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Correlated magnetic impurities in a superconductor: electron density profiles and robustness of superconductivity

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Abstract
The insertion of magnetic impurities in a conventional superconductor leads to various effects. In this work we show that the electron density is affected by the spins (considered as classical) both locally and globally. The charge accumulation is solved self-consistently. This affects the transport properties along magnetic domain walls. Also, we show that superconductivity is more robust if the spin locations are not random but correlated.

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

1. Introduction

Magnetic impurities in conventional superconductors have been studied for a long time [1]. Their effect is expressed through a spin coupling to the spin density of the conduction electrons. If the coupling is weak, the impurities may be considered as classical spins. In general, we should consider the Kondo effect due to the internal dynamics of the impurity spins. This is a difficult problem and the results are qualitatively the same as for classical spins (particularly if the coupling is antiferromagnetic [2]) which in this case is equivalent to the effect of local magnetic fields coupled to the electrons. N_i impurities induce $2N_i$ bound states due to the capture of electrons by the impurities. The addition of extra sub-gap states has been studied using scanning tunneling spectroscopy [3, 4]. As the coupling increases, various level crossings take place where the spin content is changed [5–8], inducing first order quantum phase transitions. Qualitatively the same happens in the case of Kondo impurities if the coupling is antiferromagnetic, where a quantum phase transition also occurs. The case of a Kondo ferromagnetic coupling is different since the bound states stay close to the band gap edge and no transition occurs. We will consider here the classical case valid if either the spin of the impurity, S, is large (with JS small) or if the Kondo temperature is small $T_K \ll \Delta$. These phase transitions may be identified in various ways (see [1] and references therein) such as changes in the total magnetization of the electron spin density, local spin density, local order parameter, local density of states [7, 6, 8], or through various quantum information measures such as entanglement and mutual information [9] or partial state fidelity [10].

For instance, in the case of a single impurity, as the coupling varies, the total magnetization changes from a zero average value at low coupling to a value of $1/2$ at couplings larger than a critical value. Also, there is a π shift in the order parameter at the impurity site. Since the impurity spin acts as a local magnetic field, the electron spin density will align along the local spin. At the impurity site it is positive, as expected. For small values of the coupling there is a negative spin density around the impurity site. The many-body system screens the effect of the impurity, inducing fluctuations that compensate the effect of the local field in such a way that the overall magnetization vanishes. For larger couplings the spin density in the vicinity of the impurity site is positive. For a strong enough coupling, the many-body system becomes magnetized in a discontinuous fashion. One interpretation is that, if J is strong enough, the impurity breaks a Cooper pair and captures one of the electrons, leaving the other electron unpaired, and thus the overall electronic system becomes polarized.

In this work we consider the effect of the impurities on the electron density, both overall and local densities. At half-

filling, the density is not affected by the impurity spins [7]. We find here that at general fillings the density is changed by the impurity spins. Considering the case of a single impurity, its effect on the average density (global density) is very small. However, the local density is changed in the vicinity of the impurity. If we have a larger number of impurities present, the average density is significantly affected in a way that reveals interference effects, since it is not simply cumulative. In general, as the coupling grows the density increases. At a fixed chemical potential (open system) the impurities capture electrons that are added to the system from the reservoir to preserve a maximal number of Cooper pairs.

We note that a change of the local electron density also occurs in the vicinity of a vortex in a superconductor [11]. Due to the circulating currents around the vortex line, an electrostatic potential is needed to compensate the centrifugal force due to the circular motion [12]. It has been claimed that the charge of the vortex has been measured using NMR in high temperature superconductors [13]. Usually a universal charge depletion is predicted at the vortex cores. Taking into account the competition in the d-wave case with other order parameters, it has been determined that in some circumstances the vortices may be negatively charged (charge accumulation with respect to the bulk value) [14, 15]. When two vortices are close together, strong fluctuations appear in the shared region of the vortices, inducing a smaller charge accumulation. Also, the addition of impurities changes the charge profiles. A small to moderate attractive potential also changes the sign of the vortex charge, since it locally renormalizes the chemical potential in a straightforward way [16].

We should recall that, as the number of impurities grows, superconductivity is destroyed. The case of random impurities was solved long ago [17, 18], where it was shown that the critical temperature decreases linearly at small concentrations and vanishes for relatively small values of the impurity concentration, as also found experimentally [19]. However, we find that if the spin impurity locations are correlated, superconductivity is more robust and extends to higher concentrations.

The paper is organized as follows. In section 2 we present the model and main equations. Section 3 contains the results for the electron density profile. In section 4 we consider self-consistently the effect of electron–electron interaction, taking into account the Hubbard onsite interaction as well as electron correlations at different sites. The problem of the critical concentration of correlated magnetic impurities in superconductors is discussed in section 5. In section 6 we consider a simplified one-dimensional model through which a current is applied and we study the I–V characteristics in the presence of a magnetic domain wall. The conclusions are presented in section 7.

2. Model

In this work we are interested in a situation where the classical spin distribution may be dense (see [8] and references therein). At either few or basically at all sites of the two-dimensional system (plane x–z) we place classical spins parametrized like $\frac{\vec{S}_l}{S} = \cos\varphi_l \vec{e}_x + \sin\varphi_l \vec{e}_z$, where S is the modulus of the spin. Thus, we assume that the spins lie in the x–z plane so that the orbital effect is absent (no superconducting vortices). We are interested here in superconducting films and consider that superconductivity is stabilized by some small interplane coupling. The Hamiltonian of the system is given by

$$\begin{aligned} H = &- \sum_{\langle i,j\rangle,\sigma} t_{i,j} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} \\ &+ \sum_i (\Delta_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \Delta^*_i c_{i\downarrow} c_{i\uparrow}) \\ &- \sum_{i,l,\sigma,\sigma'} J_{i,l} [\cos\varphi_l c^\dagger_{i\sigma} \sigma^x_{\sigma,\sigma'} c_{i\sigma'} + \sin\varphi_l c^\dagger_{i\sigma} \sigma^z_{\sigma,\sigma'} c_{i\sigma'}], \end{aligned} \quad (1)$$

where the first term describes the hopping of electrons between different sites on the lattice, μ is the chemical potential, the third term corresponds to the superconducting s-pairing with the site-dependent order parameter Δ_i, and the last term is the exchange interaction of the spin density of the electrons with the magnetic impurities. The sign of interaction is irrelevant in this case [1]. The hopping matrix is given by $t_{i,j} = t\delta_{j,i+\delta}$, where δ is a vector to a nearest-neighbor site, and we will take units such that $t = 1$. Note that both the indices l and i, j specify sites on a two-dimensional system (here identified as the x–z plane). The indices $i, j = 1, \ldots, N$, where N is the number of lattice sites. We take $J_{i,l} = J\delta_{i,l}$ and therefore the last sum is over the sites, l, where a spin is located. We assume that the spin configuration is fixed and static. Defining the vector

$$\psi_n(i) = \begin{pmatrix} u_n(i,\uparrow) \\ v_n(i,\downarrow) \\ u_n(i,\downarrow) \\ v_n(i,\uparrow) \end{pmatrix} \quad (2)$$

the Bogoliubov–de Gennes (BdG) equations can be written as $\mathcal{H}\psi_n = \epsilon_n \psi_n$, where the matrix $\mathcal{H}$ at site i is given by

$$\mathcal{H} = \begin{pmatrix} A_\uparrow & C_{\uparrow,\downarrow} \\ C_{\downarrow,\uparrow} & A_\downarrow \end{pmatrix}, \quad (3)$$

where

$$A_{\uparrow,\downarrow} = \begin{pmatrix} -h - \mu \mp J_{i,l}\sin\varphi_l & \Delta_i \\ \Delta^*_i & h + \mu \mp J_{i,l}\sin\varphi_l \end{pmatrix} \quad (4)$$

and $C = C_{\uparrow,\downarrow} = C_{\downarrow,\uparrow}$ is given by

$$C = \begin{pmatrix} -J_{i,l}\cos\varphi_l & 0 \\ 0 & -J_{i,l}\cos\varphi_l \end{pmatrix}, \quad (5)$$

where $h = t\hat{s}_\delta$ with $\hat{s}_\delta f(i) = f(i+\delta)$. A sum over nearest neighbors, δ, is implicit. The solution of these equations gives both the energy eigenvalues and eigenstates. The problem involves the diagonalization of a $(4N) \times (4N)$ matrix. The solution of the BdG equations is performed self-consistently, imposing at each iteration that $\Delta_i = \frac{g}{2}[\langle c_{i\uparrow} c_{i\downarrow}\rangle - \langle c_{i\downarrow} c_{i\uparrow}\rangle]$, where $g > 0$ is the effective attractive interaction between the electrons. We take $g = 2$ and the chemical potential $\mu = -1$. In most cases we take a lattice of size 15×15. Changing the lattice size does not qualitatively change the results, as discussed previously [8].

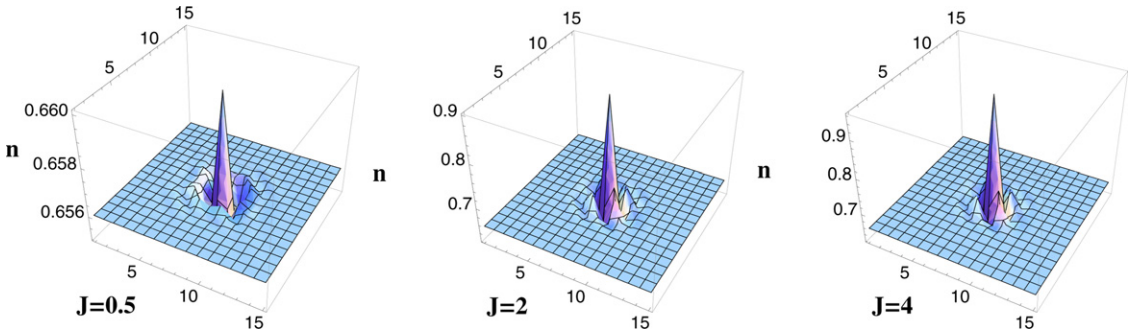

Figure 1. Local density around a single impurity as a function of J.

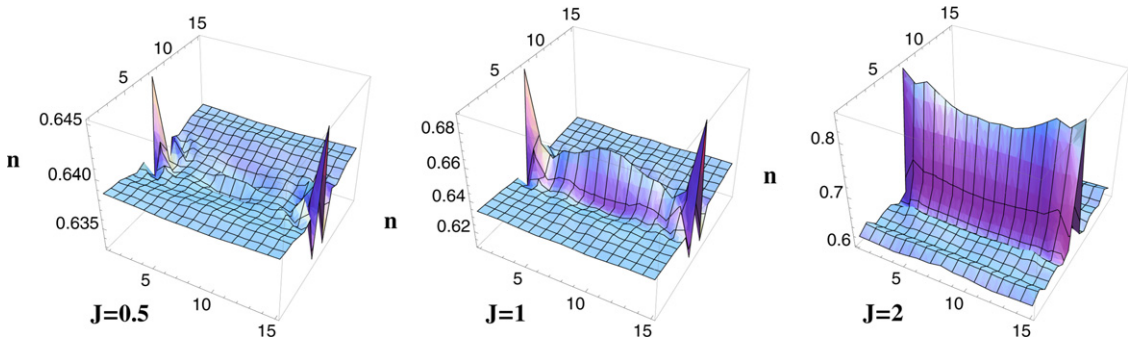

Figure 2. Local density for a domain wall (DW) as a function of J. The domain wall is of the Néel type and is composed of a line of spins in the center of the system (x_c) with $\varphi_l = \frac{\pi}{2} + \frac{\pi}{2}\tanh\frac{x-x_c}{\lambda}$. We take $\lambda = 3$ in lattice units.

3. Electron density

The particle density is calculated using

$$n_{i,\sigma} = \langle c^{\dagger}_{i,\sigma} c_{i,\sigma}\rangle = \sum_n (f_n |u_n(i,\sigma)|^2 + (1-f_n)|v_n(i,\sigma)|^2), \tag{6}$$

where f_n is the Fermi function for the energy ϵ_n. We begin by considering the cases of a single impurity located at the center of the two-dimensional system and a one-dimensional domain wall of spin orientations along the center line of the system. In figures 1 and 2 we show the electron density profiles resulting from the presence of one or various impurities, respectively. The effect is particularly noticeable for larger couplings. In this case the number of electrons captured by the impurities (and injected in the system to preserve the chemical potential) is large. This number grows with the number of impurities, as expected. We note that something similar occurs even if there is no superconducting order. While in the superconducting case the magnetization has a discontinuous change at the critical point, in the case of the normal system ($g = 0$) the magnetization increases but it is a crossover. Increasing the system size does not alter the crossover of the normal case. The location of the crossover point (or critical point in the superconducting case) changes slightly with the system size, but the width of the crossover region in the normal case actually increases as the system size increases.

As stated above, it has been argued before [7] that, at half-filling, the total density is not changed by the impurities. However for general band-filling, as the various quantum phase

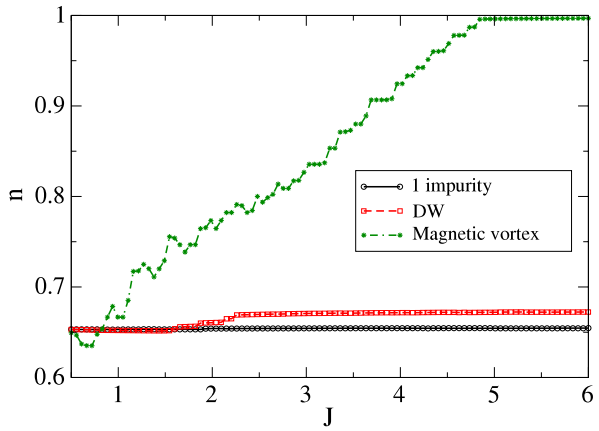

Figure 3. Density evolution as a function of the spin coupling for the single impurity, one-dimensional domain wall and magnetic vortex.

transitions occur the total band-filling also changes. We show in figure 3 the change of the average density (global density) as the spin coupling varies. In the case of one impurity, the increase is very small (and smaller by about one order of magnitude with respect to the expectation of one electron being captured by the impurity spin). As the number of impurities grows, the increase in the band-filling is more noticeable. Here we consider the Néel domain wall described in figure 2 but we also consider the case of a much denser distribution of impurity spins. In particular, we consider a magnetic vortex where the spin orientations go around the central point of the

two-dimensional system. In this case there is a spin at every site except at the central point (which acts like a defect). For such a dense distribution of spins (concentration close to one) superconductivity is expected to be destroyed for quite small values of the spin coupling (for a system size of 15×15 superconductivity is destroyed for a spin coupling between $J = 0.5$ and 1). Therefore most of the increase of the band-filling in the case of the magnetic vortex occurs in the normal phase. Note, however, that for values of J between $J = 0.5$ and 1 there is a decrease in the electron density. For larger coupling values the density increases significantly and saturates to the half-filling situation (note that these results were obtained by fixing the chemical potential at $\mu = -1$). We stress however that both in the single impurity case and in the one-dimensional domain wall case, the system remains a superconductor. In the magnetic vortex case there is a vacancy at the center of the system (absence of impurity spin). As shown before [20], if the coupling is strong enough, a localized superconducting region (shown to be a localized mode) appears at the vacancy site (and in similar situations [20]). As a consequence there is a sharp decrease of the electron density at the vacancy site and therefore a decrease in the global density at small values of J. This result is dual to the density increase due to the presence of the strong coupling spins.

4. Self-consistent solution of charge accumulation

Since the impurity spins change, locally and globally, the electron density, the charge accumulation may counteract the effect of the buildup of charge around the impurities. The same problem has been addressed before for ferromagnetic metals with a domain wall, where charging effects are also predicted to occur [21]. To simplify, we consider here the case of a single impurity inserted at the center of the superconductor. The results may be generalized to the case of a domain wall. We will see that the effect remains with renormalized amplitudes and stronger Friedel like oscillations. Something similar occurs in the case of the vortex charge [22].

We have to include two extra terms in the Hamiltonian, one with respect to the Hartree contribution to the normal self-energy due to the effective attractive interaction (usually neglected since it only renormalizes the chemical potential locally) and a term that is the renormalized repulsive Coulomb term due to the charge accumulation. The mean-field Hamiltonian is changed by adding

$$-\sum_i (g\langle c^\dagger_{i,\downarrow} c_{i,\downarrow}\rangle c^\dagger_{i,\uparrow} c_{i,\uparrow} + g\langle c^\dagger_{i,\downarrow} c_{i,\downarrow}\rangle c^\dagger_{i,\uparrow} c_{i,\uparrow}) \tag{7}$$

and

$$\sum_i \Phi_i (c^\dagger_{i,\uparrow} c_{i,\uparrow} + c^\dagger_{i,\downarrow} c_{i,\downarrow}), \tag{8}$$

where

$$\Phi_i = g_c \sum_{j\neq i} \frac{e^{-\lambda_c |\vec{r}_i - \vec{r}_j|}}{|\vec{r}_i - \vec{r}_j|} (\langle (c^\dagger_{j,\uparrow} c_{j,\uparrow} + c^\dagger_{j,\downarrow} c_{j,\downarrow})\rangle - n). \tag{9}$$

Here λ_c is a screening length valid in the low momentum limit, such as in the Thomas–Fermi approximation, g_c is the Coulomb coupling and n is the average density. The longer range Friedel like contribution is obtained through the self-consistent solution of the effect of these two extra terms. The BdG equations are changed adding the diagonal terms

$$\tilde{A}_{\uparrow,\downarrow} = \begin{pmatrix} \Phi_i - g\langle c^\dagger_{i;\downarrow,\uparrow} c_{i;\downarrow,\uparrow}\rangle & 0 \\ 0 & -\Phi_i + g\langle c^\dagger_{i;\uparrow,\downarrow} c_{i;\uparrow,\downarrow}\rangle \end{pmatrix}. \tag{10}$$

Due to the renormalization of the chemical potential by the Hartree term and the Coulomb repulsion, we choose in this section a chemical potential $\mu = -1.5$. Also, we will consider a larger system to decrease the effect of the finite size, and we have chosen $\lambda_c = 2$, leading to a relatively short range e–e interaction as in a real metallic system.

We have calculated various quantities such as Δ, n, Φ_i and the local chemical potentials renormalized by the Hartree interaction for both spin orientations $\mu_+ = \mu_\uparrow = \mu + g\langle c^\dagger_{i;\uparrow} c_{i;\uparrow}\rangle$ and $\mu_- = \mu_\downarrow = \mu + g\langle c^\dagger_{i;\downarrow} c_{i;\downarrow}\rangle$. Here we considered a larger system size (25×25) to minimize finite size effects near the border of the system.

We consider two values of the coupling J, one below the quantum phase transition and the other above the quantum phase transition. Even though the various quantities are renormalized with respect to the case where the two charge terms are not considered, the quantum phase transition prevails as the total magnetization still has a discontinuous change from zero to 1/2 and the order parameter has a π shift. The overall behavior is the same, but we can see in figure 4 that there are stronger oscillations that extend to larger distances. In the case of $g_c = 2$ the oscillations are quite strong. For these parameters $J = 1$ is smaller than the critical value and $J = 4$ is above the quantum phase transition (evidenced for instance by the π shift at the impurity location). In figure 4 we present the local density for the same set of parameters.

The self-consistent solution of the local 'Coulomb' potential is shown for a typical case in figure 5 together with the local chemical potentials for up and down spins.

5. Critical concentration

Increasing the number of spins one expects that for very moderate spin couplings superconductivity should be destroyed. However, some unexpected results were obtained in [20]. Besides the interesting reappearance of superconducting order at large couplings due to vacancies of some kind, either by removing spins or due to singular points at domain walls or magnetic vortices [20], it was also found that in some cases the magnetic impurities may induce superconducting correlations in systems where the effective pairing interaction is *repulsive* [20], even though the systems are dense. It is therefore interesting to revisit the suppression of superconductivity as the impurity concentration increases.

This was studied long ago for the case when the impurity distribution and orientations are random [17, 19]. At relatively small concentration values, superconductivity is depressed. Refining the theory to take into account the Kondo effect [18] the same is observed qualitatively and quantitatively in most concentration regimes. Close to the critical concentration

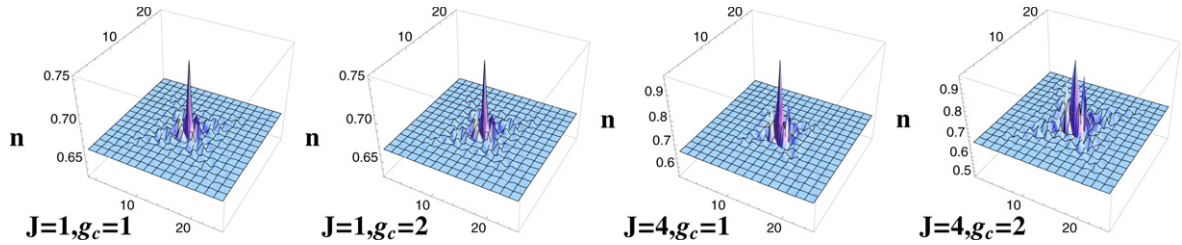

Figure 4. Electron density n around a single impurity for $J = 1, 4$ and $g_c = 1, 2$ for a 25×25 lattice.

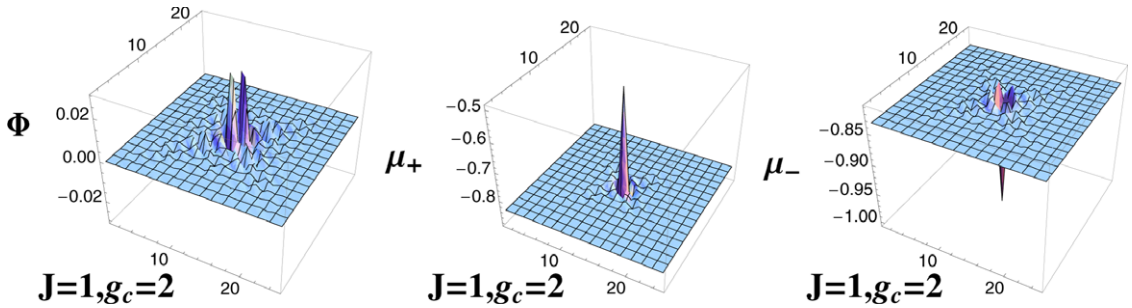

Figure 5. Parameters Φ, μ_+ and μ_- around a single impurity for $J = 1$ and $g_c = 2$ for a 25×25 lattice.

(where the critical temperature goes to zero) some reentrant superconductivity was obtained but, except near the critical concentration, the results are quite similar, providing further evidence that a reasonable description of these systems is obtained by considering the spins as classical.

In this work we have first considered the case of random impurities as a function of concentration. As shown in figure 6(a), the averaged value of the zero temperature order parameter (which is related to the critical temperature) decreases linearly from the clean limit with a slope that increases considerably as the coupling increases. For a very weak coupling, even though the system is rather dense, superconductivity prevails. However, a small increase of the coupling leads to a strong depression of the order parameter. We see that at half-filling $\mu = 0$ superconductivity prevails for concentrations up to 0.4. However, if we decrease the band-filling by lowering the chemical potential to $\mu = -1$, the drop in the order parameter is much faster, and concentrations of the order of 0.1 are enough to destroy superconductivity. Note that these results are obtained for systems of size 15×15 and an average using about 100 configurations is performed. We expect some finite size effects but this system size is illustrative of the effects.

We have also considered a regular distribution of the spins to see their effect on the order parameter. As an extreme case we have considered a set of spins distributed regularly in a superlattice commensurate with the space lattice of the electron sites and with their directions parallel, in a ferromagnetic like arrangement. As shown in the left panel of figure 6(b) superconductivity is much more robust in this case. We have considered the case of a chemical potential $\mu = 0$. It is clear that even for a concentration of 0.5 (obtained by placing one spin at every site along one direction and every other site along the other direction) superconducting order prevails. Only when the concentration is close to 1 does the order parameter vanish (we have not considered concentrations between 0.5 and 1 due to requirement of commensurability). These results show that superconductivity is much more robust if the magnetic impurities are correlated. In the right panel of figure 6(b) we considered a regular distribution of the impurity spins but with random orientations. The results also show that superconductivity is more robust, showing that the correlated spatial disorder is the dominant effect.

We note that similar results have been obtained in the context of Anderson localization in disordered one-dimensional systems, where correlated disorder may lead to a metallic state [23, 24].

6. Transport along a one-dimensional domain wall

The charge accumulation along the domain walls affects the transport properties. In this section we consider the effect of the impurity spins on a current flowing through the superconductor. To simplify, we consider here transport along a one-dimensional wire on which we place the impurity spins.

The Bogoliubov–de Gennes (BdG) equations determine both the equilibrium states and the scattering states when a current is passing through. We use a lattice formulation and define a spinor field at each location in the wire as $\psi_i = (u(i,\uparrow), v(i,\downarrow), u(i,\downarrow), v(i,\uparrow))^{\mathrm{T}}$. We use a transfer matrix, M_i, to relate the wave functions in neighboring sites i and $i+1$ as [25]:

$$\begin{pmatrix} \psi_{i+1} \\ \psi_i \end{pmatrix} = M_i \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix}, \tag{11}$$

with

$$M_i = \begin{pmatrix} T^{-1}(\epsilon - H_i) & -I \\ I & 0 \end{pmatrix}, \tag{12}$$

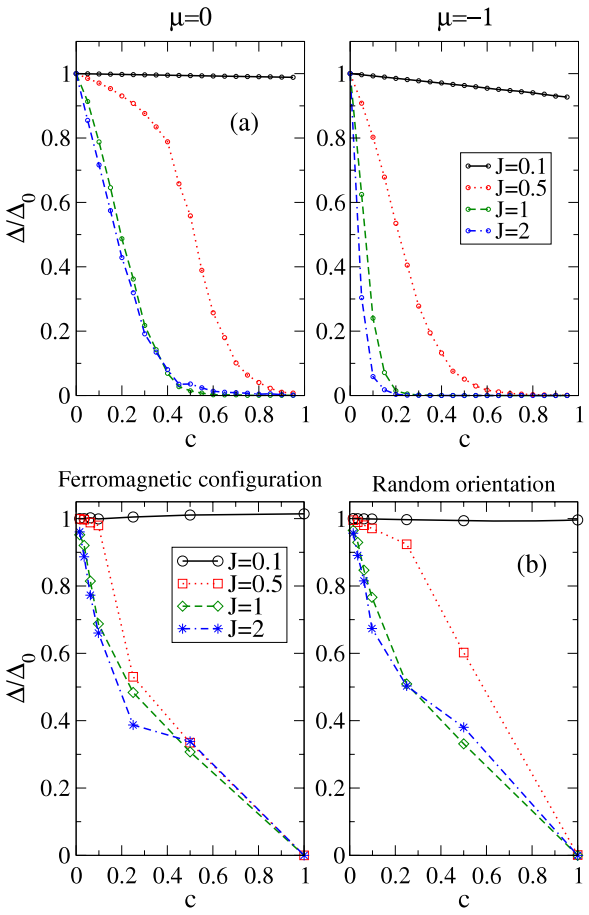

Figure 6. (a) Influence of impurity concentration on the order parameter for random locations and random orientations (upper panels) and (b) for a regular spatial distribution and fixed direction of the impurity spins (left panel) and random orientation (right panel). The lines are just guides to the eye.

where

$$T^{-1}(\epsilon - H_i) = \begin{pmatrix} A_i^- & B_i \\ B_i & A_i^+ \end{pmatrix} \tag{13}$$

and

$$A_i^{\pm} = \begin{pmatrix} \frac{-\tilde{\epsilon}_i \pm b_i - \epsilon}{t} & \frac{\Delta_i}{t} \\ -\frac{\Delta_i^*}{t} & \frac{-\tilde{\epsilon}_i \mp b_i + \epsilon}{t} \end{pmatrix}. \tag{14}$$

$B_i = -\sigma_z(J_i^x)/t$, where σ_z denotes the Pauli matrix. The energy of the incident particle is given by ϵ, t is the hopping between neighbors, $\tilde{\epsilon}_i = -U_i + \mu$ and $b_i = J_i^z$. The BdG equations are solved self-consistently, in a structure of length N of two normal leads and a superconducting region in the middle, to find the profile of the gap function inside the superconductor, Δ_i, which is then used as input in the transfer matrix (the proximity effect is thus taken into account). Here U_i is the barrier strength at the interfaces ($U = 0$ is a transparent interface and $U \to \infty$ is the tunneling regime [26]), the chemical potential we set at $\mu = 0$ and we take $t = 1$, as above. J_i^x, J_i^z are the x, z components of the local field due to the magnetic moments with magnitude J. We will only consider here the case of a transparent interface to isolate the effect of the spins. The superconducting region extends from site $N_{\rm SL}$ to $N_{\rm SR}$ and includes the magnetic

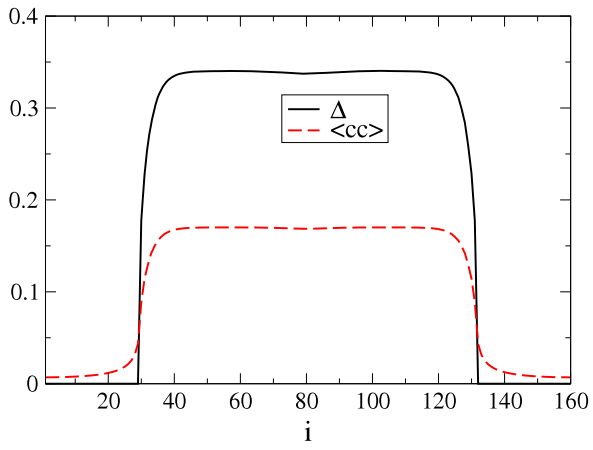

Figure 7. Order parameter and correlation function $\langle cc \rangle$ profiles for a domain wall with $J = 0.1$.

moments that constitute the domain wall. We take $N = 160$, $N_{\rm SL} = 30$, $N_{\rm SR} = 130$. Let $N_{\rm L}$ ($N_{\rm R}$) label a site in the left (right) lead, sufficiently far from the superconductor to neglect any proximity effects.

In figure 7 we show the order parameter profile along the leads and the superconducting wire together with the correlation function $\langle cc \rangle$ ($g = 2$ in the wire and $g = 0$ in the leads and $J = 0.1$). The coherence length is estimated to be $\xi \sim 15$, in lattice units.

To illustrate the procedure of the calculation of the transport properties [25], consider the scattering state for a particle with spin up incident from the left. We write

$$\psi_{N_{\rm L}} = (1 + r_z, r_{\rm A}, \bar{r}, r_{\rm A}^z)^{\rm T}, \tag{15}$$

$$\psi_{N_{\rm R}} = (t_z, t_{\rm A}, \bar{t}, t_{\rm A}^z)^{\rm T}, \tag{16}$$

and

$$\begin{aligned} \psi_{N_{\rm L}-1} &= (e^{-iq_1^l a} + r_z e^{iq_1^l a}, r_{\rm A} e^{-iq_2^l a}, \bar{r} e^{iq_3^l a}, r_{\rm A}^z e^{-iq_4^l a})^{\rm T}, \\ \psi_{N_{\rm R}+1} &= (t_z e^{iq_1^r a}, t_{\rm A} e^{-iq_2^r a}, \bar{t} e^{iq_3^r a}, t_{\rm A}^z e^{-iq_4^r a})^{\rm T}. \end{aligned} \tag{17}$$

This takes into account reflection of the particle with the same (opposite) spins r_z ($\bar{r}$), and reflection as hole due to Andreev process with the opposite (same) spin $r_{\rm A}$ ($r_{\rm A}^z$). The transmission amplitudes $t_z, t_a, \bar{t}, t_{\rm A}^z$ have the same meanings. The momenta are obtained far from the superconducting region where the solution of the BdG equations is easily obtained. Using the product of transfer matrices to relate the points $N_{\rm L}$ and $N_{\rm R}$, one can solve for the various reflection and transmission amplitudes. An identical procedure is carried out for a particle with spin down and for incident holes from the right. For an incident spin up particle the charge current is given by $j_{\rm L}(\uparrow) = \sin q_1^l a - |r_z|^2 \sin q_1^l a + |r_{\rm A}|^2 \sin q_2^l a - |\bar{r}|^2 \sin q_3^l a + |r_{\rm A}^z|^2 \sin q_4^l a$ on the left side (the sine functions are the velocities). The current on the right is given by $j_{\rm R}(\uparrow) = |t_z|^2 \sin q_1^r a - |t_{\rm A}|^2 \sin q_2^r a + |\bar{t}|^2 \sin q_3^r a - |t_{\rm A}^z|^2 \sin q_4^r a$. The differential conductance is given by the currents divided by the velocity of the incident particle.

In experiments, a potential difference, V, is imposed between the two sides of the heterostructure in a standard

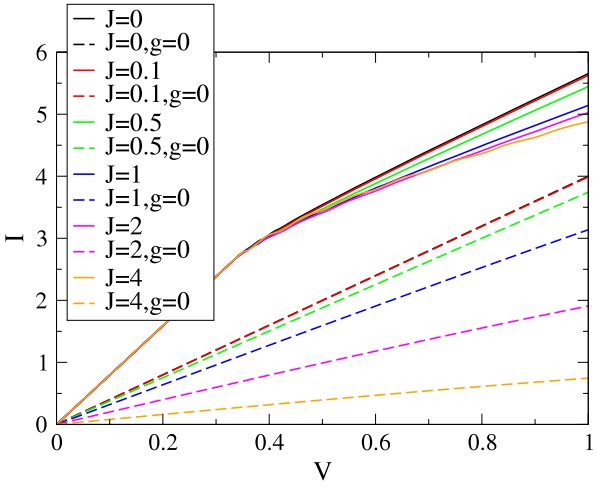

Figure 8. I–V characteristics for a single impurity, $g = 0$ is the case of a normal metal.

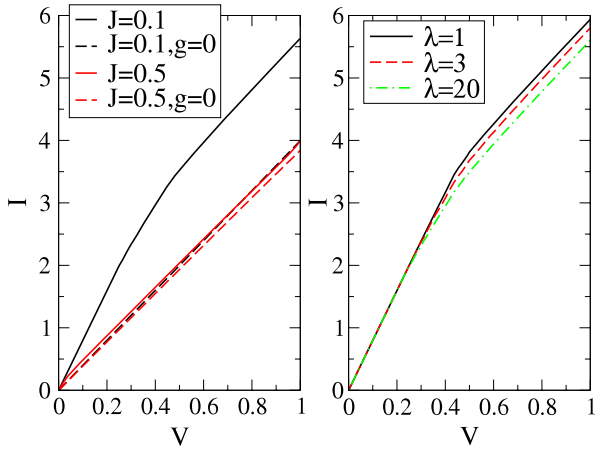

Figure 9. I–V characteristics for a dense domain wall. In the left panel we consider $\lambda = 10$.

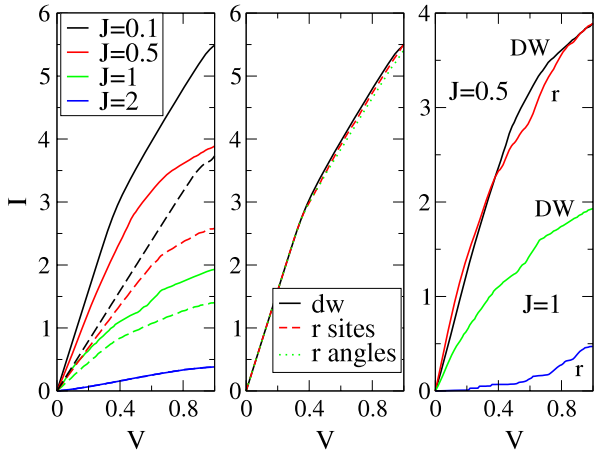

Figure 10. I–V characteristics for a domain wall with $1/3$ density. ('r' stands for random). In the left panel the dashed lines are for the normal system ($g = 0$) for the same J values. The ordering is the same: for larger values of J the current decreases.

way [27, 28]. Taking into account the contributions from particles incident from the left and holes incident from the right, one gets the expression for the current on the left side

$$I_\sigma^{\mathrm{e}} + I_\sigma^{\mathrm{h}} = \frac{e}{h}\int_0^\infty \mathrm{d}\epsilon \left[f\left(E - \frac{eV}{2}\right) - f\left(E + \frac{eV}{2}\right)\right] \times [1 - R^{\mathrm{ee}} + R^{\mathrm{he}} - T^{\mathrm{eh}'} + T^{\mathrm{hh}'}], \quad (18)$$

where R^{ee} is the reflection coefficient of an electron as an electron, R^{he} the reflection of an electron as a hole, $T^{\mathrm{eh}'}$ the transmission of a hole from the right into an electron on the left and $T^{\mathrm{hh}'}$ transmission of a hole from the right into a hole on the left. These coefficients are given by products of reflection or transmission coefficients (absolute value squared) times relative velocities to the incident particle.

In figure 8 we show results for the current as a function of the bias potential, V, for various cases. We compare the cases of a clean superconductor and a normal metal and study the difference due to the presence of a magnetic impurity in the center of the superconductor, as a function of the spin coupling, J. Due to the Andreev reflection at the interface between the lead and the superconductor the differential conductance is larger by about a factor of 2 for energies below the superconducting gap. Therefore, the current at small voltages is considerably larger in the superconductor in comparison to the case of the normal metal ($g = 0$). Inserting a magnetic impurity, the current in general decreases due to the scattering effect. Note, however, that the decrease is much stronger in the normal case. Also, for voltages smaller than the gap (here about 0.4) the impurity effect is not noticeable in the case of the superconductor.

Increasing the number of magnetic impurities their effect is stronger. Consider first the extreme case where at each lattice site we place a magnetic moment and consider, for instance, that the spins are oriented as in the Néel domain wall of figure 2. In this case the spin concentration is 1, and therefore a small spin coupling is enough to destroy superconductivity, as we have seen in section 5. For a spin coupling $J = 0.1$ superconductivity prevails, but for $J = 0.5$ it is almost destroyed. Then the superconductor and the normal metal have almost the same current characteristics, as shown in the left panel of figure 9. In the right panel of figure 9 we compare domain walls with $J = 0.1$ and different widths, $\lambda = 1, 3, 20$. As expected as the width increases the current decreases.

In order to consider the effect of an increasing spin coupling in a collection of magnetic moments one needs to decrease the density of the impurities. In figure 10 we consider a situation where only one in every three sites is occupied by a magnetic moment. In the left panel we consider that the spins are correlated like in a domain wall of width $\lambda = 10$ and compare different spin couplings in the superconductor and a normal metal. For this impurity density a spin coupling $J = 2$ destroys superconductivity. For the other couplings we find results that are qualitatively similar to those for a single impurity: the current is larger in the superconducting case and it decreases as J increases. In the middle panel we consider a small coupling $J = 0.1$ and compare the cases of a regular domain wall, impurities placed randomly and regularly spaced

but with random orientations. Since the coupling is small, the differences in the current are also small, but the results show that introducing randomness the current decreases, as expected. The effect is stronger if the orientations of the magnetic moments are random. This is considered specifically in the right panel of the same figure where we compare the case of the domain wall with the random orientations case, for two couplings. The case of $J = 1$ clearly shows that the current decreases considerably if the orientations are random.

Considering the case of magnetic impurities inserted in a superconductor, in general these will not be aligned if their mutual interactions are not strong enough, for instance if the concentration is not too high. Applying a magnetic field to orient the magnetic moments will then lead to a significant increase in the current. The signal is particularly stronger in the superconductor as compared to a normal metal. Note that, in contrast, the robustness of the superconducting order is mildly affected by the orientations of the spins but strongly affected by the randomness in their locations.

7. Conclusions

We have considered the effect of regular distributions of magnetic impurities in conventional superconductors. A reasonable description is obtained taking the impurities as classical (or local magnetic fields), since the Kondo effect is in most cases of no importance, particularly for weak couplings. We should note, however, that we have extended the range of the spin coupling between magnetic impurities and electron spin density to rather large values. In this regime it is probably more appropriate to consider superconducting films under the influence of external magnetic fields, or systems where the Kondo temperature is very small. The first case can be achieved, for instance, using magnetic dots in the vicinity of the superconducting film with their easy axis oriented parallel to the surface and with a thickness of the film smaller or of the order of the penetration length.

The magnetic impurities affect the system in various ways and, in particular, they change locally and globally the electron density. In the case of the domain wall considered here, this implies that the domain wall is charged, as predicted previously in the context of ferromagnetic metals with magnetic domain walls [21]. If the domain walls have a quasi-one-dimensional nature this will lead to lines of preferred charge accumulation which may be of relevance in the context of transport properties.

One can imagine the establishment of quasi-one-dimensional charged lines (impurity domain walls) in a two-dimensional background that may be switched on and off by the change of the local magnetic fields (or magnetizations of the quantum dots). For instance, the domain walls (which may be just a collection of parallel oriented fields) may be 'switched' on by the application of an external magnetic field, changing in this way the transport properties (one can also imagine various of these one-dimensional structures assembled in a circuit like manner). We have shown here that aligning the spins noticeably increases the current. At the very least we may consider quasi-one-dimensional organic superconductors and expect changes in the transport properties.

We have also revisited the problem of the suppression of superconductivity due to the possible increase of the impurity concentration. Usually, small concentrations are enough to destroy superconductivity in the traditional case of random impurities placed inside the superconductor. We have found here that superconductivity is much more robust if the impurity spins are correlated and placed in regular ways. In particular, one-dimensional structures in the two-dimensional system lead to small enough concentrations that in the framework of the model used here does not lead to the destruction of superconductivity.

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