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Exact energy spectrum for models with equally spaced point potentials

V. Caudrelier [*], N. Crampé

Department of Mathematics, University of York, Heslington York, YO10 5DD, United Kingdom

In memory of Daniel Arnaudon

Abstract

We describe a non-perturbative method for computing the energy band structures of one-dimensional models with general point potentials sitting at equally spaced sites. This is done thanks to a Bethe ansatz approach and the method is applicable even when periodicity is broken, that is when Bloch's theorem is not valid any more. We derive the general equation governing the energy spectrum and illustrate its use in various situations. In particular, we get exact results for boundary effects. We also study non-perturbatively the effects of impurities in such systems. Finally, we discuss the possibility of including interactions between the particles of these systems.

1. Introduction

The study of the so-called point or contact interactions covers an impressively large number of areas ranging from pure mathematics, where the main goal consists in defining and understanding them rigorously, to applied physics, where either they serve as good approximations for physical situations or they are created to control the behaviour of certain quantum systems. One particular case of such contact interactions, but certainly the most well-known, is the δ potential which

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[*] Corresponding author.

E-mail addresses: vc502@york.ac.uk (V. Caudrelier), nc501@york.ac.uk (N. Crampé).

played a crucial role in two specific areas of special interest for us in this paper: solid state physics and exactly solvable and integrable models (in one spatial dimension). Indeed, in the first context, the δ potential was used by Kronig and Penney [1] to model a free electron moving in periodic external potential created by a crystal lattice and is now a standard of textbooks in solid state physics [2]. As for the second context, it has become one of the cornerstones of exactly solvable and integrable systems through the works of McGuire, Lieb and Liniger and Yang [3–5] where it was used to describe interactions between identical particles.

These two quantum mechanical problems can be solved to get the energy spectrum. More precisely, in the Kronig–Penney model, the periodicity of the potential and of the boundary conditions on the wavefunction allows to use the famous Bloch's theorem [6] which actually fixes the form of the eigenfunctions. In the Lieb–Liniger model, one assumes that the wavefunctions can be expanded on plane waves with appropriate coefficients that must be found. These approaches combined with the various conditions imposed on the wavefunctions of the problem lead to the allowed energy states of the models. Depending on the context, this gives rise to the famous energy band structures or to the famous Bethe ansatz equations [7].

Several generalizations of the two previous problems have been considered over the past decades. For instance, in [8,9], the Kronig–Penney model is extended to the case where the δ potential is replaced by a more general point potential. In [10], boundary Bethe ansatz equations were derived by putting bosons with δ interactions in a box while in [11], impurity Bethe ansatz equations appeared by including a general external contact potential in a system of particles with δ interactions.

With the advent of nanostructures and the ever increasing need for controlling quantum devices, the standard assumption of periodicity is no longer accurate enough. But then, Bloch's theorem no longer applies and, to the best of our knowledge, only approximate methods are used. In this paper, we mainly address the above problem and propose a general method to investigate the energy spectrum in one-dimensional models with equally spaced but otherwise arbitrary point potentials. Let us note that the breaking of periodicity can have various origins. For example, one can simply imagine that the periodic boundary conditions are replaced by Dirichlet or Neumann boundary conditions. Or, one could replace the δ potential at one or more sites by a different point potential. We will see that the Bethe ansatz approach brings an elegant and more general alternative to Bloch's theorem in order to treat such problems. In all cases, we reduce the problem to finding roots of polynomials and solving Bethe ansatz equations. We also discuss the possibility of including interactions between bosons moving in such general potentials.

The paper is organised as follows. In Section 2, we discuss the general setup for treating free particles in an arbitrary equally spaced, external point potential. Then, in Section 3, we validate our method in the context of periodic potentials by deriving a general result which encompasses previous results in the literature and in particular the well-known features of the Kronig–Penney model. Section 4 illustrates the use of our method in a context where periodicity is broken by the boundary conditions. This provides non-perturbative results for the boundary effects. This is further illustrated in Section 5 where we introduce impurities at one or several sites of the potential. Again the results are non-perturbative and this allows for a study of the effects of impurities with arbitrary strength. Finally, in Section 6, we discuss the extension of our method to the case of bosons with δ interactions moving in a general point potential.

2. The general problem

We study a one-dimensional system of free particles moving in the interval $[-ML, ML]$, $M \geqslant 1$ being an integer and L a length scale, with an external point potential sitting at each site $x_j^0 = (M - 2j + 1)L$, $j = 1, \dots, M$. It is sufficient to consider the one-particle Hamiltonian which takes the following form[1]

$$H = -\frac{d^2}{dx^2} + \sum_{j=1}^{M} v_j(x - x_j^0),$$ (2.1)

where, for $j = 1, \dots, M$,

$$v_j(x) = c_j \delta(x) + 4\lambda_j \frac{d}{dx} \delta(x) \frac{d}{dx} + 2(\gamma_j + i\eta_j) \frac{d}{dx} \delta(x) - 2(\gamma_j - i\eta_j) \delta(x) \frac{d}{dx},$$ (2.2)

and $c_j, \lambda_j, \gamma_j, \eta_j \in \mathbb{R}$. These very singular point potentials find their origin in the self-adjoint extensions of the free Hamiltonian $-\frac{d^2}{dx^2}$ on the space $C_0^\infty(\mathbb{R} \setminus \{0\})$ of C^∞ functions with compact support separated from the origin. Written in this way, they are in fact quite formal but it is known that they are equivalent to imposing appropriate boundary conditions on the wavefunction at each site x_j^0 parametrized by $U(2)$ matrices (see, for example, [12] and references therein).

In each region $R_j^\pm$: $(M - 2j + \frac{1 \pm 1}{2})L < x < (M - 2j + \frac{3 \pm 1}{2})L$, the particle is actually free and we denote the wavefunction by $\phi_j^\pm(x)$ (see Fig. 1). Now the idea is to impose all the boundary conditions (those corresponding to the potential at each x_j^0 and those at the ends of the interval) in a compact form by extending the approach of [11]. To do so, we collect all the pieces of the wavefunction into a single $2M$-component vector defined for $x \in \,]ML - L, ML[$

$$\Phi(x) = \sum_{j=1}^{M} \phi_j^+ (x + 2L(j - 1)) e_j \otimes \hat{e}_+ + \phi_j^- (-x + 2L(M - j)) e_j \otimes \hat{e}_-,$$ (2.3)

where $\{e_j \mid 1 \leqslant j \leqslant M\}$ is the canonical basis of $\mathbb{C}^M$ and $\{\hat{e}_+, \hat{e}_-\}$ is that of $\mathbb{C}^2$. We are now ready to formulate the problem. As we said, this is just the free problem in each region $R_j^\pm$. In terms of Φ this reads,

$$-\frac{d^2}{dx^2} \Phi(x) = E \Phi(x), \qquad ML - L < x < ML.$$ (2.4)
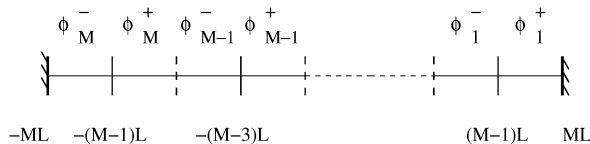

Fig. 1. The non-trivial potential lies at the points $-(M - 1)L, -(M - 3)L, \dots, (M - 1)L$ (solid lines). The dashed lines correspond to a trivial potential used for convenience.

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[1] In this paper, we use units such that $\hbar = 1 = 2m$.

Then, following for example [13], the M conditions corresponding to the general point potential are written as follows

$$(\mathcal{U}^+ - \mathbb{I})\Phi(x) + i(\mathcal{U}^+ + \mathbb{I})\frac{d}{dx}\Phi(x) = 0 \quad \text{for } x \to ML - L, \tag{2.5}$$

where $\mathbb{I}$ is the $2M \times 2M$ identity matrix and

$$\mathcal{U}^+ = \begin{pmatrix} U_1 & & \\ & \ddots & \\ & & U_M \end{pmatrix}. \tag{2.6}$$

Each submatrix U_j of $\mathcal{U}^+$ corresponds to the potential v_j in (2.2). It is a $U(2)$ matrix parametrized by

$$U_j = e^{i\xi_j} \begin{pmatrix} \mu_j & v_j \\ -v_j^* & \mu_j^* \end{pmatrix}, \quad \xi_j \in [0, \pi), \ \mu_j, v_j \in \mathbb{C} \quad \text{such that } |\mu_j|^2 + |v_j|^2 = 1, \tag{2.7}$$

where the symbol * stands for complex conjugation. The parameters of the potential v_j given in (2.2) are related to those in the matrix U_j by (see e.g. [9] and references therein)[2]

$$c_j = 2\frac{\cos\xi_j - \operatorname{Re}\mu_j}{\sin\xi_j - \operatorname{Im}v_j}, \qquad \lambda_j = -\frac{1}{2}\frac{\cos\xi_j + \operatorname{Re}\mu_j}{\sin\xi_j - \operatorname{Im}v_j}, \tag{2.8}$$

$$\gamma_j = -\frac{\operatorname{Im}\mu_j}{\sin\xi_j - \operatorname{Im}v_j}, \qquad \eta_j = \frac{\operatorname{Re}v_j}{\sin\xi_j - \operatorname{Im}v_j}. \tag{2.9}$$

Finally, the boundary conditions at the ends of the interval can be written in the same form as before

$$(\mathcal{U}^- - \mathbb{I})\Phi(x) + i(\mathcal{U}^- + \mathbb{I})\frac{d}{dx}\Phi(x) = 0 \quad \text{for } x \to ML, \tag{2.10}$$

where

$$\mathcal{U}^- = \begin{pmatrix} e^{i\xi_q}\mu_q & & & & & e^{i\xi_q}v_q \\ & 0 & 1 & & & \\ & 1 & 0 & & & \\ & & & \ddots & & \\ & & & & 0 & 1 & \\ & & & & 1 & 0 & \\ -e^{i\xi_q}v_q^* & & & & & e^{i\xi_q}\mu_q^* \end{pmatrix}. \tag{2.11}$$

The four coefficients at the corners of $\mathcal{U}^-$ also form a $U(2)$ matrix

$$U_q = e^{i\xi_q} \begin{pmatrix} \mu_q & v_q \\ -v_q^* & \mu_q^* \end{pmatrix}, \tag{2.12}$$

with the same constraints as in (2.7). They represent very general boundary conditions encompassing the usual periodic, anti-periodic and box boundary conditions. These coefficients encode the behaviour of the wavefunction on the boundaries $x = -ML$ and $x = ML$ (see Fig. 1). The

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[2] The case $\sin\xi_j - \operatorname{Im}v_j = 0$ signals the fact that the parametrization (2.5), (2.7) is slightly more general than the formal expression (2.2).

submatrices $\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ of $\mathcal{U}^-$ correspond to the dashed lines in Fig. 1. They are introduced for mere convenience in our approach.

It is now obvious that one cannot use Bloch's theorem to solve this problem as explained in the introduction. The potential, albeit sitting on equally spaced sites, is certainly not periodic and we impose quite general boundary conditions.

Instead, we formulate a *Bethe ansatz* [7] for Φ

$$\Phi(x) = e^{ikx}\mathcal{A}_I + e^{-ikx}\mathcal{A}_R \quad \text{where} \quad \begin{cases} \mathcal{A}_I = \sum_{j=1}^{M}\sum_{\epsilon=\pm} A_{I,j}^{\epsilon} e_j \otimes \hat{e}_\epsilon, \\ \mathcal{A}_R = \sum_{j=1}^{M}\sum_{\epsilon=\pm} A_{R,j}^{\epsilon} e_j \otimes \hat{e}_\epsilon. \end{cases} \quad (2.13)$$

In this form, $\Phi(x)$ is automatically a solution of (2.4) with

$$E = k^2. \tag{2.14}$$

Inserting the ansatz in (2.5) and (2.10), we find that Φ is the eigenfunction we look for if and only if the $4M$ amplitudes $A_{I,j}^{\epsilon}$ and $A_{R,j}^{\epsilon}$ satisfy the following relations

$$\mathcal{A}_R = e^{2ik(M-1)L} Z^+(-k)\mathcal{A}_I, \tag{2.15}$$

$$\mathcal{A}_R = e^{2ikML} Z^-(-k)\mathcal{A}_I, \tag{2.16}$$

where

$$Z^\pm(k) = -\big[\mathcal{U}^\pm - \mathbb{I} - k(\mathcal{U}^\pm + \mathbb{I})\big]^{-1}\big[\mathcal{U}^\pm - \mathbb{I} + k(\mathcal{U}^\pm + \mathbb{I})\big]. \tag{2.17}$$

These $2M \times 2M$ matrices characterize the type of potential and boundary conditions one is considering. Requiring a non-trivial solution for the wavefunction, one finds the following equation

$$\det\big(Z^+(-k) - Z^-(-k)e^{2ikL}\big) = 0. \tag{2.18}$$

This type of equation is usually called Bethe ansatz equations. To our knowledge, it is the first time that the Bethe equations have been established in this context. They impose constraints on the allowed values of k which incorporate the effect of the potential and of the boundary conditions. Solving in k as a function of the parameters controlling the potential and the boundary conditions allows one to determine the energy spectrum and to study how one can modify it by tuning these parameters. As we will see, this has consequences on the energy band structure of the associated model.

The above Bethe ansatz equations together with the method to get them for the very general model we are considering constitute the main result of this paper. They replace Bloch's theorem when periodicity is broken and provide a non-perturbative means to get the energy spectrum in such situations.

3. Periodic potential

Before exploring some applications of our method to more complicated cases in the following, we first show in this section that our approach consistently reproduce well-known results for periodic potentials and in particular for the Kronig–Penney model. We also obtain information on the bound states which are less studied. Finally, we compute the spectrum for an asymmetric potential which, to our knowledge, is not studied in the literature.

3.1. General case

In our language, a periodic potential with periodic boundary conditions is obtained by setting

$$U_1 = \cdots = U_M = e^{i\xi} \begin{pmatrix} \mu & \nu \\ -\nu^* & \mu^* \end{pmatrix} \equiv U \quad \text{and} \tag{3.1}$$

$$U_q = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{3.2}$$

In this case, the Bethe equations (2.18) reduce to

$$\begin{vmatrix} R^+ & T^+ & & & & & & -e^{2ikL} \\ T^- & R^- & -e^{2ikL} & & & & & \\ & -e^{2ikL} & R^+ & T^+ & & & & \\ & & T^- & R^- & -e^{2ikL} & & & \\ & & & & \ddots & & & \\ & & & T^- & R^- & -e^{2ikL} & & \\ & & & & -e^{2ikL} & R^+ & T^+ \\ -e^{2ikL} & & & & & T^- & R^- \end{vmatrix} = 0, \tag{3.3}$$

where, for $\mu = \mu_R + i\mu_I$ and $\nu = \nu_R + i\nu_I$ ($\mu_R, \mu_I, \nu_R, \nu_I \in \mathbb{R}$)[3]

$$R^+ = \frac{(\cos\xi + \mu_R)k^2 - 2i\mu_I k - \cos\xi + \mu_R}{(\cos\xi + \mu_R)k^2 + 2ik\sin\xi + \cos\xi - \mu_R},$$

$$T^+ = \frac{-2\nu k}{(\cos\xi + \mu_R)k^2 + 2ik\sin\xi + \cos\xi - \mu_R}, \tag{3.4}$$

$$R^- = \frac{(\cos\xi + \mu_R)k^2 + 2i\mu_I k - \cos\xi + \mu_R}{(\cos\xi + \mu_R)k^2 + 2ik\sin\xi + \cos\xi - \mu_R},$$

$$T^- = \frac{2\nu^* k}{(\cos\xi + \mu_R)k^2 + 2ik\sin\xi + \cos\xi - \mu_R}. \tag{3.5}$$

The determinant can be seen as a polynomial in e^{2ikL} of order $2M$ whose roots are functions of k of the form

$$X_p^\pm = \frac{1}{2}\left[\omega^{*p}T^+ + \omega^p T^- \pm \sqrt{\left(\omega^{*p}T^+ - \omega^p T^-\right)^2 + 4R^+R^-} \right],$$

$$p = 0, \ldots, M - 1, \tag{3.6}$$

where $\omega = e^{\frac{2i\pi}{M}}$ is the Mth root of unity. For $M = 1$, we recover the result given in [11]. To get the spectrum, one has to solve in k the following equations

$$e^{2ikL} = X_p^\pm, \quad p = 0, \ldots, M - 1. \tag{3.7}$$

Let us introduce the shift operator $\hat{P}f(x) = f(x + 2L)$. In the case under consideration, this operator commutes with the Hamiltonian and can therefore be diagonalized in the same basis.

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[3] In comparison with the notation of [11], $R^+ = R^+(-k)$, $T^+ = T^+(-k)$, $R^- = R^-(k)$ and $T^- = T^-(k)$.

When acting on Φ, this operator is represented by the following $2M \times 2M$ matrix

$$\hat{P} = \begin{pmatrix} & \begin{vmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{vmatrix} \\ \begin{matrix} 1 & \\ & 1 \end{matrix} & \end{pmatrix}. \tag{3.8}$$

Let us note that the eigenfunctions (2.13) constrained by relation (3.7) for a given p are actually common eigenfunctions of H and $\hat{P}$ as one can see from

$$\hat{P}\Phi(x) = \omega^p \Phi(x). \tag{3.9}$$

This relation allows us to give a simple physical interpretation for p. Indeed, p is the usual crystal momentum[4] carried by the particle. In the usual approach, it labels the Bloch's functions and we recover here by our different approach that it is indeed a good quantum number for a very general periodic potential. We also remark that Eq. (3.7) is M-periodic in terms of p. This statement is equivalent to the standard restriction of the range of the crystal momentum to the first Brillouin zone.

3.2. Kronig–Penney model

We now turn to the Kronig–Penney model to show that Eq. (3.7) consistently reproduce the standard equations of this model. In this case, all the v_j's are given by a δ potential with the same coupling constant c. This is obtained from (3.1) by taking

$$U = -e^{i\xi} \begin{pmatrix} \cos(\xi) & i\sin(\xi) \\ i\sin(\xi) & \cos(\xi) \end{pmatrix}, \quad \xi \in [0, \pi) \quad \text{and} \quad \tan(\xi) = \frac{2}{c}. \tag{3.10}$$

Therefore, we get

$$T^+ = T^- = \frac{ik\tan(\xi)}{1 + ik\tan(\xi)} \quad \text{and} \quad R^+ = R^- = \frac{-1}{1 + ik\tan(\xi)}. \tag{3.11}$$

After some algebra, we see that Eq. (3.7) become, for $p = 0, \dots, M - 1$ and real k

$$\cos(2kL) + \frac{1}{k\tan(\xi)}\sin(2kL) = \cos\left(\frac{2\pi p}{M}\right). \tag{3.12}$$

These are the equations obtained by using Bloch's theorem (see, for example, [2]). They give the well-known plots that we show in Fig. 2.[5] The plots represent the energy spectrum in terms of the crystal momentum p (restricted to the first Brillouin zone) for various values of ξ (here $M = 32$ and $L = 1$). For $\xi = 0$ (circle on Fig. 2), the coupling constant, c, tends to $+\infty$ and the energy does not depend on p. The states are localized in the regions $R_{j-1}^- \cup R_j^+$, $j = 2, \dots, M$, which are separated by purely reflecting walls (there is no transmission). The choice $\xi = \pi/2$ (box on Fig. 2) correspond to another particular case where the coupling constant vanishes. The states are delocalized and this is just the free particle model. The energy varies like the square of p. For an intermediate case, here $\xi = 0.2$ (cross on Fig. 2), the well-known energy band structure appears.

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[4] We choose the units so that $\hbar = 1$.

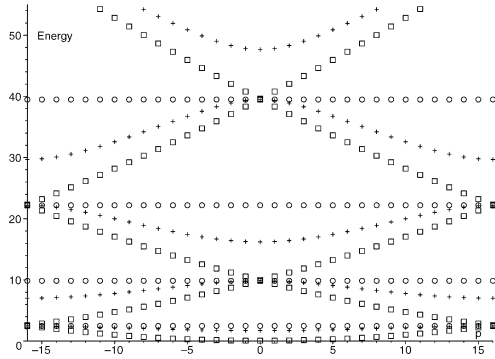[5] All the numerical resolutions and plots are realized with Maple.

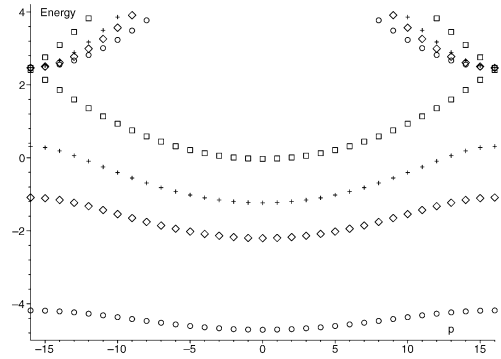Fig. 2. Lowest positive energy levels in terms of p for $\xi = 0$ (circle); 0.2 (cross); $\pi/2$ (box).

Fig. 3. Bound states and lowest positive energy levels in terms of p for $\xi = \pi/2$ (box); 2.3 (cross); 2.5 (diamond); 2.7 (circle).

Let us stress that in order to find Eq. (3.12), we assumed k real. However, to study the possible bound states we have to look for purely imaginary solutions of (3.7) of the type $k = ik_I$, $k_I \in \mathbb{R}$. In this case, we are led to solve the following equations, for $p = 0, \ldots, M - 1$

$$(1 + k_I \tan \xi)e^{2k_I L} = k_I \tan \xi \cos\left(\frac{2\pi p}{M}\right) \pm \sqrt{1 - k_I^2 \tan^2 \xi \sin^2\left(\frac{2\pi p}{M}\right)}. \tag{3.13}$$

Fig. 3 shows the solutions of this equation (for $\xi = 2.3$ (cross); 2.5 (diamond); 2.7 (circle)) which gives negative energy levels. We represent also the lowest positive energy levels solution of (3.12). The bound states appear only when $\xi > \pi/2$ (i.e. $c < 0$). For $\xi \to \pi^-$, the coupling constant tends to $-\infty$ and the states are localized around the points x_j^0.

3.3. Asymmetric potential

In this section, we study the periodic potential characterized by

$$U = \begin{pmatrix} 0 & e^{i\alpha} \\ -e^{\epsilon i\alpha} & 0 \end{pmatrix} \quad \text{where } \epsilon = -1 \quad \text{(respectively, } \epsilon = 1\text{).} \tag{3.14}$$

This particular form of U for $\epsilon = -1$ (respectively, $\epsilon = +1$) is obtained from (3.1) by setting $\mu = 0, \xi = 0$ and $\nu = e^{i\alpha}$ (respectively, $\mu = 0$, $\nu = 1$ and $\xi = \alpha$). In this case, one gets

$$R^+ = \frac{k^2 - 1}{k^2 + 1} = R^- \quad \text{and} \quad T^\pm = \frac{\mp 2ke^{\pm i\alpha}}{k^2 + 1} \tag{3.15}$$

$$\left(\text{respectively, } R^+ = \frac{k^2 - 1}{k^2 + 2ik\tan\alpha + 1} = R^- \quad \text{and} \quad T^\pm = \frac{\mp 2k}{\cos\alpha(k^2 + 2ik\tan\alpha + 1)} \right). \tag{3.16}$$

For $k \in \mathbb{R}$, Eq. (3.7) reduces to

$$(k^2 + 1)\sin(2kL) = 2k \sin\left(\frac{2\pi p}{M} - \alpha\right) \tag{3.17}$$

$$\left(\text{respectively, } (k^2 + 1)\cos\alpha \sin(2kL) + 2k \sin\alpha \cos(2kL) = 2k \sin\left(\frac{2\pi p}{M}\right) \right). \tag{3.18}$$
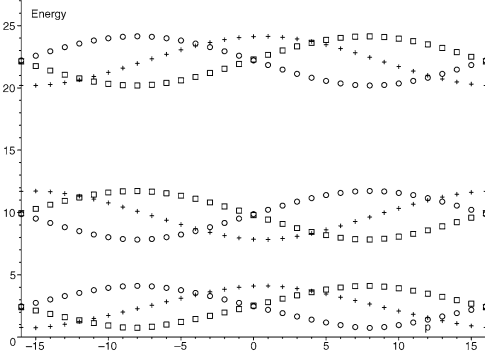
Fig. 4. Lowest positive energy levels in terms of p ($\epsilon = -1$) for $\alpha = 0$ (circle); $\pi/2$ (cross); π (box)
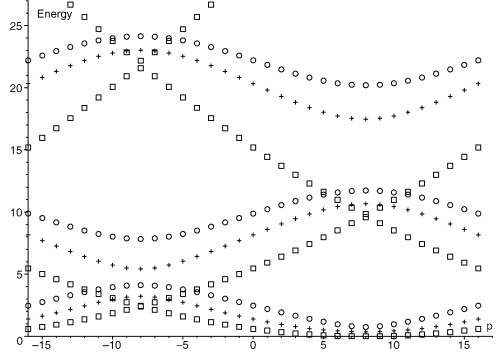
Fig. 5. Lowest positive energy levels in terms of p ($\epsilon = +1$) for $\alpha = 0$ (circle); $\pi/4$ (cross); $\pi/2$ (box).

Fig. 4 (respectively, Fig. 5) shows the behavior of the solutions of Eq. (3.17) (respectively, Eq. (3.18)). Let us remark that, for a generic α, these potentials break the symmetry of the spectrum under the transformation $p \to -p$. We also remark that the behaviors of the two spectra are completely different. For $\epsilon = -1$, the gaps between the energy bands are independent of the parameters α whereas, for $\epsilon = +1$, they decrease when α increases.

4. Dirichlet or Neumann conditions

In this section, we want to study the behavior of the energy band structure when we modify the boundary conditions. To illustrate this on a simple example we take the same potential as in (3.1) and simply change U_q in (3.2) to

$$U_q = \varepsilon \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{where } \varepsilon = -1 \quad (\text{respectively, } \varepsilon = +1). \tag{4.1}$$

This implements the Dirichlet (respectively, Neumann) boundary condition:

$$\phi(0) = 0 = \phi(L) \quad \left(\text{respectively, } \phi'(0) = 0 = \phi'(L) \right), \tag{4.2}$$

and breaks the periodicity of the model. This constitutes a basic example where our method still holds while Bloch's theorem breaks down. In this case the Bethe equations given in (2.18) are equivalent to

$$\begin{vmatrix} R^+ - \varepsilon e^{2ikL} & T^+ \\ T^- & R^- & -e^{2ikL} \\ & -e^{2ikL} & R^+ & T^+ \\ & & T^- & R^- & -e^{2ikL} \\ & & & \ddots \\ & & & T^- & R^- & -e^{2ikL} \\ & & & & -e^{2ikL} & R^+ & T^+ \\ & & & & & T^- & R^- - \varepsilon e^{2ikL} \end{vmatrix} = 0. \tag{4.3}$$

Again, this determinant is a polynomial of order $2M$ in e^{2ikL} whose roots read

$$Y_q^{\pm} = \sqrt{T^+ T^-} \cos\left(\frac{\pi q}{M}\right) \pm \sqrt{R^+ R^- - T^+ T^- \sin^2\left(\frac{\pi q}{M}\right)}, \quad 1 \leqslant q \leqslant M - 1, \tag{4.4}$$

$$Y^{\pm} = \frac{1}{2}\left[-\varepsilon(R^+ + R^-) \pm \sqrt{(R^+ - R^-)^2 + 4T^+ T^-} \right]. \tag{4.5}$$

The Bethe equations governing the spectrum then read

$$e^{2ikL} = Y_q^{\pm}, \quad 1 \leqslant q \leqslant M - 1, \tag{4.6}$$

$$e^{2ikL} = Y^{\pm}. \tag{4.7}$$

Let us make a few remarks before showing the influence of the boundary on the energy spectrum for a particular example. First, the parameter q cannot be interpreted as the crystal momentum any more (the shift operator $\hat{P}$ does not commute with the Hamiltonian). It does not label all the energy states since it is absent from Eq. (4.7). On the other hand, only Eq. (4.7) depends on the parameter ε characterizing the type of boundary conditions under consideration. We also stress that, although they look different, the roots in (3.6) and those in (4.4) can be written in the same form provided one replaces M by $M/2$ in (4.4) and relabels q appropriately. From all this, we conclude that Eq. (4.7) give the energy states arising from the presence of the boundary while the rest of the spectrum will be identical to that of the periodic case. In particular, the boundary effects become negligible as M becomes large.

Example

We take once again the matrix U given by (3.10) to define the potential at each site but now, we impose Neumann boundary conditions. The Bethe equations (4.6) and (4.7) become respectively (for k real)

$$\cos(2kL) + \frac{1}{k \tan \xi} \sin(2kL) = \cos\left(\frac{\pi q}{M}\right), \quad \text{for } 1 \leqslant q \leqslant M - 1, \tag{4.8}$$

$$\cos(2kL) - k \tan(\xi) \sin(2kL) = 1. \tag{4.9}$$

On Fig. 6 below, we plot solutions of Eqs. (4.8) and (4.9) for $M = 16$ and $\xi = 0.2$. The solutions of (4.8) are represented by circles and those of (4.9) by boxes which we displayed at $q = 0$
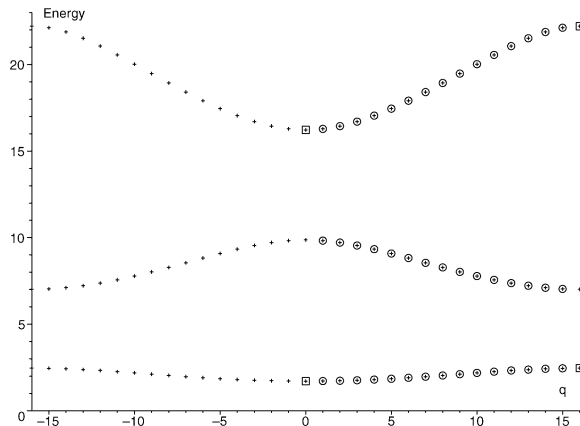

Fig. 6. Lowest positive energy levels in terms of q for $\xi = 0.2$.

and $q = 16$ for convenience. To make the comparison even easier, we have also represented the energy band structure of the periodic case for $M = 32$ (crosses on Fig. 6). We see that for the first and third energy band, the allowed energy levels coincide with the periodic case as the solutions of (4.9) nicely complete those of (4.8). However, the effect of the boundary conditions shows up in the second energy band where two states are "missing" with respect to the periodic case.

5. Impurities

So far, we have considered homogeneous potentials in the sense that the potential was the same at each site. As illustrated above, even with non-periodic boundary conditions, this does not deviate drastically from the periodic case as only local boundary effects arise.

In this section, we want to explore very different situations which cannot be approached by perturbing the periodic case and therefore, show the advantages of our approach. Such situations occur when one modifies the potential at only one or several sites. Thus, these sites appear as what we call impurities. These models can be useful for describing localized defects in materials with one dimensional behavior (nanowires, etc.).

We illustrate this in the following by considering one such impurity and then a subset of equally spaced identical impurities in a given periodic potential.

5.1. One impurity

We restrict ourselves to the case of periodic boundary conditions and we imagine that the impurity is sitting at site 1 with a potential v_1 given as in (2.2) while all the other sites have the same potential $v_2 = \cdots = v_M = v$. This model is obtained in our language by taking

$$U_1 = e^{i\xi_1} \begin{pmatrix} \mu_1 & v_1 \\ -v_1^* & \mu_1^* \end{pmatrix}, \qquad U_2 = \cdots = U_M = U = e^{i\xi} \begin{pmatrix} \mu & v \\ -v^* & \mu^* \end{pmatrix} \quad \text{and}$$

$$U_q = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{5.1}$$

where U_1 and U characterize respectively v_1 and v. In this case, the Bethe equations given in (2.18) reduce to

$$\begin{vmatrix} R_1^+ & T_1^+ & & & & & & -e^{2ikL} \\ T_1^- & R_1^- & -e^{2ikL} & & & & & \\ & -e^{2ikL} & R^+ & T^+ & & & & \\ & & T^- & R^- & -e^{2ikL} & & & \\ & & & & \ddots & & & \\ & & & & T^- & R^- & -e^{2ikL} & \\ & & & & & -e^{2ikL} & R^+ & T^+ \\ -e^{2ikL} & & & & & & T^- & R^- \end{vmatrix} = 0 \tag{5.2}$$

where R_1^+, T_1^+, T_1^- and R_1^- are given by relations (3.4) and (3.5) substituting ξ, μ and v by ξ_1, μ_1 and v_1, respectively.

To simplify the expression of these Bethe equations, we consider the case of symmetric potentials i.e. $R^+ = R^- = R$, $T^+ = T^- = T$, $R_1^+ = R_1^- = R_1$ and $T_1^+ = T_1^- = T_1$. In this particular
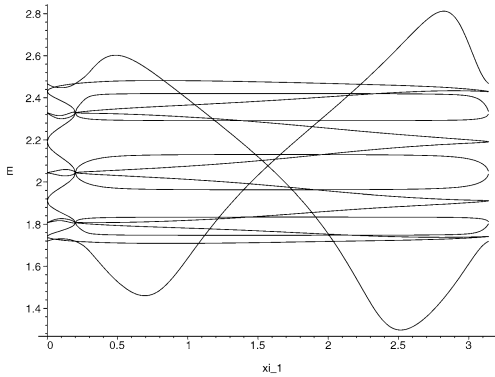
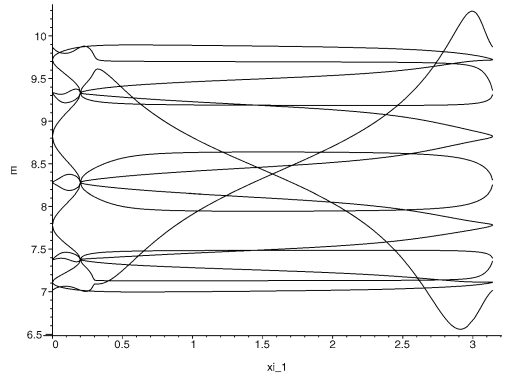Fig. 7. Energy levels of the first band in terms of ξ_1 for $\xi = 0.2$.

Fig. 8. Energy levels of the second band in terms of ξ_1 for $\xi = 0.2$.

case, relation (5.2) is equivalent to the following equations

$$2e^{2ikL} = \left(y + \frac{1}{y}\right)T \pm \sqrt{\left(y - \frac{1}{y}\right)^2 T^2 + 4R^2} \tag{5.3}$$

where y is any root of one of the following polynomials

$$T^2(T_1 \mp R_1)\left(y^{2M} + 1\right) + T\left(R^2 - T^2 - R_1^2 - T_1^2 \pm 2T_1 R\right)y^M$$

$$+ R\left(2T_1(R - R_1) \pm (R - R_1)^2 \pm T_1^2 \mp T^2\right)\sum_{j=1}^{M-1} y^{2j}. \tag{5.4}$$

Note that we consistently recover the periodic case when $R_1 = R$ and $T_1 = T$ since the polynomials (5.4) simply reduce to $(y^M - 1)^2$.

Example

We imagine that both the impurity and the bulk potential are given by a δ potential but with different coupling constants (i.e. the matrices U and U_1 are given by (3.10) with parameter ξ and ξ_1, respectively). We study the behavior of the spectrum when the coupling constant of the impurity is varied while ξ is kept fixed (we choose here $\xi = 0.2$).

Figs. 7 and 8 show the behavior of the energy levels of the first and second positive energy bands as functions of ξ_1 for $M = 8$. In the case where $\xi_1 = \xi = 0.2$, we remark a degeneracy as the impurity becomes identical to the bulk potential. The corresponding energy levels coincide with those represented by crosses on Fig. 2. Generally speaking, the effect of the impurity is far from being trivial. We see that in each band, two energy levels are severely modified depending on the strength of the impurity. This can have strong consequences on the corresponding system (if we think of conducting or insulating materials, for instance).

5.2. N identical impurities

Here, we introduce periodically N identical impurities ($N \in \mathbb{N}$) in a given periodic potential. From now on, let M be a multiple of N i.e. $M = M_1 N$ with $M_1 > 1$. The impurities have potential v_1 and the bulk potential is v. In this case, the matrices U_j take the following particular

form

$$U_1 = U_{M+1} = \cdots = U_{(N-1)M+1} = e^{i\xi_1} \begin{pmatrix} \mu_1 & \nu_1 \\ -\nu_1^* & \mu_1^* \end{pmatrix}, \qquad (5.5)$$

$$U_2 = \cdots = U_{M_1} = U_{M_1+2} = \cdots = U_{(N-1)M_1+2} = \cdots = U_M = e^{i\xi} \begin{pmatrix} \mu & \nu \\ -\nu^* & \mu^* \end{pmatrix}. \qquad (5.6)$$

As before, we restrict ourselves to the case of symmetric potentials for simplicity ($R^+ = R^- = R$, $T^+ = T^- = T$, $R_1^+ = R_1^- = R_1$ and $T_1^+ = T_1^- = T_1$). The Bethe equations take the form

$$2e^{2ikL} = T\left(y + \frac{1}{y}\right) \pm \sqrt{T^2\left(y - \frac{1}{y}\right)^2 + 4R^2}. \qquad (5.7)$$

Again, y is any root of one of the following polynomials, for $0 \leqslant q \leqslant N - 1$

$$4\gamma^{2q} P_q^+(y) P_q^-(y) + y^{2M_1}(\gamma^q - 1)^2(\gamma^q + 1)^2 T^2 (R^2 - T^2 + T_1^2 - R_1^2)^2, \qquad (5.8)$$

where we have introduced

$$P_q^\pm(y) = T^2(T_1 \mp R_1)(y^{2M_1} + 1) + \frac{1}{2}\left(\gamma^q + \frac{1}{\gamma^q}\right) T (R^2 - T^2 - R_1^2 - T_1^2 \pm 2T_1 R) y^{M_1}$$

$$+ R\left(2T_1(R - R_1) \pm (R - R_1)^2 \pm T_1^2 \mp T^2\right) \sum_{j=1}^{M_1-1} y^{2j}, \qquad (5.9)$$

and $\gamma = e^{\frac{2i\pi}{N}}$ is the Nth root of unity. The presence of γ accounts for the inclusion of N identical impurities. In the case $N = 1$, one has $\gamma = 1$ and the set of coupled equations (5.7), (5.8) reduces to (5.3), (5.4).

6. $\mathcal{N}$ bosons with contact interaction

In this section, the general method of Section 2 is extended to $\mathcal{N}$ bosons with δ-interaction in presence of the potential defined in (2.1), (2.2). We restrict ourselves to the case of bosons for the sake of clarity but a treatment analogous to that in [5,11], where the statistics is not given a priori, is possible. Our aim is to derive the corresponding Bethe ansatz equations which can be used then as above to get information on the energy spectrum of the model. However, we will not go into the details of exploring particular cases as the essential features of our approach have already been discussed in the previous sections. Instead, we trust that the interested people will adapt the general equations to their specific needs in order to study the influence of interactions in particular models with point potentials.

We first need some definitions and notations. Let $\mathfrak{S}_{\mathcal{N}}$ and $\mathfrak{W}_{\mathcal{N}}$ denote the permutation group and the Weyl group associated to the Lie algebra $B_{\mathcal{N}}$, respectively. The group $\mathfrak{S}_{\mathcal{N}}$ consists of $\mathcal{N}$ generators: the identity Id and $\mathcal{N} - 1$ elements $T_1, \ldots, T_{\mathcal{N}-1}$ satisfying

$$T_j T_j = Id, \qquad T_j T_\ell = T_\ell T_j \quad \text{for } |j - \ell| > 1, \qquad (6.1)$$

$$T_j T_{j+1} T_j = T_{j+1} T_j T_{j+1}. \qquad (6.2)$$

In particular, the last relation gives rise to the famous Yang–Baxter equation [5,14]. For convenience, we denote a general transposition of $\mathfrak{S}_{\mathcal{N}}$ by T_{ij}, $i < j$, given by

$$T_{ij} = T_{j-1} \cdots T_{i+1} T_i T_{i+1} \cdots T_{j-1}. \qquad (6.3)$$

The Weyl group $\mathfrak{W}_{\mathcal{N}}$ contains $2^{\mathcal{N}} \mathcal{N}!$ elements generated by Id, $T_1, \ldots, T_{\mathcal{N}-1}$ and R_1 satisfying (6.1), (6.2) and

$$R_1 R_1 = Id, \tag{6.4}$$

$$R_1 T_1 R_1 T_1 = T_1 R_1 T_1 R_1, \tag{6.5}$$

$$R_1 T_j = T_j R_1 \quad \text{for } j > 1. \tag{6.6}$$

Let us define also R_j, $j = 2, \ldots, N$, as

$$R_j = T_{j-1} \cdots T_1 R_1 T_1 \cdots T_{j-1}. \tag{6.7}$$

Let $x_1, \ldots, x_{\mathcal{N}}$ be the positions of the particles. Like in the previous case without interactions, the wavefunction is not defined at the sites x_j^0. Here, in addition, it is not defined at the points where the interaction takes place. As we shall see, it satisfies the boundary conditions describing the external potential and conditions describing the point interaction between two particles. The natural generalization of (2.3) leads to represent the wavefunction as follows

$$\phi(x_1, \ldots, x_{\mathcal{N}}) = \phi_{j_1, \ldots, j_{\mathcal{N}}}^{\epsilon_1, \ldots, \epsilon_{\mathcal{N}}}(x_1, \ldots, x_{\mathcal{N}}) \tag{6.8}$$

in the regions, for $1 \leqslant k \leqslant \mathcal{N}$,

$$\left(M - 2j_k + \frac{\epsilon_k + 1}{2} \right) L < x_k < \left(M - 2j_k + \frac{\epsilon_k + 3}{2} \right) L. \tag{6.9}$$

Then, for $x_1, \ldots, x_{\mathcal{N}}$ two by two different, one defines the following $(2M)^{\mathcal{N}}$-component vector

$$\Phi(x_1, \ldots, x_{\mathcal{N}})$$
$$= \sum_{\substack{1 \leqslant j_1, \ldots, j_{\mathcal{N}} \leqslant M \\ \epsilon_1, \ldots, \epsilon_{\mathcal{N}} = \pm}} \phi_{j_1, \ldots, j_{\mathcal{N}}}^{\epsilon_1, \ldots, \epsilon_{\mathcal{N}}} \left(f_{j_1}^{\epsilon_1}(x_1), \ldots, f_{j_{\mathcal{N}}}^{\epsilon_{\mathcal{N}}}(x_{\mathcal{N}}) \right) e_{j_1} \otimes \hat{e}_{\epsilon_1} \otimes \cdots \otimes e_{j_{\mathcal{N}}} \otimes \hat{e}_{\epsilon_{\mathcal{N}}} \tag{6.10}$$

where, for $1 \leqslant k \leqslant \mathcal{N}$,

$$f_k^{\pm}(x) = \pm(x + 2kL - L - ML) - L + ML. \tag{6.11}$$

As before, the advantage of the vector $\Phi(x_1, \ldots, x_{\mathcal{N}})$ is that it contains all the information on the wavefunction for $x_1, \ldots, x_{\mathcal{N}}$ running only in the interval $]ML - L, ML[$ of length L. This allows to impose all the conditions for interactions between particles and with the external potential in a very compact form.

Given a tensor product of spaces, $(\mathbb{C}^{2M})^{\otimes \mathcal{N}}$, we define the action of a matrix $A \in \text{End}(\mathbb{C}^{2M})$ on the kth space by

$$A^{[k]} = \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{k-1} \otimes A \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{\mathcal{N}-k}. \tag{6.12}$$

We are now in position to write all the conditions the wavefunction of the problem has to satisfy:

- Shrödinger equation: for $x_i \in]ML - L, ML[$ and $x_1, \ldots, x_{\mathcal{N}}$ two by two different

$$-\sum_{k=1}^{\mathcal{N}} \partial_{x_k}^2 \Phi(x_1, \ldots, x_{\mathcal{N}}) = E \Phi(x_1, \ldots, x_{\mathcal{N}}). \tag{6.13}$$

- External point potential: for $1 \leqslant k \leqslant \mathcal{N}$

$$\big[(\mathcal{U}^+ - \mathbb{I})^{[k]} + i(\mathcal{U}^+ + \mathbb{I})^{[k]} \partial_{x_k}\big]\Phi(x_1, \ldots, x_{\mathcal{N}}) = 0 \quad \text{for } x_k \to ML - L, \tag{6.14}$$

$$\big[(\mathcal{U}^- - \mathbb{I})^{[k]} + i(\mathcal{U}^- + \mathbb{I})^{[k]} \partial_{x_k}\big]\Phi(x_1, \ldots, x_{\mathcal{N}}) = 0 \quad \text{for } x_k \to ML. \tag{6.15}$$

- Interactions between particles: for $Q \in \mathfrak{S}_{\mathcal{N}}$ and $1 \leqslant i \leqslant \mathcal{N} - 1$,

$$\Phi(x_1, \ldots, x_N)\big|_{x_{Qi} = x_{Q(i+1)}^+} = \tilde{Q}\tilde{T}_i\tilde{Q}^{-1}\Phi(x_1, \ldots, x_N)\big|_{x_{Qi} = x_{Q(i+1)}^-}, \tag{6.16}$$

$$(\partial_{x_{Qi}} - \partial_{x_{Q(i+1)}})\Phi(x_1, \ldots, x_N)\big|_{x_{Qi} = x_{Q(i+1)}^+}$$

$$= \tilde{Q}\tilde{T}_i\tilde{Q}^{-1}\big[(\partial_{x_{Qi}} - \partial_{x_{Q(i+1)}}) + 2g\big]\Phi(x_1, \ldots, x_N)\big|_{x_{Qi} = x_{Q(i+1)}^-}, \tag{6.17}$$

where $\tilde{Q}$ is the usual representation of the element $Q \in \mathfrak{S}_{\mathcal{N}}$ on $(\mathbb{C}^{2M})^{\otimes \mathcal{N}}$. Namely, denoting by $E_{ij}, i, j = 1, \ldots, 2M$, the matrices with 1 at position (i, j) and 0 elsewhere, one has

$$\tilde{T}_j = \sum_{k,\ell=1}^{2M} \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{j-1} \otimes E_{k\ell} \otimes E_{\ell k} \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{\mathcal{N}-j-1}. \tag{6.18}$$

Then using $\widetilde{T_i T_j} = \tilde{T}_i \tilde{T}_j$ and (6.3), it is easy to get $\tilde{Q}$ for any $Q \in \mathfrak{S}_{\mathcal{N}}$ since an arbitrary permutation can always be decomposed in transpositions.

For bosons, the wavefunction $\phi(x_1, \ldots, x_{\mathcal{N}})$ should be symmetric under the exchange of any two particles. In terms of Φ, this reads, for $1 \leqslant i < j \leqslant N$,

$$\Phi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_{\mathcal{N}}) = \tilde{T}_{ij}\Phi(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_{\mathcal{N}}). \tag{6.19}$$

Therefore, we can order the positions of the particles without loss of generality. In the following, we take $ML - L < x_1 < \cdots < x_{\mathcal{N}} < ML$. The ansatz consists in representing Φ by

$$\Phi(x_1, \ldots, x_{\mathcal{N}}) = \sum_{P \in \mathfrak{W}_{\mathcal{N}}} e^{i(k_{P1}x_1 + \cdots + k_{P\mathcal{N}}x_{\mathcal{N}})}\mathcal{A}_P, \tag{6.20}$$

where

$$\mathcal{A}_P = \sum_{\substack{1 \leqslant j_1, \ldots, j_{\mathcal{N}} \leqslant M \\ \epsilon_1, \ldots, \epsilon_{\mathcal{N}} = \pm}} A_{P, j_1, \ldots, j_{\mathcal{N}}}^{\epsilon_1, \ldots, \epsilon_{\mathcal{N}}} e_{j_1} \otimes \hat{e}_{\epsilon_1} \otimes \cdots \otimes e_{j_{\mathcal{N}}} \otimes \hat{e}_{\epsilon_{\mathcal{N}}} \tag{6.21}$$

and, for any $v = (v_1, \ldots, v_{\mathcal{N}})$,

$$v_{T_i} = (v_1, \ldots, v_{i-1}, v_{i+1}, v_i, v_{i+2}, \ldots, v_{\mathcal{N}}), \tag{6.22}$$

$$v_{R_1} = (-v_1, v_2, \ldots, v_{\mathcal{N}}). \tag{6.23}$$

We need to determine the $2^{\mathcal{N}} \mathcal{N}! (2M)^{\mathcal{N}}$ parameters $A_{P, j_1, \ldots, j_{\mathcal{N}}}^{\epsilon_1, \ldots, \epsilon_{\mathcal{N}}}$ to find the solution of our problem. Inserting the ansatz (6.20) in conditions (6.14) and (6.15), one gets

$$\mathcal{A}_{PR_1} = \big(Z^+(-k_{P1})\big)^{[1]} e^{2ik_{P1}(M-1)L}\mathcal{A}_P, \tag{6.24}$$

$$\mathcal{A}_{PR_{\mathcal{N}}} = \big(Z^-(-k_{P\mathcal{N}})\big)^{[\mathcal{N}]} e^{2ik_{P\mathcal{N}}ML}\mathcal{A}_P, \tag{6.25}$$

where $Z^{\pm}$ is given by (2.17). Similarly, from conditions (6.16) and (6.17), we get, for $1 \leqslant j \leqslant \mathcal{N} - 1$,

$$\mathcal{A}_{PT_j} = y(k_{Pj} - k_{P(j+1)})\mathcal{A}_P, \tag{6.26}$$

where

$$y(k) = \frac{k - ig}{k + ig}.$$ (6.27)

Since our construction is based on $\mathfrak{W}_{\mathcal{N}}$, the Bethe ansatz is consistent if and only if $y(k)$ satisfies the Yang–Baxter equation [5,14] and $Z^+(k)$ and $y(k)$ satisfy the reflection equation [15,16] (see, for example [11], for details). These relations hold true by direct computation, implying the exact solvability of the model.

The non-vanishing of the wavefunction implies the following constraints, for $1 \leqslant j \leqslant \mathcal{N}$,

$$\det\left[\left(Z^+(-k_j)\right)^{[1]} - \prod_{m \neq j} y(k_j + k_m) y(k_j - k_m) \left(Z^-(-k_j)\right)^{[\mathcal{N}]} e^{2ik_j L} \right] = 0.$$ (6.28)

These relations are the Bethe equations associated to our problem. We recover the results of [11] by setting $M = 1$ and $U_q = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$. As in the previous section, to get the spectrum of a given model with δ interaction, one chooses the corresponding matrices U_j and U_q and solves these equations in k_j. The energy of the corresponding state is given by $E = \sum_{j=1}^{\mathcal{N}} k_j^2$.

7. Conclusions

In this paper, we have presented a general method to address the question of the energy spectrum for a large class of one-dimensional models with equally spaced point potentials. We also described how to extend the method to the case where particle interactions are present. The main results consist in Bethe ansatz equations which allow a non-perturbative treatment of these issues.

We have illustrated the method in various typical situations of interest and have obtained exact results on the effects of boundaries and impurities in such models. In view of the importance of the Kronig–Penney model in solid state physics, we believe that our method will serve as a useful toolbox to treat even more realistic situations which now occur in experimental situations with the advent of the "quantum technology".

Acknowledgements

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