Closing of the spin gap and ferromagnetism induced by magnetic impurities

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The Hubbard chain with attractive U and a finite concentration of magnetic impurities of spin S is studied using the Bethe *Ansatz* technique. The impurities weaken the singlet bound states of the Hubbard model reducing the spin gap. The spin gap is closed at a critical concentration which depends on the spin and the coupling strength. A ferromagnetic phase is induced for concentrations of impurities larger than the critical one, where a fraction of singlet pairs is broken up giving rise to a Fermi sea of spin-polarized itinerant electrons. [S0163-1829(98)01418-0]

I. INTRODUCTION

Magnetic impurities in superconductors break the time-reversal symmetry and are unfavorable to the formation of Cooper pairs. Consequence of the pair breaking or weakening is a gradual reduction of the superconducting gap and the transition temperature with the concentration of impurities.[1,2] The gap closes before superconductivity is completely suppressed, a phenomenon known as gapless superconductivity.[2] In addition the impurity forms a bound state inside the gap, which also contributes to the closing of the gap.[3]

A possible explanation for the pseudogap or spin-gap anomaly observed in underdoped cuprate superconductors is that they are in an intermediate regime between a BCS superconductor and a condensation of preformed bosons. The purpose of this paper is to study the effect of magnetic impurities on the preformed bosons of the one-dimensional (1D) Hubbard model with attractive U, in particular the closing of the spin-gap as a function of the impurity concentration and ferromagnetic phase that arises when the gap is ''negative.'' The magnetic impurities weaken the singlet pair boundstates, reducing in this way the gap. This is in contrast to the pair-breaking mechanism that leads to suppression of superconductivity in a BCS superconductor by magnetic impurities.[1–3]

The exact solution of the 1D Hubbard model has been obtained via nested Bethe *Ansätze* long ago[4] and numerous properties are known for both, repulsive and attractive interaction U.[5] An impurity embedded into the Hubbard model usually destroys the integrability. In recent papers we succeeded in constructing 1D integrable correlated electron lattice models with a magnetic impurity via the quantum inverse scattering method.[6–9] Several combinations of hosts, e.g., two variants of the supersymmetric t-J models and the Hubbard model, and impurities, e.g., exchange and intermediate valence impurities, have been considered. The scattering matrix of electrons in the host and the scattering matrix of electrons with the impurity have to satisfy the triangular Yang-Baxter relation. This is the necessary and sufficient condition for the integrability, which imposes restrictions on the impurity. For the Hubbard model with attractive interaction the mixed valent hybridization impurity with two magnetic configurations satisfies these conditions.[9] This impurity with undercompensated Kondo properties is considered here.

The rest of the paper is organized as follows. The definition of the scattering matrices and technical aspects, such as the triangular relation and the extension of the monodromy matrix to an arbitrary number of impurities, are presented in the Appendix. In Sec. II we briefly discuss the interaction Hamiltonian of an isolated impurity with the itinerant electrons and state the discrete Bethe *Ansatz* equations diagonalizing the lattice problem with a finite concentration of impurities. The two-strings leading to the singlet bound states are introduced and the contribution of the impurities on the dressed energy potentials is derived. The dressed energies determine the spin-gap as a function of impurity concentration. Results and conclusions follow in Sec. III.

II. GENERAL FORMULATION

A. Bethe *Ansatz* equations

Consider the Hubbard model with N_e itinerant electrons and N_i impurities in a box of N_a sites with periodic boundary conditions. The system is defined via the scattering matrices, Eqs. (A1) and (A3), and is integrable by construction as shown in the Appendix. The transfer matrices can be diagonalized simultaneously in terms of two sets of rapidities, $\{x_j\}$, $j=1,\ldots,N_e$, for the charges and $\{\Lambda_\alpha\}$, $\alpha=1,\ldots,M^*$, (M^* is the number of down-spin electrons) for the spins, which satisfy the following discrete Bethe *Ansatz* equations:

$$e^{ik_jN_a}\left[\frac{x_j-x_0+i(2S+1)U/4}{x_j-x_0-i(2S+1)U/4}\right]^{N_i}=\prod_{\beta=1}^{M^*}\frac{x_j-\Lambda_\beta+iU/4}{x_j-\Lambda_\beta-iU/4},$$

$$j=1,\ldots,N_e, \qquad (1)$$

$$\left[\frac{\Lambda_\alpha-x_0+iUS/2}{\Lambda_\alpha-x_0-iUS/2}\right]^{N_i}\prod_{j=1}^{N_e}\frac{\Lambda_\alpha-x_j+iU/4}{\Lambda_\alpha-x_j-iU/4}$$

$$=-\prod_{\beta=1}^{M^*}\frac{\Lambda_\alpha-\Lambda_\beta+iU/2}{\Lambda_\alpha-\Lambda_\beta-iU/2}, \quad \beta=1,\ldots,M^*. \qquad (2)$$

The rapidities x_j are related to the quasimomenta of the electrons k_j via $x_j=\sin k_j$. The magnetization is given by $S_z=\frac{1}{2}N_e-M^*+SN_i$ and the energy of the system is

$$E=-2\sum_{j=1}^{N_e}\cos k_j+N_iE_{\rm imp}, \tag{3}$$

where $E_{\rm imp}$ is the energy per impurity which is discussed below. Each impurity acts as a charged particle of spin S. The second factor on the left-hand side of Eq. (1) and the first factor in Eq. (2) arise from the impurities. The impurity is defined as a function of two parameters, namely, the spin S and the rapidity x_0. For $N_i=0$ Eqs. (1)–(3) reduce to Lieb and Wu's solution[4] of the Hubbard model. If $N_i=1$ we recover the single impurity embedded in the Hubbard model studied in Ref. 9.

B. Impurity Hamiltonian

The lattice Hamiltonian is the 1D Hubbard model

$$H_0=-\sum_{i\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma}+c_{i+1\sigma}^{\dagger}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{4}$$

where $c_{i\sigma}^{\dagger}$ creates an electron of spin σ at site i and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ is the corresponding number operator. The on-site interaction is attractive if $U<0$ and the hopping parameter has been equated to 1.

The *lattice impurity* Hamiltonian is complicated and its general form has been discussed in Refs. 9,10. It can in principle be obtained as the derivative of the logarithm of the transfer matrix (see Appendix). As for the algebraic Bethe *Ansatz* for the Hubbard model this involves cumbersome operations with 16×16 matrices.[11] From the definition of the transfer matrix it follows that the impurity is located on a link of the Hubbard chain and interacts with both neighboring sites. The impurity couples to states of both, even and odd parity about the impurity site.

The impurity Hamiltonian acquires a more appealing form in the *continuum limit*. When the lattice constant tends to zero, we can linearize the kinetic energy in the momentum around the Fermi level and restrict ourselves to low-energy excitations (Luttinger liquid). The interaction with the impurity is then a contact potential, so that in this limit the impurity only couples to states with even parity (s waves) with respect to the impurity site. States with odd parity affect the impurity indirectly via the Luttinger liquid. The scattering matrix (A3) corresponds to a mixed valent impurity with two magnetic configurations of spins S and $S_1=S+\frac{1}{2}$, respectively, hybridized via a conduction electron, and the Hamiltonian is[13–15]

$$H_{\rm imp}=\epsilon\sum_{M_1}|S_1M_1\rangle\langle S_1M_1|+V\sum_{\sigma MM_1}(M\sigma|M_1)\int dx\,\delta(x)\times[c_{\sigma}^{\dagger}(x)|SM\rangle\langle S_1M_1|+\text{H.c.}], \tag{5}$$

where the bra and ket denote the impurity states, $M_1=M+\sigma$, and $(M\sigma|M_1)$ is a Clebsch-Gordan coefficient defined in the Appendix. The completeness condition for the impurity requires

$$\sum_{M_1}|S_1M_1\rangle\langle S_1M_1|+\sum_M|SM\rangle\langle SM|=1. \tag{6}$$

The parameter $\epsilon=|x_0|/v$ represents the energy difference between the two configurations relative to the Fermi level, v is the Fermi velocity, and $V^2=(2S+1)|U|/(2v)$. The impurity is capable of temporarily absorbing the spin of one conduction electron to form an effective spin $S_1=S+\frac{1}{2}$, i.e., the ground state wave function is a linear superposition of two different spin configurations.[13–15] Note that for $S=0$ the Clebsch-Gordan coefficients are equal to 1 and the impurity is the $U\to\infty$ limit of the Anderson model, except that the host is now a Luttinger liquid.

While in a free electron host the Anderson impurity has two parameters (ϵ and V), the integrability in the interacting host fixes V, so that there is only one free parameter, which in Eqs. (1) and (2) is the impurity rapidity x_0. This rapidity determines both, the valence admixture and the impurity screening, which then in a host without spin gap occur on the same energy scale $t\exp(-2\pi|x_0/U|)$ (Kondo temperature). In contrast, for an impurity in a free electron gas the charge and spin fluctuations occur on different energy scales. $|x_0|$ is then related to the Kondo exchange coupling.

For a single impurity the thermodynamic properties do not depend on the sign of x_0 (chirality). The sign of x_0 only affects the mesoscopic part of the finite size corrections to the ground state energy, e.g., it changes the initial phase of persistent currents. The interaction of the impurity with itinerant electrons on the two neighboring sites is different for the two sites, since the impurity couples to states with even and odd symmetry with respect to the impurity site. For $x_0\neq0$ the impurity on the *lattice* then breaks the time-reversal (T) and parity (P) symmetries separately, but TP is conserved. On the other hand, P and T are separately conserved in the continuum limit.

C. Ground state equations

The attractive interaction ($U<0$) pairs the electrons into Cooper-like singlet states without off-diagonal long-range order even at $T=0$.[16,17] The singlet pairs introduce a spin gap (binding energy) in the excitation spectrum of unpaired electrons.

For the ground state the solutions of the Bethe *Ansatz* equations are organized as spin-charge pairs, $x^{\pm}=\Lambda\pm iU/4$, and unbound electrons with real x.[18] We introduce distribution densities for the two classes of rapidities and their holes, i.e., $\rho(k)$ and $\rho_h(k)$ for the unbound electrons, and $\sigma'(\Lambda)$ and $\sigma_h'(\Lambda)$ for the pair rapidities, which satisfy the following integral equations:[16,17]

$$\rho_h(k)+\rho(k)+\cos(k)\int_{-Q}^{Q}d\Lambda\,a_1(x-\Lambda)\sigma'(\Lambda)=\frac{1}{2\pi}+\frac{N_i}{N_a}\cos(k)a_{2S+1}(x-x_0), \tag{7}$$

$$\sigma_h'(\Lambda)+\sigma'(\Lambda)+\int_{-Q}^{Q}d\Lambda'\,a_2(\Lambda-\Lambda')\sigma'(\Lambda')=-\int_{-B}^{B}dk\,a_1(\Lambda-x)\rho(k)+\frac{1}{\pi}\,\mathrm{Re}\left[1-\left(\Lambda-i\frac{U}{4}\right)^2\right]^{-1/2}+\frac{N_i}{N_a}a_{2S+2}(\Lambda-x_0), \tag{8}$$

where $a_n(x)=(|U|n/4\pi)/[x^2+(Un/4)^2]$ and Re denotes real part. The driving terms proportional to N_i arise from the impurities. The energy, the total number of electrons, and the magnetization are given by

$$\frac{E}{N_a}=\frac{N_i}{N_a}E_{\rm imp}-2\int_{-B}^{B}dk\ \cos(k)\rho(k)$$
$$-4\ {\rm Re}\ \int_{-Q}^{Q}d\Lambda[1-(\Lambda-iU/4)^2]^{1/2}\sigma'(\Lambda),$$
$$\frac{N_e}{N_a}=n=\int_{-B}^{B}dk\rho(k)+2\int_{-Q}^{Q}d\Lambda\sigma'(\Lambda),$$
$$\frac{S_z}{N_a}=S\frac{N_i}{N_a}+\frac{1}{2}\int_{-B}^{B}dk\rho(k). \tag{9}$$

The number of electrons and the magnetization of the host determine the integration limits Q and B. Q increases monotonically with the band filling from 0 for the empty band to ∞ for one electron per site (half-filled band).

As discussed above, the sign of x_0 introduces a chirality into the system, i.e., a forward to backward asymmetry. The phase shifts due this chirality are additive (modulo 2π). We neutralize the chirality by incorporating as many impurities with backward as with forward chirality, i.e., by replacing the impurity driving term in Eq. (7) $a_{2S+1}(x-x_0)$ by

$$\frac{1}{2}[a_{2S+1}(x-x_0)+a_{2S+1}(x+x_0)], \tag{10}$$

and similarly for the impurity driving term in Eq. (8). This choice is not a unique one, but any distribution of signs of x_0 gives qualitatively the same answer.

D. Isolated impurity

A single impurity corresponds to $N_i=1$. Equations (7) and (8) are linear in the densities, and the driving terms of host and impurity are additive. We can then separate the contributions to the densities for the host and the impurity, i.e., $\rho(k)=\rho_{\rm host}(k)+N_a^{-1}\rho_{\rm imp}(k)$ and $\sigma'(\Lambda)=\sigma'_{\rm host}(\Lambda)+N_a^{-1}\sigma'_{\rm imp}(\Lambda)$. The impurity ground state energy is given by[9]

$$E_{\rm imp}=-2\int_{-B}^{B}dk\ \cos(k)\rho_{\rm imp}(k)$$
$$-4\ {\rm Re}\ \int_{-Q}^{Q}d\Lambda[1-(\Lambda-iU/4)^2]^{1/2}\sigma'_{\rm imp}(\Lambda), \tag{11}$$

where the limits of integration B and Q are governed by the host. The properties of the Hubbard model with attractive U are well known,[16,17] and we limit ourselves to summarize the results for the impurity.

The impurity manifests charge fluctuations characteristic of an intermediate valent regime.[9] This is in part a consequence of the correlations in the host, which drive the valence of the impurity. The valence is maximum if the impurity rapidity x_0 lies in the continuum of the charge rapidities, and decreases monotonically with increasing $|U|$. The valence of the impurity decreases if its rapidity gets off resonance with the Fermi sea states.

The spin fluctuations are suppressed by the spin gap of the host. There is no response to a magnetic field smaller than the critical field H_c (corresponding to the depairing energy of Cooper singlet bound states) and the magnetization of the impurity equals S. For fields slightly larger than H_c, the magnetic susceptibility of the impurity has a square-root divergence,[9] revealing the van Hove singularity of the empty unpaired electron band of the host. This behavior differs drastically from the ordinary Kondo effect.

A magnetic impurity introduces a bound state inside the gap of a BCS superconductor. The spin gap represents the energy required to form Cooper bound states, although without long-range order. The impurity considered here is a forward-scatterer only as required by the integrability, and hence does not form a bound state. An impurity that includes both forward and backward scattering would give rise to a bound state in the spin gap. This aspect of our impurity is nongeneric, imposed by the condition of integrability. We expect, however, that most of the properties of the impurity, e.g., the lack of spin screening and the pair weakening, are valid generally.

For a generic impurity the situations of an even and an odd number of electrons in the system have to be distinguished, e.g., if the number of electrons is odd, one electron remains unpaired and binds with the impurity. This difference does, of course, not play any role for a finite concentration of impurities.

E. Gap equation

A finite concentration of impurities modifies on the one hand the densities of rapidities according to Eqs. (7) and (8) and on the other hand the dressed energies of the excitations. To calculate the latter we need the expression for the total energy, which in principle can be derived from the algebraic Bethe *Ansatz*. Since the transfer matrix has (N_e+N_i) factors, the energy has (N_e+N_i) terms. The calculation of the remaining N_i factors is very cumbersome due to the double occupied sites, e.g., the host L operator is a 16×16 matrix with complicated structure.[11] We have succeeded in deriving an expression for the energy of the impurities for the supersymmetric t-J model,[12] where there are only three states per site (rather than four as for the Hubbard model). The double occupation of a site in Hubbard's model is the source of numerous complications in the algebraic Bethe *Ansatz*.[11]

For an isolated impurity the energy is given by Eq. (11), which trivially can be rewritten as

$$E_{\rm imp}=-2\int_{-B}^{B}dk\ \cos(k)R_\rho\ \rho_{\rm host}(k)-4\ {\rm Re}\ \int_{-Q}^{Q}d\Lambda$$
$$\times[1-(\Lambda-iU/4)^2]^{1/2}R_{\sigma'}\sigma'_{\rm host}(\Lambda), \tag{12}$$

where

$$R_\rho=\frac{\rho_{\rm imp}(k)}{\rho_{\rm host}(k)},\quad R_{\sigma'}=\frac{\sigma'_{\rm imp}(\Lambda)}{\sigma'_{\rm host}(\Lambda)}, \tag{13}$$

are the ratios of the densities for the isolated impurity and the pure host, obtained by solving Eqs. (7) and (8). Expressions (12) and (13) are exact only in the limit $c=N_i/N_a\to 0$. Unfortunately, we do not have an exact expression for the impurity energy if the concentration is finite. Here we will use an approximate expression for the energy valid for $c=N_i/N_a\ll 1$,

$$\frac{E}{N_a}=-2\int_{-B}^{B}dk\ \cos(k)[1+cR_\rho]\rho(k)-4\ \mathrm{Re}\int_{-Q}^{Q}d\Lambda \times[1-(\Lambda-iU/4)^2]^{1/2}[1+cR_{\sigma'}]\sigma'(\Lambda), \tag{14}$$

where R_ρ and $R_{\sigma'}$ are still given by Eq. (13). Equation (14) contains the exact first two terms of the power expansion in c of the exact energy of the system, but the term proportional to c^2 and higher order terms are only approximate.

The standard procedure to calculate the dressed energies can now be followed and we obtain

$$\varepsilon(k)=-2\cos(k)[1+cR_\rho]-\mu-\frac{1}{2}H -\int_{-Q}^{Q}d\Lambda a_1(\Lambda-\sin k)\psi(\Lambda), \tag{15}$$

$$\psi(\Lambda)=-4\ \mathrm{Re}[1-(\Lambda-iU/4)^2]^{1/2}\left[1+\frac{N_i}{N_a}R_{\sigma'}\right] -2\mu-\int_{-Q}^{Q}d\Lambda' a_2(\Lambda-\Lambda')\psi(\Lambda') -\int_{-B}^{B}dk\ \cos(k)a_1(\Lambda-\sin k)\varepsilon(k). \tag{16}$$

The integration limits B and Q are determined as a function of magnetic field and chemical potential by the Fermi surface, i.e., by the zeroes of the dressed energies, $\varepsilon(\pm B)=0$ and $\psi(\pm Q)=0$. B and Q in turn determine the number of electrons and the magnetization. Note that the integrations are over occupied states, i.e., the intervals in which ε and ψ are negative. The spin gap is the smallest energy required to depair a singlet bound state and in zero magnetic field it is given by

$$\mathrm{gap}=-2[1+cR_\rho]-\mu-\int_{-Q}^{Q}d\Lambda a_1(\Lambda)\psi(\Lambda), \tag{17}$$

where ψ is the solution of Eq. (16) for $B=0$.

Since impurities localize electrons and the total number of electrons is conserved, the integration limits B and Q are renormalized as a function of the impurity concentration c. Hence, also the distributions of rapidities for the host and the impurity change as a function of c. Numerically, we found this effect to be small within the range of concentrations used here.

III. RESULTS AND CONCLUSIONS

The integral equations (7), (8), and (16) have been solved numerically for the nonchiral situation (half of the impurities have rapidity $+x_0$ and the other half $-x_0$) for a fixed number of electrons and zero magnetic field ($B=0$). This solution has then been used to evaluate the magnitude of the spin gap as a function of impurity concentration and impurity rapidity x_0. The spin gap decreases with the impurity concentration as a consequence of the R_ρ term in Eq. (17) which in general is larger than the change of the chemical potential as a function of c (note that $d\mu/dc$ is negative). The decrease is linear with the concentration and deviations from linearity are less than 1% for impurity concentrations of up to 10%. The dependence of the spin gap on the concentration is then completely described in terms of the gap of the pure system and the slope $d\mathrm{gap}/dc$, which in turn determine the critical concentration c_{cr} at which the gap closes. c_{cr} is inversely proportional to the slope.

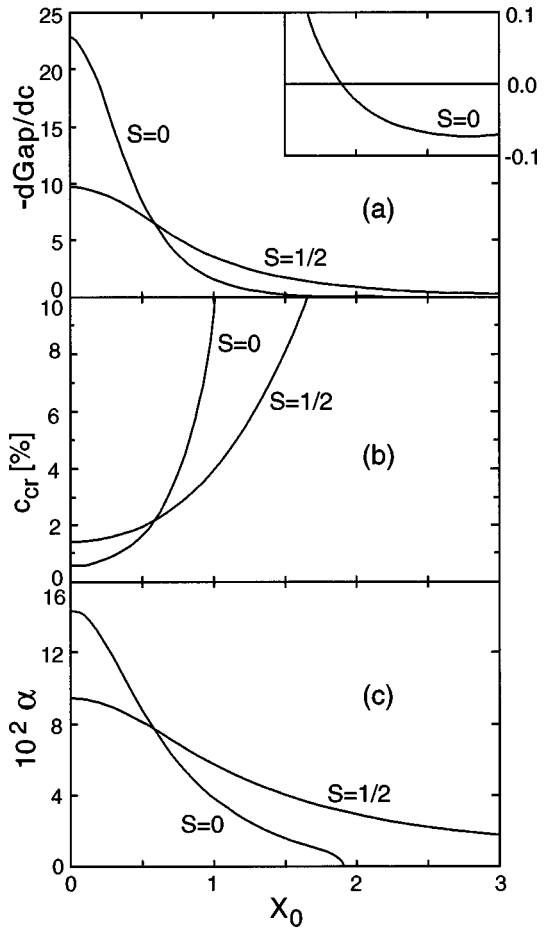

FIG. 1. (a) Rate of decrease of the spin gap with the impurity concentration, (b) critical concentration at which the spin-gap is closed, and (c) coefficient α of the spontaneous magnetization defined in Eq. (18) as a function of the rapidity of the impurity for $S=0$ and $S=1/2$. The inset shows the change of sign of $-d\mathrm{gap}/dc$ for $S=0$ for large x_0.

The slope and the critical concentration as a function of x_0 are shown in Figs. 1(a) and 1(b) for $S=0$ and $S=1/2$ and $U=-2$. $d\mathrm{gap}/dc$ decreases monotonically with x_0 (except for $S=0$ and very large x_0) and correlates with the number of electrons localized at the impurity site. For $|x_0|<Q$ the impurity rapidity lies in the continuum of charge rapidities and the isolated impurity is in a mixed valent regime, localizing a fraction of an electron, $n_{\mathrm{imp}}=2\int_{-Q}^{Q}d\Lambda\sigma'_{\mathrm{imp}}(\Lambda)$. With increasing x_0 the quantity n_{imp} gradually decreases to zero as

the rapidity gets off-resonance with the ''Cooper-pair'' continuum. The mechanism reducing the spin gap is then of the pair-weakening type and not pair breaking as for magnetic impurities in a BCS superconductor. No unpaired electrons are generated as long as there is a spin gap. The pair weakening decreases with increasing spin for small x_0, while this trend is reversed for large x_0 (off resonance).

The above can be understood in the light of the impurity Hamiltonian in the continuum limit. According to Eq. (5) the impurity rapidity plays the role of the energy difference between the two configurations relative to the Fermi level. Increasing $|U|$ and the spin, increases the hybridization matrix element and hence drives the impurity further into the mixed-valence regime. But increasing $|U|$ also increases the spin-gap. Due to the spin-gap the ground state impurity magnetization is always $N_i S$ (for $H<H_c$).

For $S=0$ and very large x_0 the rate of change of the chemical potential $d\mu/dc$ is larger than $2R_\rho$. As a consequence, $d\text{gap}/dc$ is positive and the spin gap slightly increases with the impurity concentration. This is seen in the inset of Fig. 1(a). But in this limit the impurity is nonmagnetic and the magnetic configuration of spin $S_1=1/2$ is only weakly admixed.

For impurity concentrations larger than $c_{\rm cr}$ a fraction of the itinerant electrons is (a) depaired and (b) spontaneously magnetized. The former follows from the fact that the dressed energy $\varepsilon(k)$ is now negative in an interval around $k=0$. Hence $B\neq 0$ and $\int_{-B}^{B} dk\rho(k)$ is nonzero. The ferromagnetic order of the itinerant electrons (b) is more subtle and requires an analysis of the string excitations of the Hubbard model with attractive interaction. There are two types of string excitations:[17,18] (i) bound states of Cooper pairs, which require large energies and are unfavorable for small concentrations, and (ii) spin strings, which represent spin excitations in the system. Their dressed energies are positive for the pure system, and a small concentration of impurities does not change their sign. Hence, these states are not populated in the ground state. From the zeroes of the dressed ε potential we have that to leading order $B\propto\sqrt{c-c_{\rm cr}}$. The total magnetization of the Hubbard chain with impurities is then approximately given by

$$S_z = SN_i + \alpha(c-c_{\rm cr})^{1/2},$$

$$\alpha = \rho_{\rm host}(0)\left(\frac{1}{2}\frac{d\text{gap}}{dc}[1+c_{\rm cr}R_\rho]\right)^{1/2}, \tag{18}$$

for c slightly above $c_{\rm cr}$. The expression for the coefficient α is only approximate (the error is about 10%), since here we neglected the feedback of the finite B on the dressed energy ψ. α as a function of x_0 is shown in Fig. 1(c). It essentially tracks the dependence of the slope and the fraction of localized electrons (valence) $n_{\rm imp}$. While the slope and α are determined by the driving term of $\rho_{\rm imp}$, $n_{\rm imp}$ follows the dependence of the driving term of $\sigma'_{\rm imp}$. Both driving terms are similar Lorentzians, explaining the similar trends of these quantities.

As mentioned earlier, the lack of a bound state inside the spin gap is an artifact of our impurity model and nongeneric. It is the consequence of the suppressed backward scattering, a requirement for the integrability of the model. All other properties are believed to be valid in general and nonspecific to the integrability.

In the Hubbard chain with attractive U, the impurities effectively act similarly to a magnetic field, closing the gap and polarizing the depaired electrons. On the other hand, a finite concentration of magnetic impurities introduced into a correlated host without spin gap, e.g., the supersymmetric t-J model, are antiferromagnetically correlated as experimentally found for most heavy fermion compounds.[12] The ground state in this case is always a magnetic singlet.

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APPENDIX

For the Hubbard model the scattering matrix for two electrons has the form[4]

$$\hat{X}(x_1-x_2) = \frac{(x_1-x_2)\hat{I} + i(U/2)\hat{P}}{(x_1-x_2)+iU/2}, \tag{A1}$$

where $\hat{I}=\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}$ and $\hat{P}=\delta_{\sigma_1'\sigma_2}\delta_{\sigma_2'\sigma_1}$ are the identity and permutation operators, respectively, where the unprimed (primed) indices refer to the incoming (outgoing) states. Here the x_i are rapidities. The two-electron scattering matrix $\hat{X}$ satisfies the triangular Yang-Baxter relation, which is the necessary condition for the integrability of the model. We consider an attractive interaction, i.e., $U<0$.

The impurity is introduced via its scattering matrix with the itinerant electrons $\hat{S}$. If the integrability of the model is to be preserved, $\hat{S}$ has to satisfy the triangular Yang-Baxter relation with $\hat{X}$:

$$\begin{aligned} &X^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}(x_1-x_2)S^{\sigma_1'\sigma_1''}_{MM'}(x_1-x_0)S^{\sigma_2'\sigma_2''}_{M'M''}(x_2-x_0) \\ &\quad = S^{\sigma_2\sigma_2'}_{MM'}(x_2-x_0)S^{\sigma_1\sigma_1'}_{M'M''}(x_1-x_0)X^{\sigma_1'\sigma_1''}_{\sigma_2'\sigma_2''}(x_1-x_2), \end{aligned} \tag{A2}$$

where the sum over repeated indices is implicit. The index M refers to the spin component of the magnetic impurity. An impurity scattering matrix satisfying Eq. (A2) is[13,14]

$$\begin{aligned} \hat{S}^{\sigma\sigma'}_{MM'}(x) &= \delta_{\sigma\sigma'}\delta_{MM'} + (M\sigma|M+\sigma)(M'\sigma'|M'+\sigma') \\ &\quad \times \frac{iU(2S+1)/2}{x-iU(2S+1)/4}P^{\sigma\sigma'}_{MM'}, \end{aligned} \tag{A3}$$

where $P^{\sigma\sigma'}_{MM'}=\delta_{\sigma\sigma'}\delta_{MM'}+\delta_{-\sigma\sigma'}\delta_{M'M+2\sigma}$. The Clebsch-Gordan coefficient $(M\sigma|M+\sigma)$, which is a short-hand notation for

$$(SM;\tfrac{1}{2}\sigma|S\tfrac{1}{2}(S+\tfrac{1}{2})M+\sigma), \tag{A4}$$

selects the way the impurity couples to the itinerant electrons. Here x_0 is the impurity rapidity which controls the degree of ''valence admixture.'' Note that both Eqs. (A1) and (A3) are unitary.

We now define the monodromy matrix[15,19] for N_e electrons and N_i impurities, $N=N_e+N_i$,

$$L^{\{\sigma_1' \ldots \sigma_N'\}\tau'}_{\{\sigma_1 \ldots \sigma_N\}\tau}(\alpha;\alpha_1,\ldots,\alpha_N) = Y^{\tau'\mu_1}_{\sigma_1'\sigma_1}(\alpha_1-\alpha)Y^{\mu_1\mu_2}_{\sigma_2'\sigma_2}(\alpha_2-\alpha)\ldots Y^{\mu_{N-1}\tau}_{\sigma_N'\sigma_N}(\alpha_N-\alpha), \tag{A5}$$

with the implicit summation over all the μ_j indices and Y denotes a scattering matrix. Here α is the spectral parameter. Equation (A5) consists of a product of N_e scattering matrices of the $\hat{X}$ type and N_i electron-impurity scattering matrices, which can be arranged in arbitrary order. The indices σ_i generically denote electron or impurity spins. With respect to the indices τ and τ' the monodromy matrix forms a 2×2 matrix, which we write $\hat{L}^{\tau'}_{\tau}(\alpha)$ omitting the spin indices and the parameters α_j.

From the Yang-Baxter relations it follows that the monodromy matrix satisfies the identity[15,19]

$$X^{\tau_1\tau_1'}_{\tau_2\tau_2'}(\alpha-\alpha')\hat{L}^{\tau_1'}_{\tau_3}(\alpha')\hat{L}^{\tau_2'}_{\tau_3'}(\alpha)=\hat{L}^{\tau_2}_{\tau_2'}(\alpha)\hat{L}^{\tau_1}_{\tau_1'}(\alpha') \times X^{\tau_1'\tau_3}_{\tau_2'\tau_3'}(\alpha-\alpha'), \tag{A6}$$

where the sum over repeated indices is implicit. The transfer matrix is defined as $\hat{T}(\alpha)=\Sigma_\tau \hat{L}^{\tau}_{\tau}(\alpha)$. Using Eq. (A6) and the unitarity of $\hat{X}(\alpha)$, it is straightfoward to show that transfer matrices at different α values commute and can all be diagonalized simultaneously. The procedure to diagonalize the transfer matrices is standard and yields the discrete Bethe *Ansatz* equations given in Sec. II.

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