} - JS \cdot \sigma^{\text{SP}} \quad \hat{\mathcal{G}}_0^{-1} = i0\sigma_3^{\text{CC}} - \hat{\zeta}_p \sigma_3^{\text{PH}} + \frac{i}{2\tau} Q \sigma_3^{\text{PH}}.$$

2.4. Intermediate energy saddle-point: the non-linear σ -model

To make further progress it is necessary to employ a saddle-point approximation. Following [17], it is convenient to implement a two-step procedure making use of the hierarchy of energy scales which place the superconductor in the quasi-classical and dirty limits,

$$\epsilon_F \gg \frac{1}{\tau} \gg \left\{ \frac{1}{\tau_s}, |\Delta| \right\} \gg \delta$$

where $\delta = 1/(L^d \nu)$ is the single-particle level spacing. To implement the quasi-classical approximation, we therefore temporarily suspend the energy source, ϵ , order parameter, $|\Delta|$, and magnetic impurity potential, JS , and seek an intermediate energy scale saddle-point. Such an analysis is discussed in detail in the literature [18] and here we only recapitulate the results. A variation of the action with respect to Q obtains the saddle-point equation

$$Q(\mathbf{r}) = \frac{i}{\pi\nu} \sigma_3^{\text{PH}} \langle \mathbf{r} | \hat{\mathcal{G}}_0 | \mathbf{r} \rangle.$$

Taking into account the analytical properties of the Green function, in the pole approximation, one obtains the conventional saddle-point solution $Q_{\text{SP}} = \sigma_3^{\text{PH}} \otimes \sigma_3^{\text{CC}}$. However, the saddle-point solution is not unique but spans the non-linear manifold $Q^2 = \mathbb{I}$: in the absence of the external symmetry breaking perturbations, the saddle-point equation admits an entire manifold of homogeneous solutions parametrized by transformations $Q = T Q_{\text{SP}} T^{-1}$, where T is a supermatrix, constant in space, and compatible with the charge conjugation symmetry properties of Q , (2).

Fluctuations of Q transverse to the saddle-point manifold are massive and may be integrated out within the saddle-point approximation, justified by the large parameter $1/\tau\delta$. By contrast, fluctuations which preserve the non-linear constraint $Q^2 = \mathbb{I}$ are massless and must be integrated exactly. In the same quasi-classical approximation $\epsilon_F \tau \gg 1$, the matrix Green function takes the form

$$\mathcal{G}_0(\mathbf{r}_1, \mathbf{r}_2) = -i\pi\nu f_d(|\mathbf{r}_1 - \mathbf{r}_2|) \sigma_3^{\text{PH}} Q \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right)$$

where the Friedel function $f_d(r) = \langle \operatorname{Im} G^A(\mathbf{r}, 0) \rangle_V / \langle \operatorname{Im} G_0^A(0, 0) \rangle_V$ denotes the impurity averaged single-particle Green function.

To determine the intermediate energy scale action, we now restore the symmetry breaking parameters ϵ , $|\Delta|$ and JS . Expanding the term $\operatorname{str} \ln \hat{\mathcal{G}}^{-1}$ appearing in (3), to leading order in ϵ and $|\Delta|$, one obtains

$$\ln \hat{\mathcal{G}}^{-1} \simeq \ln \hat{\mathcal{G}}_0^{-1} + [\hat{\mathcal{G}}_0 (\epsilon \sigma_3^{\text{CC}} - |\Delta| \sigma_2^{\text{PH}})] + \ln (\mathbb{I} - \hat{\mathcal{G}}_0 JS \cdot \sigma^{\text{SP}}) \quad (4)$$

where, importantly, the magnitude of the magnetic impurity potential has been left unrestricted and where the neglected terms turn out to be of order $\epsilon\tau \ll 1$ or $|\Delta|\tau \ll 1$. Taking into account slow fluctuations $Q(\mathbf{r}) = T^{-1}(\mathbf{r}) \sigma_3^{\text{PH}} \otimes \sigma_3^{\text{CC}} T(\mathbf{r})$, a gradient expansion of the first

two terms of the series (4) to leading order in $|\Delta|\tau$ and $\epsilon\tau$ recovers the familiar non-linear σ -model action for the disordered superconductor,

$$S_0[Q] = -\frac{\pi\nu}{8} \int d\mathbf{r} \operatorname{str}[D(\nabla Q)^2 + 4(i\epsilon_+\sigma_3^{\text{PH}} \otimes \sigma_3^{\text{CC}} + |\Delta|\sigma_1^{\text{PH}})Q] \quad (5)$$

where $D = v_F^2\tau/d$ represents the classical diffusion constant associated with the non-magnetic impurities. Taken together with the spin scattering contribution, the average generating functional assumes the form

$$\langle \mathcal{Z}[0] \rangle_V = \int_{Q^2=\mathbb{I}} DQ e^{-S_0[Q]-S_S[Q]}$$

where

$$S_S[Q] = \frac{1}{2} \int d\mathbf{r} \operatorname{str}(\mathbf{r} | \ln(\mathbb{I} - \hat{\mathcal{G}}_0 J \mathbf{S} \cdot \boldsymbol{\sigma}^{\text{SP}}) | \mathbf{r}).$$

To make sense of the spin scattering component of the action, it is now necessary to implement the magnetic impurity average.

2.5. Magnetic impurity averaging

If we restricted ourselves to the limit of Born scattering, we would be free to expand the action $S_S[Q]$ to second order⁵ in \mathbf{S} . In this case, once ensemble averaged over the magnetic impurity distribution, we would obtain the weak coupling action $S[Q] \simeq S_0[Q] + S_S^{\text{BA}}[Q]$, where

$$S_S^{\text{BA}} = \frac{n_s(\pi\nu L^d J S)^2}{4d_n} \int d\mathbf{r} \operatorname{str}[\sigma_3^{\text{PH}} \otimes \boldsymbol{\sigma}^{\text{SP}} Q(\mathbf{r})]^2.$$

With the identification ($d_n = 3$)

$$2\alpha n_s = \frac{\pi\nu}{\tau_s} \quad (6)$$

where $1/\tau_s$ represents the magnetic impurity scattering rate, $\alpha = (\pi\nu J L^d S)^2$, and n_s is the magnetic impurity concentration; this result coincides with that obtained by [16]. However, in the unitarity scattering limit, we are not at liberty to freely take the impurity potential from underneath the logarithm.

To simplify the action $S_S[Q]$, let us recall that the typical separation of magnetic impurities, ℓ_s , is greatly in excess of the mean-free path associated with the non-magnetic impurities, ℓ . (In the opposite limit, superconductivity would, in any case, be fully suppressed.) In this case, we may affect the approximation

$$\mathcal{G}_0(\mathbf{r}_i, \mathbf{r}_j) \simeq -i\pi\nu\sigma_3^{\text{PH}} Q(\mathbf{r}_i)\delta_{ij}.$$

Making use of this relation, an expansion and re-summation of the logarithm leads to the result

$$S_S[Q] \simeq \frac{1}{2} \sum_i \operatorname{str} \ln [\mathbb{I} + (i\pi\nu J L^d)\sigma_3^{\text{PH}} Q(\mathbf{r}_i) \mathbf{S}_i \cdot \boldsymbol{\sigma}^{\text{SP}}].$$

In this approximation, the functional has become separable in the individual magnetic impurity scatterers. In principle, we could proceed directly by subjecting the generating functional to an ensemble average over the random Poissonian distributed magnetic impurity distribution. However, for a general supermatrix Q , without expanding the logarithm, the average over the independent spin degrees of freedom is laborious and not illuminating. Instead, we will follow a different programme.

⁵ Note that the term linear in \mathbf{S} generated by the expansion vanishes when projected onto the singlet saddle-point (7), considered below.

Firstly, by taking into account the symmetry of the soft degrees of freedom, we can further simplify the analysis: specifically, from the previous analysis of the Born scattering theory, it is evident that fluctuations of Q which are not proportional to \mathbb{I}^{SP} will be rendered massive by the magnetic impurity potential. Since we are interested in the low-energy content of the theory, we may therefore specialize our considerations to the singlet degrees of freedom of Q , i.e. $Q \mapsto Q \otimes \mathbb{I}^{\text{SP}}$. In this case, if we undertake the trace over the spin degrees of freedom of Q , one obtains

$$S_S[Q] = \frac{1}{2} \sum_i \text{str}_8 \ln [\mathbb{I} - \alpha_i \sigma_3^{\text{PH}} Q(\mathbf{r}_i) \sigma_3^{\text{PH}} Q(\mathbf{r}_i)]$$

where the constant $\alpha_i = (\pi v J L^d |\mathcal{S}_i|)^2 \mapsto \alpha$, is the dimensionless scattering amplitude associated with each magnetic impurity, and the notation str_8 indicates that we have carried out the trace over the spin indices.

Secondly, the structure of the non-linear σ -model action (5) shows that the dominant contributions to the generating functional arise from field configurations which vary slowly at the scale of the coherence length. Therefore, in the dense magnetic impurity limit, where the typical separation between magnetic impurities, $\ell_s = v_F \tau_s$, is much smaller than ξ , one can expect the density of spin scatterers, $\rho(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$, to be dominated by its smooth average⁶, n_s . In this approximation, where $\xi \gg \ell_s \gg \ell$, one obtains

$$\tilde{S}_S[Q] = \frac{n_s}{2} \int d\mathbf{r} \text{str}_8 \ln [\mathbb{I} - \alpha \sigma_3^{\text{PH}} Q(\mathbf{r}) \sigma_3^{\text{PH}} Q(\mathbf{r})].$$

Note that the invariance properties of Q on the saddle-point manifold imply a symmetry of the action under the transformation $\alpha \mapsto 1/\alpha$: the weak (or Born) scattering limit is therefore ‘dual’ to the strong scattering limit.

This concludes the construction of the field theory of the disordered superconducting system. Single quasi-particle properties of the superconductor are presented as a functional field integral $\langle \dots \rangle_Q = \int DQ \dots e^{-S_{\text{eff}}[Q]}$ involving the effective non-linear σ -model action

$$S_{\text{eff}}[Q] = S_0[Q] + \tilde{S}_S[Q].$$

In particular, the local quasi-particle DoS can be obtained from the functional integral

$$\langle \nu(\epsilon, \mathbf{r}) \rangle_{v,s} = \frac{\nu}{16} \text{Re} \langle \text{str}_8 [\sigma_3^{\text{BF}} \otimes \sigma_3^{\text{PH}} \otimes \sigma_3^{\text{CC}} Q(\mathbf{r})] \rangle_Q.$$

Although the soft mode action is stabilized by the large parameter $\epsilon_F \tau \gg 1$, the majority of field fluctuations of the action are rendered massive: the energy source ϵ , order parameter $|\Delta|$ and the magnetic impurity potential all lower the symmetry of the intermediate energy scale theory. To assimilate the effect of these terms, and to establish contact with the Abrikosov–Gor’kov theory [2] in the Born approximation limit, and with [5] in the unitarity limit, in the following section, we will proceed by exploring the low-energy saddle-point structure of the theory.

2.6. Low-energy saddle-point

To explore the low-energy structure of the theory we proceed by varying the action $S_{\text{eff}}[Q]$ with respect to Q subject to the non-linear constraint $Q^2 = \mathbb{I}$. In doing so, one obtains the saddle-point equation

$$D\nabla(Q\nabla Q) + [i\epsilon_+ \sigma_3^{\text{PH}} \otimes \sigma_3^{\text{CC}} + |\Delta| \sigma_1^{\text{PH}}, Q] - \frac{1}{2\tau_s} \left[\frac{1}{\mathbb{I} - \alpha \sigma_3^{\text{PH}} Q \sigma_3^{\text{PH}} Q} \sigma_3^{\text{PH}}, Q \sigma_3^{\text{PH}} Q \right] = 0$$

⁶ Such an approximation circumvents the need to implement the averaging over the Poisson distribution explicitly. Later, we will see that this brings with it considerable simplification in the instanton analysis, while leaving the mean-field analysis unchanged.

where the scattering rate $1/\tau_s$ is related to the magnetic impurity concentration n_s and the scattering amplitude α through relation (6). The latter must be supplemented by the self-consistency condition

$$\frac{1}{g_\Delta} |\Delta| = \frac{\pi}{8\beta\delta} \sum_n \text{str}_8[\sigma_1^{\text{PH}} \otimes \sigma_3^{\text{BF}} Q] \Big|_{i\epsilon_n = -\epsilon_n}$$

where g_Δ is the BCS coupling constant and Q represents the solution of the mean-field equation taken at the Matsubara frequencies $\epsilon \mapsto i\epsilon_n = i(2n+1)\pi/\beta$. Applying the ansatz for the saddle-point,

$$Q(\mathbf{r}) = \sin \hat{\theta}(\mathbf{r}) \sigma_1^{\text{PH}} + \cos \hat{\theta}(\mathbf{r}) \sigma_3^{\text{PH}} \otimes \sigma_3^{\text{CC}} \quad (7)$$

where the matrix $\hat{\theta} = \text{diag}(i\theta_{\text{BB}}, \theta_{\text{FF}})_{\text{BF}}$ is diagonal in the superspace and independent of the other indices, one obtains the saddle-point equation

$$D\nabla^2 \hat{\theta} + 2(i\epsilon \sin \hat{\theta} - |\Delta| \cos \hat{\theta}) - \frac{1}{\tau_s} \frac{\sin 2\hat{\theta}}{\mathbb{I} + \alpha^2 + 2\alpha \cos 2\hat{\theta}} = 0. \quad (8)$$

As expected, in the limit $\alpha \ll 1$, by an expansion of the spin scattering term one obtains the Born scattering equation analysed in [16]. Here, taking the saddle-point solution to be homogeneous in space and symmetric in the superspace, $i\theta_{\text{BB}} = \theta_{\text{FF}} \equiv \theta$, one recovers the Abrikosov–Gor’kov mean-field equations. Similarly, in the strong scattering limit $\alpha \gg 1$, the action coincides with that obtained in the Born scattering limit. This coincidence reflects the duality seen on the level of the action and can be understood qualitatively in the following way: when the local spin scattering potential is very strong, the wavefunction for the low-energy quasi-particle states is strongly suppressed at the impurity centre. As a result, the matrix element for the effect spin scattering rate is itself strongly suppressed. However, our main interest is in the crossover region where the dimensionless scattering rate is $\alpha \sim 1$. Here the saddle-point equation is given by (8).

As with the Born scattering limit, to analyse the saddle-point equations, we first seek a homogeneous supersymmetric solution, $\hat{\theta}_{\text{MF}} = \theta_{\text{MF}} \mathbb{I}^{\text{BF}}$. Then, defining a ‘renormalized’ energy and order parameter,

$$\begin{aligned} \tilde{\epsilon} &= \epsilon + \frac{i}{2\tau_s} \frac{\cos \theta_{\text{MF}}}{1 + \alpha^2 + 2\alpha \cos 2\theta_{\text{MF}}} \\ |\tilde{\Delta}| &= |\Delta| + \frac{1}{2\tau_s} \frac{\sin \theta_{\text{MF}}}{1 + \alpha^2 + 2\alpha \cos 2\theta_{\text{MF}}} \end{aligned} \quad (9)$$

the homogeneous saddle-point equation (8) takes a conventional BCS form, $i\tilde{\epsilon} \sin \theta_{\text{MF}} = |\tilde{\Delta}| \cos \theta_{\text{MF}}$. Defining the dimensionless parameter $u = \tilde{\epsilon}/|\tilde{\Delta}|$ such that

$$\cos \theta_{\text{MF}} = \frac{-iu}{\sqrt{1-u^2}} \quad \sin \theta_{\text{MF}} = \frac{-1}{\sqrt{1-u^2}}$$

the mean-field equation can be cast in the following form:

$$\frac{\epsilon}{|\Delta|} = g(u, \zeta, \alpha) \equiv u \left(1 - \zeta_\alpha \frac{\sqrt{1-u^2}}{\gamma^2 - u^2} \right) \quad (10)$$

where $\zeta_\alpha = \zeta/(1+\alpha)^2$ and $\gamma = |1-\alpha|/(1+\alpha)$. As expected, despite the inclusion of an additional non-magnetic impurity potential, this result coincides with that obtained in [5] by diagrammatic expansion in the T -matrix approximation. This equivalence occurs because the nature of the electron motion (diffusive or ballistic) has no effect at the homogeneous mean-field level. By contrast, soon we will see that the nature of the underlying electron dynamics does impact on the nature of the fluctuations around the saddle-point.

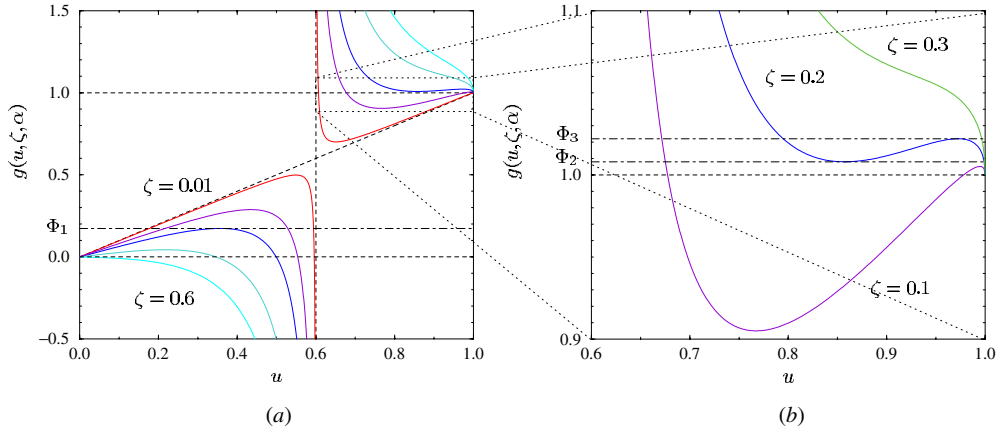


Figure 2. Function $g(u, \zeta, \alpha)$ versus u : (a) for $\alpha = 0.25$ and $\zeta = 0.01, \zeta = 0.1, \zeta = 0.2, \zeta = 0.4$ and $\zeta = 0.6$. The value of $\Phi_1 = \epsilon_g/|\Delta|$ is explicitly indicated for the case $\zeta = 0.2$. (b) The function $g(u, \zeta, \alpha)$ is plotted in the region $u > \gamma$ for $\alpha = 0.25$ and $\zeta = 0.1, \zeta = 0.2$ and $\zeta = 0.3$. The values of the edges Φ_2 and Φ_3 are explicitly indicated for the case $\zeta = 0.2$.

The homogeneous saddle-point solutions are given by the values of u satisfying equation (10). As in the Abrikosov–Gor’kov theory, a number of features of the DoS can be deduced starting from the shape of the function $g(u, \zeta, \alpha)$ when the impurity concentration ζ and the scattering amplitude α are varied. In figure 2 the typical dependence of $g(u, \zeta, \alpha)$ in u is shown. The parameter γ defines the second order pole, while for values of ζ sufficiently low the function shows one extremum in the region $u \in [0, \gamma)$ and the two extrema in the region $u \in (\gamma, 1]$, that disappear as the value of the impurity concentration increases. As will be clear later, the three extrema of g have a clear interpretation in terms of the sharp edges of the DoS.

As in the Born limit ($\alpha = 0, \gamma = 1$), the maximum of $g(u, \zeta, \alpha)$ in the interval $u \in [0, \gamma)$ has the meaning of the rescaled energy gap, $\Phi_1 = \epsilon_g/|\Delta|$, so that the set of the values of α and ζ for which ϵ_g becomes zero defines the gapless region for the superconductor in the unitarity limit:

$$g'(u, \zeta, \alpha)|_{u=0} = 0 \quad \Rightarrow \quad \zeta = \zeta_0 \equiv (1 - \alpha)^2.$$

This means that in the region $\zeta \geq (1 - \alpha)^2$ the superconductor is gapless ($\epsilon_g = 0, |\Delta| \neq 0$). Compared with the Born limit, this result shows that the concentration at which the system enters the gapless phase is renormalized by the finite scattering amplitude α .

The two extrema in the region $u \in (\gamma, 1]$, which we denote by Φ_2 and Φ_3 (see figure 2(b)), represent respectively the top of the impurity band and the bottom of the continuum of bulk states. The dependence of $\epsilon_g/|\Delta|$, Φ_2 and Φ_3 on ζ is shown in figure 3 for two representative values of α . Defining ζ_0 and ζ_1 respectively as the value of ζ at which the energy gap becomes zero and the value of ζ at which the top of the impurity band touches the bottom of the continuum, when $\zeta_1 < \zeta_0$ (figure 3(a)) the top of the impurity band touches the bottom of the continuum before the superconductor becomes gapless, while the opposite situation pertains when $\zeta_0 < \zeta_1$ (figure 3(b)).

The assigned definitions of $\epsilon_g/|\Delta|$, Φ_2 and Φ_3 become clear when we plot the normalized mean-field density of states $\langle \nu_{\text{MF}}(\epsilon) \rangle_{V,S}/\nu$ as a function of the rescaled energy, $\epsilon/|\Delta|$:

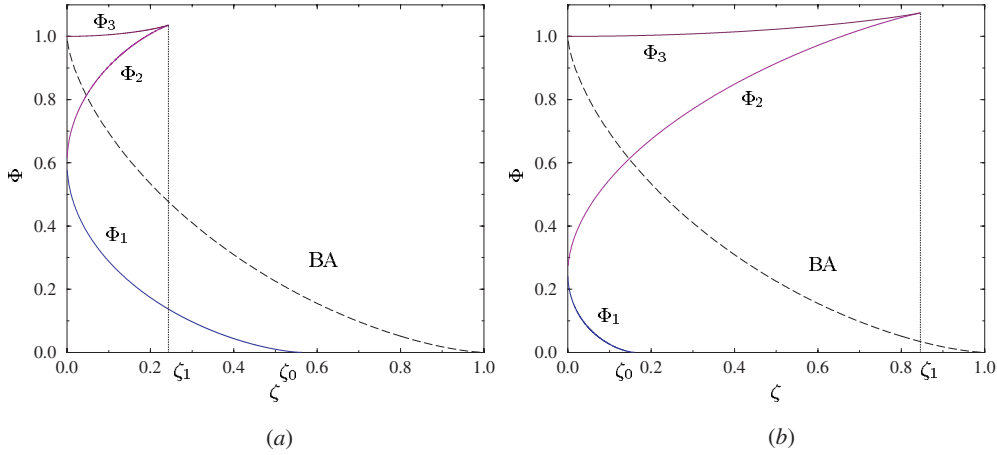


Figure 3. Rescaled energy gap $\epsilon_g/|\Delta| = \Phi_1$, edge of the impurity band Φ_2 and edge of the continuum Φ_3 versus ζ : (a) for $\alpha = 0.25$, $\zeta_1 < \zeta_0 = (1 - \alpha)^2 \simeq 0.56$ and (b) for $\alpha = 0.6$, $\zeta_1 > \zeta_0 = 0.16$. The dashed line is the energy gap in the Born approximation case that in this case coincides with the edge of the continuum.

$$\langle v_{\text{MF}}(\epsilon) \rangle_{V,S} = \frac{\nu}{16} \text{Re} \left\langle \text{str} [\sigma_3^{\text{BF}} \otimes \sigma_3^{\text{PH}} \otimes \sigma_3^{\text{CC}} Q_{\text{MF}}] \right\rangle_Q = \nu \text{Re} \cos \theta_{\text{MF}} = \text{Im} \left(\frac{u}{\sqrt{1-u^2}} \right).$$

In order to explicitly find $\langle v_{\text{MF}}(\epsilon) \rangle_{V,S}/\nu$, we have to solve equation (10), expressing u in terms of $\epsilon/|\Delta|$. For values of α and ζ at which all the edges, $\epsilon_g/|\Delta| = \Phi_1$, Φ_2 and Φ_3 , are different from zero, equation (10) has complex solutions for $\Phi_1 < \epsilon/|\Delta| < \Phi_2$ and for $\epsilon/|\Delta| > \Phi_3$. For this reason, in this case, the DoS of a single particle excitation consists of two distinct parts: over the energy range $\Phi_1 < \epsilon/|\Delta| < \Phi_2$ the system exhibits an impurity band while for $\epsilon/|\Delta| > \Phi_3$ there exists a continuum of bulk states. Within the intervening energy intervals, the mean-field DoS is zero. As ζ increases, the energy gap closes, while the top of the impurity band converges on the edge of the continuum. Which happens first depends on the value of the magnetic scattering amplitude α . Figure 1 clearly shows the phenomenon of the impurity band growth around the energy

$$\frac{\epsilon_B}{|\Delta|} = \gamma = \frac{|1 - \alpha|}{1 + \alpha}$$

corresponding to that of the bound state developed around a single isolated magnetic impurity [5, 7, 8].

This concludes our discussion of the solutions of the homogeneous mean-field equations and their ramifications on the DoS. However, as mentioned in the introduction, the integrity of a quasi-particle energy gap (or gaps) predicted by the mean-field theory does not seem tenable. Following the discussion of the Born scattering system [16], we expect optimal fluctuations of the random impurity potential to generate fluctuations in the effective spin scattering rate which in turn must lead to the nucleation of localized tail states which soften the gap edge. In [16] it was shown that such localized sub-gap quasi-particle states are reflected in spatially inhomogeneous instanton field configurations of the σ -model action. In the present case, we expect an analogous situation to persist even in the unitarity scattering limit: however, in this case, we must expect that all three of the hard edges Φ_1 , Φ_2 and Φ_3 are softened by the bounce configurations.

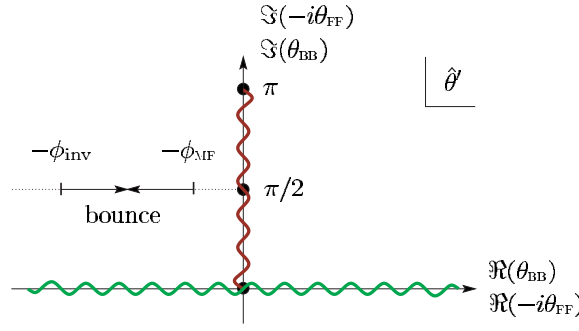


Figure 4. Integration contours for boson–boson and fermion–fermion fields in the complex $\hat{\theta}' = -i\hat{\theta}$ plane.

3. Instantons and tail states

To explore the structure of the tail state distribution, it is necessary to revisit the saddle-point equation (8) and look for inhomogeneous solutions. For this purpose, it is convenient to recast the saddle-point equation (8) in terms of its first integral

$$D(\nabla\hat{\theta})^2 - |\Delta|V(\hat{\theta}) = \text{const}$$

where

$$V(\hat{\theta}) = 4 \left(i \frac{\epsilon}{|\Delta|} \cos \hat{\theta} + \sin \hat{\theta} \right) - \frac{\zeta}{2\alpha} [\ln(\mathbb{I} + \alpha^2 + 2\alpha \cos \hat{\theta}) - \mathbb{I}]$$

represents the effective complex potential. The identification of the saddle-point solution is simplified by the observation that the homogeneous mean-field configuration (9) satisfies the condition $\theta_{\text{MF}}(\epsilon < \epsilon_g) = -\pi/2 - i\phi_{\text{MF}}$, with ϕ_{MF} real (i.e. so that the mean-field DoS, $\langle \nu_{\text{MF}}(\epsilon) \rangle_{V,S} = \nu \text{Re} \cos \theta_{\text{MF}}$, vanishes below the energy gap). One can therefore identify a ‘bounce’ solution parametrized by $\theta = -\pi/2 - i\phi$, with ϕ real, and involving the *real* potential $V_R(\phi) \equiv V(-\pi/2 - i\phi)$.

Now integration over the angles $\hat{\theta} = \text{diag}(i\theta_{\text{BB}}, \theta_{\text{FF}})_{\text{BF}}$ is constrained to certain contours [18]: the contour of integration over the boson–boson field θ_{BB} includes the entire real axis, while the fermion–fermion field $i\theta_{\text{FF}}$ runs along the imaginary axis from 0 to $i\pi$ (see figure 4). As the saddle-point solution must be accessible by a smooth deformation of the integration contour, the bounce solution is accessible only to the boson–boson field,

$$i\theta_{\text{BB}}(r) = -\frac{\pi}{2} - i\phi(r) \quad \theta_{\text{FF}} = \theta_{\text{MF}} \quad (11)$$

i.e. the particular bounce configuration is non-trivial in the superspace. With this parametrization, the saddle-point equation assumes the form $(\nabla_{r/\xi}\phi)^2 + V_R(\phi) = V_R(\phi_{\text{MF}})$, where

$$V_R(\phi) = 4 \left(\frac{\epsilon}{|\Delta|} \sinh \phi - \cosh \phi \right) - \frac{\zeta}{2\alpha} [\ln |1 + \alpha^2 - 2\alpha \cosh 2\phi| - 1]. \quad (12)$$

Typical shapes of the potential for a fixed value of the scattering amplitude ($\alpha = 0.25$) and the magnetic impurity concentration ($\zeta = 0.05$) and in two different regions of the energy are shown in figure 5. A bounce solution with minimum action exists in the regions $\epsilon < \epsilon_1 = \epsilon_g$ (figure 5(a)) and $\epsilon_2 < \epsilon < \epsilon_3$ (figure 5(b)), where $\Phi_l \equiv \epsilon_l/|\Delta|$, while outside both, the unique solution is the homogeneous one, $\phi = \phi_{\text{MF}}$. In fact when the energy approaches one of the hard edges predicted by the mean-field theory, $\epsilon \rightarrow \epsilon_1^-$, $\epsilon \rightarrow \epsilon_2^+$ or $\epsilon \rightarrow \epsilon_3^-$, the maximum

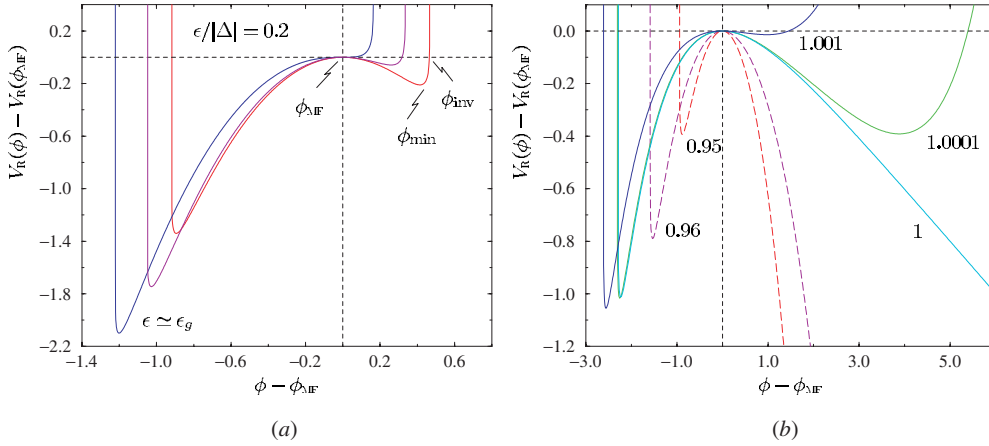


Figure 5. Rescaled potential $V_R(\phi) - V_R(\phi_{MF})$ versus the variable $\phi' = \phi - \phi_{MF}$ for $\alpha = 0.25$, $\zeta = 0.05$: (a) $\epsilon/|\Delta| = 0.2$, $\epsilon/|\Delta| = 0.3 < \epsilon_g/|\Delta|$ and $\epsilon/|\Delta| = 0.37622 \simeq \epsilon_g/|\Delta|$. The inversion point is indicated with ϕ_{inv} , while the minimum of the potential is indicated with ϕ_{min} . (b) $\epsilon/|\Delta| = 0.95 \gtrsim \Phi_2$, $\epsilon/|\Delta| = 0.96$, $\epsilon/|\Delta| = 1$, $\epsilon/|\Delta| = 1.0001$ and $\epsilon/|\Delta| = 1.001 \lesssim \Phi_3$.

of the potential for $\phi = \phi_{MF}$ merges with the minimum of the potential corresponding to the lowest value of the action.

Now, for simplicity, let us first focus on the quasi-one-dimensional case. Later we will generalize the discussion to the d -dimensional case. The symmetry broken solution (11) involves the real instanton action

$$S_{inst} = 4\pi\nu|\Delta|\xi S_\phi \quad S_\phi = \int_{\phi_{MF}}^{\phi_{inv}} d\phi \sqrt{V_R(\phi_{MF}) - V_R(\phi)} \quad (13)$$

where ϕ_{inv} represents the ‘classical turning point’, $V_R(\phi_{inv}) = V_R(\phi_{MF})$. As the energy approaches one of the three edges ($\epsilon \rightarrow \epsilon_1^-$, $\epsilon \rightarrow \epsilon_2^+$ or $\epsilon \rightarrow \epsilon_3^-$), the minimum of the potential (12) corresponding to the lowest value of the instanton action (13) disappears, merging with the maximum at the mean-field point ϕ_{MF} . Developing the function $g(u, \zeta, \alpha)$ (10) around one of the extrema $\epsilon_l/|\Delta|$,

$$u - u_0^l = (-1)^l \sqrt{\frac{2}{|g''(u_0^l, \zeta, \alpha)|}} \left[(-1)^l \left(\frac{\epsilon - \epsilon_l}{|\Delta|} \right) \right]^{1/2}$$

it is possible to deduce the expansion of the potential $V_R(\phi)$ in powers of $(\phi - \phi_{MF})$ around each edge:

$$V_R(\phi) - V_R(\phi_{MF}) \simeq -A_l \left[(-1)^l \left(\frac{\epsilon - \epsilon_l}{|\Delta|} \right) \right]^{1/2} (\phi - \phi_{MF})^2 - (-1)^l B_l (\phi - \phi_{MF})^3. \quad (14)$$

Here the positive dimensionless coefficients $A_l(u_0^l, \zeta, \alpha)$ and $B_l(u_0^l, \zeta, \alpha)$ depend solely on the scattering amplitude α and the magnetic impurity concentration ζ .

As the energy approaches one of the hard edges, from below or above depending on whether we are dealing with Φ_1 and Φ_3 or Φ_2 , expansion (14) permits one to obtain an analytic solution for S_ϕ ,

$$S_\phi = \frac{4}{15} \frac{A_l^{5/2}}{B_l^2} \left[(-1)^l \left(\frac{\epsilon - \epsilon_l}{|\Delta|} \right) \right]^{5/4}$$

and the bounce solution

$$\phi(x) - \phi_{\text{MF}} = \frac{A_l}{B_l} \frac{1}{\cosh^2 x/2r_0}$$

where the extent of the instanton is set by

$$r_0(\epsilon) = \frac{\xi}{A_l^{1/2}} \left[(-1)^l \left(\frac{|\Delta|}{\epsilon - \epsilon_l} \right) \right]^{1/4}.$$

Therefore, on approaching the edge from the ‘gapped region’ (i.e. $\epsilon \rightarrow \epsilon_{1,3}^-$ or $\epsilon \rightarrow \epsilon_2^+$) the size of the ‘droplet’ $r_0(\epsilon)$ goes to infinity. Moreover, the coefficient A_1 goes to zero at the gapless point and analogously A_2 and A_3 go to zero when the impurity band merges with the continuum.

When in the vicinity of the mean-field gap edges, a generalization of the quasi-one-dimensional results to higher dimensions ($1 < d < 6$) can be developed by dimensional analysis. Using approximation (14), the bounce configuration is shown to have the scaling form

$$\phi(\mathbf{r}) - \phi_{\text{MF}} = \left[\frac{\xi}{r_0(\epsilon)} \right]^2 \frac{1}{B_l} f(\mathbf{r}/r_0(\epsilon)).$$

Substituting this relation into the expression of the instanton action, one finds that

$$S_{\text{inst}} = 4a_d \pi g \left(\frac{\xi}{L} \right)^{d-2} B_l^{-2} A_l^{(6-d)/2} \left[(-1)^l \left(\frac{\epsilon - \epsilon_l}{|\Delta|} \right) \right]^{(6-d)/4} \quad (15)$$

where $g = \nu DL^{d-2}$ is the bare dimensionless conductance and a_d is a numerical constant⁷. This closes our discussion of the particular saddle-point solution together with the corresponding action. However, to complete the analysis it is necessary to explore the influence of fluctuations around the instanton solution.

Here we only sketch the important aspects of the fluctuation analysis, referring to [16] for a more detailed discussion in the context of the Born scattering limit. Generally, field fluctuations around the instanton solution 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 an important role.

Dealing first with the angular fluctuations, supersymmetry breaking of the bounce is accompanied by the appearance of a Grassmann zero mode separated by an energy gap from higher excitations. This Goldstone mode restores the global supersymmetry of the theory. Crucially, this mode ensures that the saddle-point respects the normalization condition $\langle \mathcal{Z}[0] \rangle_{W,V} = 1$. Associated with radial fluctuations around the bounce, there exists a zero mode due to translational invariance of the solution, and a negative energy mode (cf [19]).

Combining these contributions, one obtains the following expression for the local complex DoS in the tail regions ($\epsilon \lesssim \epsilon_g$, $\epsilon \gtrsim \epsilon_2$ and $\epsilon \lesssim \epsilon_3$):

$$\langle \nu(\epsilon) \rangle_{V,S} \underset{\epsilon \approx \epsilon_l}{\sim} \nu \int d\mathbf{r} [\sinh \phi(\mathbf{r}) - \sinh \phi_{\text{MF}}] |\chi_0(\mathbf{r})|^2 \sqrt{\frac{LS_\phi}{\xi}} e^{-S_{\text{inst}}}$$

where $\chi_0(\mathbf{r})$ represents the eigenfunction for the Grassmann zero mode, $\sqrt{LS_\phi/\xi}$ is the Jacobian associated with the introduction of the collective coordinate [19] and S_{inst} denotes

⁷ Specifically, $a_d = \int d\mathbf{u} [(\nabla_{\mathbf{u}} f)^2 + f^2(\mathbf{u}) - f^3(\mathbf{u})]$.

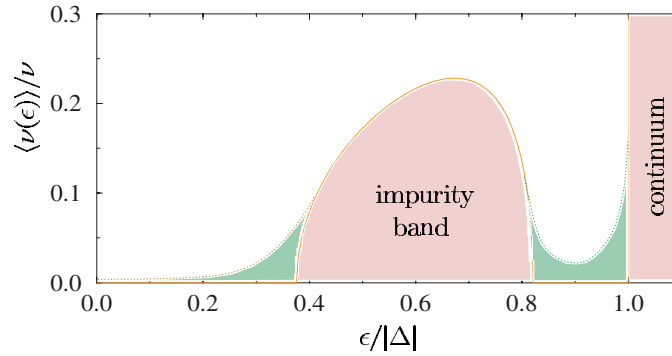


Figure 6. Smearing of the gap edges due to optimal configurations of the random impurity potentials. The three edges ϵ_g , ϵ_2 and ϵ_2 become the mobility edges separating the regions of bulk delocalized states from the localized tail states.

the instanton action (15). Thus, to exponential accuracy, the complex local DoS in the tail region becomes non-zero only in the vicinity of the bounce.

4. Discussion

This concludes our investigation of the role of quenched classical magnetic impurities on the weakly disordered superconducting system. The results above show that the gap structure predicted by the mean-field theory for magnetic impurities in both the unitarity and Born scattering limit is untenable. The hard gap edge(s) predicted by the mean-field theory are softened by the nucleation of domains or ‘droplets’ of localized tail states. The mean-field gap edges become mobility edges separating bulk delocalized quasi-particle states from localized tail states (see figure 6). The latter are induced by optimal fluctuations of the non-magnetic random impurity potential which increase the effective spin scattering rate.

How significant are these results for experiment? The nucleation of sub-gap states will lead to the softening of the transition from the metallic to the superconducting phase which would be revealed in measurements of the heat capacity close to the bulk T_c . Similarly, since the tail state regions are broad on the scale of the coherence length (and broaden close to the quasi-particle energy gap), one can expect the existence of sub-gap states to be revealed in measurements of the tunnelling density of states close to the mean-field gap. However, it should be noted that the strength arising from the sub-gap states will compete with the weight arising from dynamical spin fluctuations. The latter will typically give rise to power law tails in the sub-gap density of states [20].

Finally, our considerations of the density of states focussed largely on energy scales $\epsilon \sim \epsilon_g$. Here the generating function is dominated by the homogeneous mean-field and bounce configurations of the non-linear σ -model action. However, within the gapless phase (i.e. as $\epsilon \rightarrow 0$), field fluctuations Q which commute with both σ_1^{PH} and σ_3^{PH} become massless. These fluctuations, which are parametrized by transformations $Q = T Q_{\text{MF}} T^{-1}$ where $T = \mathbb{I}_{\text{PH}} \otimes \mathbb{I}_{\text{SP}} \otimes t$ and $t = \gamma(t^{-1})^T \gamma^{-1}$, are controlled by a non-linear σ -model defined on the manifold $T \in \text{OSp}(2 | 2) / \text{GL}(1 | 1)$ (symmetry class D in the classification of [21]). The latter reflect quantum interference effects in the particle/hole channel and substantially modify the low-energy, long-range spectral and transport properties of both the bulk system and the low-energy states inside a localized domain. For a comprehensive discussion of their effect, we refer to the comprehensive discussions in [11–14, 16].

Acknowledgments

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