Topological Confinement and Superconductivity

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We derive a Kondo Lattice model with a correlated conduction band from a two-band Hubbard Hamiltonian. This mapping allows us to describe the emergence of a robust pairing mechanism in a model that only contains repulsive interactions. The mechanism is due to topological confinement and results from the interplay between antiferromagnetism and delocalization. By using Density-Matrix-Renormalization-Group (DMRG) we demonstrate that this mechanism leads to dominant superconducting correlations in a 1D-system.

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The origin of unconventional superconductivity remains as one of the most important open problems of condensed matter physics. Physicists do not agree on the mechanism that pairs the electrons to form the superconducting condensate. To a very good approximation, electrons only interact via the repulsive Coulomb interaction. Consequently, as it was pointed out recently by Anderson [1], the crucial question is: “How can this repulsion between electrons be eliminated in favor of electron pair binding?” The problem becomes even more puzzling if we consider that the Coulomb interaction is bigger than the bandwidth for most of the unconventional superconductors. Then, the first challenge is to demonstrate that a “pairing force” can exist in model Hamiltonians that only contain strongly repulsive interactions. Although different pairing mechanisms have been proposed over the last twenty years, it is not always clear if those mechanisms actually work or if they are robust under the presence of long range Coulomb interactions. This is mainly due to the lack of controlled approximations for solving models of strongly interacting electrons in 2D or 3D.

Another aspect that is quite ubiquitous in unconventional superconductors is the proximity of the superconducting state to an antiferromagnetic (AFM) phase. This observation suggests that antiferromagnetic correlations are related to the pairing mechanism. However, although several “magnetic” pairing mechanisms have been proposed [2], it is still unclear how the interplay between AFM correlations and itinerancy leads to a “glue” that is strong enough to hold the two electrons together. It is the purpose of this Letter to show how a robust pairing mechanism emerges out of this interplay and to demonstrate that it leads to dominant superconducting correlations in a two-band Hubbard chain. Moreover, we will see that the pairing is still robust in the proximity of the AFM region, i.e., when there are large AFM fluctuations but no AFM order. What makes the mechanism robust is the fact that it is driven by confinement of topological defects (solitons) that are attached to each carrier (holes). In particular, as we will see below, this implies that the binding energy and the size of the pair are determined by different energy scales.

We start by deriving an extended Kondo lattice (KL) chain with a correlated \((t - J)\) conduction band as the low-energy effective model \(\tilde{H}\) of the original two-band Hubbard Hamiltonian \(H\). The correlated nature of the conduction band is the main difference with the standard KL chain that was extensively studied in previous works [3]. With a simple analytical treatment of the fully anisotropic (Ising-like) limit of \(\tilde{H}\), we show the origin of the two-hole bound state and the corresponding binding energy in the dilute limit. Our DMRG calculations allow us to extend these results to the fully isotropic (Heisenberg) limit and to finite hole concentrations. Moreover, we show that the superconducting pair-pair correlations are the dominant ones over an extended and relevant region of the quantum phase diagram. Interestingly enough, the pairing remains robust in the absence of long-range AFM order (fully isotropic limit) indicating that a long enough AFM correlation length is sufficient for stabilizing the pairing mechanism that we discuss below.

We will consider the following two-band Hubbard chain:

\[
H = \sum_{j\sigma} (\epsilon_j - \mu) n_{j\sigma} + t \sum_{j\sigma} (c_{j+1\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{j+1\sigma}) + \sum_{j\sigma} \Delta_{u} n_{j\sigma} n_{j\bar{\sigma}}.
\]

where \(1 \leq j \leq L\), \(L\) is even, \(L + 1 \equiv 1\) [periodic boundary conditions (PBC)], \(\eta = \{t, u\}\) denotes the lower and upper bands, and \(\sigma = \{\uparrow, \downarrow\}\). The diagonal energies are \(\epsilon_u = \Delta_{ul}/2\) and \(\epsilon_l = -\Delta_{ul}/2\) with \(\Delta_{ul} > 0\), and the density operators are \(n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}\).

From now on, we will assume that the mean number of electrons per unit cell is \(1 \leq n \leq 2\). For \(t_{\eta\eta'} = 0\) and \(U_u > \Delta_{ul}\), the ground state subspace, \(S\), consists of states containing one electron per site in the lower band (only spin remains as a degree of freedom). In contrast, the sites of the upper band can be empty or singly occupied. In the strong coupling limit, \(U_u, U_l, \Delta_{ul} \gg t_{\eta\eta'}\) and \(U_l - \Delta_{ul} \gg t_{ul}\), the low-energy spectrum of \(H\) is described by the effective Hamiltonian, \(\tilde{H}\), that acts on the subspace \(S\) and results from applying degenerate perturbation theory to second order in the hopping terms:

\[
\tilde{H} = U_u \sum_{j\sigma} (\tilde{c}_{j+1\sigma}^\dagger \tilde{c}_{j\sigma} + \tilde{c}_{j\sigma}^\dagger \tilde{c}_{j+1\sigma}) + \sum_{j\sigma} (\epsilon_u - \tilde{\mu}) n_{j\sigma} + \sum_{j\nu} \sum_{\eta} J_{\eta}^\nu S_{\nu, j\eta}^\nu S_{j+1\eta}^\nu + \sum_{j\nu} \sum_{\eta} J_{\eta}^{\nu} S_{\nu, j\eta}^{\nu} S_{j\eta}^{\nu},
\]
where $c^\dagger_{j\sigma u} = c^\dagger_{j\sigma u}(1 - n_{j\sigma u})$ (constraint of no double-occupancy), $\nu = \{x, y, z\}$, $J^\nu_u = 4t^2_{u\nu}/U_u$, and $J^\nu_K = 2t^2_{u\nu}/(U_u - \Delta_{ul}) + 2t^2_{u\nu}/(U_u + \Delta_{ul})$. Although the exchange interactions are isotropic ($J^\nu_u = J^\nu$ and $J^\nu_K = J_K$), we split the Heisenberg terms for reasons that will become clear later.

Note that we have neglected the attractive, $-\frac{J}{4} n_{j\uparrow} n_{j+1}$, and the correlated hopping terms that also appear to second order in $t_{uu}$ to keep $\bar{H}$ simple and because they are not relevant for the pairing derived below. A more extensive study including the effect of these terms will be presented elsewhere [4]. To simplify the notation, we will introduce $\beta$. Where $0 \leq \alpha, \beta \leq 1$ determine the exchange anisotropies. $\bar{H}$ is an extension of the Kondo Lattice chain: the localized spins of the lower band are coupled via a Kondo interaction, $J_K$, to the itinerant electrons of the upper band which are described by a $t - J$ model. In contrast to the usual Kondo Lattice, the itinerant electrons are strongly correlated and the local spins are AFM coupled via $J_H$.

In the following, we set $t = 1$ as the energy scale and use $J = 0.4$, $J_H = 0.5$. These values correspond for instance to $U_u = 10, U_l = 16$ and $t_{ll} = \sqrt{2}$. We will start by assuming an Ising-like ($\beta = 0$) coupling between the localized spins to stabilize long-range antiferromagnetic order at $T = 0$. The fully isotropic case $\alpha = \beta = 1$ will be considered in the second part of the manuscript, so $\beta = 0$ unless its value is explicitly specified. Below we will drop the band index in the definition of the different correlation functions because they are always applied to the conduction band. We will only compute the ground state properties.

We use the DMRG method [5] to study systems up to 100 unit cells at $T = 0$. The PBC increase substantially the computational effort. In the finite-system step, we keep up to $M = 1400$ states per block and perform up to 12 sweeps. The weight of the discarded states is kept to the order $10^{-10} - 10^{-10}$ for $\beta = 0$, and $10^{-5}$ for $\beta = 1$ [7].

We first consider the simplest case of Ising-like exchange interactions ($\alpha = 0$) and a Kondo coupling much smaller than the rest of the terms in $\bar{H}$. In this situation, the exchange $J_H$ forces the localized spins to be AFM ordered in the ground state. For the $J_K = 0$ ground state, each hole added to the conduction band carries a soliton or anti-phase domain wall (ADW) for the AFM order parameter [8]. For $J_K \neq 0$, the single hole quasiparticle becomes a spinon-holon bound state [see Fig. 1(a)] to avoid an energy increase of order $L J_K$ [9]. The single added hole is topologically neutral: the holon and the spinon carry solitons with opposite “charge” (kink and anti-kink). We also note that unless the spinon and the holon are on the same site, the ferromagnetic link associated to the spinon increases the magnetic energy by $J/2$. This provides an additional attractive force between the spinon and the holon. In this fully anisotropic limit, the spinon is immobile and the holon is localized around it [10].

The situation is qualitatively different for the two-hole ground state [see Fig. 1(b)]. The spinons attached to each holon cancel each other (they have opposite spins and topological charges) leading to a bound state of two holons attached by a magnetic string. The cancellation of the two spinons lowers the magnetic energy by $\sim J$. Consequently, we expect the two-holon bound state to be more stable than two independent spinon-holon pairs. This statement can be quantified by computing the exact ground state energies for one and two holes (this can be done for $\alpha = 0$ because the spins are not exchanged by $\bar{H}$). In particular, for $J_K = 0.1$, we get a binding energy $\Delta_B = E_\theta(N_h) + E_\theta(N_h - 2) - 2E_\theta(N_h - 1) \approx -0.25$ for $N_h = 2$, where $E_\theta(N_h)$ is the ground state energy for $N_h$ holes. The holon-holon pair formation is illustrated in Fig. 1(c). The mutual cancellation of the two spinons leaves the two holons attached by a magnetic string.

This simple picture for one and two holes has been discussed previously in the context of a $t - J$ model in a staggered magnetic field [11]. In our case, the staggered magnetic field $h$ is not artificial because it is self-generated by the AFM ordering of the localized spins. As it was pointed out in [11], the limit $h \to 0$ ($J_K \to 0$ in our case) is singular: $\text{lim}_{h \to 0} \Delta_B = -J$ while the mean distance between the two holes diverges as $h^{-1/3} (J_K^{-1/3})$. This singular behavior is
manifestation of the qualitative difference between the single- and two-hole states: the binding energy $\Delta_B$ and the size of the two-hole bound state, $l_p$, are determined by two independent energy scales. While $\Delta_B \sim -J$ for small enough $h (J_K, l_p)$ only depends on $h (J_K)$ as long as $J$ is nonzero. In particular, this shows that a negative binding energy, $\Delta_B < 0$, does not imply the formation of a two-hole bound state. The negative value of $\Delta_B$ for $h \to 0 (J_K \to 0)$ just indicates that a single hole always creates a spinon [see Fig.1(a)] while this is not true for the two-hole state as shown in Figs.1(b) and (c). An infinitesimal field $h (J_K)$ is enough for stabilizing the bound state due to the topological nature of the two-hole state: each hole carries a soliton and the two solitons become confined for any finite $h$. This remarkable property makes the pairing robust against the inclusion of a more realistic longer range Coulomb interaction in $H$. We will see below that this pairing mechanism survives in the absence of long range AFM order, i.e., when the effect of the localized spins cannot be replaced by a staggered mean field $h$ because $\langle S_{i\sigma} \rangle = 0$. This is a very important qualitative difference relative to the case considered in [11].

The above picture remains valid away from the Ising limit ($\alpha > 0$). However, the hole can now move coherently in one sublattice. The process involves the exchange of the two spins on adjacent nearest and next-nearest neighbor sites of the hole via the $\alpha J$ term followed by two hoppings in the same direction. This coherent motion of the hole leaves the magnetic background unchanged. For $0 \leq \alpha \leq 1$, the holon and spinon form a bound state. The magnetic structure of this quasiparticle is shown schematically in Fig.1(a). To confirm the above picture, we compute the hole-spin correlation function $C_{hS}(r) = \langle \hat{S}_{i\uparrow} \hat{n}_{i+1\downarrow} \hat{S}_{j\uparrow} \rangle$, where $n_{ij} = 1 - (n_{ij} + n_{ji})$ is the hole density at site $j$. Figure 1(d) shows $C_{hS}(r)$ in the isotropic limit ($\alpha = 1$) with one hole in the conduction band. The correlator shows the spinon (indicated by the arrow) separated from the holon (at $r = 1$) by a finite distance. $C_{hS}$ shows clearly that the holon and spinon carry an ADW. When a second hole is added to the conduction band, the spinons cancel each other, as explained above, leaving the two holons attached to ADW’s of opposite sign. This is also confirmed by the calculation of $C_{hh}$ [see Fig.1(e)]. The reference holon is at $r = 1$ while the average position of the second holon is indicated by the arrow (note that this average distance is artificially increased due to the PBC). To the left side of the second holon, the spins at even numbered sites ($r = 2$ for example) are antiparallel to the reference spin; whereas to its right, they are parallel (e.g. $r = 32$).

In the following we present numerical evidence of pairing and dominant superconducting correlations as a function of hole density $\nu = N_h/L$. Figure 2(a) shows the pairing energy $\Delta_B = E_g(2) + E_g(0) - 2E_g(1)$ in the dilute limit $\nu \to 0$ versus $1/L$ and for different values of $J_K$ and $\alpha$. The finite size scaling of $\Delta_B$ shows robust pairing in the thermodynamic limit for all values of $\alpha$. Figure 2(b) shows the density-density correlation function $C_{hh}(r) = \langle n_{ij} \hat{n}_{i+1j+1\uparrow} \rangle$ for $J_K = 0.1$ and different values of $\alpha$. $C_{hh}$ shows a clear maximum at a finite distance confirming that the two holons are bound. As expected, the distance between the two holons increases with $\alpha$. In the Ising limit, $\alpha = 0$, the DMRG results are compared to the exact solution and the agreement is excellent.

So far we have only considered the limit $\beta = 0$ because the pairing mechanism is easier to identify in the presence of long-range AFM order. It is natural to ask if the pairing survives in the fully isotropic limit ($\alpha = \beta = 1$) relevant for our original Hamiltonian $\tilde{H}$. In the absence of holes, the ground state of $\tilde{H}$ only exhibits short-range AFM correlations due to the gap induced by the relevant $J_K$ coupling. The $C_{hh}$ correlator for the two-hole ground state shown in Fig. 2(c) provides clear evidence of the formation of a two-hole bound state. Moreover, the pair size $l_p$ decreases monotonically with increasing $J_K$ (slope of the confining potential) indicating that the pairing mechanism remains the same.
A few comments are in order. We verified that the pairing ($\Delta_B < 0$) persists for smaller values of $J_B$ such as $J_B = J_K = 0.1$. The small $J_B$ regime of $H$ is relevant for describing lanthanide and actinide based compounds in which localized f-electrons interact via Kondo exchange with electrons in the conduction band. Conduction bands with strong $3d$ character are correlated and would provide a natural realization of our $H$. If the $t-J$ conduction band of $H$ is replaced by the original Hubbard upper band of $H$, one can study the evolution of our pairing mechanism as a function of $U_{\nu}/t$ (the standard KL model is recovered for $U_{\nu}/t = 0$).

In contrast to pairing mechanisms driven by an attractive short range interaction (like the AFM exchange $J$), our mechanism is robust under the inclusion of a more realistic longer range Coulomb interaction. This results from the fact that $\Delta_B$ and $l_p$ are determined by two independent energy scales ($J$ and $J_K$). In other words, a big enough value $l_p$ reduces the effect of longer range Coulomb terms without reducing the value of $\Delta_B$ (note that $l_p$ and $\Delta_B$ are anticorrelated when the pairing is produced by a short range attractive potential).

Finally, our pairing mechanism should also persist for weakly coupled chains (small inter-chain hopping) due to its topological nature. While single-particle coherent inter-chain hopping is not possible due to the soliton that is attached to each hole, a pair can hop coherently between chains because it is topologically neutral (soliton-antisoliton bound state). Such coherent pair hopping should stabilize a superconducting state below a finite critical temperature. A detailed study of this extension to higher-dimensional systems will be presented elsewhere.

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