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Localized Magnetic Moments Interacting with Superconductors outside the Kondo Regime

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Abstract

The Anderson model has been of utmost importance in the understanding of the presence of a magnetic impurity in metals. In this work we investigate the properties of a superconductor in the presence of the magnetic impurity interacting with the conduction electrons, using the mean field formalism. We observe the particle-hole symmetry of the superconductor to be broken by the impurity. The boundary between magnetic and non-magnetic configurations, contrary to what occurs in metal, is asymmetric around $-\varepsilon_d / U = 0.5$. *The spectrum of* $\Delta(T)/\Delta_0$ *as a function of* T/T_c *maintains the universal behavior as was found in the Bardeen-Cooper-Schrieffer theory. The critical temperature decreases with the increase in* Γ *and tends to zero as* $\Gamma >> \Delta_0$.

Key words: localized magnetic moments, superconductors, Kondo Regime

1. INTRODUCTION

Impurities have often been the main obstacle in revealing the beautiful physics that exists in cleaner systems. However, several properties are either caused or probed with the use of various impurities and are sometimes crucial in unraveling the science, for e.g the billion dollar semiconducting electronics industry is one of them. The physics of superconductors still remains unexplained and is still shrouded in mystery despite intense research over the past several decades and is never pure. The substitutional impurities allow us to study the superconductivity over a wide range of parameters paving the way thereby to check the validity of the existing theories (BCS) [1] as well as the new ones (high T_c). The study of disorder has gained an impetus recently in strongly correlated electron systems. The impurities in conventional metal lead to higher resistivity and the magnetic impurities destroy the coherence of the superconducting state. The high temperature superconductors still remain the primary focus of our study. However, there is no complete microscopic description and certainly no consensus on the mechanism of the pair formation. The reaction of the system to the introduction of impurities can be an important test of order, or even growing correlations towards such an order in the superconducting state. The prerequisite for such a test is the detailed understanding of the behavior of the simple superconductors with impurities. After intense research in the early BCS years, the subject was considered closed in the mid-60s. However, recently there has been a revival of the interest in s-wave superconductors with magnetic impurities – with many new theoretical and experimental results changing our perspective of the knowledge. The s-wave properties in the presence of the impurities continue to be investigated [2] and can play vital role in the understanding of the new superconductors.

The classic problem of the impurities in s-superconductors was considered long back in the works of [3, 4]. The direct measurements of the quasi-particle excitations around a magnetic impurity obtained by Yazdani et. al. [5] reinvigorated the field. Later the scanning tunneling microscopy (STM) measurements were used to study the electronic properties of exotic materials with impurities [6, 7, 8]. The substitution of the divalent metals [Zn, Ni] for Cu in CuO_2 planes offers an important way of introducing impurities in unconventional superconductors [9, 10, 11]. More recently, we observe a revival of interest of the study of the impurity in a conventional superconductor motivated in part by possible applications to topological quantum computation [12, 13, 14, 15]. The interplay between the magnetic moments and superconductivity can lead to emergence of exotic phases and excitations and thus provide special advantages. Recent experimental investigations of the problem have been of utmost importance opening a new chapter in superconductivity [16]. Various works have been performed to study the effect of the impurities in conventional $s-$wave superconductors [17, 18, 19, 20, 21, 22]

In this work we revisit the problem of localized magnetic moments interacting with a superconductor. We also consider a Coulomb interaction U that breaks the particle hole symmetry. A realistic model for an impurity site is the Anderson model [23, 24]. The model is extremely rich in behavior and allows a natural interpolation between the potential and the magnetic scattering [25]. The model has been analyzed thoroughly using the numerical renormalization group technique [26]. However, analytical study still lacks. In this case the impurity electrons couple to the conduction band and may modify the spin configuration. Studies on various superconductors for e.g Al doped $SrRuO_4$ [27], Ce based "115" heavy fermion materials [28], Mn, Gd and Ag atoms on Nb [5] have been of utmost importance in our understanding of the superconductors. STM has been further developed to probe the quasiparticle scattering around a single impurity in $Bi_2Sr_2CaCu_{1-x}Zn_xO_{8+\delta}$ with a spatial and energy resolution [7]. The question of the localization continues to be investigated both in s and d superconductors. Recently the Anderson model has been considered for the magnetic impurity study of the cuprates [29, 30, 31].

In this article we study the effect of a single impurity on superconductors. The Anderson model in the presence of the Coulomb interaction has been used within a mean-field formalism to study phase diagram of the superconductors in the presence of disorder. The Greens's function technique is used to study the properties of the superconductor. The outline of the paper is as follows. In section 2 we describe the Anderson impurity model suitable for the superconductors in detail. The calculated superconducting properties for the above model have been described in section 3. We discuss our results on the phase diagram, susceptibility, critical temperature and also the temperature dependence of the gap parameter in section 4.

Finally we summarize our results in section 5.

2. THE MODEL

The Anderson model has been used in various problems as can be found in ref. [24, 23]. It is often used to describe magnetic impurities embedded in metallic hosts and applied to the description of Kondo-type problems, such as heavy fermion systems and Kondo insulators. In order to study superconductivity we use the Bardeen-Cooper-Schrieffer (BCS) Hamiltonian [1]. The theory describes superconductivity as a microscopic effect caused by a condensation of Cooper pairs BCS theory and assumes that there is some attraction between electrons, which can overcome the Coulomb repulsion. In conventional superconductors, the above attraction is brought about indirectly by the coupling of electrons to the crystal lattice. The evidence of a gap at the Fermi level, exponential dependence of the specific heat on temperatures, Meissner effect are some of the important facts that BCS theory could predict.

The Hamiltonian of a magnetic impurity coupled to a superconductor can be modeled by an Anderson impurity [23] hybridized with the conduction band. The superconducting tight binding model along with the impurity Hamiltonian can be written as

$$H = H_{SC} + H_{imp} + H_{hyb}, \qquad (1)$$

where H_{SC} is the tight binding superconducting Hamiltonian, H_{imp} represents the impurity Hamiltonian and H_{hyb} denotes the hybridization of the impurity orbital with the conduction band. The superconducting Hamiltonian is given by

$$H_{SC} = \sum_k \xi_k c^\dagger_{k\sigma} c_{k\sigma} - \sum_k \Delta_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - \sum_k \Delta^*_k c_{-k\downarrow} c_{k\uparrow} \qquad (2)$$

where $c^\dagger_{k\sigma}(c_{k\sigma})$ creates (annihilates) an electron with momentum k, spin σ ($\uparrow$ or $\downarrow$) and energy ξ_k (with respect to the chemical potential μ) in the conduction band. The chemical potential is set to be zero just as the case of half filling. Δ_k is the superconducting gap. Since electrons obey Fermi statistics, the creation and annihilation operators $c^\dagger_{k\sigma}(c_{k\sigma})$ satisfy the anticommutation relations

$$[c_{k\sigma}, c^{\dagger}_{k'\sigma'}]_{+} = \delta_{kk'}\delta_{\sigma\sigma'}$$
$$[c_{k\sigma}, c_{k'\sigma'}]_{+} = [c^{\dagger}_{k\sigma}, c^{\dagger}_{k'\sigma'}]_{+} = 0$$

and particle number operator is given by $n_{k\sigma} = c^{\dagger}_{k\sigma}c_{k\sigma}$.

The impurity Hamiltonian is given by

$$H_{imp} = \sum_{\sigma}\varepsilon_d c^{\dagger}_{d\sigma}c_{d\sigma} + Un_{d\uparrow}n_{d\downarrow}, \qquad (3)$$

where $c^{\dagger}_{d\sigma}(c_{d\sigma})$ creates (annihilates) an electron with spin $\sigma = \uparrow, \downarrow$, $n_{d\sigma} = c^{\dagger}_{d\sigma}c_{d\sigma}$ is the impurity occupation number operator, ε_d is the energy in the impurity orbital and U is the Coulomb repulsion between the electrons in this orbital. The creation and annihilation operators $c^{\dagger}_{d\sigma}(c_{d\sigma})$ satisfy the anticommutation relations

$$[c_{d\sigma}, c^{\dagger}_{d\sigma'}]_{+} = \delta_{\sigma\sigma'}$$
$$[c_{d\sigma}, c_{d\sigma'}]_{+} = [c^{\dagger}_{d\sigma}, c^{\dagger}_{d\sigma'}]_{+} = 0.$$

For simplicity we adopt a mean-field approximation to the electronic correlations to obtain $Un_{d\uparrow}n_{d\downarrow} = U\sum_{\sigma}\langle n_{d-\sigma}\rangle c^{\dagger}_{d\sigma}c_{d\sigma} - U\langle n_{d\uparrow}\rangle\langle n_{d\downarrow}\rangle$. Hence,

$$H_{imp} = \sum_{\sigma}\varepsilon_{d\sigma}c^{\dagger}_{d\sigma}c_{d\sigma} \qquad (4)$$

where $\varepsilon_{d\sigma} = \varepsilon_d + U\langle n_{d-\sigma}\rangle$.

The hybridization of the impurity orbital with the conduction band is represented by

$$H_{hyb} = V\sum_{k,\sigma}\left(c^{\dagger}_{k\sigma}c_{d\sigma} + c^{\dagger}_{d\sigma}c_{k\sigma}\right), \qquad (5)$$

where V is the hybridization interaction between the electron in the impurity orbital and the electrons in the conduction band.

3. THE FORMALISM

The tight binding superconducting Hamiltonian can be diagonalized by defining new Fermi operators [32]. The transformations can be obtained using the Bogoliubov operators and is given by

$$c_{k\sigma} = u_k\gamma_{k\uparrow} - v_k\gamma^{\dagger}_{-k\downarrow}$$
$$c^{\dagger}_{-k\sigma} = v^{\dagger}_k\gamma_{k\uparrow} + u^{\dagger}_k\gamma^{\dagger}_{-k\downarrow} \qquad (6)$$

where the numerical coefficients u_k and v_k satisfy $|u_k|^2 + |v_k|^2 = 1$.

Substituting the above operators, the Hamiltonian H (Eq. (1)) can be written in terms of the Bogoliubov operators $\gamma_{k\uparrow}$ and $\gamma^{\dagger}_{-k\downarrow}$ as

$$H = \sum_{k\sigma} E_k \gamma^{\dagger}_{k\sigma}\gamma_{k\sigma} + \sum_{\sigma}\varepsilon_{d\sigma} c^{\dagger}_{d\sigma} c_{d\sigma} + V\sum_{k}\left[\left(u^{*}_{k}\gamma^{\dagger}_{k\uparrow} - v^{*}_{k}\gamma_{-k\downarrow}\right)c_{d\uparrow} + \left(v^{*}_{-k}\gamma_{-k\uparrow} + u^{*}_{-k}\gamma^{\dagger}_{k\downarrow}\right)c_{d\downarrow} + h.c\right], \tag{7}$$

where $\left|u_k\right|^2 = (1+\xi_k / E_k)/2$, $\left|v_k\right|^2 = (1-\xi_k / E_k)/2$, $\left|u_k v_k\right| = \Delta_k / 2E_k$ and $E_k = \sqrt{\xi_k^2 + \left|\Delta_k\right|^2}$.

The impurity density of states given by $ImG^r\left(c_{d\sigma},\omega\right)$, can be obtained from the Fourier transformed retarded Green's function [24]

$$G^r\left(c_{d\sigma}, t-t'\right) = -i\theta(t-t')\left\langle\{c_{d\sigma}(t), c^{\dagger}_{d\sigma}(t')\}\right\rangle.$$

Various physical observables can be written in terms of retarded Green's functions and the correlation functions that involves the calculation of the the time-dependence of these functions. Equation of motion method is one of the several methods that could be useful for this purpose [33]. The main principle of this method is to produce a series of coupled differential equations by differentiating the relevant correlation function a number of times. Hence, using the above method , we obtain

$$G^r\left(c_{d\sigma},\omega\right) = \left\{\omega - i\eta - \varepsilon_{d\sigma} - V^2\Sigma_{ii} - V^4\frac{\left(\Sigma_{12}-\Sigma_{21}\right)\left(\Sigma'_{12}-\Sigma'_{21}\right)}{\omega - i\eta - \varepsilon_{d-\sigma} - V^2\Sigma'_{ii}}\right\}^{-1}, \tag{8}$$

where η is an infinitesimal number to ensure proper convergence and

$$\begin{bmatrix}\Sigma_{11} & \Sigma_{12}\\ \Sigma_{21} & \Sigma_{22}\end{bmatrix} = \begin{bmatrix}\sum_k \frac{\left|v_k\right|^2}{\omega+i\eta+E_k} & \sum_k \frac{u_k v_k}{\omega+i\eta+E_k}\\ \sum_k \frac{u_k v_k}{\omega+i\eta-E_k} & \sum_k \frac{\left|u_k\right|^2}{\omega+i\eta-E_k}\end{bmatrix} \tag{9}$$

$$\begin{bmatrix}\Sigma'_{11} & \Sigma'_{12}\\ \Sigma'_{21} & \Sigma'_{22}\end{bmatrix} = \begin{bmatrix}\sum_k \frac{\left|v_{-k}\right|^2}{\omega+i\eta-E_k} & \sum_k \frac{u^{*}_{-k} v^{*}_{-k}}{\omega+i\eta+E_k}\\ \sum_k \frac{u^{*}_{-k} v^{*}_{-k}}{\omega+i\eta-E_k} & \sum_k \frac{\left|u_{-k}\right|^2}{\omega+i\eta+E_k}\end{bmatrix} \tag{10}$$

and the repeated indices in Σ_{ii} and Σ'_{ii} mean a sum over its allowed values(1 and 2). The term $(\Sigma_{12}-\Sigma_{21})$ that appears in Eq. (8) can be calculated transforming the sum over k to integral in ξ_k by the relation $\sum_k = \rho(\xi_F)\int_{-D}^{D} d\xi_k$, where $\rho(\xi_F)$ denotes the density of states at Fermi energy [24, 32, 33]. Hence, adopting this procedure for Σ_{12} and Σ_{21} we obtain,

$$\Sigma_{12} = \frac{1}{2}\rho(\xi_F)\int_{-D}^{D} d\xi_k \frac{|\Delta_k|}{E_k\left(\omega + E_{\vec{k}}\right)} - i\frac{\pi\rho(\xi_F)|\Delta_k||\omega|}{\left(\omega^2 + \left|\Delta_{\vec{k}}\right|^2\right)\sqrt{\omega^2 - |\Delta_k|^2}} \tag{11}$$

$$\Sigma_{21} = \frac{1}{2}\rho(\xi_F)\int_{-D}^{D} d\xi_k \frac{|\Delta_k|}{E_k\left(\omega - E_{\vec{k}}\right)} - i\frac{\pi\rho(\xi_F)|\Delta_k||\omega|}{\left(\omega^2 + \left|\Delta_{\vec{k}}\right|^2\right)\sqrt{\omega^2 - |\Delta_k|^2}}, \tag{12}$$

where $\rho(\xi_F)$ is the density of states of the conduction band at the Fermi level and $2D$ is the conduction band width. From Eqs. (11) and (12), $Im(\Sigma_{12} - \Sigma_{21}) = 0$ and $Re(\Sigma_{12} - \Sigma_{21}) = \rho(\xi_F)\int_{-D}^{D} d\xi_{\vec{k}} |\Delta_k| / (\omega^2 - \xi_k^2 - |\Delta_k|^2)$, which is also zero in the limit $D \to \infty$. In this limit, substituting $\Sigma_{12} - \Sigma_{21} = 0$ into Eq. (8), $G^r\left(d_\sigma, \omega\right)$ reduces to

$$G^r\left(d_\sigma, \omega\right) = \left[\omega - i\eta - \varepsilon_{d\sigma} - V^2\Sigma_{ii}(\omega)\right]^{-1}. \tag{13}$$

The impurity density of states $\rho_{d\sigma}(\omega)$ is given by

$$\rho_{d\sigma}(\omega) = -(1/\pi) Im G^r\left(d_\sigma, \omega\right) = \frac{1}{\pi}\frac{V^2 Im\Sigma_{ii}(\omega)}{\left[\omega - \varepsilon_{d\sigma} - V^2 Re\Sigma_{ii}(\omega)\right]^2 + \left[V^2 Im\Sigma_{ii}(\omega)\right]^2}, \tag{14}$$

with

$$Re\Sigma_{ii}(\omega) = \begin{cases} \dfrac{2\rho(\xi_F)\omega}{\sqrt{\omega^2 - \Delta^2}} \ln\left(\dfrac{D + \sqrt{\omega^2 - \Delta^2}}{D - \sqrt{\omega^2 - \Delta^2}}\right) & if\ |\omega| \geq \Delta \\ \\ \dfrac{4\rho(\xi_F)\omega}{\sqrt{\Delta^2 - \omega^2}} tg^{-1}\left(\dfrac{\sqrt{\Delta^2 - \omega^2}}{D}\right) & if\ |\omega| < \Delta \end{cases} \tag{15}$$

$$Im\Sigma_{ii}(\omega)=\begin{cases} -2\pi\rho(\xi_F)\dfrac{|\omega|}{\sqrt{\omega^2-\Delta^2}} & if\ |\omega|\geq\Delta \\ \\ -2\pi\rho(\xi_F)\dfrac{|\omega|}{\sqrt{\Delta^2-\omega^2}} & if\ |\omega|<\Delta \end{cases}, \qquad (16)$$

where we consider $\Delta_k=\Delta$. In the limit $D ? \sqrt{|\omega^2-\Delta^2|}$, $\mathrm{Re}\Sigma_{ii}\to 0$, and the impurity density of states $\rho_{d\sigma}(\omega)$ becomes

$$\rho_{d\sigma}(\omega)=\frac{2}{\pi}\Gamma\frac{|\omega|}{\sqrt{\omega^2-\Delta^2}}\times\frac{1}{\left[\omega-\varepsilon_{d\sigma}\right]^2+\Gamma^2\dfrac{|\omega|^2}{\omega^2-\Delta^2}} \quad for\,|\omega|\geq\Delta \qquad (17)$$

and zero for $|\omega|\leq\Delta$, with $\Gamma=\pi\rho(\xi_F)V^2$. In contrast to the impurity in metal, the density of states of the impurity embedded in a superconductor is not a conventional Lorentzian, due to its anomalous broadening of the frequency by the factor $|\omega|/\sqrt{\omega^2-\Delta^2}$.

The superconducting gap is given by $\Delta_k=\Sigma_{k'}V_{sc}\left\langle c_{-k\downarrow}c_{k\uparrow}\right\rangle$, where V_{sc} is the pairing interaction. It can be obtained using the equation of motion technique for the Matsubara function. The Matsubara Green's functions technique [34] has been developed to describe many-body systems in equilibrium at finite temperature [24, 35]. By Fourier transformation and exploiting the Fermionic symmetry one can obtain all the necessary information contained in the Green's functions defined for a discrete set of energies proportional to the Matsubara frequencies. We define the two Green's functions

$$\mathrm{G}(c_{k\uparrow},\tau)=-\left\langle Tr\left(c_{k\uparrow}(\tau)c^{\dagger}_{k'\uparrow}(0)\right)\right\rangle \qquad (18)$$

$$\mathrm{G}(d_{\uparrow},\tau)=-\left\langle Tr\left(d_{\uparrow}(\tau)c^{\dagger}_{k'\uparrow}(0)\right)\right\rangle \qquad (19)$$

and the two anomalous Green's functions

$$\mathrm{F}\,(c^{\dagger}_{-k\downarrow},\tau)=-\left\langle Tr\left(c^{\dagger}_{-k\downarrow}(\tau)c^{\dagger}_{k'\uparrow}(0)\right)\right\rangle \qquad (20)$$

$$\mathrm{F}\,(d^{\dagger}_{\downarrow},\tau)=-\left\langle Tr\left(d^{\dagger}_{\downarrow}(\tau)c^{\dagger}_{k'\uparrow}(0)\right)\right\rangle. \qquad (21)$$

where Tr is the time-ordering operator. Performing the Fourier transformation of the the equation of motion of the above Green's functions to Matsubara frequency space $i\omega_n$, and taking into account that $\xi_k = \xi_{-k}$ and $\sum_k \mathrm{F}\,(c^{\dagger}_{k\downarrow}, i\omega_n) = \sum_k \mathrm{F}\,(c^{\dagger}_{-k\downarrow}, i\omega_n)$, we obtain

$$(i\omega_n - \xi_k)\mathrm{G}(c_{k\uparrow}, i\omega_n) = \delta_{kk'} - \Delta_k \mathrm{F}\,(c^{\dagger}_{-\vec{k}\downarrow}, i\omega_n) + V\mathrm{G}(d_{\uparrow}, i\omega_n) \qquad (22)$$

$$(i\omega_n - \varepsilon_{d\uparrow})\mathrm{G}(d_{\uparrow}, i\omega_n) = V\sum_k \mathrm{G}(c_{k\uparrow}, i\omega_n) \qquad (23)$$

$$(i\omega_n + \xi_k)\mathrm{F}\,(c^{\dagger}_{-k\downarrow}, i\omega_n) = -\Delta_k^* \mathrm{G}(c_{k\uparrow}, i\omega_n) - V\mathrm{F}\,(d^{\dagger}_{\downarrow}, i\omega_n) \qquad (24)$$

$$(i\omega_n + \varepsilon_{d\downarrow})\mathrm{F}\,(d^{\dagger}_{\downarrow}, i\omega_n) = -V\sum_k \mathrm{F}\,(c^{\dagger}_{-k\downarrow}, i\omega_n). \qquad (25)$$

Solving the above equations for $\mathrm{F}\,(c^{\dagger}_{-k\downarrow}, i\omega_n)$ we find

$$\mathrm{F}\,(c^{\dagger}_{-k\downarrow}, i\omega_n) = -\frac{\Delta_k^*}{(i\omega_n)^2 - E_k^2} - \Delta_k^* V^2 \sum_{s=\pm 1} Z_s \left[\frac{|u_k|^2}{i\omega_n - sE_k} + \frac{|v_k|^2}{i\omega_n + sE_k}\right]^2, \qquad (26)$$

where

$$Z_s = \frac{1}{(i\omega_n + s\xi_k)(i\omega_n - s\varepsilon_{ds} - V^2\Omega_1)}$$

$$\Omega_1 = \sum_k \left[\frac{u_k^2}{i\omega_n + E_k} + \frac{v_k^2}{i\omega_n - E_k}\right]$$

and $\varepsilon_{d+(-)} = \varepsilon_{d\uparrow(\downarrow)}$. The first term corresponds to the contribution from the pure case and the last term appears from the interaction of the conduction electron with the impurity, neglecting terms of fourth order in V. The superconducting order parameter Δ_k is defined as

$$\Delta_k = V_{sc} \sum_k^{|\xi_k|<\omega_D} \left\langle c_{-k\downarrow} c_{k\uparrow} \right\rangle = V_{sc} \sum_k^{|\xi_k|<\omega_D} \mathrm{F}^{\,*}(c^{\dagger}_{-k\downarrow}, \tau = 0^+), \qquad (27)$$

where ω_D is the Debye energy and $\mathrm{F}^{\,*}(c^{\dagger}_{-k\downarrow}, \tau = 0^+)$ is the Fourier transform of $\mathrm{F}^{\,*}(c^{\dagger}_{-k\downarrow}, i\omega_n)$ with the Matsubara frequency $i\omega_n$. Substituting Eq. (26) into Eq. (27) and carrying out the Matsubara summation, taking Δ_k independent of k, we obtain

$$\frac{1}{\rho(\xi_F)V_{sc}} = -\sum_{s=\pm 1} s\left\{\int_{-\omega_D}^{\omega_D}\frac{d\xi_k}{2E_k}n_F(sE_k)+V^2\sum_{s'=\pm 1}s'\int_{-\omega_D}^{\omega_D}\frac{d\xi_k(\xi_k+s'sE_k)n_F(s'E_k)}{[2E_k(E_k-\varepsilon_{ds})]^2}\right. \qquad (28)$$
$$\left. +V^2\int_{-\omega_D}^{\omega_D}\frac{d\xi_k(\varepsilon_{ds}+\xi_k)n_F(s\varepsilon_{ds})}{\left(\varepsilon_{ds}^2-E_k^2\right)^2}\right\}$$

where $n_F(\varepsilon)=1/(\exp(\beta\varepsilon)+1)$ is the Fermi distribution and $\beta=1/k_BT$.

4. RESULTS AND DISCUSSION

The impurity magnetization is defined as $m=\langle n_{d\uparrow}\rangle-\langle n_{d\downarrow}\rangle$, where $\langle n_{d\sigma}\rangle$ is the occupation number of the impurity, given by $\int\rho_{d\sigma}(\omega)n_F(\omega)d\omega$. The impurity is magnetic when $\langle n_{d\uparrow}\rangle\neq\langle n_{d\downarrow}\rangle$. All our results in this work are in eV, unless mentioned otherwise. In Fig. (1) we present the boundary between the magnetic and nonmagnetic impurity states at zero temperature as a function of the parameters $-\varepsilon_d/U$ and $\pi\Gamma/U$. The solid line represents the boundary for the impurity embedded in a metal and the remaining curves represent that of a s-wave superconductor, with different values of $\Delta/\Gamma=0.1, 0.2, 0.5$, and 1.0 (dashed, dotted, dashed-dotted, and dashed-double-dotted line, respectively). The impurity is magnetic inside and non-magnetic outside the boundary. For metal, the transition curve is symmetric around $-\varepsilon_d/U=0.5$. On the contrary, in the superconductor the symmetry is broken by the presence of the impurity. In metal the boundary is always less than $-\varepsilon_d/U=1$ and in superconductor it can assume values greater than one due to the broadening of the impurity density of states for energy close to Δ by a factor $|\omega|/\sqrt{\omega^2-\Delta^2}$. In the limit $\pi\Gamma/U \to 0$ the boundary in the superconductor converges to one or zero, as in metal, indicating the maintenance of the electron-hole symmetry in this limit. Thereby the quantum mechanical fluctuations like the Kondo effect which should be important at low-temperatures is beyond the scope of this scenario and the temperature considered is above the Kondo temperature [4]. It exhibits a sharp transition between the nonmagnetic states and the magnetic states of an impurity. The transition should be gradual as the fluctuation effect are indeed important near the transition.

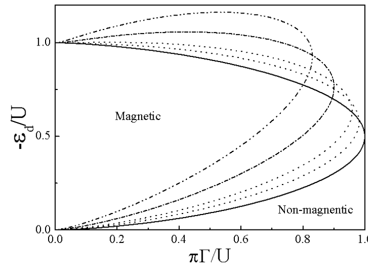

Figure 1: The transition curve between the magnetic and non magnetic region hybridized with the conduction electrons of a metal (solid line) and a superconductor with different values of $\Delta = 0.1$ (dashed line), 0.2 (dotted line), 0.5 (dashed dotted line) and 1.0 (dashed dotted dotted line).

The occupation number and the magnetic susceptibility as a function of Δ_0, the gap at $T = 0$, are shown in Fig. (2) for $\varepsilon_d = -0.02$, $\Gamma = 0.002$ and $U = 0.016$. For $\Delta_0 = 0$, representing an impurity in metal, $n_{d\uparrow} = n_{d\downarrow}$, the impurity is nonmagnetic. However, for the same parameters, in a s-wave superconductor, depending on the value of the gap Δ_0, $n_{d\uparrow} \neq n_{d\downarrow}$ and the impurity becomes magnetic. Varying Δ_0 the occupation number splits at $\Delta_0 = \left|\varepsilon_d + U\langle n_{d\uparrow}\rangle\right|$ and collapses at $\Delta_0 = \left|\varepsilon_d + U\langle n_{d\downarrow}\rangle\right|$ (with the convention $\langle n_{d\uparrow}\rangle < \langle n_{d\downarrow}\rangle$), and the impurity is magnetic for specific values of Δ_0. The magnetization of the impurity varies between these two values. The behavior of the magnetic susceptibility at the zero-field limits, $\chi = \mu_B \sum_\sigma \sigma (dn_\sigma / dB)_{B=0}$ (μ_B is the Bohr magneton and B is an applied magnetic field) can be written as

$$\chi = -\mu_B^2 \sum_{\sigma=\uparrow\downarrow} \frac{dn_\sigma}{d\varepsilon_{d\sigma}} \frac{1 - U\dfrac{dn_{-\sigma}}{d\varepsilon_{d-\sigma}}}{1 - U^2 \dfrac{dn_{-\sigma}}{d\varepsilon_{d-\sigma}} \dfrac{dn_\sigma}{d\varepsilon_{d\sigma}}}. \qquad (29)$$

In Fig. 2(b) the magnetic susceptibility presents two peaks, at Δ_0 close to the two different energies $\left|\varepsilon_d + U\langle n_{d\uparrow}\rangle\right|$ and $\left|\varepsilon_d + U\langle n_{d\downarrow}\rangle\right|$. The fact that the impurity becomes magnetic between $\left|\varepsilon_{d\uparrow}\right|$ and $\left|\varepsilon_{d\downarrow}\right|$ values of

Δ_0 is evident from Fig. (3), where for $\varepsilon_d = -0.02$, $\Gamma = 0.002$ and different values of U we present the magnetization as a function of Δ_0.

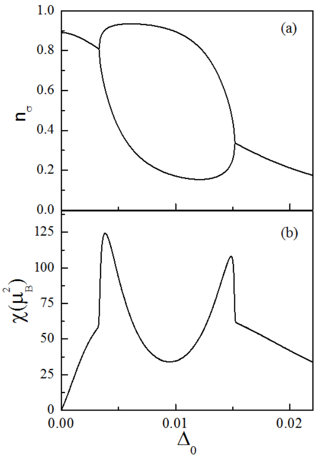

Figure 2: (a)The occupation number and (b) the magnetic susceptibility as a function of Δ_0, taking $\varepsilon_d = -0.02, \Gamma = 0.002$ and $U = 0.016$.

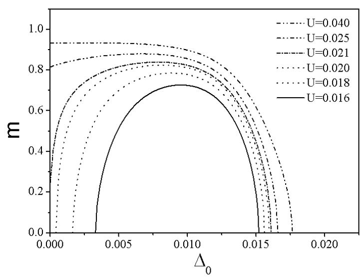

Figure 3: Magnetization as a function of Δ_0 for $\varepsilon_d = -0.02, \Gamma = 0.002$ and different values of U.

In Fig. (4) we present the gap $\Delta(T)$ as a function of temperature T for $\varepsilon_d = -0.2$, $\Gamma = 0.002$, $V_{sc} = -0.15$ and different values of U ($0.0, 0.1$ and 0.3). Scaling $\Delta(T)$ by Δ_0 and T by T_c the gap presents an universal behavior. Increase in U decreases the critical temperature T_c and Δ_0 as shown in the insert (a) of this figure. Curiously the universal curve approaches the function

$$\frac{\Delta(T)}{\Delta_0} = \sqrt{1-\left(\frac{T}{T_c}\right)^3} \tag{30}$$

as is presented in insert (b). In the limit $T \approx T_c$,

$$\frac{\Delta(T)}{\Delta_0} \approx \sqrt{3}\left(1-\frac{T}{T_c}\right)^{1/2}, \tag{31}$$

which is very close to the asymptotic result for BCS model ([32]), where instead of $\sqrt{3}$ we observe 1.74.

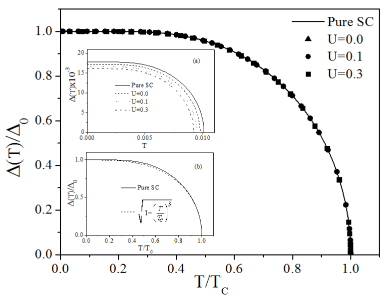

Figure 4: The gap $\Delta(T)$ as a function of temperature T for $\varepsilon_d = -0.2$, $\Gamma = 0.002$, $V_{sc} = -0.15$ and different values of $U = 0.0$, 0.1, 0.3.

In Fig. (5) we show $\Delta(T)$ as a function of T for $\varepsilon_d = -0.2$, $U = 0.1$, $V_{sc} = -0.15$ and different values of $\Gamma = 0.002$, 0.010, 0.02. The gap and the critical temperature decrease with the increase in Γ as can be seen in 5(a). As is shown in Fig. 5(b), the universal behavior is maintained as Γ varies. In the insert in 5(b) we present the critical temperature as a function of Γ. It decreases linearly with small Γ and presents an inflection around $\Gamma / \Delta(\Gamma = 1)$. For $\Gamma >> \Delta(\Gamma=0)$ the critical temperature goes to zero, the gap disappears, and the system behaves as a metal.

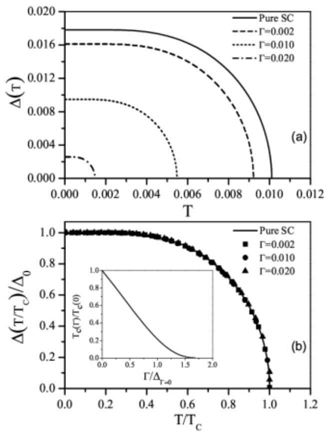

Figure 5: (a) $\Delta(T)$ as a function of T for $\varepsilon_d = -0.2$, $U = 0.1$, $V_{sc} = -0.15$ and different values of Γ. (b) Universal behavior of $\dfrac{\Delta(T)}{\Delta_0}$ with Γ In the insert, the critical temperature decreases and goes to zero as $\Gamma >> \Delta(\Gamma=0)$.

5. CONCLUSION

We studied a magnetic impurity embedded in a superconductor. The magnetic impurity breaks the electron-hole symmetry, as was shown by the asymmetry of the boundary between the magnetic and non-magnetic regimes, for various values of Δ_0. The ground state of the impurity is magnetic for Δ_0 in the interval between $\left|\varepsilon_d + U\langle n_{d\uparrow}\rangle\right| \leq \Delta_0 \leq \left|\varepsilon_d + U\langle n_{d\downarrow}\rangle\right|$. The universal behavior is maintained with the inclusion of impurity, as observed in the spectrum of $\Delta(T)$ normalized by Δ_0 as a function of T/Tc for different values of U and Γ. The gap decreases with the increase in Γ and finally disappears recovering the behavior of a metal.

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