Solvable model for an impurity spin coupled to a one-dimensional superconductor

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A solvable model for a magnetic impurity in a one-dimensional superconductor is proposed. The model consists of the impurity spin coupled to the edge of a quantum wire. The electron gas in the wire is dominated by attractive mutual interactions and forms a gapped state with a short-range superconducting order. In a restricted (but nontrivial) region of parameters, the model is solved by means of bosonization methods. The spectrum and thermodynamic functions are calculated. [S0163-1829(96)01846-2]

I. INTRODUCTION

Since the pioneering paper by Abrikosov and Gor'kov[1] and the discovery of the Kondo effect,[2] the problem of magnetic impurities is a superconductor has been extensively discussed in the literature. Apart from conventional materials, this problem is of interest for high-T_c and heavy fermion superconductors. It was studied for classical impurity spins,[3] approached by perturbative methods,[4] by means of various decoupling schemes,[5,6] and by numerical methods.[7] Yet, even for the case of a single impurity, the physics has not been completely understood, because of the complexity of local dynamic correlations in superconductors. Below the superconducting transition temperature, the conduction electrons density of states is removed from the vicinity of the Fermi level. One might think that there are, therefore, no infrared divergences associates with spin-flip processes—hence no Kondo effect. That would certainly be true for a rigid-band insulator. In the superconductor the situation is more complicated, since the condensate wave function needs to be relaxed to a chosen impurity spin direction. Upon lowering the temperature, we are dealing with a competition of the two infrared effects: the Kondo effect and the building up of the superconducting state. Thus, the interplay of the Kondo effect with the superconducting ordering is, by nature, a crossover phenomenon. For this kind of phenomena exact solutions are particularly useful.

In this paper such an exactly solvable model is proposed. Normally, solvability requires considerable simplifications and/or modifications of realistic models. Though the model described below is not free of these disadvantages it still captures some generic features of a realistic situation. Namely, I consider an impurity spin, $\vec{\sigma}$, coupled to the edge of an interacting one-dimensional (1D) electron gas (quantum wire). The electron-electron interaction is assumed to be attractive thus resulting in what is called a superconducting phase (a phase characterized by gapped spin excitations spectrum and enhanced pairing correlations, though without a long-range superconducting order.[8]) There is an exact solution for this phase devised by Luther and Emery applying bosonization methods,[9] which still goes through in the case of systems with boundaries.[10] On the other hand, there is a bosonization solution of the Kondo problem at the Toulouse limit.[11] It is shown in what follows that the two solutions, the Luther-Emery solution and the Toulouse limit solution, can be combined.[12] Hence the exactly solvable model for the magnetic impurity in the superconductor. Additionally, in response to a recent progress in the nanofabrication technology, the problem of a magnetic impurity in quantum wires attracted considerable attention[13,10] but it has been so far only studied for repulsive bulk interactions.

The layout of the paper is as follows. In Sec. II the model is formulated. The bosonization technique for an isolated semi-infinite electron system is highlighted. The exchange coupling is studied in Sec. III, where it is shown that the model can be refermionized on the Luther-Emery line and then exactly solved in the Toulouse limit. The spectrum and the free energy are found.

II. MODEL AND BOSONIZATION

The proposed model describes the impurity spin situated at the edge of a quantum wire. Thus, the Hamiltonian of the model consists of two parts:

$$H = H_W + H_K .$$

Here

$$H_K = I \sum_{s,s'} \vec{\sigma} \psi_s^\dagger(0) \vec{\tau}_{ss'} \psi_{s'}(0) \tag{1}$$

is the exchange coupling of the impurity spin to conduction electrons, $\psi_s(0)$, at the edge of the wire ($\vec{\tau}$ being Pauli matrices, $s = \uparrow, \downarrow$), and

$$H_W = H_{\mathrm{kin}} + H_{\mathrm{int}},$$

where the first term represents the kinetic energy,

$$H_{\mathrm{kin}} = \sum_s \int_0^\infty dx \, \psi_s^\dagger(x) \varepsilon(-i\partial_x) \psi_s(x), \tag{2}$$

of conduction electrons in a semi-infinite wire ($0 < x < \infty$), $\varepsilon(k)$ being the dispersion relation, and the second term, H_{int}, is responsible for electron-electron interactions. This term will be specified shortly.

Since the system is semi-infinite, the momentum k takes only positive values and the single-particle eigenstates of Eq.

(2) are standing waves. Being interested in the low-energy properties of the system one linearizes the spectrum in a standard manner,

$$\varepsilon(k) \simeq v_F(k-k_F),$$

where k_F is the Fermi momentum and v_F is the Fermi velocity, and defines slowly varying right- and left-moving fields:

$$\psi_s(x)=\int_0^\infty \frac{dk}{\pi}\sin(kx)c_{sk}=e^{ik_Fx}\psi_{sR}(x)+e^{-ik_Fx}\psi_{sL}(x), \tag{3}$$

where the operators c_{sk}, conventionally normalized as $\{c_{sk}^\dagger, c_{s'k'}^\dagger\}=2\pi\delta_{ss'}\delta(k-k')$, create electron states with the spin s and momentum k, and

$$\psi_{sR}(x)=-i\int \frac{dp}{2\pi}e^{ipx}c_{s,k_F+p},$$

$$\psi_{sL}(x)=i\int \frac{dp}{2\pi}e^{-ipx}c_{s,k_F+p}. \tag{4}$$

Because the system is semi-infinite, these fields are not independent, but satisfy

$$\psi_{sL}(x)=-\psi_{sR}(-x). \tag{5}$$

The formal trick behind the open boundary bosonization of Ref. 10 is to let the variable x take all values on the real axes, $-\infty<x<\infty$, and regard Eq. (5) as the definition of the right moving field $\psi_{sR}(x)$ for the negative values of x. The Hamiltonian should then be expressed in terms of this right-moving field only, so the kinetic energy takes the form

$$H_0=v_F\sum_s \int_{-\infty}^{\infty} dx\,\psi_{sR}^\dagger(x)(-i\partial_x)\psi_{sR}^\dagger(x).$$

The advantage of treating $\psi_{sR}(x)$ as a usual chiral field is that it can now be straightforwardly bosonized:

$$\psi_{sR}(x)=\frac{1}{\sqrt{2\pi\alpha}}e^{i\phi_s(x)}, \tag{6}$$

where α is a high-energy cutoff and the phase fields $\phi_s(x)$ are defined by

$$\phi_s(x)=\int_0^\infty \frac{dq}{\sqrt{2\pi q}}e^{iqx-\alpha q/2}b_{sq}+\text{H.c.}, \tag{7}$$

b_{sq} being canonical Bose operators, $[b_{sq}^\dagger, b_{s'q'}^\dagger]=2\pi\delta_{ss'}\delta(q-q')$. Equations (6) and (7) are totally standard; see Ref. 8 for the discussion of the conventional bosonization. [Strictly speaking, one should assign Majorana fermions—statistical factors—to each field Eq. (6), in order to assure correct anticommutation relations for different spin electron fields. These factors, however, cancel out in the following calculations, so I have dropped them to simplify the formulas.] In terms of the phase fields Eq. (7), the density of right-moving electrons is given by

$$\rho_{sR}(x)=\frac{1}{2\pi}\partial_x\phi_s(x), \tag{8}$$

whereas

$$\rho_{sL}(-x)=\rho_{sR}(x), \tag{9}$$

and the kinetic energy is simply

$$H_0=\sum_s \int_0^\infty \frac{dq}{2\pi}q b_{sq}^\dagger b_{sq}. \tag{10}$$

For further usage, the bosonic variables corresponding to the charge and spin excitations are defined as

$$b_{\rho(\sigma)q}=\frac{1}{\sqrt{2}}(b_{\uparrow q}\pm b_{\downarrow q}),$$

and analogously for $\rho_{\rho(\sigma)}(x)$ and $\phi_{\rho(\sigma)}(x)$.

Equations (8)–(10) complete the bosonization of the noninteracting semi-infinite electron system. As in the case of the infinite system,[8] the interaction part of the Hamiltonian,

$$H_{\text{int}}=H_q+H_{bs},$$

contains different processes—those which are quadratic in the electron densities:

$$\begin{aligned} H_q=&\frac{g_{\rho(\sigma)}}{2}\int_0^\infty dx[\rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)R}(x)+\rho_{\rho(\sigma)L}(x)\rho_{\rho(\sigma)L}(x)]\\ &+\tilde{g}_{\rho(\sigma)}\int_0^\infty dx\,\rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)L}(x)\\ =&\frac{g_{\rho(\sigma)}}{2}\int_{-\infty}^\infty dx\,\rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)R}(x)\\ &+\frac{1}{2}\tilde{g}_{\rho(\sigma)}\int_{-\infty}^\infty dx\,\rho_{\rho(\sigma)R}(x)\rho_{\rho(\sigma)R}(-x), \end{aligned} \tag{11}$$

and those which are not:

$$\begin{aligned} H_{bs}=&\frac{g_{bs}}{2}\sum_s \int_0^\infty dx[\psi_{sR}^\dagger(x)\psi_{sL}(x)\psi_{\bar{s}L}^\dagger(x)\psi_{\bar{s}R}(x)\\ &+(R\to L)]\\ =&\frac{g_{bs}}{2}\sum_s \int_{-\infty}^\infty dx\,\psi_{sR}^\dagger(x)\psi_{sR}(-x)\psi_{\bar{s}R}^\dagger(-x)\psi_{\bar{s}R}(x). \end{aligned} \tag{12}$$

The latter are referred to in the literature as the spin-backscattering processes.[8] ($g_{\rho(\sigma)}$, $\tilde{g}_{\rho(\sigma)}$, g_{bs} stand for the interaction constants.) The former, even though nonlocal in terms of the right-moving electron densities, can be brought to a diagonal form by a canonical (Bogoliubov) transformation:

$$U_0(H_0+H_q)U_0^\dagger=\sum_\nu H_0[\phi_\nu]=\sum_\nu \frac{v_\nu}{4\pi}\int_{-\infty}^\infty dx[\partial_x\phi_\nu(x)]^2, \tag{13}$$

where the charge and spin sound velocities are given by

$$v_\nu = \frac{v_\nu^0}{\cosh(2\varphi_\nu)}$$

with

$$v^0_{\rho(\sigma)} = v_F + \frac{g_{\rho(\sigma)}}{2\pi}$$

and Bogoliubov's rotation angles

$$\tanh(2\varphi_\nu) = -\frac{\tilde{g}_\nu}{2\pi v_\nu^0}. \tag{14}$$

The unitary operator U_0 is of the form

$$U_0 = \exp\left\{ \sum_\nu \int_0^\infty \frac{dq}{4\pi} \varphi_\nu (b^\dagger_{\nu q} b^\dagger_{\nu q} - b_{\nu q} b_{\nu q}) \right\}. \tag{15}$$

Applying this transformation to the electron field operator, one arrives at

$$U_0 \psi_s(x) U_0^\dagger = \frac{1}{\sqrt{2\pi\alpha}} \exp\left\{ i k_F x + \frac{i}{\sqrt{2}} \sum_\nu \varepsilon_{\nu s} [c_\nu \phi_\nu(x) - s_\nu \phi_\nu(-x)] \right\} - (x \to -x), \tag{16}$$

where $\varepsilon_{\nu s}$ is $+1$ unless $s=\downarrow$ and $\nu=\sigma$, when its value is -1, and

$$c_\nu = \cosh(\varphi_\nu), \quad s_\nu = \sinh(\varphi_\nu)$$

are related to the conventional spin and charge exponents

$$K_\nu = \exp(2\varphi_\nu).$$

The conduction electron Hamiltonian thus takes the form

$$H_W = H_\rho + H_\sigma,$$

with $H_\rho = H_0[\phi_\rho]$. The charge degrees of freedom decouple, whereas the spin ones are described by

$$H_\sigma = H_0[\phi_\sigma] + H_{bs}.$$

In terms of bosonic fields, the spin-backscattering interaction reads

$$H_{bs} = \frac{g_{bs}}{(2\pi\alpha)^2} \int_{-\infty}^{\infty} dx e^{-i\sqrt{2K_\sigma}\phi_\sigma(x)} e^{i\sqrt{2K_\sigma}\phi_\sigma(-x)} e^{-i\pi K_\sigma s(x)}, \tag{17}$$

$s(x)$ being the sign function.

For $K_\sigma > 1$ the operator Eq. (17) is irrelevant—it scales to the weak coupling under the renormalization-group transformations. This paper deals with the opposite case of $K_\sigma < 1$ when the operator Eq. (17) is relevant and generates the spin gap. The singlet pairing fluctuations are then dominating the bulk properties if $K_\rho > 1$.[14]

So far I have outlined the particular bosonization scheme for semi-infinite electron systems; for more details the reader is referred to Ref. 10. The impurity spin interacts with the electron system via the Kondo coupling Eq. (1); this coupling is discussed in the following section.

III. REFERMIONIZATION, RESULTS, AND DISCUSSION

Utilizing the bosonized expression for the electron field operator Eq. (16), one obtains the exchange coupling Eq. (1) in the form

$$H_K = \frac{J_\perp}{4\pi\alpha}[\sigma_+ e^{i\sqrt{2/K_\sigma}\phi_\sigma(0)} + \text{H.c.}] + \frac{J_z \sigma_z \nabla \phi_\sigma(0)}{2\sqrt{2K_\sigma}\pi}, \tag{18}$$

where $J_\perp$ and J_z are the effective exchange couplings of the bosonized version of the model.[15]

I now focus on the Luther-Emery line, $K_\sigma = 1/2$. Then, a standard unitary transformation[11]

$$U = \exp[i\sigma_z \phi_\sigma(0)]$$

brings the Hamiltonian to a form containing only simple exponentials of ϕ_σ (while H_{bs} can be shown to stay invariant under U):

$$\tilde{H} = U(H_\sigma + H_K)U^\dagger = H_0[\phi_\sigma] - \frac{i g_{bs}}{(2\pi\alpha)^2}\int_{-\infty}^{\infty} s(x) dx e^{-i\phi_\sigma(x)} e^{i\phi_\sigma(-x)} + \frac{J_\perp}{4\pi\alpha}[\sigma_+ e^{i\phi_\sigma(0)} + \text{H.c.}] + \frac{\lambda}{2\pi}\sigma_z \nabla \phi_\sigma(0),$$

where $\lambda = J_z - \pi v_F$.

It is now convenient to refermionize the problem. Defining new Fermi operators

$$\psi_\sigma(x) = \frac{1}{\sqrt{2\pi\alpha}} \exp[i\phi_\sigma(x)] \quad \text{and} \quad d = \sigma_-,$$

one arrives at

$$\tilde{H} = \tilde{H}_\sigma + \tilde{H}_K,$$

with

$$\tilde{H}_\sigma = v_\sigma \int_{-\infty}^{\infty} dx [\psi^\dagger_\sigma(x)(-i\partial_x)\psi_\sigma(x) - i\Delta s(x) \psi^\dagger_\sigma(x)\psi_\sigma(-x)], \tag{19}$$

where

$$\Delta = \frac{g_{bs}}{2\pi\alpha}$$

is the gap in the spin-excitation spectrum, and

$$\tilde{H}_K = \frac{J_\perp}{2\sqrt{2\pi\alpha}}[d^\dagger \psi_\sigma(0) + \text{H.c.}] + \lambda \psi^\dagger_\sigma(0)\psi_\sigma(0)\left(d^\dagger d - \frac{1}{2}\right). \tag{20}$$

The value $\lambda = 0$ defines the Toulouse limit at which the Hamiltonian is quadratic in the new Fermi operators and the problem can therefore be exactly solved.

It is instructive to first diagonalize the bulk Hamiltonian:

$$\widetilde{H}_\sigma = \sum_\mu \int_0^\infty \frac{dp}{2\pi} \mu \epsilon_p c_{p\mu}^\dagger c_{p\mu}, \tag{21}$$

where

$$\epsilon_p = \sqrt{(v_\sigma p)^2 + \Delta^2}$$

is the usual gapped spectrum and $\mu = \pm 1$. This can be achieved by means of the transformation:

$$\psi_\sigma(x) = \chi_0(x) c_0 + \sum_\mu \int_0^\infty \frac{dp}{2\pi} \chi_{p\mu}(x) c_{p\mu}, \tag{22}$$

where $c_{p\mu}$ and c_0 are Fermi operators, and χ's are normalized wave functions. For Eq. (22) to diagonalize Eq. (19), these wave functions should satisfy a (nonlocal) Schrödinger-type equation

$$\epsilon \chi(x) = -i v_\sigma \partial_x \chi(x) - i \Delta s(x) \chi(x). \tag{23}$$

Notice that the operator c_0 in Eq. (22) creates a zero-energy state, which corresponds to the solution of Eq. (23) localized at the edge of the system:

$$\chi_0(x) = \sqrt{\frac{\Delta}{v_\sigma}} e^{-\Delta |x|/v_\sigma}. \tag{24}$$

The existence of such localized states has been predicted in Ref. 10; it derives from the particle-hole symmetry of the problem. The scattering wave functions $\chi_{p\mu}(x)$ form, together with Eq. (24), the complete orthogonal set of solutions to Eq. (23). The full x dependence of the functions $\chi_{p\mu}(x)$ is not of an immediate interest, so I only quote, for further usage, their $x=0$ values:

$$\chi_{p\mu}(0) = \frac{2\Delta(v_\sigma p)}{(\mu \epsilon_p + v_\sigma p + i\Delta)\sqrt{(\mu \epsilon_p - v_\sigma p)^2 + \Delta^2}}. \tag{25}$$

Upon substituting Eq. (22) into Eq. (20), the exchange part of the Hamiltonian becomes a resonant-level type term:

$$\widetilde{H} = \sum_\mu \int_0^\infty \frac{dp}{2\pi} \mu \epsilon_p c_{p\mu}^\dagger c_{p\mu} + \frac{J_\perp}{2\sqrt{2\pi\alpha}} \times \left\{ d^\dagger \left[\chi_0(0) c_0 + \sum_\mu \int_0^\infty \frac{dp}{2\pi} \chi_{p\mu}(0) c_{p\mu} \right] + \text{H.c.} \right\},$$

($\lambda = 0$ is set in the above). Green's functions can easily be found in the Toulouse limit. (See, e.g., Ref. 11 for the diagonalization of the resonant level model.) So, the impurity Green function,

$$D(t) = -i \langle T\{d(t) d^\dagger(0)\}\rangle,$$

takes (in the frequency domain) the form

$$D(i\omega_n) = \frac{1}{i\omega_n - \Lambda(i\omega_n)}.$$

Here ω_n are fermionic Matsubara frequencies and the characteristic function Λ, which defines the single-particle excitation spectrum of the system, is given by

$$\Lambda(i\omega_n) = \frac{J_\perp^2}{8\pi\alpha} \left\{ \frac{|\chi_0(0)|^2}{i\omega_n} + \sum_\mu \int_0^\infty \frac{dp}{2\pi} \frac{|\chi_{p\mu}(0)|^2}{i\omega_n - \mu \epsilon_p} \right\}. \tag{26}$$

Substituting Eq. (25) into Eq. (26) and taking the momentum integral, one finds a rather simple expression for the characteristic function:

$$\Lambda(i\omega_n) = \Gamma \frac{\sqrt{\omega_n^2 + \Delta^2} + \Delta^2}{i\omega_n}, \tag{27}$$

where the resonance width, Γ, is defined as

$$\Gamma = \frac{J_\perp^2}{16\pi\alpha v_\sigma}.$$

Notice that there can be bound states which are determined from the characteristic equation

$$\omega = \Lambda(\omega). \tag{28}$$

The bound states, $\omega = \pm \omega_b$, only exist for weak coupling $\Gamma < \Delta$. Due to the remarkably simple result Eq. (27) for the characteristic function, the solution to Eq. (28) can be explicitly found:

$$\omega_b = \sqrt{2\Delta\Gamma - \Gamma^2}.$$

At $\Gamma = \Delta$ the bound states verge on the edge of the continuum spectrum and disappear for larger couplings. Physically, these bound states are due to the hybridization of the resonant level and the zero-energy state localized at the boundary of the wire. Put another way, the latter is composed from the spin degrees of freedoms; it may be interpreted as a "bound spinon." Due to the exchange coupling this bound spinon forms a singlet with the impurity spin. Notice that this scenario is completely different from a usual interpretation of bound states in superconductors based on the BCS divergency of the density of states. One might expect that this divergency should lead to additional bound states, which would be close in the energy to the gap (for the weak-coupling case). This is, however, incorrect. The reason is that, though the density of states indeed diverges, this divergency is compensated by vanishing of the hybridization matrix elements (coherence factors): $|\chi_{p\mu}(0)|^2 \sim p^2$ at small p^2.

The impurity contribution to the free energy can be calculated in a standard way by averaging H_K and integrating over the coupling constant:

$$\delta F_{\text{imp}}(T) = \int_0^1 dg \langle \widetilde{H}_K \rangle_g = \int_0^1 dg T \sum_{\omega_n} \frac{\Gamma(\sqrt{\omega_n^2 + \Delta^2} + \Delta)}{\omega_n^2 + g\Gamma(\sqrt{\omega_n^2 + \Delta^2} + \Delta)}.$$

Representing in a standard manner the sum over the Matsubara frequencies as a contour integral, shifting the contour of integration to infinity, and explicitly computing the integral over the coupling constant g, one finds ($\Gamma < \Delta$)

$$\delta F_{\mathrm{imp}}(T)=-2T\ln\left[\cosh\left(\frac{\omega_b}{2T}\right)\right]+\int_{\Delta}^{v_\sigma/\alpha}\frac{d\omega}{\pi}\tanh\left(\frac{\omega}{2T}\right)\arctan\left(\frac{\Gamma\sqrt{\omega^2-\Delta^2}}{\omega^2+\Gamma\Delta-2\Delta^2}\right). \tag{29}$$

The first term in Eq. (29) represents the contribution of the bound states, whereas the second one is due to the excitations above the gap. At low temperatures, the bound state contribution dominates the thermodynamics. So, the impurity specific heat is

$$C_{\mathrm{imp}}(T)\simeq 2(\omega_b/T)^2 e^{-\omega_b/T}.$$

To conclude, a model describing an impurity spin coupled to a 1D superconductor is proposed in this paper. It is shown that the solvable limit for the spin-backscattering interaction (responsible for the spin gap) in the bulk and the solvable limit for the spin impurity in a normal metal can be matched to describe the interplay of the Kondo effect and the superconductivity in one dimension.

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[15] That means that if the exchange coupling in Eq. (1) is taken as nonlocal, $I=I(x)$ (though still confined to the vicinity of the edge of the wire), then the effective coupling in Eq. (18) is calculated as $J=(2k_F)^2\int dx x^2 I(x)$.