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LETTER TO THE EDITOR

New boundary bound states in an open quantum spin chain

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Abstract. New boundary bound states (BBS) are found for an integrable model with magnetic impurities located at the edges of an open Heisenberg spin chain. These bound states carry the real energy and are formed by three or five imaginary modes of the rapidities. These imaginary modes of the rapidities give non-zero antisymmetric wave functions and the moments of the centres of the bound states are zero. This indicates that these bound states result from the magnetic impurities and are localized at the edges of the correlated system. Kondo screening occurs for the antiferromagnetic spin chain with ferromagnetic-impurity–electron exchange interaction.

Magnetic impurities in one-dimensional (1D) strongly correlated electron systems or quantum spin chains have been the focus of intense investigation. These strongly correlated systems can be described in terms of a Luttinger liquid [1], and the behaviour of the impurities in these 1D quantum systems is rather different from their behaviour in a Fermi liquid [2, 3]. The availability of nonperturbative techniques has supplied us with a means for detailed understanding of the relevant physics, and some very interesting phenomena have been revealed, such as the Kondo problem [4, 2] and the pinning of bound states in low-dimensional strongly correlated electron systems and quantum spin chains. Experimentally, magnetic impurities implanted in carbon nanotubes or quantum wires and analogical phenomena (for example, x-ray boundary effects, metal point-contact spectroscopies, etc) have renewed interest in investigations of these problems.

The quantum inverse scattering method (QISM) and the Bethe ansatz (BA) techniques are very effective tools for the study of magnetic impurities in a 1D quantum system. These methods have been used successfully to deal with the Kondo impurity in a free electron host, the magnetic impurities in spin chains and the mixed valent behaviour of hybridization (Anderson-like, with hybridized impurity and host wave functions) [5–7]. Recently, the properties of magnetic impurities in correlated electron hosts have been studied in a series of very interesting papers [8, 9]. *Periodic* boundary conditions were imposed on the electron host and spin chains for all these cases. Kane and Fisher investigated a 1D repulsive interacting system in the presence of a potential barrier and pointed out that it corresponds to a chain disconnected at the barrier site at low energy scales [10]. This can be effectively described by *open* boundary conditions, which have been extensively investigated using the boundary conformal field theory [11] and the BA methods [12, 13]. Zvyagin found that the low-energy magnetic behaviour of an impurity in a chain with periodic boundary conditions and a chain with open boundary conditions coincides up to mesoscopic corrections of order of L^{-1}, where L is the length of the system [9]. We know that several methods have been used for introducing impurities into the integrable models of correlated electrons and quantum spin chains with the *open* boundary conditions. The first method for the construction of impurity models is dependent mainly on the idea that the spectral parameters in the scattering matrix of the

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model rely on the differences in the particles' rapidities. This method has been used by Eckle, Punnoose and Römer [7] to create the impurity model of 1D quantum lattice gases with periodic conditions, where the integrable condition continues to be satisfied under an arbitrary local shift of the related parameter (see, for example [14]). The second method depends on the fact that the scattering matrix of the bulk of the $t - J$ model relies on the tangent (or cotangent) functions of the half moments of the electrons [15]. The interesting thing is that the Hamiltonian corresponding to the magnetic impurities has a simple and compact form [16], which is different from its form in the open Hubbard impurity model [17]. The boundary scattering matrix between the impurity and the electron can be factorized into two terms: one is similar to the R matrix and the other is similar to the inverse of the R matrix with an inverse spectral parameter, as correctly obtained by Zvyagin and Johannesson in their very interesting study [18]. Zvyagin and Johannesson revealed the existence of a hidden Kondo effect driven by forward electron scattering from the impurity related to this property of the boundary scattering matrix.

As is well known, bound states can be formed for strongly correlated electron systems and quantum spin chains within the charge or spin sectors, and they are very important for the determination of the thermodynamical and low temperature properties of the system. Despite the success of the QISM and BA approaches to the investigation of the magnetic impurities in a correlated system, it is not very clear whether the impurities contribute to the bound states of the strongly correlated system with *open* boundary conditions. In this letter, we discuss this problem in detail.

In general, a bound state can be formed by several complex rapidities of particles, such as charges or spins. The total energy and the total moments of these complex modes should be real. Under open boundary conditions, the rapidities u_j of the charges or spins should satisfy also that $u_j \neq \pm u_l$ when $j \neq l$. Otherwise, the wave function is zero, which means that formation of a bound state is forbidden. When the complex rapidities form a bound state, the above three conditions should be satisfied for the correlated system under the open boundary conditions. For clarity we focus here on the case of the quantum Heisenberg model. When the two impurities with arbitrary spins are coupled to this open quantum spin chain, the Hamiltonian of the system can be written as

$$H = \frac{J}{2} \sum_{j=1}^{N-1} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + J_L \vec{\sigma}_1 \cdot \vec{S}_L + J_R \vec{\sigma}_N \cdot \vec{S}_R \tag{1}$$

where $\vec{\sigma}_j$ are the Pauli matrices and $\vec{S}_{L,R}$ are the impurity moments with arbitrary spins $S_{L,R}$. The site number of the bulk is N. $J_{L,R}$ are two arbitrary real constants which describe the coupling between the bulk, and the impurities and can be parameterized as

$$J_{L,R} = \frac{J}{\left(S_{L,R} + \frac{1}{2}\right)^2 - c_{L,R}^2} \tag{2}$$

with the arbitrary constants $c_{L,R}$. This Hamiltonian can be diagonalized using the standard Bethe ansatz scheme. The eigenvalue of the energy of this impurity system is

$$E(\lambda_1, \lambda_2, \ldots, \lambda_M) = \sum_{j=1}^{M} \frac{-J}{\lambda_j^2 + \frac{1}{4}} + \sum_{l=L,R} J_l S_l + \frac{J(N-1)}{2}$$

with the following Bethe ansatz equation:

$$\left(\frac{\lambda_j + \frac{\mathrm{i}}{2}}{\lambda_j - \frac{\mathrm{i}}{2}}\right)^{2N} \prod_{l=L,R} \prod_{r=\pm 1} \frac{\lambda_j + \mathrm{i}\,(S_l + r c_l)}{\lambda_j - \mathrm{i}\,(S_l + r c_l)}$$

$$= \prod_{l=1(l\neq j)}^{M} \prod_{r=\pm 1} \frac{\lambda_j + r\lambda_l + \mathrm{i}}{\lambda_j + r\lambda_l - \mathrm{i}}. \tag{3}$$

Now we study the boundary bound states in detail for the above Heisenberg impurity model. From equation (2) we know that $-c_{L,R}$ is equivalent to $c_{L,R}$ because they give the same Hamiltonian (equation (1)). So, without losing generality, we restrict the parameters $c_{L,R}$ to non-negative values in the following discussion.

When the coupling in the bulk is antiferromagnetic ($J > 0$) and the coupling between the bulk and the impurity is ferromagnetic, the system has the following boundary bound states (BBS):

$$\lambda_{3,1} = \mathrm{i}(S_{L,R} - c_{L,R}) \tag{4}$$

$$\lambda_{3,2} = -\frac{\mathrm{i}}{2}(S_{L,R} - c_{L,R} - 1) \tag{5}$$

$$\lambda_{3,3} = -\frac{\mathrm{i}}{2}(S_{L,R} - c_{L,R} + 1) \tag{6}$$

where $S_{L,R} + 1/2 < c_{L,R} < S_{L,R} + 1$. These two BBS, one BBS for each end (L and R) of the chain, are formed by the three imaginary modes of λ. They carry the energy

$$E^{(3)}_{L,R} = \frac{12J\left[3(S_{L,R} - c_{L,R})^2 - 2\right]}{\left[4(S_{L,R} - c_{L,R})^2 - 1\right]\left[(S_{L,R} - c_{L,R})^2 - 4\right]}. \tag{7}$$

The moments of the centres of the BBS are $\sum_{j=1}^{3} \lambda_{3,j} = 0$. This means that these kinds of bound state are localized at the edges of the system. Of course, the energy and the moments of the centres of the BBS are all real and the spin rapidities satisfy $\lambda_{3,1} \neq \pm\lambda_{3,2} \neq \lambda_{3,3} \neq \pm\lambda_{3,1}$, which ensures that the antisymmetric wave functions of the system are not zero. Therefore, these BBS satisfy all the physical demands. The BBS for the three imaginary modes can also be obtained for the Heisenberg impurity model with $S_{L,R} + 1/2 < c_{L,R} < S_{L,R} + 1$ by making the transformations $\lambda_{3,j} \to -\lambda_{3,j}$ ($j = 1, 2, 3$) in the relations (4–6). They also carry energy in the form described by equation (7).

When the coupling in the bulk is antiferromagnetic ($J > 0$) and the coupling between the bulk and the impurity also falls into the antiferromagnetic regime, the above BBS (equations (4–6)) with the three imaginary modes are formed under the condition $1/3 + S_{L,R} < c_{L,R} < 1/2 + S_{L,R}$. The corresponding imaginary modes with the transformations $\lambda_{3,j} \to -\lambda_{3,j}$ ($j = 1, 2, 3$) are also the BBS in this case. The energy expression (7) does not change the forms and the moments of the centres of the bound states are also zero. By taking the logarithm of the Bethe ansatz equation (3) and introducing the distribution functions of the spin rapidities, we can get the integral equations of the impurity model for the ground state. Thus we find that the self-magnetization of the ground state is $S_L + S_R - 1$ for the two up impurity spins, or $1 - S_L - S_R$ for the two down impurity spins, or $\pm(S_L - S_R)$ for the one up and one down impurity spins. A similar procedure gives the result that the self-magnetization of the ground state is also $\pm(S_L - S_R)$ when the coupling in the bulk is antiferromagnetic but the coupling between the bulk and the impurity is ferromagnetic. When the parameters $c_{L,R}$, which describe the coupling between the impurities and the bulk, satisfy $S_{L,R} < c_{L,R} < S_{L,R} + 1/3$, there exist the BBS formed by the three imaginary modes as described by relations (4–6) and the BBS formed by the transformations $\lambda_{3,j} \to -\lambda_{3,j}$ ($j = 1, 2, 3$). They carry the energy described by equation (7) and have the zero moments of the centres of the BBS. In this case, the coupling between the bulk and the impurities is in the antiferromagnetic regime if the exchange interaction in the bulk is antiferromagnetic also. Furthermore, in the case where $S_{L,R} < c_{L,R} < S_{L,R} + 1/3$ there are two bound states (one for each end of the chain) formed by the following five imaginary modes of λ

$$\lambda_{5,1} = \mathrm{i}(S_{L,R} - c_{L,R}) \tag{8}$$

$$\lambda_{5,2} = \mathrm{i}(S_{L,R} - c_{L,R} + 1) \tag{9}$$

$$\lambda_{5,3} = \mathrm{i}(S_{L,R} - c_{L,R} - 1) \tag{10}$$

$$\lambda_{5,4} = -\frac{\mathrm{i}}{2}(3S_{L,R} - 3c_{L,R} - 1) \tag{11}$$

$$\lambda_{5,5} = -\frac{\mathrm{i}}{2}(3S_{L,R} - 3c_{L,R} + 1). \tag{12}$$

They carry the energy

$$E^{(5)}_{L,R} = \frac{20J\left[7(S_{L,R} - c_{L,R})^2 - 6\right]}{\left[9(S_{L,R} - c_{L,R})^2 - 4\right]\left[4(S_{L,R} - c_{L,R})^2 - 9\right]}. \tag{13}$$

The moments of the centres of the above bound states formed by the five imaginary modes of λ are $\sum_{j=1,2,\ldots,5} \lambda_{5,j} = 0$. Therefore, they localize at the two edges of the Heisenberg spin chain and $\lambda_{5,j} \neq \pm\lambda_{5,l}$ if $j \neq l$ ($j, l = 1, 2, \ldots, 5$), which ensures that the system has a non-zero antisymmetric wave function. Similar to the case of the BBS of the three imaginary modes, the transformations $\lambda_{5,j} \to -\lambda_{5,j}$ ($j = 1, 2, \ldots, 5$) also give the boundary bound states of the system; they do not change the expression of the energy and the moments of the centres of the bound states are also zero. Using the method mentioned above, we find that the self-magnetization of the model is the same as for the situation $1/3+S_{L,R} < c_{L,R} < 1/2+S_{L,R}$. The above BBS satisfy the three conditions for the complex modes.

In the following section, we describe simply the self-magnetization and the BBS of the ferromagnetic Heisenberg impurity model. By solving the Bethe ansatz equations in the thermodynamic limit, we find that the self-magnetization of the system is $S_L + S_R + N/2$ when the coupling between the impurities and the bulk is also ferromagnetic. Otherwise, the self-magnetization is $-S_L - S_R + N/2$ for the antiferromagnetic exchange interaction between the impurities and the bulk. When one impurity has a ferromagnetic interaction with the bulk and another impurity has an antiferromagnetic interaction with the bulk, the self-magnetization of the system has the form $\pm(S_L - S_R) + N/2$. When $S_{L,R} + 1/2 < c_{L,R} < S_{L,R} + 1$, the system has the BBS formed by the three imaginary modes (equations (4–6)) and the BBS carry the energy given by equation (7). If the transformations $\lambda_{3,j} \to -\lambda_{3,j}$ ($j = 1, 2, 3$) are made, the corresponding bound states are also the BBS of the system. They satisfy all of the three conditions and the coupling between the bulk and the impurities is antiferromagnetic. When the coupling between the bulk and the impurities is ferromagnetic, the system has BBS which can be formed by the three imaginary modes (equations (4–6)) or the five imaginary modes (equations (8–12)) with $S_{L,R} < c_{L,R} < S_{L,R} + 1/3$. They have energies as described by expressions (7) and (13). Of course, the corresponding imaginary modes with transformations $\lambda_{3,j} = -\lambda_{3,j}$ ($j = 1, 2, 3$) and $\lambda_{5,l} = -\lambda_{5,l}$ ($l = 1, 2, \cdots, 5$) form also the BBS of the impurity model. When $1/3 + S_L < c_L < S_L + 1/2$ we have the BBS of equations (4–6) or the inverse of the rapidities, and the exchange interaction between the bulk and the impurities is ferromagnetic. Notice that the system may have other forms of the impurity bound states in the above restricted range of the impurity couplings $J_{L,R}$. It is also an open problem to find out the impurity bound states for other values of the impurity couplings for the strongly correlated system.

The above discussion shows that the ferromagnetic and antiferromagnetic Heisenberg spin chains with magnetic impurities always have BBS resulting from the impurities when the strengths of the interactions between the bulk and the impurities are chosen properly. These bound states carry real energy and the moments of the centres of the BBS are zero.

They satisfy all three conditions of the imaginary modes. For the ferromagnetic Heisenberg model where the coupling between the bulk and the impurities is ferromagnetic the system has BBS formed by the three imaginary modes and the five imaginary modes of the spin rapidities. When the coupling between the bulk and the impurities is antiferromagnetic, the system has only BBS contained in the three imaginary modes of the rapidities. For the antiferromagnetic Heisenberg model, the system has BBS formed by the three imaginary modes and the five imaginary modes of the spin rapidities when the coupling between the bulk and the impurities is antiferromagnetic. When the coupling between the bulk and the impurities is ferromagnetic, the system has only the BBS contained in the three imaginary modes of the rapidities. Kondo screening—as predicted by Furusaki and Nagaosa [2]—exists for the antiferromagnetic Heisenberg model with ferromagnetic coupling between the bulk and the impurities. At zero impurity couplings ($J_{L,R} = 0$), the system has impurity bound states (although trivial ones), which correspond to the $2S_{L,R}+1$ spin states of the impurity. By turning on the boundary coupling, the BBS can be formed by the imaginary modes of the rapidities and the number of BBS might change. The BBS can affect the ground state of the whole system when the boundary coupling is strong enough; this is under investigation. New properties of the specific heat, excited state, dressed energy, etc, can be introduced due to the impurity couplings. We point out that similar BBS with three or five imaginary modes contributed by the magnetic impurities can be found also for strongly correlated electron systems such as the Hubbard model and the $t - J$ model with open boundary conditions in the charge sectors. The BBS carry energy and satisfy the three conditions of the imaginary modes. Finally, the way the string affects the distribution of the rapidities is also the interesting subject for the further investigation.

To conclude, we have found that BBS result from magnetic impurities in a correlated host under open boundary conditions. These BBS are formed by three or five imaginary modes such as charges or spins. The imaginary modes of the bound states due to the magnetic impurities satisfy that: (i) the total energy is real; (ii) the total moment of the imaginary modes is real (zero); (iii) the absolute values of the imaginary modes are different. These BBS carry energy and are localized at the edges of the system. Kondo screening exists for the antiferromagnetic Heisenberg model with ferromagnetic coupling between the bulk and the impurities.

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