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LETTER TO THE EDITOR

XXZ model as an effective Hamiltonian for generalized Hubbard models with broken η -symmetry

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Abstract. We consider the limit of strong Coulomb attraction for generalized Hubbard models with η -symmetry. In this limit these models are equivalent to the ferromagnetic spin- $\frac{1}{2}$ Heisenberg quantum spin chain. In order to study the behaviour of the superconducting phase in the electronic model under perturbations which break the η -symmetry we investigate the ground state of the ferromagnetic non-critical XXZ-chain in the sector with fixed magnetization. It turns out to be a large bound state of N magnons. We find that the perturbations considered here lead to the disappearance of the off-diagonal long-range order.

There has been a lot of activity in the past few years in the investigation of electronic models for superconductivity. In particular, the so-called η -pairing mechanism introduced by Yang [1] has been quite fruitful for the construction of models with superconducting ground states (see e.g. [2]). Although the ground state of the Hubbard model is not of the η -pairing type [1] one can construct such models by adding nearest-neighbour interaction terms. The first example was found in [3, 4]. In [2] it has been shown that, for a large class of generalized Hubbard models, the ground state in the limit $U \rightarrow -\infty$ is the simplest η -pairing state $(\eta^\dagger)^N|0\rangle$ with $\eta^\dagger = \sum_j c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger$. For the supersymmetric Hubbard model [3, 4] and a special case of the Hirsch model with a correlated hopping interaction [5] the complete phase diagram in arbitrary dimensions has been found. It shows two phases with η -pairing ground states. Since these states have off-diagonal long-range order (ODLRO) they are also superconducting [6].

The main aim of this letter is to clarify the effect of η -symmetry-breaking perturbations on the superconducting ground state. In order to keep the problem as simple as possible we restrict ourselves to the one-dimensional case and the limit $U \rightarrow -\infty$. For strong coupling limits, spin models often turn out to be effective Hamiltonians for models of correlated electrons. For example, the antiferromagnetic Heisenberg model is known to be the effective Hamiltonian for the Hubbard model in the limit $U \rightarrow \infty$ at half-filling. In our case the effective Hamiltonian is found to be the ferromagnetic Heisenberg chain.

We perturbate the supersymmetric Hubbard model by changing the value of the nearest-neighbour Coulomb interaction V in such a way that the effective Hamiltonian in the limit of large attraction will be a ferromagnetic non-critical XXZ model ($\Delta \geq 1$, see equation (6)). In this regime the ground state is simply the fully polarized ferromagnetic state $|\uparrow \cdots \uparrow\rangle$,

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and the spectrum has a gap which vanishes in the limit $\Delta \rightarrow 1^+$. The question of stability of the superconducting ground state of the electronic model thus turns out to be closely related to the form of the ground state of the ferromagnetic XXZ model at fixed magnetization.

In the following we will be interested in the large- U limit of generalized Hubbard models with Hamiltonian

$$\begin{aligned} \mathcal{H} = & -t \sum_{j=1}^L \sum_{\sigma=\uparrow,\downarrow} (c_{j\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j\sigma}) + V \sum_{j=1}^L (n_j - 1)(n_{j+1} - 1) \\ & + X \sum_{j=1}^L \sum_{\sigma} (c_{j\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j\sigma}) (n_{j,-\sigma} + n_{j+1,-\sigma}) \\ & + Y \sum_{j=1}^L (c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j+1,\downarrow} c_{j+1,\uparrow} + c_{j+1,\uparrow}^\dagger c_{j+1,\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow}) + \frac{J_{xy}}{2} \sum_{j=1}^L (S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) \\ & + J_z \sum_{j=1}^L S_j^z S_{j+1}^z + U \sum_{j=1}^L (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}). \end{aligned} \quad (1)$$

Here $c_{j\sigma}^\dagger$ and $c_{j\sigma}$ are the usual electron creation and annihilation operators, i.e. $\{c_{j\sigma}, c_{l\sigma'}^\dagger\} = \delta_{jl}\delta_{\sigma\sigma'}$, $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$ is the corresponding number operator and the components of the spin operators are given by $S_j^z = \frac{1}{2}(n_{j\uparrow} - n_{j\downarrow})$, $S_j^x = \frac{1}{2}(S_j^+ + S_j^-)$ and $S_j^y = \frac{1}{2i}(S_j^+ - S_j^-)$ with $S_j^+ = c_{j\uparrow}^\dagger c_{j\downarrow}$, $S_j^- = c_{j\downarrow}^\dagger c_{j\uparrow}$.

In [2] the conditions under which the Hamiltonian (1) has an η -pairing ground state of the form

$$|\psi_N\rangle = (\eta^\dagger)^N |0\rangle \quad (2)$$

with $\eta^\dagger = \sum_{j=1}^L \eta_j^\dagger = \sum_{j=1}^L c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger$ were investigated. They were found to occur for $t = X$, $2V = Y$, $V \leq 0$ and

$$-U \geq 2 \max(V - \frac{1}{4}J_z, V + \frac{1}{4}J_z + |\frac{1}{2}J_{xy}|, 2V + 2|t|). \quad (3)$$

Note that the first two conditions also guarantee the η -symmetry of the Hamiltonian (1) with $U = 0$, i.e. $[\mathcal{H}(U=0), \eta^\dagger] = 0$.

For the supersymmetric Hubbard model in [3,4] only the Coulomb interaction U is a free parameter. The other interaction constants have fixed values: $X = t$, $V = -t/2$, $Y = -t$, and $J_{xy} = J_z = 2t$. The other integrable model (1) has—apart from the Coulomb interaction U —only two non-vanishing interactions constants, namely $t = X$ [5].

In the limit of strong attraction ($U \rightarrow -\infty$) in the Hamiltonian (1) one expects†, for the single-particle excitations, a gap which is proportional to $|U|$. This means that only the motion and interactions of the doubly occupied sites are important. Therefore, all the terms in (1) can be dropped except for the pair-hopping term Y and nearest-neighbour Coulomb interaction V . Setting $Y = -1$ (since the η -symmetry implies $Y \leq 0$) we then obtain the effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = - \sum_{j=1}^L \left(\frac{\Delta}{2} (n_j - 1)(n_{j+1} - 1) + c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j+1,\downarrow} c_{j+1,\uparrow} + c_{j+1,\uparrow}^\dagger c_{j+1,\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \right) \quad (4)$$

with $\Delta = 2V/Y = 1$. Allowing for an interaction constant $\Delta \neq 1$ thus gives a perturbation of the original model. In this letter we want to investigate the effects of $\Delta > 1$ (i.e. $2V > Y$). Note that this perturbation destroys the η -symmetry of the original Hamiltonian.

† This can be shown explicitly for the exactly solvable cases [7,5].

In order to derive an effective spin Hamiltonian we first make a partial particle-hole transformation $c_{j\uparrow}^\dagger \rightarrow c_{j\uparrow}^\dagger$ and $c_{j\downarrow}^\dagger \rightarrow c_{j\downarrow}$ on the \downarrow -spins only. This changes $n_{j\uparrow} \rightarrow n_{j\uparrow}$ and $n_{j\downarrow} \rightarrow 1 - n_{j\downarrow}$ and transforms doubly-occupied sites into \uparrow -spins and empty sites into \downarrow -spins. The transformed effective Hamiltonian (4) now reads:

$$\mathcal{H}_{\text{eff}} = - \sum_{j=1}^L \left(\frac{\Delta}{2} (n_{j\uparrow} - n_{j\downarrow})(n_{j+1,\uparrow} - n_{j+1,\downarrow}) + c_{j\uparrow}^\dagger c_{j\downarrow} c_{j+1,\downarrow}^\dagger c_{j+1,\uparrow} + c_{j\downarrow}^\dagger c_{j\uparrow} c_{j+1,\uparrow}^\dagger c_{j+1,\downarrow} \right). \quad (5)$$

Using the spin operators introduced above and $S_j^\alpha = \frac{1}{2} \sigma_j^\alpha$ (where σ_j^α are the Pauli matrices, $\alpha = x, y, z$) the Hamiltonian (5) becomes

$$\mathcal{H}_{\text{eff}} = -\frac{1}{2} \sum_{j=1}^L (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z). \quad (6)$$

Under the particle-hole transformation—which maps the fermionic vacuum $|0\rangle$ onto the ferromagnetic state $|\downarrow \cdots \downarrow\rangle = \prod_{j=1}^L c_{j\downarrow}^\dagger |0\rangle$ —the η -pairing state (2) translates into

$$|\psi_N\rangle = (S^+)^N |\downarrow \cdots \downarrow\rangle \quad (7)$$

which is the ground state of the isotropic Heisenberg ferromagnet in the sector with fixed magnetization $S^z = N - \frac{L}{2}$.

In the following we will determine how the form (7) of the ground state changes for $\Delta > 1$ by proving a conjecture by Gaudin [8].

Hamiltonian (6) has long been known to be solvable by means of the Bethe ansatz [9, 10]. In the sector with a fixed number N of upturned spins, the eigenvalues are determined by the equations [10–12]

$$\left(\frac{\sin(\lambda_j + \frac{i\gamma}{2})}{\sin(\lambda_j - \frac{i\gamma}{2})} \right)^L = - \prod_{l=1}^N \frac{\sin(\lambda_j - \lambda_l + i\gamma)}{\sin(\lambda_j - \lambda_l - i\gamma)} \quad (8)$$

$$E = -\frac{L\Delta}{2} + 2 \sum_{j=1}^N \frac{\sinh^2 \gamma}{\cosh \gamma - \cos 2\lambda_j}. \quad (9)$$

We will consider all possible types of string solutions:

$$\lambda_{\alpha,k}^{(n)} = \lambda_\alpha^{(n)} - \frac{1}{2}i\gamma(n+1-2k) \quad (k = 1, 2, \dots, n \text{ with } n \in \mathbb{Z}_+). \quad (10)$$

Periodicity along the real axis allows one to take the real centre of the string, $\lambda_\alpha^{(n)}$, in the restricted range $(-\pi/2, \pi/2]$. As usual, it is possible to reduce (8) to a set of equations for the string centres. Choosing

$$\phi(\lambda, \alpha) \doteq i \log \left(-\frac{\sin(\lambda + i\alpha)}{\sin(\lambda - i\alpha)} \right) = 2 \arctan(\tan \lambda \coth \alpha) \quad (11)$$

we find

$$\frac{1}{2\pi} t_n(\lambda_\alpha^{(n)}) - \frac{1}{2\pi L} \left[\sum_{m \neq n} \sum_{\beta=1}^{M_m} \Theta_{n,m}(\lambda_\alpha^{(n)} - \lambda_\beta^{(m)}) + \sum_{\beta=1}^{M_n} \Theta_{n,n}(\lambda_\alpha^{(n)} - \lambda_\beta^{(n)}) \right] = \frac{I_\alpha^{(n)}}{L} \quad (12)$$

where M_m denotes the number of m -strings, $I_\alpha^{(n)}$ is integer (half-odd) if $L + M_n + 1$ is even (odd) and

$$t_n(\lambda) = \phi\left(\lambda, \frac{n\gamma}{2}\right)$$

$$\Theta_{n,m}(\lambda) = \phi\left(\lambda, \frac{\gamma}{2}(n+m)\right) + \phi\left(\lambda, \frac{\gamma}{2}|n-m|\right) + \sum_{k=1}^{\min(m,n)-1} 2\phi\left(\lambda, \frac{\gamma}{2}(n+m-2k)\right)$$

$$\Theta_{n,n}(\lambda) = \phi(\lambda, n\gamma) + \sum_{k=1}^{n-1} 2\phi(\lambda, k\gamma). \quad (13)$$

The energy of an n -string, derived from (9), is

$$e_n(\lambda) = 2 \sinh \gamma \frac{\sinh n\gamma}{\cosh n\gamma - \cos 2\lambda} \quad (14)$$

and, therefore, the total energy, neglecting the immaterial additive constant, is

$$E = 2 \sinh \gamma \sum_{n=1}^{\infty} \sum_{\beta=1}^{M_n} \frac{\sinh n\gamma}{\cosh n\gamma - \cos 2\lambda_{\beta}^{(n)}} \quad (15)$$

where $\{\lambda_{\beta}^{(n)}\}$ are the real string centres. We are interested in the ground state in a sector of fixed magnetization where

$$\sum_{n=1}^{\infty} nM_n = N \quad \lim_{L \rightarrow \infty} \frac{N}{L} = a \quad 0 < a \leq \frac{1}{2}. \quad (16)$$

In principle one should find all solutions of the Bethe ansatz equations for the string centres $\lambda_{\alpha}^{(n)}$ which are compatible with (16) and compare the respective energies. Yet, for a string of length n , the lower and upper bounds of the energy (14) are given by

$$2 \sinh \gamma \frac{\sinh n\gamma}{\cosh n\gamma + 1} \leq 2 \sinh \gamma \frac{\sinh n\gamma}{\cosh n\gamma - \cos 2\lambda} \leq 2 \sinh \gamma \frac{\sinh n\gamma}{\cosh n\gamma - 1} \quad (17)$$

for $\lambda = \pi/2$ and $\lambda = 0$ respectively. We conclude that the ground state must contain exactly one string of length N if we can show that, for any other string configuration $(M_1, M_2, \dots, M_{N-1}, 0)$ with $\sum_{n=1}^{N-1} nM_n = N$, we have

$$\frac{\sinh N\gamma}{\cosh N\gamma - 1} < \sum_{n=1}^{N-1} M_n \frac{\sinh n\gamma}{\cosh n\gamma + 1}. \quad (18)$$

First we observe that, in the sector under consideration, any configuration $(M_1, M_2, \dots, M_{N-1}, 0)$ can be obtained starting from one of the configurations where only two strings are present, $M_n = 1$, $M_m = 1$, $n+m = N$, and performing the steps in which a string is broken into two smaller strings:

$$(M_1, \dots, M_{n_1}, \dots, M_{n_2}, \dots, M_n, \dots) \rightarrow (M_1, \dots, M_{n_1}+1, \dots, M_{n_2}+1, \dots, M_n-1, \dots) \quad (19)$$

with $n_1 + n_2 = n$. In each step the RHS of (18) increases since

$$\frac{\sinh n_1\gamma}{\cosh n_1\gamma + 1} + \frac{\sinh n_2\gamma}{\cosh n_2\gamma + 1} \geq \frac{\sinh n\gamma}{\cosh n\gamma + 1} \quad (n_1 + n_2 = n). \quad (20)$$

This inequality is guaranteed by the fact that $f(0) = 0$ and $f''(x) < 0$ in $(0, +\infty)$, where $f(x) = \sinh \gamma x / (\cosh \gamma x + 1)$, and consequently $f(x_1) + f(x_2) \geq f(x_1 + x_2)$. We conclude that, to demonstrate (18), it is sufficient to consider configurations on the RHS made up of two strings only. Again concavity of $f(x)$ shows that it is sufficient to have

$$\frac{\sinh N\gamma}{\cosh N\gamma - 1} < \frac{\sinh \gamma}{\cosh \gamma + 1} + \frac{\sinh(N-1)\gamma}{\cosh(N-1)\gamma + 1} \quad (21)$$

and, for fixed γ , this is certainly the case for N large enough[†]. This concludes the proof that the ground state is given by a solution of the Bethe ansatz equations with only one N -string, confirming a result predicted by Gaudin [8]. For the isotropic case $\Delta = 1$ a similar result had already been obtained by Bethe [9].

The string centre $\lambda^{(N)}$ of the Bethe state with a single N -string (10) can easily be determined from (12). On a finite lattice there are L solutions

$$\lambda^{(N)} = \arctan \left(\tanh \frac{N\gamma}{2} \tan \frac{\pi I^{(N)}}{L} \right)$$

$$I^{(N)} = -\frac{1}{2}L + 1, -\frac{1}{2}L + 2, \dots, \frac{1}{2}L \quad (22)$$

(this holds for L both even and odd) with the ground state at $I^{(N)} = \frac{1}{2}L$ and energy given by (14). The energies of all these states become degenerate in the limit $L \rightarrow \infty$ (and consequently $N \rightarrow \infty$) with the limiting value $2 \sinh \gamma$ and energy differences vanishing like $O(e^{-N\gamma})$. Consequently we have an infinite degeneracy of the ground state.

Low-lying excitations are given by configurations where the N -string is broken into a finite number of shorter strings. In this situation, the 'interaction term' in equation (12) for the centres $\lambda_\alpha^{(n)}$ goes to zero with $1/L$. Therefore, the energy of each string coincides with the bare energy (14) and no dressing needs to be considered. In the most general excited state configuration $(M_1, M_2, \dots, M_{N-1})$ with $\sum_{n=1}^{N-1} nM_n = N$, the total number of strings $\sum_{n=1}^{N-1} M_n$ remains finite and the length of one or more strings has to diverge. Each of these diverging-length strings contributes $2 \sinh \gamma$ to the energy, regardless of its position, while the finite-length ones have energy (14). It is easily seen that the spectrum has a gap

$$\Delta E = 2(\cosh \gamma - 1) \quad (23)$$

obtained by taking $M_1 = 1, M_{N-1} = 1$.

The above results show that the ground state of the ferromagnetic XXZ chain (6) with $\Delta > 1$ at fixed magnetization $S^z = N - \frac{1}{2}L$ is a bound state of the form

$$|\psi_N\rangle = \sum_{\{x_1, \dots, x_N\}} \psi(x_1, \dots, x_N) \prod_{j=1}^N \sigma_{x_j}^+ |\downarrow \dots \downarrow\rangle. \quad (24)$$

Here $\psi(x_1, \dots, x_N)$ is a bound-state wavefunction, i.e. it decays exponentially with respect to all coordinate differences $|x_j - x_l| \rightarrow \infty$ ($j, l = 1, \dots, N$ with $j \neq l$) [8]. The wavefunction $\psi(x_1, \dots, x_N)$ for $x_1 < x_2 < \dots < x_N$ is given by the Bethe ansatz expression

$$\psi(x_1, \dots, x_N) = \sum_{P \in S_N} \prod_{j=1}^N \left[\frac{\sin(\lambda_{P(j)} - i\frac{\gamma}{2})}{\sin(\lambda_{P(j)} + i\frac{\gamma}{2})} \right]^{x_j} \prod_{\substack{j < l \\ P(j) > P(l)}} \frac{\sin(\lambda_{P(l)} - \lambda_{P(j)} + i\gamma)}{\sin(\lambda_{P(l)} - \lambda_{P(j)} - i\gamma)} \quad (25)$$

where S_N denotes the permutation group. We now specialize to the state containing exactly one N -string. It can easily be seen that only the term where P is the identity has a non-vanishing contribution. Introducing the new variables $z_0 = \frac{1}{N} \sum_{j=1}^N x_j$ and $z_j = x_{j+1} - x_j$ ($j = 1, \dots, N-1$), i.e.

$$x_j = z_0 + \frac{1}{N} \sum_{k=1}^{N-1} k z_k - \sum_{k=j}^{N-1} z_k$$

[†] Note that for large N the difference

$$\frac{\sinh(N-1)\gamma}{\cosh(N-1)\gamma + 1} - \frac{\sinh N\gamma}{\cosh N\gamma - 1}$$

is of order $e^{-N\gamma}$.

we can finally rewrite the wavefunction as

$$\psi(x_1, \dots, x_N) = C(\lambda, z_0, N) \prod_{l=1}^{N-1} \left[\left(\frac{\sin(\lambda - \frac{i\gamma}{2}(N-2l))}{\sin(\lambda - \frac{i\gamma}{2}N)} \right) \left(\frac{\sin(\lambda - \frac{i\gamma}{2}N)}{\sin(\lambda + \frac{i\gamma}{2}N)} \right)^{l/N} \right]^{z_l} \quad (26)$$

where the constant $C(\lambda, z_0, N)$ depends only on λ , z_0 and N . The form (26) shows directly that the wavefunction describes a bound state since it decays exponentially as a function of the coordinate differences $z_j = x_{j+1} - x_j$.

For the fermionic model the ground state is then of the form

$$|\psi_N\rangle = \sum_{\{x_1, \dots, x_N\}} \psi(x_1, \dots, x_N) \prod_{j=1}^N (c_{x_j \downarrow}^\dagger c_{x_j \uparrow}^\dagger) |0\rangle. \quad (27)$$

This state has no ODLRO, i.e.

$$\frac{\langle \psi_N | c_{j \downarrow}^\dagger c_{j \uparrow}^\dagger c_{l \uparrow} c_{l \downarrow} | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} \xrightarrow{|j-l| \rightarrow \infty} 0.$$

This can be seen as follows.

Using the $SU(2)$ commutation relations for $\eta_j = c_{j \uparrow} c_{j \downarrow}$ [3] it is easy to see that

$$\frac{\langle \psi_N | \eta_j^\dagger \eta_l | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} = \mathcal{N} \sum_{\{x\}} \psi^*(x_1, \dots, x_{N-1}, j) \psi(x_1, \dots, x_{N-1}, l) \quad (28)$$

where \mathcal{N} is a normalization constant. Since $\psi(x_1, \dots, x_N)$ decays exponentially as a function of all coordinate differences there is only a significant contribution to the sum in (28) from $x_1 \approx x_2 \approx \dots \approx x_{N-1} \approx j$ and $x_1 \approx x_2 \approx \dots \approx x_{N-1} \approx l$. This means that for $|j-l| \rightarrow \infty$ at least one of the factors in each term and thus the whole sum decays exponentially.

This argument shows that superconductivity in the one-dimensional supersymmetric Hubbard model is destroyed by a perturbation with $\Delta > 1$. Instead, the form of the ground state suggests a tendency to phase separation. This is not surprising since numerical investigations have shown that superconducting phases in electronic models appear quite generally in the vicinity of phase separation [13]. In higher dimensions, however, the situation is somewhat different. By analogy with the non-ideal Bose gas and preliminary results from perturbation theory [14] we expect the superconducting ground state to be stable under the type of perturbation considered here.

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