

Superconductivity and antiferromagnetism: Hybridization impurities in a two-band spin-gapped electron system

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We present the exact solution of a one-dimensional model of a spin-gapped correlated electron system with hybridization impurities exhibiting both magnetic and mixed-valence properties. The host supports superconducting fluctuations with a spin gap. The localized electrons create a band of antiferromagnetic spin excitations *inside the gap* for concentrations x of the impurities below some critical value x_c . When $x = x_c$, the spin gap closes and a ferrimagnetic phase appears. This is an example of an exactly solvable model with coexisting superconducting and antiferromagnetic fluctuations, which in addition supports a quantum phase transition to a (compensated) ferrimagnetic phase. We discuss the possible relevance of our results for experimental systems, in particular the U-based heavy fermion materials. [S0163-1829(99)01345-4]

There has recently been a renewed interest in the role of impurities in spin-gapped electron systems. Examples include magnetic or mixed-valent impurities in ordinary BCS-like superconductors,¹ heavy fermion alloys,² and underdoped high- T_c cuprates,³ as well as disorder driven quantum phase transitions in superconducting thin films.⁴ While many effects from impurities in these systems are well understood, such as the pair breaking in an ordinary superconductor due to the violation of time-reversal symmetry by magnetic impurities,⁵ others remain to be clarified—the coexistence of superconductivity and antiferromagnetism in certain U-based heavy fermion compounds^{6,7} being a prime example.

In this paper we study an exactly solvable model of a finite concentration of hybridization impurities in a one-dimensional (1D) multiband correlated electron host with a spin gap. Our choice of a multiband model is in part inspired by recent experiments on the heavy fermion compound $U_{1-x}\text{Th}_x\text{Be}_{13}$, which show a scattering of electrons off impurities in two channels.⁸ Equally important, multiband electron models are intrinsically interesting, in particular when allowing for interactions with defects, when they generically exhibit non-Fermi liquid behavior.⁹ Here we address the question how this behavior gets influenced by electron correlations in a spin-gapped host.

The exact solution of our model—to be defined below—reveals several remarkable properties. Most interestingly, for a finite concentration of impurities, too weak to destroy the spin gap in the host, there is an impurity-induced band of antiferromagnetic spin excitations living *inside the gap*, suggestive of a coexistence of superconducting and antiferromagnetic fluctuations. As the impurity concentration increases, the gap closes, signaling a quantum phase transition to a fully compensated ferrimagnetic phase. Since our model is exactly solvable, with antiferromagnetic fluctuations of localized electrons *and* superconducting fluctuations of itinerant electrons taken into account simultaneously, we can per-

form a fully nonperturbative analysis of the relevant physics.

As Hamiltonian for the electron host we take¹⁰

$$\mathcal{H}_{\text{host}} = \int dx \left(-\psi_{m\sigma}^\dagger(x) \partial_x^2 \psi_{m\sigma}(x) + c \int dx' \delta(x-x') \right. \\ \left. \times \psi_{m\sigma}^\dagger(x) \psi_{m'\sigma'}^\dagger(x') \psi_{m'\sigma}(x') \psi_{m\sigma}(x) \right), \quad (1)$$

where the electron fields $\psi_{m\sigma}$ carry band $m = 1, 2$, and spin $\sigma = \pm 1/2$ indices, with repeated indices in Eq. (1) summed over. The screened electron-electron interaction is here simulated by a local exchange potential with strength $c > 0$, with electrons in the same band (and opposite spin) experiencing an attraction while electrons in different bands (with the same spin) repel each other. This interaction, which is integrable,¹⁰ produces Cooper-like singlet pairing bound states at any temperature, but since the model is one-dimensional there is no global phase coherence between pairs, and hence no long-range order. However, the pairing implies a critical field H_c at zero temperature below which there is no magnetic response, reminiscent of the Meissner effect (although there is, of course, no manifest Meissner effect in the system).

Next, we introduce a Hamiltonian term describing a (band-neutral) hybridization of itinerant electrons with impurities, with N_i counting their number:¹¹

$$\mathcal{H}_{\text{imp-el}} = \sum_j^{N_i} \sum_{m,\sigma,M} \left[\frac{\theta}{4} |SMm\rangle \langle SMm| \right. \\ \left. + \sum_{M'} A_{M,M'} (\psi_{m\sigma}^\dagger(x_j) |SMm\rangle \langle S'M'm| + \text{H.c.}) \right]. \quad (2)$$

Here $|SMm\rangle$ denotes an impurity state with spin S and projection M ($S' = S - 1/2 \geq 0$) satisfying the constraint $\sum_{M'} |S'M'm\rangle \langle S'M'm| + \sum_M |SMm\rangle \langle SMm| = 1$, θ measures the off-resonance shift of the impurity from the Fermi level, $A_{M,M'}^2 = -2Sc(M\sigma|M')^2$, with the Clebsch-Gordan coefficients selecting states with $M' = M + \sigma$ as $(M\sigma|M') \equiv (S\frac{1}{2}; M\sigma|S(S-\frac{1}{2}); \frac{1}{2}M')$. Each impurity can temporarily absorb the spin of one itinerant electron to form an effective spin $(S-\frac{1}{2})$, i.e., it exists in two spin configurations.¹¹ Note that the spin sector of \mathcal{H}_{imp-el} corresponds to a local antiferromagnetic exchange $2c\mathbf{S}_j \cdot \boldsymbol{\tau}(x)$ between the impurity spin \mathbf{S}_j and the electron-spin density $\boldsymbol{\tau}(x)$. The two-particle scattering matrices of the model in Eqs. (1) and (2) satisfy the Yang-Baxter relations, thus providing for complete integrability.¹² The model remains integrable for any distributions of S_j and θ_j , but for simplicity we here focus on the case where all impurities carry the same spin, with an equal number of positive and negative shifts $\pm\theta$.

The energies and eigenstates of the model are parameterized by three sets of rapidities: charge rapidities $\{k_j\}_{j=1}^N$ (with N the number of itinerant electrons), spin rapidities $\{\lambda_\alpha\}_{\alpha=1}^M$ (with M the number of ‘‘down spins’’), and band rapidities $\{\xi_\beta\}_{\beta=1}^n$ (with n the number of electrons in the $m=1$ band). [Note that a crystalline field will lift the degeneracy in Eq. (1), with the bands becoming unequally populated.] Each eigenstate corresponds to a solution of the Bethe Ansatz equations, here obtained on a periodic interval of length L :

$$e^{ik_j L} = \prod_{f=1}^M e_1(k_j - \lambda_f) \prod_{q=1}^n e_1^{-1}(k_j - \xi_q),$$

$$\prod_{\pm} e_{2S}^{N_i/2}(\lambda_\alpha \pm \theta) \prod_{j=1}^N e_1(\lambda_\alpha - k_j) = - \prod_{f=1}^M e_2(\lambda_\alpha - \lambda_f),$$

$$\prod_{j=1}^N e_1(\xi_\beta - k_j) = - \prod_{\gamma=1}^n e_2(\xi_\beta - \xi_\gamma), \quad (3)$$

where $e_n(y) = (2y - inc)/(2y + inc)$, $j = 1, \dots, N$, $\alpha = 1, \dots, M$, and $\beta = 1, \dots, n$, and with the energy given by $E = \sum_{j=1}^N k_j^2$. To model a Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in a real system we add an antiferromagnetic coupling between neighboring impurities.¹³ While Eq. (3) is insensitive to this addition, it does cause a shift of the energy: $E \rightarrow E - 2\pi x \sum_{\alpha}^N a_{2S}(\lambda_\alpha - \theta)$, where $x = N_i/L$ is the impurity concentration, and $a_n(y)$ is the Fourier transform of $\exp(-n|pc|/2)$. The structure of the impurity-impurity interaction is similar to that of Eqs. (1) and (2), but with impurity state operators replacing electron fields. In the case when all electrons are localized, it collapses to the well-known Takhtajan-Babujian spin-exchange Hamiltonian.¹⁴ The fact that energies and eigenstates are blind to the spatial distribution of impurities is an artifact of integrability. One should note, however, that real systems, including certain heavy fermion alloys and doped superconductors,^{2,15} often exhibit a large quasidegeneracy of the states as a function of the distribution of impurities for stoichiometric compounds. Seen from this perspective, the exact degeneracy in our model can be turned to an advantage.

Within the framework of the standard ‘‘string hypothesis,’’¹² the rapidities satisfying Eq. (3) fall into four classes in the thermodynamic limit (with continuous distributions): (i) real charge rapidities of unbound itinerant electrons; (ii) pairs of complex conjugated charge rapidities representing Cooper-like singlet spin pairs; (iii) spin bound states (λ strings); and (iv) interband bound states (ξ strings). Since in 1D the most interesting behavior appears in the ground state (corresponding to the low-temperature phases of higher-dimensional analogs), we focus on this in the following.

The ground state is obtained by filling up the Dirac seas of the low-lying excitations, i.e., by populating all possible states with negative energies. An analysis shows that when $x=0$, only unbound electrons, Cooper-like spin-singlet pairs, and interband strings of lengths 1 and 2 have negative energies, and thus make up the Dirac seas defining the ground state. The introduction of a finite concentration $x \neq 0$ of hybridization impurities drastically affects the ground state (and in fact all states that are effectively present at a temperature $T \ll H$, in the case that an external magnetic field H is applied): The spin levels of the localized electrons now form a low-lying *band of spin excitations inside the spin gap of the host*, given by spin strings of length $2S$. To see how this comes about, we study the integral equations for the dressed energies of the excitations (where the ‘‘dressing’’ is due to interactions¹²), which, in the case of degenerate bands (zero band splitting) can be done analytically. We first integrate the equations for the dressed energies of the interband excitations, as these do not feel the presence of the impurities. Then the set of equations for the dressed energies of unbound electrons (ε), Cooper-like pairs (ψ), and spin $2S$ strings (ϕ_{2S}) has the form:

$$(1 - G_1) * \varepsilon = k^2 - \mu - \frac{H}{2} - G_0 * \psi + a_{2S} * \phi_{2S},$$

$$\psi = 2 \left(\lambda^2 - \frac{c^2}{4} - \mu \right) - G_0 * \varepsilon - x \pi \sum_{\pm} a_{2S}(\lambda \pm \theta),$$

$$W * \phi_{2S} = 2SH - xV - a_{2S} * \varepsilon, \quad (4)$$

where μ is the chemical potential, $*$ denotes the convolution over the appropriate Dirac seas, $G_n(y)$ and $W(y)$ are the Fourier transforms of $\exp(-n|pc|/2)/2 \cosh(pc/2)$ and $\coth(pc/2)[1 - \exp(-2S|pc|)]$, respectively, and $V(p) = \cos(p\theta) \coth(pc/2)[G_0(p) - G_{4S}(p)]$. As revealed by Eq. (4), for $H=0$ and for sufficiently small concentrations of the impurities, the Dirac sea of spin- $2S$ strings is filled completely. The value of the spin gap (the gap for unbound electron excitations) is the smallest energy required to depair the Cooper-like spin-singlet state. The gap renormalizes in the presence of a small finite concentration of hybridization impurities, and we find that

$$\Delta(x) = \Delta(0) - \frac{xS}{2} \sum_{\pm} \left(\int_{|\lambda| \geq Q} \frac{d\lambda \operatorname{sech}(\pi\lambda/c)}{(\lambda \pm \theta)^2 + (cS)^2} + \frac{cS}{(Q \pm \theta)^2 + (cS)^2} [(2/\pi) \tan^{-1} \sinh(\pi Q/c) - 1] \right), \quad (5)$$

where Q is the Fermi level for paired electrons. The spin gap decreases due to localized electrons (with their number given by $(N_i/\pi)\Sigma_{\pm}\tan^{-1}[(Q\pm\theta)/cS]$) and closes at a critical concentration x_c [i.e., $\Delta(x_c)=0$]. As seen from Eq. (5), the smallest value of x_c is obtained when $S=1/2$, with x_c increasing with increasing S . As also follows from Eq. (5), the gap persists for larger impurity concentrations when the number of paired electrons ($\propto Q$) is large. However, and this is important, there are no additional unbound electron excitations appearing when the gap is present (i.e., for $x < x_c$). Hence, the presence of the hybridization impurities does not lead to a pair breaking for these concentrations, in contrast to the suppression of superconductivity in ordinary BCS-like superconductors.⁵ The presence of the spin 2S strings in the gapped phase indeed suggests a coexistence of antiferromagnetic and superconducting fluctuations. It is important to note that the charge and magnetic subsystems are effectively disconnected for $x < x_c$, as revealed by Eq. (4): The low-energy (conformal) limit corresponds to a direct sum of free bosons (hard-core pairs) with scaling dimension $\eta=1$, and antiferromagnetic spin strings with $\eta=r(r+2)/4(S+1)$, $r=1,2,\dots$ (spinons with the minimal $\eta=1/2$ when $S=1/2$).¹⁶

The gap, and hence the energies of unbound electrons, may become negative when $x > x_c$. Thus, a Fermi sea for unbound electron excitations (with $k_F \propto \sqrt{x-x_c}$) opens up in the absence of a magnetic field, signaling a quantum phase transition. For $H=0$ there are no holes in the distribution of spin 2S strings, and hence the total magnetization of the system remains zero. The appearance of itinerant electrons correlates with the number of localized electrons, with both particle numbers scaling with $\sqrt{x-x_c}$, thus producing a compensated ferrimagnetic phase of the total system. (Note that there are two kinds of magnetic excitations in the system: spin 2S strings and unbound electrons which carry spin 1/2.) This compensating effect is due to the RKKY type interactions between the impurities [which were absent in the attractive Hubbard model with hybridization impurities recently studied in (Ref. 13), where instead a ferromagnetic phase appears]. However, Cooper-like pairs are still present for $x > x_c$, reminiscent of gapless superconductivity, where the gap closes before superconductivity is destroyed.⁵ We here note that this is different from the supersymmetric $t-J$ model with hybridization impurities,¹³ since for that model all low-lying excitations are gapless also with no impurities present.

Let us briefly discuss the model in the presence of a magnetic field H . For H smaller than some critical field $H_c(x)$, the spin gap persists for $x < x_c$, and there are no unbound electrons in the system. The critical field $H_c(x)$ decreases with increasing concentration x and vanishes when x approaches x_c . Thus, as expected, the spin gap decreases with the growth of a magnetic field and the concentration of impurities. The critical line separating the gapless and gapped (ferrimagnetic) phases manifests itself in the van Hove singularity of the opening of the band of unbound electron excitations. The critical behavior at the quantum phase transition point $x=x_c, H=0$ also shows up in the scaling dimensions. Since an additional band of unbound electron excitations now appears, the dressed charge matrix¹² gets enlarged from 2×2 to 3×3 with the off-diagonal compo-

nents proportional to $\sqrt{x-x_c}$. The emergence of 2S-spin strings when $S > 1/2$, together with the fact that their bandwidth is relatively narrow [$\propto x$, see Eq. (4)], for this case implies the appearance of an additional critical magnetic field H_{c1} at which the band of spin strings becomes empty (provided that the concentration of impurities is finite, since for $x=0$ $H_{c1}=H_c$). In addition, there is the possibility of an additional quantum phase transition for $H=0$ at $x_{c1} > x_c$, where the band of spin strings may become empty, with the impurities spin polarized, analogous to the case of the attractive Hubbard chain with noninteracting hybridization impurities.¹³ The additional band (of spin strings) increases the effective mass of the electrons, producing a larger coefficient for the low-temperature specific heat ($\propto T$). In contrast, at the critical lines, the van Hove singularities of empty bands (of unbound electrons or spin strings) produce a \sqrt{T} behavior of the specific heat.

To summarize, in this paper we have studied an exactly solvable model of spin- S hybridization impurities embedded into a two-band correlated electron host with a spin gap. A finite fraction of the electrons localize, producing a mixed valence of the impurities. These magnetic impurities interact, giving rise to a band of low-lying antiferromagnetic excitations appearing inside the spin gap of unbound conduction electrons. The simultaneous presence of Cooper pairs and spin-density waves in the spin gap suggests that superconducting and antiferromagnetic fluctuations in fact coexist in this system. This is an important result, more so since it is obtained by an exact method taking *all* possible fluctuations into account, with no *a priori* assumption of a (local) symmetry breaking. We predict that the spin gap closes for concentrations of impurities above some critical value, at which unbound itinerant (and localized) electrons appear. However, the total magnetization of the system remains zero for $H=0$, implying a quantum phase transition to a compensated ferrimagnetic phase. A nonzero magnetic field less than the critical field H_c does not destroy the coexistence of superconducting and antiferromagnetic fluctuations (provided that also the impurity concentration is smaller than the critical concentration x_c).

Finally, let us briefly discuss the possible relevance of our results for real multiband systems with hybridization impurities. It is clear that the one-dimensionality of the model—required for its exact solvability—introduces features not seen in higher dimensions. In particular, spin-charge separation, implying no response of the paired system to an external field coupled to the current operator, is believed to be an intrinsically one-dimensional phenomenon. On the other hand, our model shares a number of important characteristics with real materials such as the U-based heavy fermion compounds, the alloy $U_{1-x}\text{Th}_x\text{Be}_{13}$ (Refs. 6–8) being a case in point. Common properties include (i) an enhancement of the effective mass;¹⁷ (ii) non-Fermi-liquid behavior in the normal (nongapped) phase;¹⁹ (iii) power-law behavior of the low-temperature specific heat in the presence of a spin gap;¹⁷ (iv) scattering of the electrons off two configurations of the impurity ion;^{8,18} (v) the presence of low-lying magnetic excitations in the superconducting as well as in the normal state;¹⁹ (vi) coexistence of superconducting and antiferromagnetic fluctuations for some concentrations of magnetic impurities (U ions);^{6,7} (vii) a (ferrimagnetic) phase with a

weak ferromagnetic moment for a certain range of impurity concentrations;²⁰ and (viii) (quantum) phase transitions driven by a change of the impurity concentration^{6,7,20}. Considering these similarities, it is tempting to speculate that our microscopic model supports the phenomenological Ginzburg-Landau approach of Ref. 21 for the coexistence of superconductivity and magnetism in this class of heavy fermion alloys.²² Still, the presence of possible nodes on the Fermi surface of unbound electrons in 2D or 3D may change the picture,²³ as may the fact that in our model the mechanism for superconductivity lives outside the magnetic ions—in contrast to the conventional picture of the U-based heavy fermion superconductors. It is interesting to note that while integrability imposes certain formal restrictions on possible hybridization terms, our particular choice in Eq. (2) shares some similarities with that recently proposed for $U_{1-x}Th_xBe_{13}$ on purely phenomenological grounds.¹⁸ This

compound shows an admixture of *two* low-energy configurations of U ions: the magnetic state Γ_6 of the $5f^3$ configuration of U^{3+} and the nonmagnetic doublet Γ_3 of the $5f^2$ configuration of U^{4+} . This should be compared with the special case of $S=\frac{1}{2}$ in Eq. (2), with θ chosen to remove the degeneracy between magnetic and nonmagnetic states: $\theta = 4[E(5f^3) - E(5f^2)]$, although in our case the magnetic state is fourfold degenerate, in contrast to Ref. 18 where the magnetic state has a twofold degeneracy.

Results on the effect of random distributions of impurity parameters in spin-gapped electron systems, as well as a detailed analysis of the present model will be reported elsewhere.

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- ²²Note that the local character of the attraction for the electrons due to the exchange interaction in (1) implies a short superconducting coherence length $\xi_0 \propto \pi v_F / \Delta$, which is consistent with the relatively short coherence lengths in unconventional superconductors, as compared with the ordinary BCS-like superconductors.
- ²³These nodes may, e.g., stabilize an intermediate (spin-glass-like) phase between the antiferromagnetic and superconducting phases, as in the high- T_c cuprates.