Integrable impurities for an open fermion chain

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Abstract. Employing the graded versions of the Yang-Baxter equation and the reflection equations, we construct two kinds of integrable impurities for a small-polaron model with general open boundary conditions: (a) we shift the spectral parameter of the local Lax operator at arbitrary sites in the bulk, and (b) we embed the impurity fermion vertex at each boundary of the chain. The Hamiltonians with different types of impurity terms are given explicitly. The Bethe ansatz equations, as well as the eigenvalues of the Hamiltonians, are constructed by means of the quantum inverse scattering method. In addition, we discuss the ground-state properties in the thermodynamic limit.

Revision : 1.16

PACS numbers: 71.10.Fd, 71.10.Pm, 71.55.-i, 72.10.Fk

Submitted to: *J. Phys. A: Math. Gen.*

1. Introduction

The interplay between disorder and many-body interactions continues to be one of the main topics of condensed matter physics. In one-dimensional quantum many-body systems without disorder, the Bethe ansatz (BA) has proven to be a valuable tool, giving access to the energy spectra and eigenstates of certain so-called integrable models [1, 2]. At first glance, it appears that the integrability, namely the existence of infinitely many integrals of motion, seems to preclude any applications of the method to disordered systems. However, in 1984 it was shown [3, 4] how to apply the BA method to the Kondo problem [5] of a single magnetic impurity in a bath of conduction electrons. Further developments led to the construction and solution of integrable spin chains with embedded spin defects [6, 7].

A different approach to integrable impurity models was considered in references [8] where impurity vertices are introduced by varying the *local* interaction parameters while preserving integrability. These studies have stimulated further investigations [9, 10] of such impurities in various systems. The resulting models have impurity terms with couple to the charge degrees of freedom, and look fairly similar to generic impurity terms. However, the energy spectrum is independent of the spatial distribution of the defects, and there is no localization of the ground-state wave function, unlike what is expected for generic impurities. This peculiar behaviour can be understood by the fact that integrability implies a purely forward-scattering mechanism at the impurities [10]. There is no reflection and thus no possibility of destructive quantum interference which could lead to a localization.

Back-scattering can be introduced into integrable models by choosing suitable boundary conditions (BC). Sklyanin [11] proposed a systematic approach to construct and solve integrable quantum spin systems with *open* BC. Central to his method are the so-called reflection equations (RE) [12] which are the boundary analogues of the Yang-Baxter equations (YBE) [13]. Together, the YBE and RE imply the integrability of a model which can then be constructed as usual by the algebraic approach of the quantum inverse scattering method (QISM) [14]. The finite-size corrections of the corresponding energy spectra and the asymptotic behaviour of correlation functions follow predictions based on boundary conformal field theory [15]. We remark that the BC of Sklyanin [11] are called "open" in order to distinguish them from the more often used periodic and the free BC. Although the term "open" seems to suggest particular transmission and reflection properties, this is not necessarily implied. The combination of open BC and integrable impurities has been considered in references [16, 17, 18, 19]. Of particular interest is the case where the forward-scattering impurity is directly coupled to a back-scattering open boundary [18, 19]. This combination may lead to physically relevant, yet completely integrable models.

In the present article, we construct two kinds of integrable impurities for a fermionic small-polaron model with general open BC. Due to the fermionic nature of the model, we employ the graded version of the QISM [20, 21]. For well-separated impurity vertices located within the bulk, the local interaction terms involve the two neighbouring sites as usual [8]. Placing the forward-scattering impurities at the back-scattering boundaries, we derive a Hamiltonian with rather general boundary terms which may be interpreted as sources and sinks of particles at the boundaries. Using the graded YBE and the graded RE, we derive the BA equations, and obtain expressions for the eigenvalues for special cases of the Hamiltonian. In addition, we discuss the ground-state properties in the thermodynamic limit.

The paper is organized as follows. In section 2, we introduce the small-polaron model with general open BC. In section 3, a class of integrable impurities is constructed by shifting the spectral parameters of local Lax operators at arbitrary sites in the bulk. By embedding the impurity fermion vertex at each boundary of the model, we construct a class of integrable impurities with perfect back-scattering in section 4. In section 5, we study the algebraic BA solutions for those impurity models. The ground-state properties are discussed in section 6. Section 7 is devoted to a discussion and conclusion.

2. The small-polaron model

We consider the small-polaron model [22], which describes the motion of an additional electron in a polar crystal. The Hamiltonian reads

$$\begin{aligned}\boldsymbol{H} = & -J\sum_{j=2}^{N}(\boldsymbol{a}_j^\dagger\boldsymbol{a}_{j-1}+\boldsymbol{a}_{j-1}^\dagger\boldsymbol{a}_j) + V\sum_{j=2}^{N}\boldsymbol{n}_j\boldsymbol{n}_{j-1} + W\sum_{j=1}^{N}\boldsymbol{n}_j \\ & + p_+\boldsymbol{n}_N + \alpha_+\boldsymbol{a}_N^\dagger + \beta_+\boldsymbol{a}_N + p_-\boldsymbol{n}_1 + \alpha_-\boldsymbol{a}_1^\dagger + \beta_-\boldsymbol{a}_1, \end{aligned} \tag{2.1}$$

where J is proportional to the overlap integral, V denotes the electron-phonon coupling and W is the energy of the polaron. The boundary coefficients $p_\pm$, $\alpha_\pm$ and $\beta_\pm$ are Grassmann variables, with $p_\pm$ even and $\alpha_\pm$, $\beta_\pm$ odd. Hermiticity of the Hamiltonian requires $\alpha_\pm^\dagger = \beta_\pm$ and $p_\pm^\dagger = p_\pm$. The fermionic creation and annihilation operators $\boldsymbol{a}_j^\dagger$ and $\boldsymbol{a}_j$ satisfy the usual anticommutation relations

$$\{\boldsymbol{a}_j,\boldsymbol{a}_k\} = \{\boldsymbol{a}_j^\dagger,\boldsymbol{a}_k^\dagger\} = 0, \qquad \{\boldsymbol{a}_j,\boldsymbol{a}_k^\dagger\} = \delta_{j,k}, \tag{2.2}$$

and $\boldsymbol{n}_j = \boldsymbol{a}_j^\dagger\boldsymbol{a}_j$. The R-matrix and local monodromy matrix are explicitly given as [23]

$$R_{12}(u_1,u_2) = \begin{pmatrix} a''_+ & 0 & 0 & 0 \\ 0 & -ib''_- & c'' & 0 \\ 0 & c'' & ib''_+ & 0 \\ 0 & 0 & 0 & -a''_- \end{pmatrix} \tag{2.3}$$

and

$$\boldsymbol{L}_j(u) = \begin{pmatrix} b'_+ + (ia'_+ - b'_+)\boldsymbol{n}_j & c'\boldsymbol{a}_j \\ -ic'\boldsymbol{a}_j^\dagger & a'_- - (a'_- + ib'_-)\boldsymbol{n}_j \end{pmatrix}, \tag{2.4}$$

respectively. They satisfy the graded Yang-Baxter algebra (YBA)

$$R_{12}(u_1,u_2)\overset{1}{\boldsymbol{T}}(u_1)\overset{2}{\boldsymbol{T}}(u_2) = \overset{2}{\boldsymbol{T}}(u_2)\overset{1}{\boldsymbol{T}}(u_1)R_{12}(u_1,u_2), \tag{2.5}$$

where

$$\boldsymbol{T}(u) = \boldsymbol{L}_N(u) \cdots \boldsymbol{L}_2(u)\boldsymbol{L}_1(u), \tag{2.6}$$

and

$$\overset{1}{X} \equiv X \otimes_S \mathrm{id}_{V_2}; \quad \overset{2}{X} \equiv \mathrm{id}_{V_1} \otimes_S X. \tag{2.7}$$

Here, $\otimes_S$ is the supertensor product

$$[A \otimes_S B]_{\alpha\beta,\gamma\delta} = (-1)^{[P(\alpha)+P(\gamma)]P(\beta)} A_{\alpha\gamma} B_{\beta\delta} \tag{2.8}$$

with the parity $P(1) = 0$, $P(2) = 1$ such that the R-matrix correspond to the null parity case $P(\alpha) + P(\beta) + P(\gamma) + P(\delta) = 0$ [20]. We parametrize the coupling parameters J, V and W as

$$J = 1, \tag{2.9a}$$
$$V = -2c_2(0), \tag{2.9b}$$
$$W = 2s_2(0)\tan(w) + 2c_2(0). \tag{2.9c}$$

The entries of the R-matrix (2.3) and the monodromy matrix (2.4) are

$$a''_\pm = \xi_+^{\pm 1}(u_1)\xi_+^{\mp 1}(u_2)s_2(u_1 - u_2), \tag{2.10a}$$
$$b''_\pm = \xi_+^{\pm 1}(u_1)\xi_+^{\pm 1}(u_2)s_0(u_1 - u_2), \tag{2.10b}$$
$$c'' = c' = s_2(0), \tag{2.10c}$$
$$a'_\pm = \xi_+^{\pm 1}(u)s_2(u), \tag{2.10d}$$
$$b'_\pm = \xi_+^{\mp 1}(u)s_0(u), \tag{2.10e}$$
$$\xi_\pm(u) = \frac{c_0(u \pm w)}{c_0(u)c_0(w)}, \tag{2.10f}$$

where we introduced the convenient notation

$$s_n(u) \equiv \sin(u + n\eta), \quad c_n(u) \equiv \cos(u + n\eta). \tag{2.11}$$

Throughout the paper, we therefore use η and w for the parametrization of the model parameters J, V, and W.

In a previous article [24], we proved that the model (2.1) is integrable under the conditions that the boundary $K_\pm$ supermatrices

$$K_\pm(u) = \begin{pmatrix} K_{11}^\pm & K_{12}^\pm \\ K_{21}^\pm & K_{22}^\pm \end{pmatrix} \tag{2.12}$$

take the form

$$K_{11}^- = \xi_+ s_0(u - \psi_-)\left[\xi_-^2 s_2(u) - \xi_+^2 s_{-2}(u)\right], \tag{2.13a}$$
$$K_{22}^- = \xi_- s_0(u + \psi_-)\left[\xi_-^2 s_{-2}(u) - \xi_+^2 s_2(u)\right], \tag{2.13b}$$
$$K_{12}^- = -\frac{\alpha_- s_0(\psi_-)s_0(u)}{i\xi_+\xi_- s_2^2(0)}\left[\xi_-^2 s_2(u) - \xi_+^2 s_{-2}(u)\right]\left[\xi_+^2 s_2(u) - \xi_-^2 s_{-2}(u)\right], \tag{2.13c}$$
$$K_{21}^- = -\frac{\beta_- s_0(\psi_-)s_0(u)}{i s_2^2(0)}\left[\xi_-^2 s_2(u) - \xi_+^2 s_{-2}(u)\right]\left[\xi_+^2 s_2(u) - \xi_-^2 s_{-2}(u)\right], \tag{2.13d}$$
$$K_{11}^+ = \xi_+ s_2(u - \psi_+)\left[\xi_-^2 s_4(u) - \xi_+^2 s_0(u)\right], \tag{2.13e}$$

$$K_{22}^{+}=\xi_{-}s_2(u+\psi_+)\left[\xi_+^2s_4(u)-\xi_-^2s_0(u)\right], \tag{2.13f}$$

$$K_{12}^{+}=-\frac{\alpha_+s_0(\psi_+)s_2(u)}{i\xi_+\xi_-s_2^2(0)}\left[\xi_-^2s_4(u)-\xi_+^2s_0(u)\right]\left[\xi_+^2s_4(u)-\xi_-^2s_0(u)\right], \tag{2.13g}$$

$$K_{21}^{+}=-\frac{\beta_+s_0(\psi_+)s_2(u)}{is_2^2(0)}\left[\xi_-^2s_4(u)-\xi_+^2s_0(u)\right]\left[\xi_+^2s_4(u)-\xi_-^2s_0(u)\right]. \tag{2.13h}$$

Here we would like to emphasize that although we [24] construct the general boundary K-matrices (2.12) for the small-polaron model (2.1) by the Lax pair formulation, we did not figure out the form of the RE corresponding to more general boundary K-matrices (2.12). In the above expressions, we further defined

$$p_{\pm}=s_2(0)\cot\psi_{\pm}. \tag{2.14}$$

The parameters $\psi_{\pm}$ control the strength of the boundary potential terms, whereas $\alpha_{\pm}$ and $\beta_{\pm}$ in (2.13*a*)–(2.13*h*) are the parameters characterizing the fermion sources and sinks at the boundaries. The Hamiltonian (2.1) can be obtained as usual as an invariant of the commuting family of transfer matrices $\boldsymbol{\tau}(u)$

$$\boldsymbol{\tau}(u)=\mathrm{Str}_0[K_+(u)\boldsymbol{T}(u)K_-(u)\boldsymbol{T}^{-1}(-u)] \tag{2.15}$$

by taking the derivative at a special value of the spectral parameter u. Namely,

$$-s_2(0)\left.\frac{d}{du}\boldsymbol{\tau}(u)\right|_{u=0}=2\boldsymbol{H}\boldsymbol{\tau}(0)+\mathrm{Str}_0\left(\left.\frac{d}{du}K_+(u)\right|_{u=0}\right), \tag{2.16}$$

with Str_0 denoting the supertrace with respect to the auxiliary space.

3. Integrable impurities in the bulk

In this section, we construct integrable impurities which appear in the bulk part for the fermionic small-polaron model with general open BC. If the quantum R-matrix of a fermionic system has the difference property of spectral parameters, the associated Lax operator with additional parameter also satisfies the graded YBA, i.e.,

$$R_{12}(u_1-u_2)\overset{1}{\boldsymbol{L}}(u_1+\nu)\overset{2}{\boldsymbol{L}}(u_2+\nu)=\overset{2}{\boldsymbol{L}}(u_2+\nu)\overset{1}{\boldsymbol{L}}(u_1+\nu)R_{12}(u_1-u_2). \tag{3.1}$$

Therefore one can construct a class of integrable impurities for the fermion model with both open and periodic BC by shifting the spectral parameters of local monodromy matrices at arbitrary sites in the bulk. The associated monodromy matrix is given as

$$\boldsymbol{T}(u)\quad=\boldsymbol{L}_N(u)\cdots\boldsymbol{L}_m(u+\nu_m)\cdots\boldsymbol{L}_1(u) \tag{3.2a}$$

$$\boldsymbol{T}^{-1}(-u)=\boldsymbol{L}_1^{-1}(-u)\cdots\boldsymbol{L}_m^{-1}(-u+\nu_m)\cdots\boldsymbol{L}_N^{-1}(-u), \tag{3.2b}$$

where the parameter ν_m characterizes the impurity strength at site m. Now we suppose that the supermatrices $K_{\pm}$ are the solutions of the graded RE [25, 26],

$$\begin{aligned}&R_{12}(u_1-u_2)\overset{1}{K}_-(u_1)R_{21}(u_1+u_2)\overset{2}{K}_-(u_2)=\\&\qquad\overset{2}{K}_-(u_2)R_{12}(u_1+u_2)\overset{1}{K}_-(u_1)R_{21}(u_1-u_2),\end{aligned} \tag{3.3a}$$

$$\begin{aligned}&R_{21}^{\mathrm{St_1iSt_2}}(-u_1+u_2)\overset{1}{K}{}_+^{\mathrm{St_1}}(u_1)R_{12}(-u_1-u_2-4\eta)\overset{2}{K}{}_+^{\mathrm{iSt_2}}(u_2)=\\&\qquad\overset{2}{K}{}_+^{\mathrm{iSt_2}}(u_2)R_{21}(-u_1-u_2-4\eta)\overset{1}{K}{}_+^{\mathrm{St_1}}(u_1)R_{12}^{\mathrm{St_1iSt_2}}(-u_1+u_2),\end{aligned} \tag{3.3b}$$

where $R_{21}(u) = \mathcal{P}R_{12}(u)\mathcal{P}$ with the graded permutation

$$\mathcal{P}_{\alpha\beta,\gamma\delta} = (-1)^{P(\alpha)P(\beta)}\delta_{\alpha\delta}\delta_{\beta\gamma}, \tag{3.4}$$

and iSt_α denotes the inverse operation of the supertransposition St_α in the space α. The R-matrix possesses the unitary property $R_{12}(u)R_{21}(-u) = \rho(u)I$, with $\rho(u)$ a scalar function of u. It follows that the double-row transfer matrix (2.15) may be considered as a generating function of the infinite conserved quantities such that the K-matrices are the solutions to the RE (3.3*a*) and (3.3*b*). From the relation (2.16), it is not difficult to obtain the Hamiltonian for the open fermion chain with an impurity located at site m,

$$\begin{aligned}\boldsymbol{H} = &\sum_{\substack{j=2\\ j\neq m,m-1}}^{N} \boldsymbol{H}_{j,j-1} + \frac{1}{2}\boldsymbol{L}_1(0)K'_-(0)\boldsymbol{L}_1^{-1}(0) + \frac{\mathrm{Str}_0[K_+(0)\boldsymbol{L}'_N(0)\boldsymbol{L}_N^{-1}(0)]}{\mathrm{Str}_0[K_+(0)]}\\ &+ \boldsymbol{C}_{m,m-1}\boldsymbol{B}_{m,m-1} + \boldsymbol{A}_{m,m-1}\boldsymbol{H}_{m-1,m-2}\boldsymbol{B}_{m,m-1}\end{aligned} \tag{3.5}$$

where

$$\boldsymbol{H}_{j,j-1} = \boldsymbol{L}_{j-1}(0)\,\boldsymbol{L}'_j(0)\,\boldsymbol{L}_j^{-1}(0)\,\boldsymbol{L}_{j-1}^{-1}(0), \tag{3.6a}$$

$$\boldsymbol{A}_{m,m-1} = \boldsymbol{L}_{m-1}(0)\,\boldsymbol{L}_m(\nu_m)\,\boldsymbol{L}_m^{-1}(0)\,\boldsymbol{L}_{m-1}^{-1}(0), \tag{3.6b}$$

$$\boldsymbol{B}_{m,m-1} = \boldsymbol{L}_{m-1}(0)\,\boldsymbol{L}_m(0)\,\boldsymbol{L}_m^{-1}(\nu_m)\,\boldsymbol{L}_{m-1}^{-1}(0), \tag{3.6c}$$

$$\boldsymbol{C}_{m,m-1} = \boldsymbol{L}_{m-1}(0)\,\boldsymbol{L}'_m(\nu_m)\,\boldsymbol{L}_m^{-1}(0)\,\boldsymbol{L}_{m-1}^{-1}(0). \tag{3.6d}$$

The prime denotes the derivative with respect to the spectral parameter u. The interactions of the open fermion chain with the impurity are shown schematically in figure 1.

In order to simplify the algebraic calculation for the construction of such an integrable impurity for the model (2.1), we let $w = 0$ the supermatrices (2.12) become (up to a normalization)

$$K_-(u) = \frac{1}{s_0(\psi_-)}\begin{pmatrix} -s_0(u-\psi_-) & \alpha_- s_0(2u)\\ \beta_- s_0(2u) & s_0(u+\psi_-)\end{pmatrix}, \tag{3.7a}$$

$$K_+(u) = \begin{pmatrix} s_2(u-\psi_+) & \alpha_+ s_4(2u)\\ \beta_+ s_4(2u) & s_2(u+\psi_+)\end{pmatrix}. \tag{3.7b}$$

Then we check that the supermatrices (3.7*a*) and (3.7*b*) satisfy the graded RE (3.3*a*) and (3.3*b*), respectively. From (3.5), after some algebra, we obtain the Hamiltonian for the small-polaron model with both general open BC and an integrable impurity located at site m as

$$\boldsymbol{H} = \sum_{j=2}^{N} \boldsymbol{H}_{j,j-1} + \boldsymbol{H}_1^{(\mathrm{b})} + \boldsymbol{H}_N^{(\mathrm{b})} + \boldsymbol{H}_{m,m-1,m-2}^{(\mathrm{h})} + \boldsymbol{H}_{m,m-1,m-2}^{(\mathrm{d})} + \boldsymbol{H}_{m,m-1,m-2}^{(\mathrm{c})} \tag{3.8}$$

with

$$\boldsymbol{H}_{j,j-1} = \boldsymbol{a}_j^\dagger \boldsymbol{a}_{j-1} + \boldsymbol{a}_{j-1}^\dagger \boldsymbol{a}_j + 2c_2(0)\,\boldsymbol{n}_j\boldsymbol{n}_{j-1} - 2c_2(0)\,\boldsymbol{n}_j, \tag{3.9a}$$

$$\boldsymbol{H}_1^{(\mathrm{b})} = -\frac{s_2(0)}{s_0(\psi_-)}\left[c_0(\psi_-)\,\boldsymbol{n}_1 - i\alpha_-\,\boldsymbol{a}_1^\dagger - i\beta_-\,\boldsymbol{a}_1\right], \tag{3.9b}$$

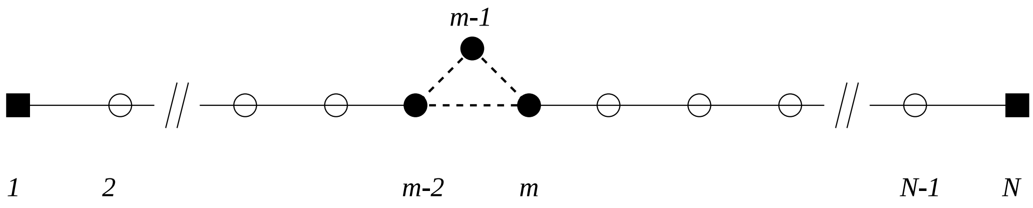

Figure 1. Graphical representation of the interactions in the chain with the impurity located at an arbitrary site m together with boundary impurities.

$$\boldsymbol{H}_N^{(\mathrm{b})} = -\frac{s_2(0)}{s_0(\psi_+)}\left[c_0(\psi_+)\,\boldsymbol{n}_N - i\alpha_+\,\boldsymbol{a}_N^\dagger - i\beta_+\,\boldsymbol{a}_N\right], \tag{3.9c}$$

$$\boldsymbol{H}^{(\mathrm{h})}_{m,m-1,m-2} = \left\{\frac{s_2(0)-s_2(\nu_m)}{s_2(\nu_m)}\left[\boldsymbol{a}^\dagger_{m-1}\boldsymbol{a}_{m-2} + \boldsymbol{a}^\dagger_m\boldsymbol{a}_{m-1}\right] + \frac{s_0(\nu_m)}{s_{-2}(\nu_m)}\boldsymbol{a}^\dagger_{m-2}\boldsymbol{a}_m\right\} + \text{h.c.}, \tag{3.9d}$$

$$\boldsymbol{H}^{(\mathrm{d})}_{m,m-1,m-2} = \frac{2c_2(0)s_0^2(\nu_m)}{\Delta(\nu_m)}\left[\boldsymbol{n}_m\boldsymbol{n}_{m-2} - \boldsymbol{n}_m\boldsymbol{n}_{m-1} - \boldsymbol{n}_{m-2}\boldsymbol{n}_{m-1} + \boldsymbol{n}_{m-1}\right], \tag{3.9e}$$

$$\boldsymbol{H}^{(\mathrm{c})}_{m,m-1,m-2} = \left\{\frac{s_0(\nu_m)s_4(0)}{\Delta(\nu_m)}\left[\boldsymbol{n}_m\boldsymbol{a}^\dagger_{m-2}\boldsymbol{a}_{m-1} - \boldsymbol{n}_{m-2}\boldsymbol{a}^\dagger_m\boldsymbol{a}_{m-1}\right] - \frac{2c_2(0)s_0^2(\nu_m)}{\Delta(\nu_m)}\boldsymbol{n}_{m-1}\boldsymbol{a}^\dagger_{m-2}\boldsymbol{a}_m\right\} + \text{h.c.}, \tag{3.9f}$$

where

$$\Delta(u) \equiv s_2(u)s_{-2}(u) \tag{3.10}$$

and h.c. denotes the hermitian conjugate with $(\psi_\pm)^* = -\psi_\pm$, $\eta^* = -\eta$, $\nu^* = \nu$. Here, $\boldsymbol{H}_1^{(\mathrm{b})}$ and $\boldsymbol{H}_N^{(\mathrm{b})}$ are the general boundary terms which are responsible for the sources and sinks with particle injection and ejection at the boundaries; $\boldsymbol{H}^{(\mathrm{h})}_{m,m-1,m-2}$ consists of nearest- and next-nearest-neighbour hopping terms involving the sites m, $m-1$ and $m-2$; $\boldsymbol{H}^{(\mathrm{d})}_{m,m-1,m-2}$ contains an onsite potential and density-density interaction terms between neighbours and next-nearest neighbours; and $\boldsymbol{H}^{(\mathrm{c})}_{m,m-1,m-2}$ involves current-density interactions (see figure 1). The Hamiltonian in the presence of more than one impurity can easily be constructed, if the two nearest impurities are still well separated. In this case, the Hamiltonian reduces to a sum over the isolated impurities like in the case of the Heisenberg periodic chain [8, 9, 10].

4. Integrable impurities coupled to the boundaries

Kondo-like impurities of local impurity spins coupled to 1D strongly correlated conduction electrons have attracted much interest [17, 19] especially in the context of the BA solution [3]. To every complex-valued K-matrix solution of the RE (3.3a) and (3.3b), one may construct a class of "regular" solutions [27], i.e.,

$$\tilde{\boldsymbol{K}}_-(u) = \boldsymbol{L}(u)K_-(u)\boldsymbol{L}^{-1}(-u), \quad \tilde{\boldsymbol{K}}_+(u) = K_+(u) \tag{4.1}$$

to the same RE. In order to study Kondo impurities for 1D electron systems [19, 27], it is better to construct "non-regular", i.e. non-trivial operator-valued, solutions, to the RE. Wang and coworkers [18] constructed a class of integrable impurities coupled to each boundary of the spin-$\frac{1}{2}$ Heisenberg XXZ chain by a special choice of boundary $K_\pm$-matrices, i.e., $K_\pm = 1$. But in their approach the parameters characterizing the strength of the magnetic impurities — related to our potential impurities via the customary Jordan-Wigner transformation [1] — disappear in the Hamiltonian as well as in the BA equations. Here we present a different approach to integrable impurities: from "regular" solutions of the graded RE (3.3a) and (3.3b), we construct a class of integrable impurities [8, 9, 10] coupled to each of the boundaries of a fermion chain with general open BC. We stress that these impurities are not Kondo-like. If we embed two fermionic impurity vertices at the boundaries,

$$\boldsymbol{T}(u) \quad = \boldsymbol{L}_r(u+\nu_r)\boldsymbol{L}_N(u)\cdots\boldsymbol{L}_m(u)\cdots\boldsymbol{L}_1(u)\boldsymbol{L}_\ell(u+\nu_\ell), \tag{4.2a}$$

$$\boldsymbol{T}^{-1}(-u) = \boldsymbol{L}_\ell^{-1}(-u+\nu_\ell)\boldsymbol{L}_1^{-1}(-u)\cdots\boldsymbol{L}_m^{-1}(-u)\cdots\boldsymbol{L}_N^{-1}(-u)\boldsymbol{L}_r^{-1}(-u+\nu_r), \tag{4.2b}$$

one can show that

$$\boldsymbol{U}_-(u) = \boldsymbol{T}(u)K_-(u)\boldsymbol{T}^{-1}(-u) \tag{4.3}$$

also satisfies (3.3a) and so does the solution $\boldsymbol{L}_\ell(u+\nu_\ell)K_-(u)\boldsymbol{L}_\ell^{-1}(-u+\nu_\ell)$. It follows that there exists a family of transfer matrices

$$\boldsymbol{\tau}(u) = \mathrm{Str}_0[K_+(u)\boldsymbol{U}_-(u)] \tag{4.4}$$

and its members commute with each other for different spectral parameters. Similarly to (2.16), we can formulate the explicit expression of the Hamiltonian for an open fermion chain with boundary impurities,

$$\begin{aligned}\boldsymbol{H} = &\sum_{j=2}^{N}\boldsymbol{H}_{j,j-1} + \frac{1}{\mathrm{Str}_0[K_+(0)]}\left\{\mathrm{Str}_0[K_+(0)\boldsymbol{L}_r'(\nu_r)\boldsymbol{L}_r^{-1}(\nu_r)]\right.\\ &\left.\qquad +\mathrm{Str}_0[K_+(0)\boldsymbol{L}_r(\nu_r)\boldsymbol{L}_N'(0)\boldsymbol{L}_N^{-1}(0)\boldsymbol{L}_r^{-1}(\nu_r)]\right\}\\ &+\frac{1}{2}\boldsymbol{L}_1(0)\boldsymbol{L}_\ell(\nu_\ell)K_-'(0)\boldsymbol{L}_\ell^{-1}(\nu_\ell)\boldsymbol{L}_1^{-1}(0) + \boldsymbol{L}_1(0)\boldsymbol{L}_\ell'(\nu_\ell)\boldsymbol{L}_\ell^{-1}(\nu_\ell)\boldsymbol{L}_1^{-1}(0).\end{aligned} \tag{4.5}$$

Substituting (3.7a) and (3.7b) into (4.5), the corresponding Hamiltonian is given as

$$\begin{aligned}\boldsymbol{H} = &\sum_{j=2}^{N}\boldsymbol{H}_{j,j-1} + \frac{s_2(0)}{\Delta(\nu_r)s_0(\psi_+)}\left[\boldsymbol{H}_N^{(\mathrm{b})} + \boldsymbol{H}_r^{(\mathrm{b})} + \boldsymbol{H}_{N,r}^{(\mathrm{i})}\right]\\ &+\frac{s_2(0)}{\Delta(\nu_\ell)s_0(\psi_-)}\left[\boldsymbol{H}_1^{(\mathrm{b})} + \boldsymbol{H}_\ell^{(\mathrm{b})} + \boldsymbol{H}_{1,\ell}^{(\mathrm{i})}\right]\end{aligned} \tag{4.6}$$

where

$$\begin{aligned}\boldsymbol{H}_N^{(\mathrm{b})} &= s_0(\nu_r)\left[s_0(\psi_+-\nu_r)\,\boldsymbol{n}_N + is_2(\nu_r)\alpha_+\,\boldsymbol{a}_N^\dagger + is_{-2}(\nu_r)\beta_+\,\boldsymbol{a}_N\right]\\ &\quad - c_2(\nu_r)s_{-2}(\nu_r)s_0(\psi_+)\,\boldsymbol{n}_N,\end{aligned} \tag{4.7a}$$

$$\boldsymbol{H}_r^{(\mathrm{b})} = s_2(0)\left[s_2(\psi_+)\,\boldsymbol{n}_r - is_2(\nu_r)\alpha_+\,\boldsymbol{a}_r^\dagger + is_{-2}(\nu_r)\beta_+\,\boldsymbol{a}_r\right], \tag{4.7b}$$

$$\boldsymbol{H}_{N,r}^{(\mathrm{i})} = -\,s_2(0)c_2(0)\left[s_0(\psi_+)\,\boldsymbol{n}_r - 2is_0(\nu_r)(\alpha_+\,\boldsymbol{a}_r^\dagger - \beta_+\,\boldsymbol{a}_r)\right]\boldsymbol{n}_N$$

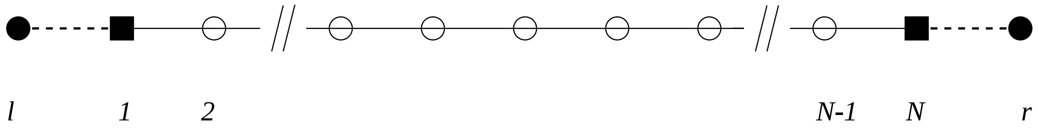

Figure 2. Impurities coupled to each of the boundaries.

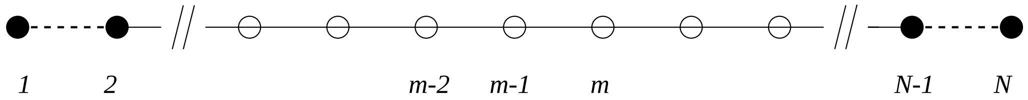

Figure 3. Integrable impurities situated at the boundaries.

$$
\begin{aligned}
&- c_2(0)\left[s_2(0)s_0(\psi_+)\,\boldsymbol{n}_N + 2is_0^2(\nu_r)(\alpha_+\,\boldsymbol{a}_N^\dagger + \beta_+\,\boldsymbol{a}_N)\right]\boldsymbol{n}_r,\\
&- s_2(0)\left[s_0(\nu_r+\psi_+)\,\boldsymbol{a}_N^\dagger\boldsymbol{a}_r - s_0(\nu_r-\psi_+)\,\boldsymbol{a}_r^\dagger\boldsymbol{a}_N\right], \qquad (4.7c)
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{H}_1^{(\mathrm{b})} &= \boldsymbol{H}_N^{(\mathrm{b})}(N\to 1, r\to\ell, \psi_+\to\psi_-, \alpha_+\to\alpha_-, \beta_+\to\beta_-, \nu_r\to-\nu_\ell), && (4.7d)\\
\boldsymbol{H}_\ell^{(\mathrm{b})} &= \boldsymbol{H}_r^{(\mathrm{b})}(N\to 1, r\to\ell, \psi_+\to\psi_-, \alpha_+\to\alpha_-, \beta_+\to\beta_-, \nu_r\to-\nu_\ell), && (4.7e)\\
\boldsymbol{H}_{1,\ell}^{(\mathrm{i})} &= \boldsymbol{H}_{N,r}^{(\mathrm{i})}(N\to 1, r\to\ell, \psi_+\to\psi_-, \alpha_+\to\alpha_-, \beta_+\to\beta_-, \nu_r\to-\nu_\ell), && (4.7f)
\end{aligned}
$$

where $\boldsymbol{H}^{(\mathrm{b})}$ can be interpreted as fermion sources and sinks with particle injection and ejection at the boundaries and at the impurity sites. However, unlike the previous Hamiltonian (3.8), the boundary parameters and impurity parameters are both involved. $\boldsymbol{H}^{(\mathrm{i})}$ describes the interaction between impurities and boundaries (see figure 2).

On the other hand, if we move the impurity in the bulk to each boundary of the chain as shown in figure 3 with the monodromy matrix

$$
\begin{aligned}
\boldsymbol{T}(u) \quad &= \boldsymbol{L}_N(u+\nu_N)\cdots\boldsymbol{L}_m(u)\cdots\boldsymbol{L}_1(u+\nu_1), && (4.8a)\\
\boldsymbol{T}^{-1}(-u) &= \boldsymbol{L}_1^{-1}(-u+\nu_1)\cdots\boldsymbol{L}_m^{-1}(-u)\cdots\boldsymbol{L}_N^{-1}(-u+\nu_N), && (4.8b)
\end{aligned}
$$

one finds that the Hamiltonian is same as (4.6) apart from the numbering

$$
r\to N, N\to N-1, \ell\to 1, 1\to 2.
$$

Although the eigenvalues of the open chain do not depend on the position of the impurities in the bulk due to the absence of back-scattering, the open boundary is a perfect back-scatterer with vanishing transmission at each end of the open chain for $\alpha_\pm = \beta_\pm = 0$. Moreover, it is easy to obtain a model with the impurities coupled to each boundary together with f well separated impurities (see figure 4) at positions m_i for $i = 1, \ldots, f$, i.e.

$$
\begin{aligned}
\boldsymbol{H} = &\sum_{j=2}^{N}\boldsymbol{H}_{j,j-1} + \frac{s_2(0)}{\Delta(\nu_r)s_0(\psi_+)}\left[\boldsymbol{H}_N^{(\mathrm{b})} + \boldsymbol{H}_r^{(\mathrm{b})} + \boldsymbol{H}_{N,r}^{(\mathrm{i})}\right]\\
&+ \frac{s_2(0)}{\Delta(\nu_\ell)s_0(\psi_-)}\left[\boldsymbol{H}_1^{(\mathrm{b})} + \boldsymbol{H}_\ell^{(\mathrm{b})} + \boldsymbol{H}_{1,\ell}^{(\mathrm{i})}\right]
\end{aligned}
$$

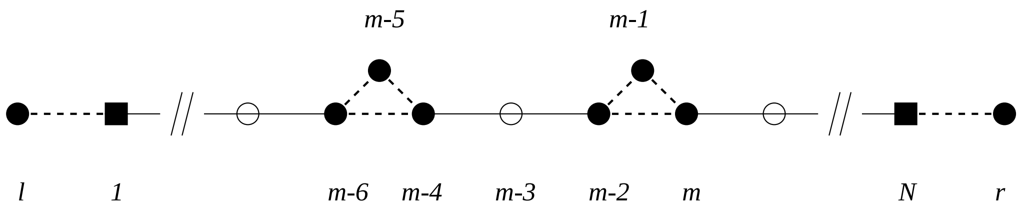

Figure 4. Two well-separated bulk impurities at sites $m_1 = m$ and $m_2 = m - 4$ together with the boundary impurities.

$$+\sum_{i=1}^{f}(\boldsymbol{H}^{(\mathrm{h})}_{m_i,m_i-1,m_i-2} + \boldsymbol{H}^{(\mathrm{d})}_{m_i,m_i-1,m_i-2} + \boldsymbol{H}^{(\mathrm{c})}_{m_i,m_i-1,m_i-2}). \qquad (4.9)$$

The terms $\boldsymbol{H}^{(\mathrm{b})}$, $\boldsymbol{H}^{(\mathrm{i})}$ are the same as in (4.7*a*)-(4.7*f*), and the terms $\boldsymbol{H}^{(\mathrm{c})}, \boldsymbol{H}^{(\mathrm{d})}$ and $\boldsymbol{H}^{(\mathrm{h})}$ are given in (3.9*d*)–(3.9*f*). To keep these Hamiltonians (3.8), (4.6) and (4.9) hermitian, the parameters η and $\psi_\pm$ must be purely imaginary, ν is real and $\alpha_\pm^\dagger = \beta_\pm$. All terms in the Hamiltonians are needed to ensure the integrability of the models. In the next section we shall proceed with the algebraic solutions for the small-polaron model with different kinds of impurities in the most interesting special case of perfectly back-scattering boundaries without sources and sinks.

5. Bethe ansatz solution for finite chains

Following the method of [11, 26], we shall study the algebraic BA solutions for the open fermion chain with different kinds of impurities. We first note that the general open BC spoil the pseudo vacuum state. Therefore it seems difficult to solve the models with general open BC by means of the QISM. We thus restrict ourselves to the simpler situation $\alpha_\pm = 0$, $\beta_\pm = 0$ in the following. In this case, the Hamiltonians (3.8), (4.6) and (4.9) do not contain any Grassmannian source and sink terms and are charge conserving. They still contain the potential impurities and are perfect back-scatterers. Thus these Hamiltonians are ideal for the proposed investigation of the interplay of forward-scattering bulk impurities with backward-scattering boundaries.

Let us for simplicity first consider the Hamiltonian (4.6). In the case $\alpha_\pm = 0$, $\beta_\pm = 0$, the Hamiltonian (4.6) comprises

$$\boldsymbol{H}^{(\mathrm{b})}_N = \left[s_2(0)c_2(0)s_0(\psi_+) - s_0^2(\nu_r)c_0(\psi_+)\right]\boldsymbol{n}_N, \qquad (5.1a)$$

$$\boldsymbol{H}^{(\mathrm{b})}_r = \left[s_2(0)c_2(0)s_0(\psi_+) + s_2^2(0)c_0(\psi_+)\right]\boldsymbol{n}_r, \qquad (5.1b)$$

$$\boldsymbol{H}^{(\mathrm{i})}_{N,r} = -\,s_2(0)\left[s_0(\nu_r+\psi_+)\,\boldsymbol{a}_N^\dagger\boldsymbol{a}_r - s_0(\nu_r-\psi_+)\,\boldsymbol{a}_r^\dagger\boldsymbol{a}_N\right] - s_4(0)s_0(\psi_+)\boldsymbol{n}_r\boldsymbol{n}_N \qquad (5.1c)$$

and $\boldsymbol{H}^{(b)}_1$, $\boldsymbol{H}^{(b)}_\ell$, and $\boldsymbol{H}^{(i)}_{1,\ell}$ follow as in (4.7*d*)–(4.7*f*). $\boldsymbol{H}^{(\mathrm{b})}$ describes the boundary impurities. $\boldsymbol{H}^{(\mathrm{i})}$ contains the interaction terms with exchange coupling between the bulk and the impurities (see figure 2). As mentioned before, this Hamiltonian conserves the particle number due to the absence of sources and sinks with particle injection and ejection at the boundaries.

Now we proceed to establish the Bethe eigenvectors for the Hamiltonian (4.6) with (5.1a)-(5.1c) by means of the algebraic BA [14]. Let

$$\boldsymbol{T}(u)=\begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad \boldsymbol{T}^{-1}(-u)=\begin{pmatrix} \bar{A} & \bar{B} \\ \bar{C} & \bar{D} \end{pmatrix}, \tag{5.2}$$

be the monodromy matrices acting on the pseudo vacuum state defined by $\boldsymbol{a}_j|0\rangle = 0$, $j=1,\cdots,N$. Then we have

$$\begin{aligned}
A|0\rangle &= s_0^N(u)s_0(u+\nu_\ell)s_0(u+\nu_r)|0\rangle, && (5.3a)\\
D|0\rangle &= s_2^N(u)s_2(u+\nu_\ell)s_2(u+\nu_r)|0\rangle, && (5.3b)\\
B|0\rangle &= 0, && (5.3c)\\
C|0\rangle &\neq 0, && (5.3d)\\
\bar{A}|0\rangle &= \frac{(-1)^N s_0^N(u)s_0(u-\nu_\ell)s_0(u-\nu_r)}{\delta\left[\boldsymbol{T}(-u)\right]}|0\rangle, && (5.3e)\\
\bar{D}|0\rangle &= \frac{(-1)^N s_2^N(u)s_2(u-\nu_\ell)s_2(u-\nu_r)}{\delta\left[\boldsymbol{T}(-u)\right]}|0\rangle, && (5.3f)\\
\bar{B}|0\rangle &= 0, && (5.3g)\\
\bar{C}|0\rangle &\neq 0, && (5.3h)
\end{aligned}$$

where the quantum determinant [28] is $\delta\left[\boldsymbol{T}(-u)\right] = \Delta^N(u)\Delta(u-\nu_\ell)\Delta(u-\nu_r)$.Let us define

$$\boldsymbol{U}_-(u)=\begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix}. \tag{5.4}$$

From (4.3), we then have

$$\begin{aligned}
\tilde{A} &= \frac{1}{s_0(\psi_-)}[-s_0(u-\psi_-)A\bar{A}+s_0(u+\psi_-)B\bar{C}], && (5.5a)\\
\tilde{D} &= \frac{1}{s_0(\psi_-)}[-s_0(u-\psi_-)C\bar{B}+s_0(u+\psi_-)D\bar{D}]. && (5.5b)
\end{aligned}$$

Noting the following form of the graded YBA

$$\overset{2}{\boldsymbol{T}}{}^{-1}(-u)R_{12}(2u)\overset{1}{\boldsymbol{T}}(u) = \overset{1}{\boldsymbol{T}}(u)R_{12}(2u)\overset{2}{\boldsymbol{T}}{}^{-1}(-u), \tag{5.6}$$

it is possible to derive the commutation relation

$$B\bar{C} = \frac{s_2(0)}{s_2(2u)}(\bar{D}D - A\bar{A}). \tag{5.7}$$

With the help of the graded RE (3.3a) we obtain — after a lengthy calculation — the commutation relations

$$\begin{aligned}
\hat{A}(u)\tilde{C}(v) &= \frac{s_2(u-v)s_4(u+v)}{s_0(u-v)s_2(u+v)}\tilde{C}(v)\hat{A}(u) - \frac{s_2(0)s_4(2u)}{s_2(2u)s_0(u-v)}\tilde{C}(u)\hat{A}(v)\\
&\quad + \frac{s_2(0)s_0(2v)s_4(2u)}{s_2(2v)s_2(2u)s_2(u+v)}\tilde{C}(u)\tilde{D}(v), && (5.8a)
\end{aligned}$$

$$\tilde{D}(u)\tilde{C}(v) = \frac{s_0(u+v)s_{-2}(u-v)}{s_0(u-v)s_2(u+v)}\tilde{C}(v)\tilde{D}(u) + \frac{s_2(0)s_0(2v)}{s_0(u-v)s_2(2v)}\tilde{C}(u)\tilde{D}(v)$$
$$- \frac{s_2(0)}{s_2(u+v)}\tilde{C}(u)\hat{A}(v), \tag{5.8b}$$

where we introduced the transformation

$$\hat{A}(u) = \tilde{A}(u) - \frac{s_2(0)}{s_2(2u)}\tilde{D}(u). \tag{5.9}$$

From (5.3a)-(5.3h) and (5.4), we can choose an M-particle excitation as

$$|\Phi(v_1 \cdots v_M)\rangle = \tilde{C}(v_1) \cdots \tilde{C}(v_M)|0\rangle. \tag{5.10}$$

Using the commutation relations (5.8a) and (5.8b), one obtains the eigenvalue Λ of the transfer matrix (4.4)

$$\tau(u)|\Phi(v_1 \cdots v_M)\rangle = \Lambda(u; v_1 \cdots v_M)|\Phi(v_1 \cdots v_M)\rangle, \tag{5.11}$$

where

$$\begin{aligned}\Lambda(u; v_1 \cdots v_M) = &-\frac{(-1)^N}{s_2(2u)\delta\left[\boldsymbol{T}(-u)\right] s_0(\psi_-)} \\ &\times \Bigg\{ s_2(u-\psi_+)s_2(u-\psi_-)s_0(u-\nu_\ell)s_0(u+\nu_\ell)s_0(2u)s_0^{2N}(u) \\ &\times s_0(u-\nu_r)s_0(u+\nu_r)\prod_{j=1}^{M}\frac{s_4(u+v_j)s_2(u-v_j)}{s_0(u-v_j)s_2(u+v_j)} \\ &+ s_0(u+\psi_+)s_0(u+\psi_-)s_2(u+\nu_\ell)s_2(u-\nu_\ell)s_4(2u)s_2^{2N}(u) \\ &\times s_2(u+\nu_r)s_2(u-\nu_r)\prod_{j=1}^{M}\frac{s_0(u+v_j)s_{-2}(u-v_j)}{s_0(u-v_j)s_2(u+v_j)}\Bigg\},\end{aligned} \tag{5.12}$$

provided that

$$\begin{aligned}&\frac{s_1(v_j-\psi_-)s_1(v_j-\psi_+)s_{-1}^{2N}(v_j)}{s_{-1}(v_j+\psi_-)s_{-1}(v_j+\psi_+)s_1^{2N}(v_j)} = \\ &\qquad \prod_{m=\ell,r}\frac{s_1(v_j+\nu_m)s_1(v_j-\nu_m)}{s_{-1}(v_j+\nu_m)s_{-1}(v_j-\nu_m)} \prod_{\substack{k=1\\k\neq j}}^{M}\frac{s_{-2}(v_j+v_k)s_{-2}(v_j-v_k)}{s_2(v_j+v_k)s_2(v_j-v_k)}\end{aligned} \tag{5.13}$$

for all $j = 1, \ldots, M$. In the above BA equations, we have shifted the parameter $v_j \to v_j - \eta$. From the relation (2.16), the eigenvalue E of the Hamiltonian (4.6) for $\alpha_\pm = \beta_\pm = 0$ follows as

$$\begin{aligned}E = -s_2(0)\Bigg[&\cot\psi_- + \cot\psi_+ + 2(N+1)\cot 2\eta - 2\cot(\nu_r - 2\eta) - 2\cot(\nu_\ell - 2\eta) \\ &-\sum_{j=1}^{M}\frac{2s_2(0)}{s_{-1}(v_j)s_1(v_j)}\Bigg].\end{aligned} \tag{5.14}$$

On the right hand side of (5.14) we have dropped a multiplicative term $1/2\cos(2\eta)$ as is customary [11]. Following the same procedure, the BA equations and the eigenvalues for the Hamiltonian (3.8) are given as

$$\frac{s_1(v_j-\psi_-)s_1(v_j-\psi_+)s_{-1}^{2(N-1)}(v_j)}{s_{-1}(v_j+\psi_-)s_{-1}(v_j+\psi_+)s_1^{2(N-1)}(v_j)} = \frac{s_1(v_j+\nu_m)s_1(v_j-\nu_m)}{s_{-1}(v_j+\nu_m)s_{-1}(v_j-\nu_m)} \prod_{\substack{k=1\\k\neq j}}^{M} \frac{s_{-2}(v_j+v_k)s_{-2}(v_j-v_k)}{s_2(v_j+v_k)s_2(v_j-v_k)} \tag{5.15}$$

for all $j=1,\dots,M$, and

$$E=-s_2(0)\left[\cot\psi_-+\cot\psi_++2N\cot 2\eta-2\cot(\nu_m-2\eta)-\sum_{j=1}^{M}\frac{2s_2(0)}{s_{-1}(v_j)s_1(v_j)}\right]. \tag{5.16}$$

For the Hamiltonian (4.9) we find

$$\frac{s_1(v_j-\psi_-)s_1(v_j-\psi_+)s_{-1}^{2(N-f)}(v_j)}{s_{-1}(v_j+\psi_-)s_{-1}(v_j+\psi_+)s_1^{2(N-f)}(v_j)} = \prod_{m=1}^{f,\ell,r}\frac{s_1(v_j+\nu_m)s_1(v_j-\nu_m)}{s_{-1}(v_j+\nu_m)s_{-1}(v_j-\nu_m)} \prod_{\substack{k=1\\k\neq j}}^{M} \frac{s_{-2}(v_j+v_k)s_{-2}(v_j-v_k)}{s_2(v_j+v_k)s_2(v_j-v_k)}, \tag{5.17}$$

where $\prod_{m=1}^{f,\ell,r}$ denotes the product over the f isolated impurities in the bulk as well as the boundary impurities. The energy spectrum is given as

$$E=-s_2(0)\left[\cot\psi_-+\cot\psi_++2(N-f+1)\cot 2\eta-2\sum_{m=1}^{f,\ell,r}\cot(\nu_m-2\eta) -\sum_{j=1}^{M}\frac{2s_2(0)}{s_{-1}(v_j)s_1(v_j)}\right]. \tag{5.18}$$

When comparing (5.17), (5.18) to (5.15), (5.16) and (5.13), (5.14), we see that using (5.17), (5.18) corresponding to the Hamiltonian (4.9), we can reproduce the results for the other two Hamiltonians (3.8) and (4.6). Namely, with $f=1$ and $\nu_r=\nu_l=0$ we get the result for (3.8) with (5.15), (5.16) and with $f=0$ and $\nu_r,\nu_l\neq 0$ we find for (4.6) the BA equations (5.13) with energy (5.14). Thus the Hamiltonian (4.9) contains the other two Hamiltonians as special cases, although the construction by QISM proceeds independently. We note that care has to be paid to the varying number of sites N when doing this procedure.

6. Ground-state properties in the thermodynamic limit

We note that the bulk terms of the Hamiltonians (3.8), (4.6) and (4.9) are equivalent to the counter part of the 1D Heisenberg XXZ model with periodic BC via a Jordan-Wigner transformation. The finite-size corrections and thermodynamics for the XXZ model with or without boundary magnetic fields have been studied in many papers [29, 30]. As mentioned before, the Jordan-Wigner transformation does not preserve the boundary terms nor the impurity terms due to its nonlocality. The BA equations we obtained provide a more meaningful description of the ground-state properties due to the presence of the boundary potential terms and the impurity parameters. In what follows, we shall study the ground-state properties for the resulting models following the scheme in [9, 18, 29, 30].

For convenience, let us first redefine the variable $v_j \to iv_j$. Then, taking the logarithm, we rewrite the BA equations (5.13) for the Hamiltonian (4.6) as follows:

$$\begin{aligned}2\pi I_j = {} & 2N\theta(v_j,\eta) + \theta(v_j,\psi_+ - \eta) + \theta(v_j,\psi_- - \eta) + \theta(v_j+\nu_r,\eta) + \theta(v_j-\nu_r,\eta)\\ & +\theta(v_j+\nu_\ell,\eta) + \theta(v_j-\nu_\ell,\eta) - \sum_{\substack{k=1\\k\neq j}}^{M} \theta(v_j-v_k,2\eta) + \theta(v_j+v_k,2\eta),\end{aligned} \tag{6.1}$$

for all $j = 1,\cdots,M$, where the two-body phase shift [2, 13, 14] is

$$\theta(v_j,\eta) = i\ln\frac{\sinh(v_j+i\eta)}{\sinh(v_j-i\eta)} = 2\mathrm{arccot}\left(\tanh v_j \cot\eta\right). \tag{6.2}$$

We now define v_{-k} as $-v_k$ and define $v_0 = 0$. Then the density of the roots $\{v_j\}$ can be defined as

$$\rho_N(v) = \frac{dZ_N(v)}{dv}, \quad Z_N = \frac{I_j}{N} \tag{6.3}$$

and the finite-size BA equation (6.1) becomes

$$Z_N(v) = \frac{1}{\pi}\left\{\theta(v,\eta) + \frac{1}{2N}\left[\theta^{(\mathrm{i})}(v) + \theta^{(\mathrm{b})}(v)\right] - \frac{1}{2N}\sum_{k=-M}^{M}\theta(v-v_k,2\eta)\right\}, \tag{6.4}$$

where

$$\theta^{(\mathrm{i})}(v) = \theta(v+\nu_r,\eta) + \theta(v-\nu_r,\eta) + \theta(v+\nu_\ell,\eta) + \theta(v-\nu_\ell,\eta), \tag{6.5a}$$

$$\theta^{(\mathrm{b})}(v) = \theta(v,2\eta) + \theta(2v,2\eta) + \theta(v,\psi_+ - \eta) + \theta(v,\psi_- - \eta). \tag{6.5b}$$

We note that the first two terms in (6.5b) arise due to the non-periodicity of the chain, whereas the last two terms are due to the boundary potentials at sites 1 and N. Taking the thermodynamic limit and differentiating (6.4) with respect to the spectral parameter v, we have

$$\rho_\infty(v) = \frac{1}{\pi}\left\{\theta'(v,\eta) + \frac{1}{2N}\left[\theta^{(\mathrm{i})\prime}(v) + \theta^{(\mathrm{b})\prime}(v)\right]\right\} - \frac{1}{2\pi}\int_{-\Lambda}^{\Lambda} du\,\rho_\infty(u)\theta'(v-u,2\eta), \tag{6.6}$$

where the integration boundary Λ is determined by

$$\int_{-\Lambda}^{\Lambda}\rho_\infty(v)dv = \frac{2M+1}{N} + O(N^{-2}). \tag{6.7}$$

The prime denotes the derivative with respect to v. Due to the linearity of (6.6), one may formally solve the following three linear integral equations:

$$\rho_\infty^{(0)}(v) = \frac{1}{\pi}\theta'(v,\eta) - \frac{1}{2\pi}\int_{-\Lambda}^{\Lambda} du \rho_\infty^{(0)}(u)\theta'(v-u,2\eta), \tag{6.8a}$$

$$\rho_\infty^{(\mathrm{i})}(v) = \frac{1}{\pi}\theta^{(\mathrm{i})\prime}(v) - \frac{1}{2\pi}\int_{-\Lambda}^{\Lambda} du \rho_\infty^{(\mathrm{i})}(u)\theta'(v-u,2\eta), \tag{6.8b}$$

$$\rho_\infty^{(\mathrm{b})}(v) = \frac{1}{\pi}\theta^{(\mathrm{b})\prime}(v) - \frac{1}{2\pi}\int_{-\Lambda}^{\Lambda} du \rho_\infty^{(\mathrm{b})}(u)\theta'(v-u,2\eta), \tag{6.8c}$$

In this way, the solution of (6.6) can be expressed as

$$\rho_\infty(v) = \rho_\infty^{(0)}(v) + \frac{1}{2N}[\rho_\infty^{(\mathrm{i})}(v) + \rho_\infty^{(\mathrm{b})}(v)], \tag{6.9}$$

where $\rho_\infty^{(0)}(v)$, $\frac{1}{2N}\rho_\infty^{(\mathrm{i})}(v)$ and $\frac{1}{2N}\rho_\infty^{(\mathrm{b})}(v)$ are the contributions of the bulk, the impurities and the boundary effect to the root density, respectively. The ground-state energy (5.14) is minimized at the cutoff Λ in the thermodynamic limit as discussed in [29, 30]. Following the argument in [29, 30], we find the cutoff $\Lambda = \infty$ such that the particle density is $M/N = 1/2$.

By using the Fourier transforms, the formal solutions to the equations (6.8a)–(6.8c) read

$$\tilde{\rho}_\infty(\omega,\eta) = \frac{2\tilde{\theta}(\omega,\eta)}{2\pi + \tilde{\theta}(\omega,2\eta)}, \tag{6.10}$$

where

$$\tilde{\theta}(\omega,\eta) = \int_{-\infty}^{\infty} \theta'(v,\eta)e^{i\omega v}dv. \tag{6.11}$$

From the residue theorem, we obtain

$$\rho_\infty^{(0)}(v) = \frac{2}{\eta\cosh\frac{\pi}{2\eta}v}, \tag{6.12a}$$

$$\rho_\infty^{(\mathrm{i})}(v) = \sum_{m=r,\ell} \frac{4\cosh\frac{\pi}{2\eta}v\cosh\frac{\pi}{2\eta}\nu_m}{\eta\cosh\frac{\pi}{2\eta}(v+\nu_m)\cosh\frac{\pi}{2\eta}(v-\nu_m)}, \tag{6.12b}$$

$$\rho_\infty^{(\mathrm{b})}(v) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\tilde{\rho}_\infty^{(\mathrm{be})}(\omega) + \tilde{\rho}_\infty^{(\mathrm{bp})}(\omega)\right]e^{-i\omega v}d\omega, \tag{6.12c}$$

where

$$\tilde{\rho}_\infty^{(\mathrm{be})}(\omega) = \frac{2\sinh(\frac{\pi}{2}-2\eta)\omega + 4\cos\frac{\pi}{4}\omega\sinh(\frac{\pi}{4}-\eta)\omega}{\sinh\frac{\pi}{2}\omega + \sinh(\frac{\pi}{2}-2\eta)\omega}, \tag{6.13a}$$

$$\tilde{\rho}_\infty^{(\mathrm{bp})}(\omega) = \frac{2\sinh(\frac{\pi}{2}+\eta-\psi_+)\omega + 2\sinh(\frac{\pi}{2}+\eta-\psi_-)\omega}{\sinh\frac{\pi}{2}\omega + \sinh(\frac{\pi}{2}-2\eta)\omega}. \tag{6.13b}$$

Here $\tilde{\rho}_\infty^{(\mathrm{be})}(\omega)$ and $\tilde{\rho}_\infty^{(\mathrm{bp})}(\omega)$ are the contributions to the root density from the boundary effect and the boundary potential terms, respectively, due to (6.5b). Then, from (5.14), we also obtain the ground-state energy in the thermodynamic limit as

$$E_{\mathrm{g}} = N\int_{-\infty}^{\infty} dv \frac{4\sin^2 2\eta}{\cosh 2v - \cosh 2\eta}\rho_\infty(v) + E_0, \tag{6.14}$$

with

$$E_0 = -p_+ - p_- - 2(N+1)\cos 2\eta + 2\sin 2\eta \sum_{m=r,\ell} \cot(\nu_m - 2\eta). \qquad (6.15)$$

The boundary energy [30] is given by

$$\begin{aligned} E_{\mathrm{b}} = & \int_{-\infty}^{\infty} dv \frac{2\sin^2 2\eta}{\cosh 2v - \cosh 2\eta}[\rho_\infty^{(\mathrm{i})}(v) + \rho_\infty^{(\mathrm{b})}(v)] \\ & - p_+ - p_- - 2\cos 2\eta + 2\sin 2\eta \sum_{m=r,\ell} \cot(\nu_m - 2\eta). \end{aligned} \qquad (6.16)$$

We thus note that the boundary potential terms do not only enter the expression for the ground-state energy explicitly as $-p_+ - p_-$, but also implicitly via $\tilde{\rho}_\infty^{(\mathrm{b})}$ of (6.12*c*).

We remark that in [18] no boundary magnetic field terms like (6.13*b*) contribute to the root density due to the lack of free boundary parameters in the boundary $K_\pm$-matrices. The presence of boundary potentials (magnetic fields) and the impurity parameters changes the asymptotic behaviour of the BA equations (6.1) resulting in string solutions different from those discussed in the papers [30]. Indeed, either the boundary parameters $p_\pm$ (or $\psi_\pm$) or the impurity strength parameters ν_m, ν_ℓ and ν_r affect the boundary string solutions to the BA equations. It is obvious that the ground-state energy of the bulk is same as in the periodic case [29]. In general, the boundary states are associated with complex roots of the BA equations.

Analogously, we obtain the ground-state energy (6.14) for the Hamiltonians (3.8) and (4.9). The differences to the ground states for these Hamiltonians are only the contributions from the impurities expressed in $\rho_\infty^{(\mathrm{i})}(v)$. Thus we get for the Hamiltonian (3.8)

$$\rho_\infty^{(\mathrm{i})}(v) = \frac{4\cosh\frac{\pi}{2\eta}v\cosh\frac{\pi}{2\eta}\nu_m}{\eta\cosh\frac{\pi}{2\eta}(v+\nu_m)\cosh\frac{\pi}{2\eta}(v-\nu_m)} - \frac{4}{\eta\cosh\frac{\pi}{2\eta}v}, \qquad (6.17)$$

$$E_0 = -p_+ - p_- - 2N\cos 2\eta + 2\sin 2\eta\,\cot(\nu_m - 2\eta). \qquad (6.18)$$

For the most general Hamiltonian (4.9), we have

$$\rho_\infty^{(\mathrm{i})}(v) = \sum_m^{f,r,\ell}\left[\frac{4\cosh\frac{\pi}{2\eta}v\cosh\frac{\pi\nu}{2\eta}\nu_m}{\eta\cosh\frac{\pi}{2\eta}(v+\nu_m)\cosh\frac{\pi}{2\eta}(v-\nu_m)}\right] - f\frac{4}{\eta\cosh\frac{\pi}{2\eta}v}. \qquad (6.19)$$

$$\begin{aligned} E_0 = & -p_+ - p_- - 2(N+1-f)\cos 2\eta \\ & + 2\sin 2\eta \sum_{m=1}^{f,r,\ell}\cot(\nu_m - 2\eta). \end{aligned} \qquad (6.20)$$

Further thermodynamic properties such as compressibilities and susceptibilities can be calculated as demonstrated previously in [8, 10, 15]. Results will be presented elsewhere.

7. Conclusions and discussion

In the present work, we have considered the interplay of integrable impurities and general open boundary conditions for the example of the small-polaron model. The impurities have been constructed via inhomogeneous shifts in the spectral parameters of the Lax operators such that the YBE are satisfied. The boundary terms are taken to obey the RE. In both cases, we dealt with the graded version of the equations due to the fermionic nature of the particles and the boundary terms. Thus by construction, the model remains integrable. We have shown that this is true even when placing the impurities directly at the boundaries.

The most general boundary terms considered in (2.1) include fermionic particle sources and sink terms as well as more standard density terms. However, these linear terms in creation and annihilation operators contain coefficients that are odd Grassmann variables. Thus a straightforward physical interpretation appears problematic. Representing these coefficients $\alpha_\pm$, $\beta_\pm$ as additional fermionic operators $\boldsymbol{a}_\pm$, $\boldsymbol{a}_\pm^\dagger$, we arrive at a chain with two additional sites but without sources and sinks.

The boundary terms coupling to the particle density can be viewed as potential impurities — much like in the Anderson model of localization [31] — situated at the boundaries. For the special case with only these potential impurities and the integrable impurities present, we solve the BA equations and compute the ground-state energy in the thermodynamic limit for half-filling. We find that the solution is possible regardless whether the integrable impurities are located within the bulk or at the boundaries.

The two types of impurities enter the expressions for the ground-state energy additively. Thus the simultaneous presence of both purely forward scattering integrable impurities and purely reflecting boundary potential terms does not seem to change the physics in a substantial way. We therefore do not expect to see the onset of localization as might be expected from the form of the boundary impurities.

An analogue of the integrable impurities can be found in the case of light waves. Consider a long strip of glass, interspersed with pieces of bifringent material of the same index of refraction as the glass. Then as circular polarized light enters the strip and reaches the first bifringent slab, its plane of polarization will be rotated by an angle $\theta \propto \alpha l_1$ where l_1 represents the length of the first slab and α is the material specific rotation angle per unit length [32]. There is no reflection at the contact due to the identical indices of refraction. After the next slab, we have $\theta = \alpha l_1 + \alpha l_2$ and so on. Thus the net effect of the bifringent slabs is a rotation of the plane of polarization, i.e., a change in the overall phase of the wave function of light just as for the electronic wave function in Ref. [8, 9, 10]. In this picture the integrable boundaries satisfying the RE then simply correspond to perfect mirrors at both ends of the strip.

Acknowledgments

The authors thank H.-P. Eckle for helpful discussions. GXW thanks H.-Q. Zhou and M. Shiroishi for their communications and also thanks the Institut für Physik, Technische Universität Chemnitz for kind hospitality. UG, RAR and MS gratefully acknowledge the hospitality of the Max-Planck-Institut für Physik komplexer Systeme (Dresden) during COOP99 where much of this manuscript was prepared. The work has been supported by the DFG via SFB393 and the Schwerpunktprogramm "Quasikristalle".

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