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A new class of solvable models in quantum mechanics describing point interactions on the line

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Abstract. We provide a detailed analysis of properties of the Schrödinger operator in $L^2(\boldsymbol{R})$ which formally can be written as

$$-\frac{d^2}{dx^2}+\sum_{y\in Y}\nu_y\delta'(\cdot-y)$$

where δ' is the derivative of Dirac's δ-function and $Y\subset\boldsymbol{R}$ is discrete. This model allows for an explicit calculation of spectral properties. Special emphasis is given to the periodic case $Y=\boldsymbol{Z}$, $\nu=\nu_j$, $j\in\boldsymbol{Z}$ where the spectrum and the density of states are explicitly computed. Also the spectrum for a half-crystal is given. We study in detail spectral consequences when various defects and impurities are added to the periodic case.

1. Introduction

Solvable models are important in the sense that they provide exact and detailed information. Furthermore they can serve as a 'laboratory' for testing one's intuition and for testing conjectures. In this paper we study a new class of solvable one-dimensional Schrödinger operators in detail in which the Hamiltonian formally can be written as

$$H=-\frac{d^2}{dx^2}+\sum_{y\in Y}\nu_y\delta'(\cdot-y) \tag{1.1}$$

where Y is a discrete subset of $\boldsymbol{R}$, finite or infinite, and δ' denotes the derivative of Dirac's δ-function. The existence of the model (1.1) was pointed out by Grossmann *et al* [1]; however, no detailed analysis has appeared so far.

Before we proceed to a description of the content of this paper, we point out some properties of the operator (1.1). First of all we observe that the interaction is concentrated on the discrete set Y, i.e. the potential is a point interaction. The corresponding model with δ' replaced by δ has been extensively studied, originating with Kronig and Penney [2]; see also the literature referred to in [3]. Whereas the δ-interaction model can be rigorously defined using quadratic forms, this approach does not work for (1.1). This is similar to the multidimensional case: the Hamiltonian corresponding to point interactions in dimensions two and three cannot be defined as a quadratic form. One way to define (1.1) rigorously (for simplicity we here take $Y=\{0\}$) is to consider the operator ($\mathscr{D}(H)$ denotes the domain of an operator H, cf [4])

$$\dot{H} = -\frac{d^2}{dx^2} \qquad \mathscr{D}(\dot{H}) = \{g \in H^{2,2}(\boldsymbol{R}) | g'(0) = 0\} \tag{1.2}$$

which has deficiency indices (1, 1) (cf [4]). Then the members of the one-parameter family of self-adjoint extensions of $\dot{H}$ serve as realisations of (1.1) with $Y = \{0\}$.

In § 2 we give a detailed description of properties of the self-adjoint realisation of (1.1), denoted by $\Xi_{\beta,Y}$, $Y = \{y_j \in \boldsymbol{R} | j \in J\}$, $\beta = (\beta_j)_{j \in J}$, with $J \subset \boldsymbol{N}$ finite, with special attention to spectral properties. The eigenvalues, of which there can be at most $|J|$ (counting multiplicities), are then determined as zeros of an explicit $|J| \times |J|$ determinant.

In § 3 we study in detail the case when Y forms a lattice $Y = a\boldsymbol{Z}$. In particular we give explicitly the spectrum of $\Xi_{\beta,a\boldsymbol{Z}}$ when β is constant. Furthermore we compute the density of states for this model. Finally we provide the spectrum of two half-crystals 'glued' together, i.e. $\sigma(\Xi_{\beta,a\boldsymbol{Z}})$ with $\beta_j = \beta^+$, $j \geq 0$, $\beta_j = \beta^-$, $j < 0$. The method used is to relate $\Xi_{\beta,a\boldsymbol{Z}}$ to a certain second-order difference operator on $l^2(\boldsymbol{Z})$, a technique introduced by Phariseau [5] for the δ-model.

For an analysis of various types of ordered alloys, both deterministic and random, for this model we refer to Gesztesy *et al* [6] where, e.g., the Saxon–Hutner conjecture [7] concerning gaps in the spectrum is proved.

In § 4 we study how the introduction of certain impurities in the crystal affects the spectrum. More precisely it is proved that the essential spectrum remains invariant and absolutely continuous, while eigenvalues may occur in gaps of the spectrum. Detailed properties are given when only one impurity or defect is added. For a comprehensive presentation of models with point interactions we refer to Albeverio *et al* [3].

2. Basic properties

We will start by giving some basic properties of the Schrödinger operator with a potential which is formally a finite sum of δ'-functions located at a set Y where

$$Y = \{y_1, \ldots, y_N\} \subset \boldsymbol{R}. \tag{2.1}$$

Consider the closed, symmetric and non-negative operator $\dot{H}_Y$ with

$$\begin{aligned} &\mathscr{D}(\dot{H}_Y) = \{g \in H^{2,2}(\boldsymbol{R}) | g'(y_j) = 0, j = 1, \ldots, N\} \\ &\dot{H}_Y = -d^2/dx^2 \end{aligned} \tag{2.2}$$

where $H^{2,2}(\boldsymbol{R})$ is the standard Sobolev space. Since formally $\dot{H}_Y$ and

$$-\frac{d^2}{dx^2} + \sum_{j=1}^{N} \nu_j \delta'(\cdot - y_j)$$

coincide on $\mathscr{D}(\dot{H}_Y)$, it is reasonable to consider certain self-adjoint extensions of $\dot{H}_Y$ as rigorous realisations of the Schrödinger operator with interaction given as a sum of δ'-functions located at Y. The adjoint of $\dot{H}_Y$ is

$$\dot{H}_Y^* = -\frac{d^2}{dx^2} \qquad \mathscr{D}(\dot{H}_Y^*) = \{g \in H^{2,2}(\boldsymbol{R} \setminus Y) | g'(y_{j^+}) = g'(y_{j^-}), j = 1, \ldots, N\}. \tag{2.3}$$

It is easily seen that

$$\phi_j(x) = \operatorname{sgn}(x-y_j)\exp(\mathrm{i}k|x-y_j|) \qquad j=1,\ldots,N \tag{2.4}$$

($\operatorname{sgn} x = x|x|^{-1}$, $x \neq 0$) span the deficiency subspaces of $\dot{H}_Y$, and hence

$$\operatorname{def}(\dot{H}_Y) = (N, N). \tag{2.5}$$

Thus there is a N^2-parameter family of self-adjoint extensions of $\dot{H}_Y$ (cf [4]).

We select the following N-parameter family $\Xi_{\beta,Y}$ which by definition will be considered as a rigorous realisation of (1.1):

$$\mathscr{D}(\Xi_{\beta,Y}) = \{g \in H^{2,2}(\boldsymbol{R}\setminus Y) | g'(y_{j^+}) = g'(y_{j^-}),\, g(y_{j^+}) - g(y_{j^-}) = \beta_j g'(y_j),\, j=1,\ldots,N\}$$

$$\begin{aligned} &\Xi_{\beta,Y} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \qquad \beta = (\beta_1,\ldots,\beta_N) \qquad Y = \{y_1,\ldots,y_n) \\ &-\infty < \beta_j \leqslant \infty \qquad y_j \in \boldsymbol{R} \qquad j=1,\ldots,N. \end{aligned} \tag{2.6}$$

Observe that $\beta_j = 0$, $j=1,\ldots,N$ gives $\Xi_{\beta,Y} = -\mathrm{d}^2/\mathrm{d}x^2$ on $H^{2,2}(\boldsymbol{R})$ and that $\beta_j = \infty$ for some $j \in \{1,\ldots,N\}$ gives a Neumann boundary condition at y_j.

The basic properties of $\Xi_{\beta,Y}$ can be summarised in the following theorem.

Theorem 2.1. (*a*) The resolvent of $\Xi_{\beta,Y}$ equals ($\rho(H) = \boldsymbol{C}\setminus\sigma(H)$ denotes the resolvent set of an operator H)

$$\begin{aligned} &(\Xi_{\beta,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\Gamma_{\beta,Y}(k)]_{jj'}^{-1} (\overline{\tilde{G}_k(\cdot - y_{j'})}, \cdot)\tilde{G}_k(\cdot - y_j), \\ &\qquad k^2 \in \rho(\Xi_{\beta,Y}),\ \operatorname{Im} k \geqslant 0] \qquad -\infty < \beta_j \leqslant \infty \qquad \beta_j \neq 0 \\ &\qquad y_j \in \boldsymbol{R} \qquad j=1,\ldots,N \end{aligned} \tag{2.7}$$

where

$$\begin{aligned} &G_k = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - k^2\right)^{-1} \qquad \operatorname{Im} k > 0 \\ &G_k(x-y) = \frac{\mathrm{i}}{2k}\exp(\mathrm{i}k|x-y|) \qquad \tilde{G}_k(x) = \operatorname{sgn}(x) G_k(x) \end{aligned} \tag{2.8}$$

and

$$\Gamma_{\beta,Y}(k) = [-(\beta_j k^2)^{-1}\delta_{jj'} + G_k(y_j - y_{j'})]_{j,j'=1}^{N}. \tag{2.9}$$

(*b*) The domain of $\Xi_{\beta,Y}$ is

$$\begin{aligned} \mathscr{D}(\Xi_{\beta,Y}) = \Bigg\{ &\psi \in L^2(\boldsymbol{R}) | \psi(x) = \phi_k(x) + \frac{\mathrm{i}}{k}\sum_{j,j'=1}^{N} [\Gamma_{\beta,Y}(k)]_{jj'}^{-1} \phi_k'(y_{j'})\tilde{G}_k(x-y_j), \\ &\phi_k \in H^{2,2}(\boldsymbol{R}),\ k^2 \in \rho(\Xi_{\beta,Y}),\ \operatorname{Im} k > 0 \Bigg\}. \end{aligned} \tag{2.10}$$

The above decomposition is unique, and we have

$$(\Xi_{\beta,Y} - k^2)\psi = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - k^2\right)\phi_k. \tag{2.11}$$

Furthermore if $\psi = 0$ in an open set $\Omega \subset \boldsymbol{R}$, then also $\Xi_{\beta,Y}\psi = 0$ in Ω.

(*c*) We have that (where $\sigma_{ess}/\sigma_{ac}/\sigma_{sc}$ denotes the essential/absolutely continuous/singularly continuous part of the spectrum σ)

$$\sigma_{ess}(\Xi_{\beta,Y}) = \sigma_{ac}(\Xi_{\beta,Y}) = [0,\infty),\ \sigma_{sc}(\Xi_{\beta,Y}) = \varnothing. \tag{2.12}$$

In addition $\Xi_{\beta,Y}$ has at most N negative eigenvalues counting multiplicities and

$$k_0^2 \in \sigma_p(\Xi_{\beta,Y}) \cap (-\infty, 0) \qquad \text{iff} \qquad \det[\Gamma_{\beta,Y}(k_0)] = 0 \qquad \operatorname{Im} k_0 > 0 \tag{2.13}$$

and the multiplicity of the eigenvalue k_0^2 equals the multiplicity of the eigenvalue zero of the matrix $\Gamma_{\beta,Y}(k_0)$. The corresponding eigenfunction is

$$\psi_{k_0^2}(x) = \sum_{j=1}^{N} c_j \tilde{G}_{k_0}(x - y_j) \tag{2.14}$$

where $(c_1, \ldots, c_N)$ is an eigenvector of $\Gamma_{\beta,Y}(k_0)$ to the eigenvalue zero. If at most one $\beta_{j_0} = \infty$, then all the eigenvalues are simple. If $\beta_j = \infty$ for at least two different $j \in \{1, \ldots, N\}$, then $\Xi_{\beta,Y}$ has in addition infinitely many eigenvalues embedded in $[0, \infty)$ accumulating at infinity.

Proof. (*a*) Define

$$h_\beta(x) = (\overline{G_k(x-\cdot)}, g) + \sum_{j,j'=1}^{N} [\Gamma_{\beta,Y}(k)]_{jj'}^{-1} (\overline{\tilde{G}_k(\cdot - y_{j'})}, g)\tilde{G}_k(x - y_j) \tag{2.15}$$

where $g \in L^2(\boldsymbol{R})$ and $\operatorname{Im} k > 0$ is such that $\det[\Gamma_{\beta,Y}(k)] \neq 0$. It is easily seen that $h_\beta \in \mathscr{D}(\Xi_{\beta,Y})$ and by explicit calculation

$$(\Xi_{\beta,Y} - k^2)h_\beta = -h_\beta'' - k^2 h_\beta = g. \tag{2.16}$$

(*b*) We have that

$$\mathscr{D}(\Xi_{\beta,Y}) = (\Xi_{\beta,Y} - k^2)^{-1} L^2(\boldsymbol{R}) \qquad \operatorname{Im} k > 0 \tag{2.17}$$

and by using

$$L^2(\boldsymbol{R}) = \left(-\frac{d^2}{dx^2} - k^2\right) H^{2,2}(\boldsymbol{R}) \qquad \operatorname{Im} k > 0$$

and (2.7) the result (2.10) follows. To prove the locality property assume ψ of the form in (2.10) vanishes in Ω, thus

$$\phi_k(x) = -\sum_{j,j'=1}^{N} [\Gamma_{\beta,Y}(k)]_{jj'}^{-1} \phi_k'(y_{j'}) \tilde{G}_k(x - y_j) \qquad x \in \Omega. \tag{2.18}$$

Consider first the case when $\Omega \cap Y = \varnothing$. Then

$$\begin{aligned}(\Xi_{\beta,Y}\psi)(x) &= \left(-\frac{d^2}{dx^2} - k^2\right)\phi_k(x) \\ &= -\sum_{j,j'=1}^{N} [\Gamma_{\beta,Y}(k)]_{jj'}^{-1} \phi_k'(y_{j'}) \left[\left(-\frac{d^2}{dx^2} - k^2\right)\tilde{G}_k(\cdot - y_j)\right](x) = 0.\end{aligned} \tag{2.19}$$

Let now $y_1 \in \Omega$. Since $\phi_k \in H^{2,2}(\boldsymbol{R})$ we see from (2.18) that

$$\sum_{j'=1}^{N} [\Gamma_{\rho,Y}(k)]_{1j'}^{-1} \phi_k'(y_{j'}) = 0 \qquad x \in \Omega \tag{2.20}$$

from which we infer that the sum in (2.19) still equals zero when j is summed from 2 to N.

(c) Weyl's theorem [8] implies that

$$\sigma_{\mathrm{ess}}(\Xi_{\beta,Y}) = \sigma_{\mathrm{ess}}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) = [0, \infty). \tag{2.21}$$

The absence of a singular continuous spectrum follows from [8], theorem X.111. Turning now to the analysis of the point spectrum we assume

$$y_1 < y_2 < \ldots < y_N. \tag{2.22}$$

If $\beta_j \in \boldsymbol{R}$, $j = 1, \ldots, N$, define

$$\psi_k(x) = \begin{cases} a_1\,\mathrm{e}^{\mathrm{i}kx} + b_1\,\mathrm{e}^{-\mathrm{i}kx} & x < y_1 \\ a_{m+1}\,\mathrm{e}^{\mathrm{i}kx} + b_{m+1}\,\mathrm{e}^{-\mathrm{i}kx} & y_m < x < y_{m+1} \qquad 1 \leqslant m \leqslant N-1 \\ a_{N+1}\,\mathrm{e}^{\mathrm{i}kx} + b_{N+1}\,\mathrm{e}^{-\mathrm{i}kx} & x > y_N; \qquad \operatorname{Im} k > 0 \qquad k \neq 0. \end{cases} \tag{2.23}$$

The boundary conditions (2.6) imply

$$\begin{gathered} a_{m+1}\,\mathrm{e}^{\mathrm{i}ky_m} - b_{m+1}\,\mathrm{e}^{-\mathrm{i}ky_m} = a_m\,\mathrm{e}^{\mathrm{i}ky_m} - b_m\,\mathrm{e}^{-\mathrm{i}ky_m} \\ a_{m+1}\,\mathrm{e}^{\mathrm{i}ky_m}(1 - \mathrm{i}k\beta_m) + b_{m+1}\,\mathrm{e}^{-\mathrm{i}ky_m}(1 + \mathrm{i}k\beta_m) = a_m\,\mathrm{e}^{\mathrm{i}ky_m} + b_m\,\mathrm{e}^{-\mathrm{i}ky_m} \\ a_1 = a \qquad b_1 = b \qquad m = 1, \ldots, N-1 \end{gathered} \tag{2.24}$$

and thus ψ_k satisfies (locally)

$$\Xi_{\beta,Y}\psi_k = k^2\psi_k. \tag{2.25}$$

Clearly $\psi_k \in L^2(\boldsymbol{R})$ iff $a_1 = b_{N+1} = 0$. Since a_m, b_m are uniquely defined (up to a common multiplicative constant) we see that the eigenvalues are simple. If $k^2 > 0$, then $\psi_k \in L^2(\boldsymbol{R})$ iff $a = b = 0$ which implies $\psi_k = 0$. Applying the same argument when $k = 0$ with the functions $\mathrm{e}^{\pm\mathrm{i}kx}$ replaced by 1 and x we infer that

$$\sigma_p(\Xi_{\beta,Y}) \subset (-\infty, 0). \tag{2.26}$$

From the explicit form of the resolvent we obtain (2.13). To infer the form (2.14) of the eigenfunctions, one has to recall that the residuum of the resolvent of a self-adjoint operator at an eigenvalue equals the projection onto the corresponding eigenspace. By applying this first to the self-adjoint matrix $\Gamma_{\beta,Y}(k)$, $\operatorname{Im} k > 0$, and then to $(\Xi_{\beta,Y} - k^2)^{-1}$ we conclude that (2.14) is valid. Observe that

$$\mathscr{D}(\dot{H}_Y) \subset \mathscr{D}(\Xi_{\beta,Y}) \tag{2.27}$$

using (2.10) thereby proving that $\Xi_{\beta,Y}$ is a self-adjoint extension of $\dot{H}_Y$. Since $\dot{H}_Y \geqslant 0$ and $\operatorname{def}(\dot{H}_Y) = (N, N)$ we infer using [4, p 247] that $\Xi_{\beta,Y}$ has at most N negative eigenvalues counting multiplicity. Consider now the case when precisely one $\beta_{j_0} = \infty$ and $N \geqslant 2$. The boundary condition in (2.6) at y_{j_0} reduces to a Neumann condition, $g'(y_{j_0}) = 0$, and hence $\boldsymbol{R}$ is decoupled into $(-\infty, y_{j_0})$ and (y_{j_0}, ∞). By essentially repeating the above argument for each of the intervals one can prove that $\Xi_{\beta,Y}$ has no non-negative eigenvalues. If however $\beta_j = \infty$ for at least two different values of $j \in \{1, \ldots, N\}$, say

$$\beta_{j_0} = \beta_{j_1} = \infty \qquad y_{j_0} < y_{j_1} \tag{2.28}$$

$\Xi_{\beta,Y}$ can be written as a direct sum of the corresponding operators on $L^2(-\infty, y_{j_0})$, $L^2(y_{j_0}, y_{j_1})$ and $L^2(y_{j_1}, \infty)$ respectively. Since the operator on $L^2(y_{j_0}, y_{j_1})$ has an empty essential spectrum, the discrete spectrum has eigenvalues accumulating at infinity, thereby proving the claim. The proof is completed.

Recall that the corresponding operator with δ-function interactions instead of δ' interactions has the resolvent (see e.g. [9] or [3])

$$(-\Delta_{\alpha,Y}-k^2)^{-1}=G_k+\sum_{j,j'=1}^{N}[\tilde{\Gamma}_{\alpha,Y}(k)]_{jj'}^{-1}(\overline{G_k(\cdot-y_{j'})},\cdot)G_k(\cdot-y_j)$$

$$\alpha=(\alpha_1,\ldots,\alpha_N)\qquad Y=\{y_1,\ldots,y_N\}\qquad -\infty<\alpha_j\leqslant\infty \tag{2.29}$$

$$y_j\in\boldsymbol{R}\qquad k^2\in\rho(-\Delta_{\alpha,Y})\qquad \operatorname{Im}k\geqslant 0$$

where the matrix $\tilde{\Gamma}_{\alpha,Y}(k)$ is now

$$\tilde{\Gamma}_{\alpha,Y}(k)=-[\alpha_j^{-1}\delta_{jj'}+G_k(y_j-y_{j'})]_{j,j'=1}^{N}. \tag{2.30}$$

Hence we see that

$$\Gamma_{\beta,Y}(k)=-\tilde{\Gamma}_{-k^2\beta,Y}(k)\qquad k^2\beta=(k^2\beta_1,\ldots,k^2\beta_N). \tag{2.31}$$

By using this, some of the spectral results in theorem 2.1 could be deduced from the corresponding results for $-\Delta_{\alpha,Y}$. We have however chosen here to give an independent treatment.

As an example of the above theorem, we consider the one-centre case, i.e. $Y=\{0\}$. It then follows that $\Xi_{\beta,0}$ has a simple, negative eigenvalue $E=-4\beta^{-2}$ provided $\beta\in(-\infty,0)$ with corresponding eigenfunction $\psi_E(x)=\tilde{\tilde{G}}_{2i/\beta}(x)$. We see from theorem 2.1(a) that eigenvalues and resonances (defined as poles of the resolvent for $\operatorname{Im}k<0$, i.e. points where $\det[\Gamma_{\beta,Y}(k)]=0$, $\operatorname{Im}k<0$) can be treated on an equal footing (cf also [10]). Returning to the one-centre case, we see that $\Xi_{\beta,0}$ has a simple resonance at $k=-2i\beta^{-1}$ iff $\beta\in(0,\infty)$.

Theorems 2.1(a) and (b) have natural extensions to the infinite centre case, i.e. when Y forms a discrete subset of $\boldsymbol{R}$. However since our main interest in this case is when Y forms a lattice, i.e.

$$Y=a\boldsymbol{Z} \tag{2.32}$$

we will only briefly discuss the general case here. Equation (2.32) will be extensively discussed in the next section.

Consider

$$Y=\{y_j\in\boldsymbol{R}\,|\,j\in\boldsymbol{Z}\}\qquad y_j<y_{j+1}\qquad j\in\boldsymbol{Z}\qquad \inf_{\substack{j,j'\in\boldsymbol{Z}\\ j\neq j'}}|y_j-y_{j'}|=d>0 \tag{2.33}$$

and define

$$I_j=(y_j,y_{j+1}]. \tag{2.34}$$

Let

$$\dot{H}_Y=-\frac{d^2}{dx^2}\qquad \mathscr{D}(\dot{H}_Y)=\{g\in H^{2,2}(\boldsymbol{R})\,|\,g'(y_j)=0, j\in\boldsymbol{Z}\}. \tag{2.35}$$

Then its adjoint is

$$\dot{H}_Y^*=-\frac{d^2}{dx^2}\qquad \mathscr{D}(\dot{H}_Y^*)=\{g\in H^{2,2}(\boldsymbol{R}\setminus Y)\,|\,g'(y_{j^+})=g'(y_{j^-}), j\in\boldsymbol{Z}\} \tag{2.36}$$

and it can be seen that the functions

$$\phi_j(x)=\tilde{G}_k(x-y_j)\qquad j\in\boldsymbol{Z}\qquad \operatorname{Im}k>0 \tag{2.37}$$

span the deficiency subspaces of $\dot{H}_Y$.

We define the self-adjoint extension $\Xi_{\beta,Y}$, $\beta=(\beta_j)_{j\in\mathbf{Z}}$, $\beta_j\in\mathbf{R}$, of $\dot{H}_Y$ by

$$\Xi_{\beta,Y}=-\frac{d^2}{dx^2}$$

$$\mathscr{D}(\Xi_{\beta,Y})=\{g\in H^{2,2}(\mathbf{R}\setminus Y)|g'(y_{j^+})=g'(y_{j^-}),\, g(y_{j^+})-g(y_{j^-})=\beta_j g'(y_j),\, j\in\mathbf{Z}\}$$
$$\beta=(\beta_j)_{j\in\mathbf{Z}} \qquad -\infty<\beta_j<\infty \qquad j\in\mathbf{Z}. \tag{2.38}$$

(Obviously $\Xi_{\beta,Y}$ is symmetric. That it is actually self-adjoint follows from, e.g., [11].) Then we have the following.

Theorem 2.2. Let $\beta_j\in\mathbf{R}\setminus\{0\}$, $j\in\mathbf{Z}$.

(*a*) The resolvent of $\Xi_{\beta,Y}$ is

$$(\Xi_{\beta,Y}-k^2)^{-1}=G_k+\sum_{j,j'\in\mathbf{Z}}[\Gamma_{\beta,Y}(k)]^{-1}_{jj'}(\overline{\tilde{G}_k(\cdot-y_{j'})},\,\cdot\,)\tilde{G}_k(\cdot-y_j)$$
$$k^2\in\rho(\Xi_{\beta,Y}) \qquad \operatorname{Im}k>0 \tag{2.39}$$

where

$$\Gamma_{\beta,Y}(k)=[-(\beta_j k^2)^{-1}\delta_{jj'}+G_k(y_j-y_{j'})]_{j,j'\in\mathbf{Z}} \tag{2.40}$$

is a closed operator on $l^2(Y)$ with

$$[\Gamma_{\beta,Y}(k)]^{-1}\in\mathscr{B}(l^2(Y)) \qquad k^2\in\rho(\Xi_{\beta,Y}) \qquad \operatorname{Im}k>0 \quad \text{large enough.} \tag{2.41}$$

(*b*) We have

$$\mathscr{D}(\Xi_{\beta,Y})=\left\{\psi\in L^2(\mathbf{R})|\psi(x)=\phi_k(x)+\frac{i}{k}\sum_{j,j'\in\mathbf{Z}}[\Gamma_{\beta,Y}(k)]^{-1}_{jj'}\phi_k'(y_{j'})\tilde{G}_k(x-y_j),\right.$$
$$\left.\phi_k\in H^{2,2}(\mathbf{R}),\,\operatorname{Im}k>0,\,k^2\in\rho(\Xi_{\beta,Y})\right\}. \tag{2.42}$$

The above decomposition is unique and

$$(\Xi_{\beta,Y}-k^2)\psi=\left(-\frac{d^2}{dx^2}-k^2\right)\phi_k. \tag{2.43}$$

If $\psi\in\mathscr{D}(\Xi_{\beta,Y})$ and $\psi=0$ in an open set $\Omega\subset\mathbf{R}$, then $\Xi_{\beta,Y}\psi=0$ in Ω.

Proof. Similar to that of theorem 2.1, see also [3].

3. The case $Y=a\mathbf{Z}$

In this section we will study various properties of the operator $\Xi_{\beta,a\mathbf{Z}}$. However the analysis will, in contrast to the previous section, be done by relating the self-adjoint operator $\Xi_{\beta,a\mathbf{Z}}$ on $L^2(\mathbf{R})$ to a second-order difference operator on $l^2(\mathbf{Z})$. This technique was introduced in [5] for operators with δ interactions and rediscovered in [12] (cf also [13]).

Theorem 3.1. Let $\beta_j \in \boldsymbol{R}$, $j \in \boldsymbol{Z}$, $a > 0$ and $k^2 \in \boldsymbol{R}$, $\operatorname{Im} k \geqslant 0$, $k \neq (\pi/a)j$, $j \in \boldsymbol{Z}$. Assume

$$\Xi_{\beta, a\boldsymbol{Z}} \psi_k = k^2 \psi_k \tag{3.1}$$

with ψ_k, ψ'_k locally absolutely continuous on $\boldsymbol{R} \backslash a\boldsymbol{Z}$, and

$$\psi'_k(aj+) = \psi'_k(aj-) \qquad \psi_k(aj+) - \psi_k(aj-) = \beta_j \psi'(aj) \qquad j \in \boldsymbol{Z}. \tag{3.2}$$

Then

$$\Phi_{j+1}(k) = M_j(k)\Phi_j(k) \tag{3.3}$$

where

$$M_j(k) = \begin{bmatrix} -\beta_j k \sin(ka) + 2\cos(ka) & -1 \\ 1 & 0 \end{bmatrix} \qquad \Phi_j(k) = \begin{bmatrix} \psi'_k(aj) \\ \psi'_k(a(j-1)) \end{bmatrix} \qquad j \in \boldsymbol{Z}. \tag{3.4}$$

Conversely any solution of (3.3) and (3.4) defines via

$$\psi_k(x) = \psi'_k(aj)k^{-1}\sin[k(x-aj)] + \{-\psi'_k(a(j+1)) + \psi'_k(aj)\cos(ka)\}\frac{\cos[k(x-aj)]}{k\sin(ka)}$$
$$x \in (aj, a(j+1)) \qquad j \in \boldsymbol{Z} \tag{3.5}$$

a solution of (3.1) and (3.2). Furthermore for $p = 2$ or $p = \infty$

$$\psi_k \in L^p(\boldsymbol{R}) \Leftrightarrow \{\psi'_k(aj)\}_{j \in \boldsymbol{Z}} \in l^p(\boldsymbol{Z}) \tag{3.6}$$

and

$$\begin{gathered} c_1\,\mathrm{e}^{\pm\delta|x|} \leqslant |\psi_k(x)| \leqslant c_2\,\mathrm{e}^{\pm\delta|x|} \\ x \in \boldsymbol{R} \Leftrightarrow c_1\,\mathrm{e}^{\pm\delta a|j|} \leqslant |\psi'_k(aj)| \leqslant c_2\,\mathrm{e}^{\pm\delta a|j|} \\ j \in \boldsymbol{Z}. \end{gathered} \tag{3.7}$$

Remark. The analogues of (3.6) and (3.7) for δ interactions can be found in [13] (cf also [3]).

Proof. Equations (3.3), (3.4) and (3.5) are verified by explicit calculations. If $\psi_k \in L^p(\boldsymbol{R})$ and thus $\psi''_k \in L^p(\boldsymbol{R})$ we can infer $\psi'_k \in L^p(\boldsymbol{R})$ for $1 \leqslant p \leqslant \infty$. Furthermore

$$\psi'_k(aj) = \psi_k(x)k\sin[k(x-aj)] + \psi'_k(x)\cos[k(x-aj)] \qquad x \in (aj, a(j+1)) \tag{3.8}$$

then proves that $\{\psi'_k(aj)\}_{j \in \boldsymbol{Z}} \in l^\infty(\boldsymbol{Z})$, and

$$[\psi_k(aj+)]^2 + k^{-2}[\psi'_k(aj)]^2 = [\psi_k(x)]^2 + k^{-2}[\psi'_k(x)]^2 \qquad x \in (aj, a(j+1)) \tag{3.9}$$

then proves that $\{\psi'_k(aj)\} \in l^2(\boldsymbol{Z})$. Assume now that $\{\psi'_k(aj)\}_{j \in \boldsymbol{Z}} \in l^p(\boldsymbol{Z})$ for $p = 2$ or ∞. Then $\psi_k \in L^\infty(\boldsymbol{R})$ from (3.5) and

$$\begin{aligned} [\psi_k(x)]^2 + k^{-2}[\psi'_k(x)]^2 = k^{-2}[\psi'_k(aj)]^2 + k^{-2}\sin^{-2}(ka)\{-\psi'_k(a(j+1)) \\ + \psi'_k(aj)\cos(ka)\}^2 \qquad x \in (aj, a(j+1)) \end{aligned} \tag{3.10}$$

then proves that $\psi_k \in L^2(\boldsymbol{R})$.

Equation (3.7) is proved as follows. From the Schrödinger equation we see that ψ_k and ψ''_k satisfy the same inequalities, and by integration ψ'_k also satisfies the same inequalities. The proof is completed.

The analysis in theorem 3.1 can be extended to the case of an arbitrary discrete subset Y. However in that case (3.6) and (3.7) are only valid as implications from the left-hand side to the right-hand side. For a more detailed study we assume

$$\beta_j = \beta \in \boldsymbol{R} \qquad j \in \boldsymbol{Z}. \tag{3.11}$$

Then the operator $\Xi_{\beta,a\boldsymbol{Z}}$, being invariant under translations by $a\boldsymbol{Z}$, can be decomposed as a direct integral. We introduce

$$\begin{aligned}
&\Xi_{\beta,a\boldsymbol{Z}}(\theta) = -\frac{\mathrm{d}^2}{\mathrm{d}\nu^2} \qquad \mathscr{D}(\Xi_{\beta,a\boldsymbol{Z}}(\theta)) = \{g(\theta) \in H^{2,2}((-\tfrac{1}{2}a, \tfrac{1}{2}a) - \{0\})\} \\
&g(\theta, -a/2+) = \mathrm{e}^{\mathrm{i}\theta a} g(\theta, a/2-) \qquad g'(\theta, -a/2+) = \mathrm{e}^{\mathrm{i}\theta a} g'(\theta, a/2-) \\
&g'(\theta, 0+) = g'(\theta, 0-) \qquad g(\theta, 0+) - g(\theta, 0-) = g'(\theta, 0)\} \\
&-\infty < \beta \leqslant \infty \qquad \theta \in [-\pi/a, \pi/a).
\end{aligned} \tag{3.12}$$

and define the operator U by

$$\begin{aligned}
&U\colon \mathscr{S}(\boldsymbol{R}) \to L^2([-\pi/a, \pi/a), (2\pi/a)\,\mathrm{d}\theta;\, L^2([-\tfrac{1}{2}a, \tfrac{1}{2}a))) \\
&(Uf)(\theta, \nu) = \sum_{j \in \boldsymbol{Z}} \mathrm{e}^{-\mathrm{i}j\theta a} f(\nu + aj)
\end{aligned} \tag{3.13}$$

extending it to a unitary operator on $L^2(\boldsymbol{R})$ by continuity.

Theorem 3.2. Let $\beta \in \boldsymbol{R}$, $a > 0$. Then

$$U \Xi_{\beta,a\boldsymbol{Z}} U^{-1} = \frac{2\pi}{a} \int_{[-\pi/a, \pi/a)}^{\oplus} \mathrm{d}\theta\, \Xi_{\beta,a\boldsymbol{Z}}(\theta). \tag{3.14}$$

Before we prove this theorem we will analyse the spectrum of $\Xi_{\beta,a\boldsymbol{Z}}(\theta)$ in detail.

Theorem 3.3. Let $\beta \in \boldsymbol{R}$, $\theta \in [-\pi/a, \pi/a)$ and $a > 0$. Then

$$\sigma_{\mathrm{ess}}(\Xi_{\beta,a\boldsymbol{Z}}(\theta)) = \varnothing. \tag{3.15}$$

The eigenvalues $E_m^{\beta,a}(\theta)$ of $\Xi_{\beta,a\boldsymbol{Z}}(\theta)$, ordered according to their magnitude, are given by

$$E_m^{\beta,a}(\theta) = [k_m^{\beta,a}(\theta)]^2 \qquad \operatorname{Im} k_m^{\beta,a}(\theta) > 0 \tag{3.16}$$

where $k_m^{\beta,a}(\theta)$ solves

$$\cos(\theta a) = \cos(ka) - \tfrac{1}{2}\beta k \sin(ka). \tag{3.17}$$

For $\beta \in \boldsymbol{R} - \{0\}$, except for $\beta = -a$, $m = 1$ and $\theta = 0$, the eigenvalues are simple with corresponding eigenfunctions

$$g_m^{\beta,a}(\theta, \nu) = \begin{cases}
\exp(\mathrm{i}k_m^{\beta,a}(\theta)\nu) + \mathrm{e}^{\mathrm{i}\theta a}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)a) \\
\quad \times \dfrac{1 - \mathrm{e}^{-\mathrm{i}\theta a}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)a)}{\mathrm{e}^{\mathrm{i}\theta a}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)a) - 1}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)\nu) & \nu \in (-\tfrac{1}{2}a, 0) \\
\mathrm{e}^{-\mathrm{i}\theta a}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)a)\exp(\mathrm{i}k_m^{\beta,a}(\theta)\nu) \\
\quad + \dfrac{1 - \mathrm{e}^{-\mathrm{i}\theta a}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)a)}{\mathrm{e}^{\mathrm{i}\theta a}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)a) - 1}\exp(-\mathrm{i}k_m^{\beta,a}(\theta)\nu) & \nu \in (0, \tfrac{1}{2}a)
\end{cases} \tag{3.18}$$

$$m \in \mathbf{N} \qquad \theta \in [-\pi/a, \pi/a) \quad \text{and} \quad m \geqslant 2 \quad \text{for} \quad \beta = -a \quad \text{and} \quad \theta = 0.$$

If $\beta=-a$, then $E_1^{-a,a}(0)=0$ is twice degenerate and

$$g_{1,1}^{-a,a}(0,\nu)=1 \qquad g_{1,2}^{-a,a}(0,\nu)=\begin{cases}1+\nu & \nu\in(-\frac{1}{2}a,0)\\ 1-a+\nu & \nu\in(0,\frac{1}{2}a)\end{cases} \tag{3.19}$$

are the corresponding eigenfunctions. Furthermore we have for $\beta>0$

$$\begin{aligned}E_1^{\beta,a}(0)=0<E_1^{\beta,a}(-\pi/a)<E_2^{\beta,a}(-\pi/a)=\pi^2/a^2<E_2^{\beta,a}(0)\\ <E_3^{\beta,a}(0)=4\pi^2/a^2<E_3^{\beta,a}(-\pi/a)<E_4^{\beta,a}(-\pi/a)=9\pi^2/a^2<\dots\end{aligned} \tag{3.20}$$

and for $\beta<0$

$$\begin{aligned}&E_1^{\beta,a}(-\pi/a)<E_1^{\beta,a}(0)<E_2^{\beta,a}(0)<E_2^{\beta,a}(-\pi/a)=\pi^2/a^2<E_3^{\beta,a}(-\pi/a)\\ &\qquad<E_3^{\beta,a}(0)=4\pi^2/a^2<E_4^{\beta,a}(0)<E_4^{\beta,a}(-\pi/a)=\tfrac{9}{4}\pi^2<\dots\\ &E_1^{\beta,a}(-\pi/a)<0 \qquad E_1^{\beta,a}(0)\begin{cases}<0 & -a<\beta<0\\ =0 & \beta\leqslant -a\end{cases}\\ &E_2^{\beta,a}(0)\begin{cases}=0 & -a\leqslant\beta<0\\ >0 & \beta<-a.\end{cases}\end{aligned} \tag{3.21}$$

All non-constant eigenvalues $E_m^{\beta,a}(\theta)$, $\theta\in[-\pi/a,\pi/a)$, $m\in\boldsymbol{N}$ are strictly decreasing with respect to $\beta\in\boldsymbol{R}$.

For $\beta=0$, $\Xi_{\beta,a}(\theta)$ equals the decomposed Laplacian and we have

$$\begin{aligned}&E_{m\pm}^{0,a}(\theta)=[\pm\theta+2(m-1)\pi/a]^2 \qquad \theta\in(-\pi/a,0) \qquad m\in\boldsymbol{N}\\ &E_m^{0,a}(0)=[2(m-1)\pi/a]^2 \qquad E_m^{0,a}(-\pi/a)=[(2m-1)\pi/a]^2 \qquad m\in\boldsymbol{N}\\ &g_{m\pm}^{0,a}(\theta,\nu)=c\,\mathrm{e}^{\mathrm{i}[\pm\theta+2(m-1)\pi/a]\nu} \qquad \theta\in(-\pi/a,0) \quad m\in\boldsymbol{N}\end{aligned} \tag{3.22}$$

$$\begin{aligned}&g_m^{0,a}(0,\nu)=c\begin{cases}\cos[2(m-1)(\pi/a)\nu] & m\in\boldsymbol{N}\\ \sin[2(m-1)(\pi/a)\nu] & m\geqslant 2\end{cases}\\ &g_m^{0,a}(-\pi/a,\nu)=c\begin{cases}\cos[(2m-1)(\pi/a)\nu]\\ \sin[(2m-1)(\pi/a)\nu]\end{cases} \qquad m\in\boldsymbol{N}.\end{aligned} \tag{3.23}$$

For $\beta=\infty$ we have

$$\begin{aligned}&E_1^{\infty,a}(\theta)=0 \qquad g_{1,1}^{\infty,a}(\theta,\nu)=\begin{cases}1 & -\frac{1}{2}a<\nu<0\\ 0 & 0<\nu<\frac{1}{2}a\end{cases}\\ &\qquad\qquad g_{1,2}^{\infty,a}(\theta,\nu)=\begin{cases}0 & -\frac{1}{2}a<\nu<0\\ 1 & 0<\nu<\frac{1}{2}a\end{cases}\\ &E_m^{\infty,a}(\theta)=(m-1)^2\pi^2/a^2\\ &g_m^{\infty,a}(\theta,\nu)=C\cos[(m-1)(\pi/a)\nu]\begin{cases}1 & -\frac{1}{2}a<\nu<0\\ (-1)^{m-1}\mathrm{e}^{-\mathrm{i}\theta a} & 0<\nu<\frac{1}{2}a\end{cases} \qquad m\geqslant 2.\end{aligned} \tag{3.24}$$

Proof. Equation (3.15) follows from the fact that $\Xi_{\beta,aZ}(\theta)$ has a compact resolvent. To prove non-degeneracy of the eigenvalues $E_m^{\beta,aZ}(\theta)$, $\theta\in(-\pi/a,\pi/a)-\{0\}$, one can follow the proof of theorem 2.1. We use (3.3) to prove (3.17). More precisely, we make the ansatz

$$\psi_k'(aj)=\mathrm{e}^{\pm\mathrm{i}\theta(k)aj} \qquad \mathrm{Im}(k)\geqslant 0 \qquad j\in\boldsymbol{Z}. \tag{3.25}$$

By inserting this in (3.3), (3.17) follows immediately. A tedious but straightforward calculation then proves the remaining statements.

With this theorem, we now turn to the proof of theorem 3.2.

Proof of theorem 3.2. Let

$$\mathscr{D}^{\alpha,a}(\theta)=[g_m^{\alpha,a}(\theta),\, m\in \boldsymbol{N}] \tag{3.26}$$

be the linear span of all the eigenvectors of $\Xi_{\beta,a\boldsymbol{Z}}(\theta)$ as described in theorem 3.3. Then $\mathscr{D}^{\alpha,a}(\theta)$ is a core for $\Xi_{\beta,a\boldsymbol{Z}}(\theta)$ and by explicit calculation one verifies that

$$(U\Xi_{\beta,a\boldsymbol{Z}}U^{-1}g_m^{\alpha,a})(\theta,\nu)=E_m^{\alpha,a}(\theta)g_m^{\alpha,a}(\theta,\nu)=(\Xi_{\beta,a}(\theta)g^{\alpha,a}(\theta))(\nu) \tag{3.27}$$

which proves (3.14).

Using now the basic relation

$$\sigma(\Xi_{\beta,a\boldsymbol{Z}})=\bigcup_{\theta\in[-\pi/a,\pi/a)}\sigma(\Xi_{\beta,a\boldsymbol{Z}}(\theta)) \tag{3.28}$$

(see e.g. [8]) and theorem 3.3 we can compute the spectrum of $\Xi_{\beta,a\boldsymbol{Z}}$.

Theorem 3.4. Let $\beta\in\boldsymbol{R}$, $a>0$. Then $\Xi_{\beta,a\boldsymbol{Z}}$ has an absolutely continuous spectrum, namely

$$\begin{aligned}&\sigma(\Xi_{\beta,a\boldsymbol{Z}})=\sigma_{\mathrm{ac}}(\Xi_{\beta,a\boldsymbol{Z}})=\bigcup_{m=1}^{\infty}[a_m^{\beta,a},b_m^{\beta,a}]\\&\sigma_{\mathrm{sc}}(\Xi_{\beta,a\boldsymbol{Z}})=\sigma_{\mathrm{p}}(\Xi_{\beta,a\boldsymbol{Z}})=\varnothing\qquad a_m^{\beta,a}<b_m^{\beta,a}<a_{m+1}^{\beta,a}\qquad m\in\boldsymbol{N}.\end{aligned} \tag{3.29}$$

We have for $\beta>0$

$$\begin{aligned}&a_m^{\beta,a}=\begin{cases}E_m^{\beta,a}(0)=(m-1)^2\pi^2/a^2 & m\text{ odd}\\ E_m^{\beta,a}(-\pi/a)=(m-1)^2\pi^2/a^2 & m\text{ even}\end{cases}\\&b_m^{\beta,a}=\begin{cases}E_m^{\beta,a}(-\pi/a) & m\text{ odd}\\ E_m^{\beta,a}(0) & m\text{ even}\end{cases}\qquad b_m^{\beta,a}<m^2\pi^2/a^2\qquad m\in\boldsymbol{N}\end{aligned} \tag{3.30}$$

and for $\beta<0$

$$\begin{aligned}&a_m^{\beta,a}=\begin{cases}E_m^{\beta,a}(-\pi/a) & m\text{ odd}\\ E_m^{\beta,a}(0) & m\text{ even}\end{cases}\qquad m\in\boldsymbol{N}\\&b_m^{\beta,a}=\begin{cases}E_m^{\beta,a}(0)=(m-1)^2\pi^2/a^2 & m\text{ odd}\\ E_m^{\beta,a}(-\pi/a)=(m-1)^2\pi^2/a^2 & m\text{ even}\end{cases}\qquad m\geqslant 2\\&a_1^{\beta,a}=E_1^{\beta,a}(-\pi/a)<0\\&a_2^{\beta,a}\begin{cases}=0 & -a\leqslant\beta<0\\ >0 & \beta<-a\end{cases}\qquad a_m^{\beta,a}>(m-2)^2\pi^2/a^2\qquad m\geqslant 2.\\&b_1^{\beta,a}\begin{cases}>0 & -a\leqslant\beta<0\\ =0 & \beta<-a.\end{cases}\end{aligned} \tag{3.31}$$

Asymptotically, as $m\to\infty$, the length of the mth gap $a_{m+1}^{\beta,a}-b_m^{\beta,a}$ and the width of the mth band $b_m^{\beta,a}-a_m^{\beta,a}$ satisfy

$$\begin{aligned}&a_{m+1}^{\beta,a}-b_m^{\beta,a}=2m\pi^2a^{-2}-\left(\frac{8a}{|a|}+\pi^2\right)a^{-2}+\frac{8}{a\beta m}+\mathcal{O}(m^{-2})\\&b_m^{\beta,a}-a_m^{\beta,a}=\frac{8}{a|\beta|}-\frac{8}{a\beta m}+\mathcal{O}(m^{-2}).\end{aligned} \tag{3.32}$$

When $\beta \in \boldsymbol{R}\backslash\{0\}$, $\Xi_{\beta,a\boldsymbol{Z}}$ has infinitely many gaps in its spectrum. When in addition $\beta \neq -a$, all gaps are open. However when $\beta = -a$, the first gap closes at zero.

For $\beta = 0$, we have $\Xi_{0,a\boldsymbol{Z}} = -\mathrm{d}^2/\mathrm{d}x^2$ on $H^{2,2}(\boldsymbol{R})$ and hence

$$\sigma(\Xi_{0,a\boldsymbol{Z}}) = [0, \infty). \tag{3.33}$$

For $\beta = \infty$, $\Xi_{\infty,a\boldsymbol{Z}}$ equals the Neumann Laplacian on $\boldsymbol{R}\backslash a\boldsymbol{Z}$ and hence $\Xi_{\infty,a\boldsymbol{Z}}$ equals the direct sum of Neumann Laplacians on $(ma, (m+1)a)$, $m \in \boldsymbol{Z}$. Thus

$$\sigma_{\mathrm{c}}(\Xi_{\infty,a\boldsymbol{Z}}) = \varnothing \qquad \sigma_{\mathrm{ess}}(\Xi_{\infty,a\boldsymbol{Z}}) = \sigma_{\mathrm{p}}(\Xi_{\infty,a\boldsymbol{Z}}) = \{m^2(\pi^2/a^2) | m \in \boldsymbol{N}_0\}. \tag{3.34}$$

Finally we have that

$$\begin{aligned} &\sigma(\Xi_{\beta,a\boldsymbol{Z}}) \subset \sigma(\Xi_{\beta',a\boldsymbol{Z}}) && 0 \leqslant \beta' < \beta \\ &\sigma(\Xi_{\beta,a\boldsymbol{Z}}) \supset \sigma(\Xi_{\beta',a\boldsymbol{Z}}) && -\infty \leqslant \beta' < \beta < -a. \end{aligned} \tag{3.35}$$

The band edges $a_m^{\beta,a}$, $b_m^{\beta,a}$, $m \in \boldsymbol{N}$, are continuous in $\beta \in \boldsymbol{R}$.

Proof. To prove the absence of eigenvalues for $\Xi_{\beta,a\boldsymbol{Z}}$, $\beta \in \boldsymbol{R}$, we differentiate (3.17) with respect to θ when $k = k_m^{\beta,a}(\theta)$, i.e.

$$\begin{aligned} -a\sin(\theta a) = \bigg\{ &-a\sin[k_m^{\beta,a}(\theta)a] - \tfrac{1}{2}\beta\sin[k_m^{\beta,a}(\theta)a] \\ &- \frac{a\beta k_m^{\beta,a}(\theta)}{2}\cos[k_m^{\beta,a}(\theta)a]\bigg\}(k_m^{\beta,a})'(\theta). \end{aligned} \tag{3.36}$$

Hence $(k_m^{\beta,a})'(\theta_0) = 0$ for some $\theta_0 \in (-\pi/a, 0)$ yields the contradiction $\sin(\theta_0 a) = 0$, and we conclude that $k_m^{\beta,a}(\theta)$ is strictly monotone in $\theta \in (-\pi/a, 0)$. Thus the set $\theta \in (-\pi/a, 0) | E_m^{\beta,a}(\theta) = E_0\}$ has zero Lebesgue measure which implies the absenco of eigenvalues using [8], theorem XIII.85. The absolute continuity of the spectrum follows from [14].

The rest of the theorem follows from a straightforward computation using (3.17) and theorem 3.3.

Remark. The above theorem exhibits two curious facts. First of all the bottom of the band spectrum of $\Xi_{\beta,a\boldsymbol{Z}}$ starts with the antiperiodic eigenvalue $E_1^{\beta,a}(-\pi/a)$ for $\beta < 0$. Clearly this is due to the fact that for $k = \mathrm{i}\kappa$, $\kappa > 0$, the right-hand side of (3.17) converges to $-\infty$ as $\kappa \to \infty$ for $\beta < 0$ (whereas it converges to $+\infty$ as $\kappa \to \infty$ for $\beta \geqslant 0$). In fact the standard non-degeneracy statement for ground states of reduced Schrödinger operators with periodic boundary conditions (i.e. with $\theta = 0$) [8] breaks down since the ground-state wavefunction of $\Xi_{\beta,a\boldsymbol{Z}}(0)$ in fact does change sign. The second curiosity concerns the fact that iff $\beta = -a$ the first gap in the spectrum of $\Xi_{\beta,a\boldsymbol{Z}}$ closes. Together with the unusual behaviour of widths and gaps in (3.32), this model serves as a counterexample to some of the standard folk wisdom in connection with one-dimensional periodic Schrödinger operators.

In figure 1 we have illustrated the function $f_\beta(E) = \cos(\sqrt{E}) - \frac{1}{2}\beta\sqrt{E}\sin(\sqrt{E})$, $\mathrm{Im}\sqrt{E} \geqslant 0$ for various values of β. Using (3.17) and (3.28) we see that

$$E \in \sigma(\Xi_{\beta,a\boldsymbol{Z}}) \qquad \text{iff} \qquad f_\beta(E) \in [-1, 1]. \tag{3.37}$$

The energy bands $E_m^{\beta,1}(\theta)$ as functions of θ are illustrated in figure 2 when $\theta \in [-\pi, \pi)$ (*reduced band scheme*). Finally in figure 3 the spectrum of $\Xi_{\beta,\boldsymbol{Z}}$ as functions of β is given.

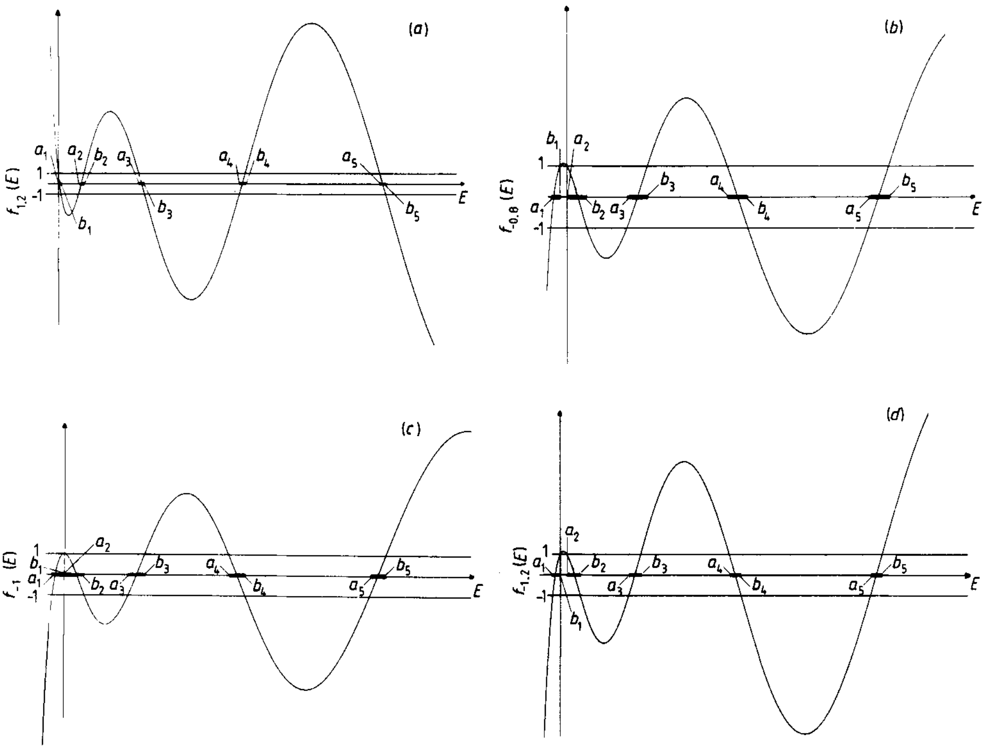

Figure 1. $f_\beta(E)=\cos(\sqrt{E})-\frac{1}{2}\beta\sqrt{E}\sin(\sqrt{E})$, $\mathrm{Im}\sqrt{E}\geqslant 0$. ($a$), $\beta=1.2$; (b), $\beta=-0.8$; (c), $\beta=-1$; (d), $\beta=-1.4$. The dependence on β, a in $a_m^{\beta,a}$, $b_m^{\beta,a}$ and $E_m^{\beta,a}(\theta)$ is for simplicity suppressed. We use $a=1$.

The density of states $\mathrm{d}\rho^{\beta,a}/\mathrm{d}E$ of $\Xi_{\beta,a\boldsymbol{Z}}$ can be explicitly computed as the next theorem shows.

Theorem 3.5. Let $\beta\in\boldsymbol{R}$, $a>0$. Then the density of states of $\Xi_{\beta,a\boldsymbol{Z}}$ at a point $E=k^2\in\sigma(\Xi_{\beta,a\boldsymbol{Z}})$ equals

$$\frac{\mathrm{d}\rho^{\beta,a}}{\mathrm{d}E}=\frac{\mathrm{sgn}(\beta)}{2\pi|k|}\frac{|\sin(ka)|}{|\sin(\theta(k)a)|}\left(1+\frac{\beta}{2a}[1+ka\cot(ka)]\right) \tag{3.38}$$

where

$$\theta(k)=\begin{cases}(-1)^{m+1}a^{-1}\cos^{-1}\left(\cos(ka)-\dfrac{\beta k}{a}\sin(ka)\right) & \\ \quad+\begin{cases}m\pi a^{-1} & m\text{ odd}\\ (m-1)\pi a^{-1} & m\text{ even}\end{cases} & \beta\geqslant 0\\ (-1)^m a^{-1}\cos^{-1}[\cos(ka-\frac{1}{2}\beta k\sin(ka)] & \\ \quad+\begin{cases}(m-1)\pi a^{-1} & m\text{ odd}\\ (m-2)\pi a^{-1} & m\text{ even}\end{cases} & \beta<0\end{cases} \tag{3.39}$$

$$k^2\in(a_m^{\beta,a},b_m^{\beta,a})\qquad \mathrm{Re}\,k\geqslant 0\qquad \mathrm{Im}\,k\geqslant 0\qquad m\in\boldsymbol{N}.$$

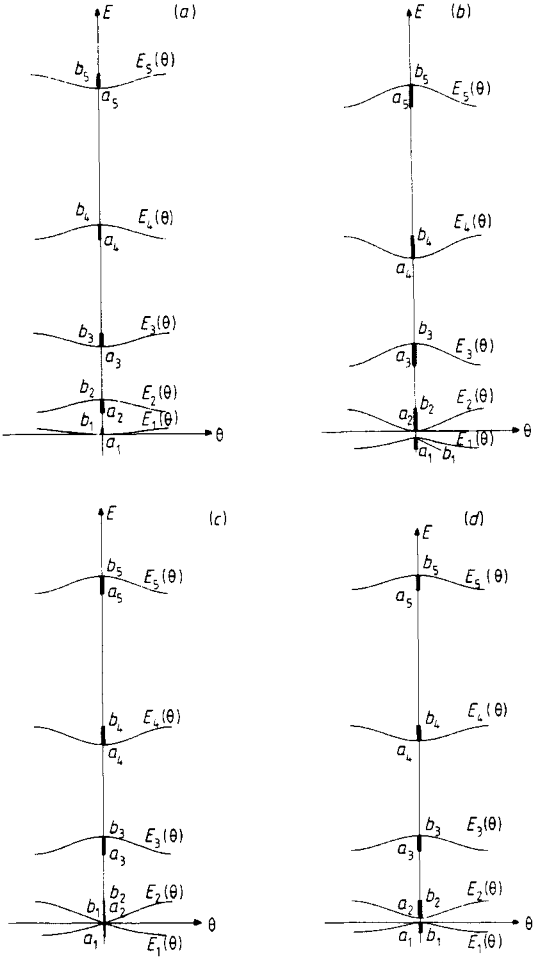

Figure 2. $E_m^{\beta,1}(\theta)$, $m \in \mathbf{N}$, as a function of $\theta \in [-\pi/a, \pi/a)$. ($a$), $\beta = 1.2$; (b), $\beta = -0.8$; (c), $\beta = -1$; (d), $\beta = -1.2$. The dependence on β, a in $a_m^{\beta,a}$, $b_m^{\beta,a}$ and $E_m^{\beta,a}(\theta)$ is for simplicity suppressed. We use $a = 1$.

Furthermore

$$\frac{d\rho^{\beta,a}}{dE} = \mathcal{O}(|E - E_m^{\beta,a}|^{-1/2}) \tag{3.40}$$

near band edges $E_m^{\beta,a} \in \{a_m^{\beta,a}, b_n^{\beta,a}\}_{m \in \mathbf{N}}$.

Proof. Equation (3.38) follows from

$$\frac{d\rho^{\beta,a}}{dE} = \frac{1}{2\pi k}\frac{d\theta(k)}{dk}. \tag{3.41}$$

Our final topic in this section concerns *half-crystals*, i.e. the analysis of $\Xi_{\beta,a\mathbf{N}}$. In fact one can study the more general operator $\Xi_{\beta^{-+},a\mathbf{Z}}$ where

$$\beta^{-+} = (\beta_j)_{j \in \mathbf{Z}} \qquad \beta_j = \begin{cases} \beta^- & j < 0 \\ \beta^+ & j \geqslant 0 \end{cases} \qquad \beta^\pm \in \mathbf{R}. \tag{3.42}$$

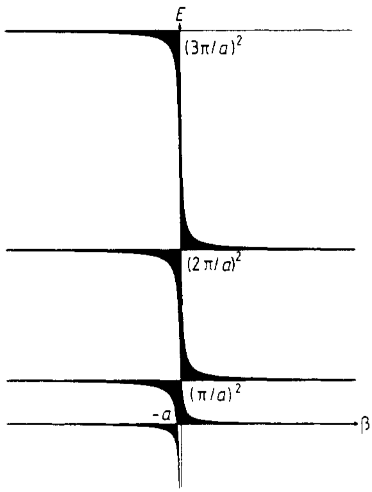

Figure 3. $\sigma(\Xi_{\beta,aZ})$ as a function of $\beta \in \boldsymbol{R}$. The dependence on β, a in $a_m^{\beta,a}$, $b_m^{\beta,a}$ and $E_m^{\beta,a}(\theta)$ is for simplicity suppressed. We use $a = 1$.

We then have the following theorem.

Theorem 3.6. Let $a > 0$ and $\beta^{\pm} \in \boldsymbol{R}$. Then

$$\begin{gathered}\sigma(\Xi_{\beta^{-+},aZ}) = \sigma_{\mathrm{ac}}(\Xi_{\beta^{-+},aZ}) = \sigma(\Xi_{\beta^{+},aZ}) \cup \sigma(\Xi_{\beta^{-},aZ}) \\ \sigma_{\mathrm{sc}}(\Xi_{\beta^{-+},aZ}) = \varnothing \qquad \sigma_{\mathrm{p}}(\Xi_{\beta^{-+},aZ}) = \varnothing.\end{gathered} \tag{3.43}$$

In particular

$$\sigma(\Xi_{\beta,aN}) = [a_1^{\beta,a}, b_1^{\beta,a}] \cup [0, \infty). \tag{3.44}$$

The spectral multiplicity of $\Xi_{\beta^{-+},aZ}$ equals two on the interior of the intersection $\sigma(\Xi_{\beta^{-},aZ}) \cap \sigma(\Xi_{\beta^{+},aZ})$ and one on the interior of the rest, i.e. on $\sigma(\Xi_{\beta^{-+},aZ}) \backslash \{\sigma(\Xi_{\beta^{-},aZ}) \cap \sigma(\Xi_{\beta^{+},aZ})\}$.

Proof. The difference equation (3.3) is now

$$\psi'_k(a(j-1)) + \psi'_k(a(j+1)) + \mu_j \psi'_k(aj) = \varepsilon \psi'_k(aj) \qquad j \in \boldsymbol{Z} \tag{3.45}$$

where

$$\psi'_k(aj) \in \boldsymbol{C} \qquad \varepsilon = \varepsilon(k) = 2\cos(ka) \qquad j \in \boldsymbol{Z} \tag{3.46}$$

and

$$\mu_j = \mu_j(k) = \begin{cases} \mu_j^+ & j \geq 0 \\ \mu_j^- & j < 0 \end{cases} \qquad \mu_j^{\pm} = \mu_j^{\pm}(k) = \beta^{\pm} k \sin(ka). \tag{3.47}$$

Let

$$\psi_j'^{+} = \begin{cases} N_-(\mathrm{e}^{\mathrm{i}\theta_- aj} - \mathrm{e}^{-\mathrm{i}\theta_- aj} R^l) & j < 0 \\ N_+ \, \mathrm{e}^{\mathrm{i}\theta_+ aj} \tilde{T}^l & j \geq 0 \end{cases} \qquad j \in \boldsymbol{Z} \tag{3.48}$$

and

$$\psi_j'^{-} = \begin{cases} M_+(\mathrm{e}^{-\mathrm{i}\theta_+ aj} - \mathrm{e}^{\mathrm{i}\theta_+ aj} R^r) & j \geq 0 \\ M_- \, \mathrm{e}^{-\mathrm{i}\theta_- aj} \tilde{T}^r & j < 0 \end{cases} \qquad j \in \boldsymbol{Z}. \tag{3.49}$$

By inserting $\psi'^{\pm}$ into the difference equation (3.45) it reduces to

$$\cos(\theta_{\pm} a) = \tfrac{1}{2}(\varepsilon - \mu^{\pm}) \qquad \operatorname{Im} \theta_{\pm} \geqslant 0 \tag{3.50}$$

for $j \leqslant -2$ and $j \geqslant 1$ respectively. By using the equations for $j = -1$ and $j = 0$ for $\psi'^{\pm}$, one finds that there exists a unique non-trivial solution for $\tilde{T}^l$, R^l and $\tilde{T}^r$, R^r respectively provided

$$\theta_- + \theta_+ \neq 0. \tag{3.51}$$

Define the bounded, self-adjoint difference operators on $l^2(\boldsymbol{Z})$ by

$$(h_0\phi)_j = \phi_{j-1} + \phi_{j+1} \qquad (h\phi)_j = (h_0\phi)_j + \mu_j \phi_j \qquad \phi \in l^2(\boldsymbol{Z}). \tag{3.52}$$

Then

$$\sigma(h_0) = \sigma_c(h_0) = [-2, 2] \qquad \sigma_p(h_0) = \varnothing \tag{3.53}$$

which implies

$$-2 + \min(\mu^-, \mu^+) \leqslant h \leqslant 2 + \max(\mu^-, \mu^+). \tag{3.54}$$

Thus (3.50) determines the values $\varepsilon \in \sigma(h)$ with $\theta_{\pm} \in \boldsymbol{R}$. Without loss of generality we may assume

$$\theta_{\pm} \in [0, \pi/a]. \tag{3.55}$$

Then

$$\varepsilon \in [-2 + \min(\mu^-, \mu^+), 2 + \max(\mu^-, \mu^+)] = \sigma(h) \tag{3.56}$$

which implies, using theorems 3.1 and 3.4, that

$$k^2 \in \sigma(\Xi_{\beta^-, a\boldsymbol{Z}}) \cup \sigma(\Xi_{\beta^+, a\boldsymbol{Z}}) \qquad \operatorname{Im} k \geqslant 0. \tag{3.57}$$

The multiplicity statement follows by noting that $\psi'^{\pm}$ are linearly independent on the interior of the intersection $\sigma(\Xi_{\beta^-, a\boldsymbol{Z}}) \cap \sigma(\Xi_{\beta^+, a\boldsymbol{Z}})$. Absence of a singular continuous spectrum follows by the standard technique (cf e.g. [15]) and to show absence of eigenvalues one has to prove the same property for h which is easily seen to be true.

4. Impurities and defects in crystals

Consider the situation where we have given

$$Y = \{y_j \in \boldsymbol{R} \mid j \in J\} \qquad y_j < y_{j+1} \qquad \inf_{\substack{j, j' \in J \\ j \neq j'}} |y_j - y_{j'}| = d > 0 \qquad j \subseteq \boldsymbol{Z} \tag{4.1}$$

and $\beta = (\beta_{y_j})_{j \in J}$, $\beta_{y_j} \in \boldsymbol{R} \backslash \{0\}$, bounded. Let

$$Z = \{z_1, \ldots, z_M) \subset \boldsymbol{R} \qquad M \in \boldsymbol{N} \tag{4.2}$$

be the location of the impurities relative to Y and let the strength of the δ' interaction in Z be given by $\gamma = (\gamma_{z_j})_{j=1, M}$, $\gamma_{z_j} \in \boldsymbol{R} \backslash \{0\}$. Let $\Xi_{\beta, Y, \gamma, Z}$ denote the total Hamiltonian with δ' interactions with strength β located at Y and with additional δ' interactions with strength γ located at Z. We then distinguish three cases.

(i) Assume

$$Y \cap Z = \varnothing. \tag{4.3}$$

Then $\Xi_{\beta,Y,\gamma,Z}$ represents the Hamiltonian with *interstitial impurities* located at Z relative to $\Xi_{\beta,Y}$.

(ii) Assume

$$Z \subset Y \qquad \gamma_z = -\beta_z \qquad \text{iff} \qquad z \in Z. \tag{4.4}$$

Then $\Xi_{\beta,Y,\gamma,Z}$ represents the Hamiltonian with *defect impurities* or *vacancies* located at Z relative to $\Xi_{\beta,Y}$.

(iii) Assume

$$Z \subset Y \qquad \gamma_y \neq -\beta_y \qquad y \in Y. \tag{4.5}$$

Then $\Xi_{\beta,Y,\gamma,Z}$ represents the Hamiltonian with *substitution impurities* located at Z relative to $\Xi_{\beta,Y}$.

We then have the following theorem.

Theorem 4.1. Let β_y, $y_z \in \boldsymbol{R}\backslash\{0\}$, $y \in Y$, $z \in Z$, $Y, Z \subset \boldsymbol{R}$, satisfy (4.1), (4.2) and one of (4.3), (4.4) and (4.5). Then

$$(\Xi_{\beta,Y,\gamma,Z} - k^2)^{-1}$$
$$= G_{k,\beta,Y} + \sum_{l,l'=1}^{M} [\Gamma_{\beta,Y,\gamma,Z}(k)]^{-1}_{ll'} (\overline{G_{k,\beta,Y}(z_{l'},\cdot)}, \cdot) G_{k,\beta,Y}(\cdot, z_l)$$
$$k^2 \in \rho(\Xi_{\beta,Y,\gamma,Z}) \qquad \operatorname{Im} k > 0 \tag{4.6}$$

where $G_{k,\beta,Y} = (\Xi_{\beta,Y} - k^2)^{-1}$, $\operatorname{Im} k \geqslant 0$, with integral kernel $G_{k,\beta,Y}(x,x')$ and

$$\Gamma_{\beta,Y,\gamma,z}(k) = [-(\gamma_{z_l} k^2)^{-1} \delta_{ll'} - G_{k,\beta,Y}(z_l, z_{l'})]_{l,l'=1}^{M}$$
$$k^2 \in \rho(\Xi_{\beta,Y}) \qquad \operatorname{Im} k > 0. \tag{4.7}$$

Furthermore

$$\sigma_{\mathrm{ess}}(\Xi_{\beta,Y,\gamma,Z}) = \sigma_{\mathrm{ess}}(\Xi_{\beta,Y}). \tag{4.8}$$

Finally if $(a, b) \subseteq \rho(\Xi_{\beta,Y})$, $-\infty \leqslant a < b \leqslant \infty$, then $\sigma(\Xi_{\beta,Y,\gamma,Z}) \cap (a, b)$ contains at most M eigenvalues counting multiplicities.

Proof. Equation (4.8) and the statement following that follows from (4.6) as in theorem 2.1. Equation (4.6) can be inferred by using Krein's formula (see e.g. [16]) and noting that both $\Xi_{\beta,Y}$ and $\Xi_{\beta,Y,\gamma,Z}$ are self-adjoint extensions of the closed, symmetric operator

$$\dot{H}_{\alpha,Y,\beta,Z} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \qquad \mathscr{D}(\dot{H}_{\alpha,Y,\beta,Z}) = \{g \in \mathscr{D}(\Xi_{\beta,Y}) | g'(z_j) = 0, j = 1, \ldots, M\} \tag{4.9}$$

with deficiency indices (M, M).

We now turn to the detailed analysis of the pure crystal with one impurity. The following lemma was shown in [17] for the model with δ interactions, see also [3].

Lemma 4.2. Let k^2 be in the mth gap of $\sigma(\Xi_{\beta,aZ})$, i.e.

$$k^2 \in (b_m^{\beta,a}, a_{m+1}^{\beta,a}) \qquad \operatorname{Im} k \geqslant 0 \qquad b_0^{\beta,a} = -\infty \qquad m \in \boldsymbol{N}_0 \tag{4.10}$$

and suppose that $K = e^{i\theta a}$ where $\theta = m\pi/a + i\delta$, $\delta > 0$, $m \in N_0$ is a solution of (3.17) such that

$$\tfrac{1}{2}(K + K^{-1}) = \cos(ka) - \frac{\beta k}{2}\sin(ka). \tag{4.11}$$

Assume that ψ_k is a solution of

$$-\psi_k''(x) = k^2\psi_k(x) \qquad k^2 \in \rho(\Xi_{\beta,aZ}) \qquad \mathrm{Im}\, k \geqslant 0 \qquad x \in (0, a) \tag{4.12}$$

satisfying

$$\psi_k'(a-) = K\psi_k'(0+) \qquad \psi_k(a-) = K[\psi_k(0+) - \beta\psi_k'(0)]. \tag{4.13}$$

(*a*) Define

$$r(k) = \frac{\psi_k(\frac{1}{2}a+)}{\psi_k'(\frac{1}{2}a)}. \tag{4.14}$$

Then $r(k)$ is a continuous, strictly decreasing function of k^2 in each gap in $\sigma(\Xi_{\beta,aZ})$, and $r(k)$ is decreasing from 0 to $-\infty$ in every even gap. If $\beta > 0$, $r(k)$ is also decreasing from $+\infty$ to 0 in every odd gap. If $\beta < 0$, $r(k)$ is decreasing from ∞ to 0 in every odd gap except the first (i.e. $m = 1$). If $-a < \beta < 0$ and $m = 1$, $r(k)$ is decreasing from 0 to $-\infty$, and if $\beta < -a$, and $m = 1$, $r(k)$ is decreasing from ∞ to 0.

(*b*) Define

$$\tilde{r}(k) = \frac{\psi_k(0+)}{\psi_k'(0+)} - \tfrac{1}{2}\beta. \tag{4.15}$$

Then $\tilde{r}(k)$ is a continuous, strictly decreasing function of k^2 in each gap of $\sigma(\Xi_{\beta,aZ})$. If $\beta > 0$, $\tilde{r}(k)$ is decreasing from 0 to $-\infty$ in every gap except the zeroth gap where $\tilde{r}(k)$ is decreasing from $-\beta/2$ to $-\infty$. If $-a < \beta < 0$, $\tilde{r}(k)$ is decreasing from ∞ to 0 in every gap except the zeroth gap where $\tilde{r}(k)$ is decreasing from $-\beta/2$ to 0 and the first gap where $\tilde{r}(k)$ is decreasing from 0 to $-\infty$. If $\beta < -a$, $\tilde{r}(k)$ is decreasing from ∞ to 0 in all gaps except the zeroth gap where $\tilde{r}(k)$ is decreasing from $-\beta/2$ to 0.

Remark. By definition the first gap in $\sigma(\Xi_{\beta,a})$ always carries $m = 1$ irrespective of whether it is open (i.e. $\beta \neq -a$) or closed (i.e. $\beta = -a$).

Proof. By explicit computation one verifies that

$$r(k) = \begin{cases} \dfrac{2}{k}\cot\left(\dfrac{ka}{2}\right)\left(\dfrac{\xi(k)-1}{\xi(k)+1}\right)^{1/2} & k > 0 \\ -\dfrac{2}{\kappa}\coth\left(\dfrac{\kappa a}{2}\right)\left(\dfrac{\xi(i\kappa)-1}{\xi(i\kappa)+1}\right)^{1/2} & k = i\kappa \qquad \kappa > 0 \end{cases} \tag{4.16}$$

and

$$\tilde{r}(k) = \begin{cases} \dfrac{\mathrm{sgn}(\xi(k))}{k\sin(ka)}(\xi(k)^2 - 1)^{1/2} & k > 0 \\ -\dfrac{\mathrm{sgn}(\xi(i\kappa))}{\kappa\sinh(\kappa a)}(\xi(i\kappa)^2 - 1)^{1/2} & k = i\kappa \qquad \kappa > 0 \end{cases} \tag{4.17}$$

with

$$\xi(k) = \cos(ka) - \tfrac{1}{2}\beta k\sin(ka) \qquad \xi(i\kappa) = \cosh(a\kappa) + \tfrac{1}{2}\beta\kappa\sinh(a\kappa). \tag{4.18}$$

Before we proceed to the detailed separate results for one substitutional, defect and interstitial impurity, we derive the basic eigenvalue equation common for these three types of impurities. We want to solve

$$-\psi_k''(x) = k^2\psi_k(x) \qquad \operatorname{Im} k \geq 0 \qquad x \in \boldsymbol{R}\backslash(a\boldsymbol{Z} \cup \{z\})$$
$$\psi_k'(ja+) = \psi_k'(ja-) \qquad \psi_k(ja+) - \psi_k(ja-) = \beta\psi_k'(ja) \qquad j \in \boldsymbol{Z} \tag{4.19}$$
$$\psi_k(z+) = \psi_k(z-) \qquad \psi_k'(z+) - \psi_k'(z-) = [\gamma + \beta\delta_{a\boldsymbol{Z}}(z)]\psi_k(z)$$

with $\delta_{a\boldsymbol{Z}}(z) = 1$ if $z \in a\boldsymbol{Z}$ and 0 otherwise.

If $x \in \boldsymbol{R}\backslash\{z\}$, $\psi_k(x)$ also solves $(\Xi_{\beta,a\boldsymbol{Z}}\psi_k)(x) = k^2\psi_k(x)$ which implies that ψ_k is a linear combination of the functions

$$\psi^{\sigma}_{k,\beta,a\boldsymbol{Z}}(x) = \psi^{\sigma}_{k,\beta,a\boldsymbol{Z}}(0)\,\tfrac{1}{2}\,\beta\,\mathrm{e}^{\mathrm{i}\theta(k)\sigma x}\,\mathrm{e}^{-\mathrm{i}\theta(k)\sigma x'}$$
$$\times\frac{\mathrm{e}^{\mathrm{i}\theta(k)\sigma a}\cos(kx') - \cos[k(x'-a)]}{\cos(\theta(k)a) - \cos(ka)}$$
$$x' = x - a]x/a[\qquad x \in \boldsymbol{R} \qquad \operatorname{Im} k \geq 0 \qquad \operatorname{Im}\theta(k) \geq 0$$
$$\operatorname{Re}\theta(k) \geq 0 \qquad \sigma = \pm 1 \tag{4.20}$$

where $]y[$ denotes the largest integer smaller than or equal to y and $\theta = \theta(k)$ satisfies (3.17). $\psi^{\sigma}_{k,\beta,a\boldsymbol{Z}}$, $\sigma = \pm 1$, satisfy

$$\Xi_{\beta,a\boldsymbol{Z}}\psi^{\sigma}_{k,\beta,a\boldsymbol{Z}} = k^2\psi^{\sigma}_{k,\beta,a\boldsymbol{Z}}. \tag{4.21}$$

A short calculation then gives

$$2\mathrm{i}\sin(\theta(k)a)\sin(ka) + k\gamma\{\sin^2(kz') + \sin^2[k(z'-a)]$$
$$-2\sin(kz')\sin[k(z'-a)]\cos(\theta(k)a)\} = 0 \tag{4.22}$$

where $z' = z - a]z/a[$, $\operatorname{Im} k \geq 0$, $\operatorname{Im}\theta(k) \geq 0$, as the equation for the possible impurity state.

Theorem 4.3. (One substitutional impurity.) Let $z \in a\boldsymbol{Z}$, $a > 0$, and β, $\gamma \in \boldsymbol{R}\backslash\{0\}$, $\gamma \neq \beta$. Then

$$\sigma_{\mathrm{ess}}(\Xi_{\beta,a\boldsymbol{Z},\gamma,z}) = \sigma_{ac}(\Xi_{\beta,a\boldsymbol{Z},\beta,z}) = \sigma(\Xi_{\beta,a\boldsymbol{Z}}) \qquad \sigma_{\mathrm{sc}}(\Xi_{\beta,a\boldsymbol{Z},\beta,z}) = \varnothing. \tag{4.23}$$

Furthermore we have below $\sigma(\Xi_{\beta,a\boldsymbol{Z}})$ (i.e. in the zeroth gap).

(i) $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has exactly one simple eigenvalue in the zeroth gap of $\sigma(\Xi_{\beta,a\boldsymbol{Z}})$ iff $\gamma < -\beta$.

For the other gaps we have the following cases.

(ii) If $\beta > 0$, $\gamma > 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has no eigenvalues.

(iii) If $\beta > 0$, $\gamma < 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in every gap.

(iv) If $-a < \beta < 0$, $\gamma > 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in all gaps except the first gap ($m = 1$).

(v) If $-a < \beta < 0$, $\gamma < 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in the first gap ($m = 1$).

(vi) If $\beta < -a$, $\gamma > 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in all gaps.

(vii) If $\beta < -a$, $\gamma < 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has no eigenvalues.

The eigenvalue satisfies the relation

$$\cot(ka) = \frac{1}{\beta k}\left(\frac{(\beta^2 - \gamma^2)k^2}{4} - 1\right) \qquad k^2 \in \boldsymbol{R}\backslash\sigma(\Xi_{\beta,a\boldsymbol{Z}}). \tag{4.24}$$

Proof. Absence of embedded eigenvalues follows from the fact that a possible eigenvector would be a linear combination of $\psi^{\sigma}_{k,\beta,a\boldsymbol{Z}}$, $\sigma = \pm 1$, which however are not decaying when $k^2 \in \sigma(\Xi_{\beta,a\boldsymbol{Z}})$. Equation (4.23) follows from (4.6), (4.8) and [8]. Equation (4.22) which in this case reduces to (4.24) is equivalent to

$$\tilde{r}(k) = \tfrac{1}{2}\gamma \tag{4.25}$$

in lemma 4.2(b) from which the theorem follows.

Theorem 4.4. (One-defect impurity.) Let $z \in a\boldsymbol{Z}$, $a > 0$, and $\beta \in \boldsymbol{R}\backslash\{0\}$. Then

$$\sigma_{\mathrm{ess}}(\Xi_{\beta,a\boldsymbol{Z},-\beta,z}) = \sigma_{\mathrm{ac}}(\Xi_{\beta,a\boldsymbol{Z},-\beta,z}) = \sigma(\Xi_{\beta,a\boldsymbol{Z}}) \qquad \sigma_{\mathrm{sc}}(\Xi_{\beta,a\boldsymbol{Z},-\beta,z}) = \varnothing. \tag{4.26}$$

Furthermore

(i) if $\beta > 0$, $\Xi_{\beta,a\boldsymbol{Z},-\beta,z}$ has one simple eigenvalue in all gaps except the zeroth;

(ii) if $-a < \beta < 0$, $\Xi_{\beta,a\boldsymbol{Z},-\beta,z}$ has one simple eigenvalue in all gaps except the zeroth and the first;

(iii) if $\beta < -a$, $\Xi_{\beta,a\boldsymbol{Z},-\beta,z}$ has one simple eigenvalue in all gaps except the zeroth. The eigenvalue satisfies the relation

$$\cot(ka) = -\frac{1}{k\beta} \qquad k^2 \in \boldsymbol{R}\backslash\sigma(\Xi_{\beta,a\boldsymbol{Z}}). \tag{4.27}$$

Proof. The theorem follows by letting $\gamma = -\beta$ in theorem 4.3.

Theorem 4.5. (One interstitial impurity.) Let $z = \frac{1}{2}a$, $a > 0$, and $\beta, \gamma \in \boldsymbol{R}\backslash\{0\}$. Then

$$\sigma_{\mathrm{ess}}(\Xi_{\beta,a\boldsymbol{Z},\gamma,z}) = \sigma_{\mathrm{ac}}(\Xi_{\beta,a\boldsymbol{Z},\gamma,z}) = \sigma(\Xi_{\beta,a\boldsymbol{Z}}) \qquad \sigma_{\mathrm{sc}}(\Xi_{\beta,a\boldsymbol{Z},\gamma,z}) = \varnothing. \tag{4.28}$$

We now have the following cases.

(i) If $\beta > 0$, $\gamma > 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in every odd gap.

(ii) If $\beta > 0$, $\gamma < 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in every even gap.

(iii) If $-a < \beta < 0$, $\gamma > 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in every odd gap starting with the third gap.

(iv) If $-a < \beta < 0$, $\gamma < 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in every even gap (including the zeroth) and in addition one simple eigenvalue in the first gap.

(v) If $\beta < -a$, $\gamma > 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in every odd gap.

(vi) If $\beta < -a$, $\gamma < 0$, $\Xi_{\beta,a\boldsymbol{Z},\gamma,z}$ has one simple eigenvalue in every even gap (including the zeroth).

The eigenvalue satisfies the relation

$$\left(\frac{\gamma k}{2}\right)^2 = \frac{\beta k[\tan(\frac{1}{2}ka)]^{-1} + 2}{\beta k \tan(\frac{1}{2}ka) - 2} \qquad k^2 \in \boldsymbol{R}\backslash\sigma(\Xi_{\beta,a\boldsymbol{Z}}). \tag{4.29}$$

Proof. The proof is similar to that of theorem 4.3 except that we now apply lemma 4.2(a).

Although we explicitly omitted the possibility that $\beta = -a$ in theorems 4.3–4.5 (implying that the first gap associated with $m = 1$ closes) this situation is easily obtained by continuity of $\sigma(\Xi_{\beta,a\boldsymbol{Z},\gamma,z})$ with respect to β and simply disregarding the statements in theorems 4.3–4.5 concerning the case $m = 1$.

The anologues of theorems 4.3–4.5 for models with δ interactions were derived in [7, 17]. With the results in theorems 4.3–4.5 one can proceed to the computation of the scattering matrix for the pair $(\Xi_{\beta,aZ,\gamma,z}, \Xi_{\beta,aZ})$. Furthermore one can study impurities in half-crystals. For a discussion of these two subjects we refer to [3].

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