Some properties of the one-dimensional generalized point interactions (a torso)

Pavel Exner[1,2] *and* Harald Grosse[3,4]

1 *Nuclear Physics Institute, Academy of Sciences, CZ–25068 Řež near Prague, Czechia*
2 *Doppler Institute for Mathematical Physics, Czech Technical University, Břehová 7, CZ–11519 Prague, Czechia*
3 *Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, A–1090 Vienna, Austria*
4 *E.Schrödinger Institute for Mathematical Physics, Boltzmanngasse 9, A–1090 Vienna, Austria*

This text is a part of an unfinished project which deals with the generalized point interaction (GPI) in one dimension. We employ two natural parametrizations, which are known but have not attracted much attention, to express the resolvent of the GPI Hamiltonian as well as its spectral and scattering properties. It is also shown that the GPI yields one of the simplest models in which a non-trivial Berry phase is exhibited. Furthermore, the generalized Kronig-Penney model corresponding to the GPI is discussed. We show that there are three different types of the high-energy behaviour for the corresponding band spectrum.

1 Introduction

Many projects have a complicated history and some never make it to a paper; most of us will find examples on our desks. The present text was conceived in the fall of 1993 as a part of a larger study. For various reasons the final result never materialized and the draft could be easily put into the bin. If we do not do that it is because it contains some results on generalized point interactions in one dimension which may be of an independent interest. We reproduce the text as it was written six years ago, updating the references and adding in places an occasional "remark 99" to reflect the current state of affairs.

* * *

The intuitively attractive idea of describing interaction of quantum particles with sharply localized objects by δ-shaped potentials was introduced in the early days of quantum mechanics [11, 15]. However, it was only in the beginning of the sixties when Berezin and Faddeev [7] suggested how such formal Schrödinger operators can be constructed as mathematically well defined objects, namely as self-adjoint extensions of a symmetric operator which coincides with the free Hamiltonian outside the support of the interaction.

Two decades later point interactions became an object of a systematic and extensive study which was summarized in the monograph [2]. At the same time, numerous generalizations has appeared with contact-type interactions on configuration spaces of a non-trivial geometric structure, for relativistic Hamiltonians, with applications to the perturbation theory of embedded eigenvalues, *i.e.*, decay and resonance models *etc.* – a list of references can be found, *e.g.*, in [4, 10].

Remark 99 - 1 *We complete the list of references with several new items – see [21]–[29] – without striving for completeness. The most exhaustive bibliography to the date can be found in the forthcoming monograph by Albeverio and Kurasov [22].*

Somehow unnoticed remained in this developments remarkable properties of one-dimensional point interactions. Recall that – as long as one stays within the standard quantum mechanical setting – the self-adjoint extension construction works for dimensions $d \leq 3$, because otherwise a restriction of the Laplacian to functions which vanish in the vicinity of a fixed point yields an *e.s.a.* operator. There is a substantial difference, however, between $d = 2, 3$ on one side and one-dimensional systems on the other coming from the fact that a one-point restriction of the one-dimensional Laplacian leads to deficiency indices $(2, 2)$, and therefore to a four-parameter family of self-adjoint extensions.

The generalized point interaction (GPI) was introduced by Šeba [19]. Until recently the only particular case of it different from the standard point (or δ) interaction which was discussed was the so-called δ'*-interaction* [2], and even this did not attract the attention of physicists because of the lack of a reasonable physical model. Recall that in distinction to δ, the δ'-interaction cannot be approximated by a family of Schrödinger operators with squeezed potentials; in this sense the name is misleading because δ' is *not* an elementary dipole.

Instead, there are other approximations. The first of them was found by Šeba [20] who demonstrated that δ' is a limit of a suitable sequence of rank-one perturbations to the free Hamiltonian. Alternatively, one can use scaled Schrödinger operators but with velocity-dependent potentials. On a formal level, this was suggested for a two-parameter family of extensions in [19]. Recently, another approximation of this type (using non-selfadjoint Schrödinger operators) for a four-parameter class of GPI's including the δ'-interaction has been suggested in [8], and a similar procedure has been proposed for another three-parameter class "almost disjoint" with the former one [9]. Still another possibility – physically a very exciting one – is based on the observation that the scattering properties of δ' can be reproduced in a fixed energy interval by a suitable many-loop graph; in this sense δ'-interactions appears to a paradigm for geometric scatterers [5].

Remark 99-2 *Another geometric scatterer with similar properties is a sphere with two leads – see [28] and [26] – although the scattering in this case is more complicated. The above claim about the impossibility of approximation by a family of Schrödinger operators with squeezed potentials is not quite correct – it was shown recently [CS] that one can do that with potentials scaled in a* nonlinear *way. A rigorous nature of this approximation, however, remains to be clarified.*

Moreover, it is known that the δ' modification of the Kronig-Penney model exhibits gaps whose widths are growing at large energies - *cf.* [2, Sec.III.3]. If a homogeneous electric field is added, this leads to rather interesting spectral properties [6] which are quite unlike those of the conventional Wannier-Stark ladder [17]. In particular, such Hamiltonians appear to have empty absolutely continuous part of the spectrum, and the rest is likely to depend substantially on the slope of the linear potential: if the latter has a rational value in suitable units, the spectrum is pure point and nowhere dense, while in an irrational case it covers the whole real line. The proof of Ref.[6] cannot be adapted for the δ Wannier-Stark ladders whose spectral properties remain still an open problem. This gives a strong motivation for study the analogous problem for the general GPI including the the cases "intermediary" between the δ and δ'.

Remark 99-3 *A part of the original plan was to extend the result about the absence of absolutely continuous spectrum to other δ'-type GPI's. The question is still there, but in the course of time other aspects of the δ' Wannier-Stark problem appeared to be more appealing. In particular, the above claim about the essential spectrum (formulated as a conjecture in [5, 6]) has been proved, and moreover, the spectrum has been shown to be pure point for a "large" set of irrational slopes [23].*

Another motivation comes from the search for simple models exhibiting a nontrivial geometric phase. Recently its existence has been demonstrated for a quantum particle on an interval with a family of boundary conditions coupling the endpoints [14]. Since the occurrence of eigenvalue crossings is essential for the effect, it cannot be achieved with a standard Schrödinger operator on *line* having a potential which is limit-point at both $\pm\infty$, because the corresponding spectrum is simple. Neither can any of the standard point interactions be used, since they have at most one eigenvalue. Unlike the δ and δ', the one-center GPI has in general two eigenvalues which *do* cross at finite values of the parameters, and therefore it might yield the simplest example of a system with a nontrivial geometric phase. We shall show that this is indeed the case.

Remark 99-4 *We intended also to look into the behaviour of the continuous spectrum when the GPI parameters change. This appeared to be less urgent after the paper [SA] was published where analogous question was discussed in a more general context. Notice, however, that the Berry phase of the example given in Section 3 is independent of the parameter loop size exhibiting thus the "homeopathic" behaviour investigated in the framework of another model in [AB].*

It is not our intention to write an exhaustive study which would constitute another chapter of [2]; we want to concentrate primarily on the two above mentioned physically interesting problems. However, since several authors have addressed already the question, each of them using his own notation, a general introduction and mutual comparison is needed.

Let us review briefly the contents of the paper. In the next section we first introduce two natural parametrizations of the GPI and compare them to those existing in the literature. Then we derive an explicit expression for the resolvent kernel and use it to discuss spectral properties of the one-center GPI Hamiltonian, in particular, its eigenvalues and eigenfunctions. We also find the corresponding scattering matrix and show how it behaves at low and high energies.

In Section 3 we present the mentioned example of a geometric phase arising when the coupling-constant vector makes a loop in the parameter space.

In Section 4 we study equidistant arrays of GPI's. We show that the spectrum of the generalized Kronig-Penney model has always infinitely many gaps, however, their behaviour depends substantially on the parameters of the GPI. In addition to the δ and δ'-type situations, where the gap-to-band width ratio is decreasing and growing, respectively, we specify a class of the GPI's for which this ratio is asymptotically constant with respect to the band number.

2 The one-center generalized point interaction

2.1 Boundary conditions

Without loss of generality, we may assume that the mass is $m = 1/2$ and the interaction is supported by the point $x = 0$. The standard construction starts from the restriction of the free Hamiltonian $H_0 := -d^2/dx^2$ with $D(H_0) := H^{2,2}(\mathbb{R})$ to the subspace $\mathcal{D} := \{ f \in D(H_0) : f(0) = f'(0) = 0 \}$, which is a symmetric operator with the deficiency indices $(2, 2)$.

The most straightforward way to get the corresponding family of self-adjoint extensions is to use the von Neumann theory as Šeba did in his pioneering paper [19], see also [9]. If the operators under consideration are ordinary differential ones, however, it is more suitable to use boundary conditions; the drawback is that they usually become singular for some values of the parameters. It is easy to write a general four-parameter family of boundary conditions. Various choices have been used in [8, 9, 12, 16, 19]; below we shall present their comparison.

Here we propose two other sets of boundary conditions which seem us to be natural for the problem under consideration. The first of them is the following

$$\begin{aligned} f'(0+) - f'(0-) &= \frac{\alpha}{2}\,(f(0+)+f(0-)) + \frac{\gamma}{2}\,(f'(0+)+f'(0-))\,, \\ f(0+) - f(0-) &= -\frac{\bar\gamma}{2}\,(f(0+)+f(0-)) + \frac{\beta}{2}\,(f'(0+)+f'(0-)) \end{aligned} \tag{2.1}$$

with $\alpha, \beta \in \mathbb{R}$ and $\gamma \in \mathbb{C}$. For brevity, denote $\mathcal{A} := \left(\begin{smallmatrix} \alpha & \gamma \\ -\bar\gamma & \beta \end{smallmatrix}\right)$. This form of the boundary conditions reduces easily to the standard cases: for $\beta = \gamma = 0$ we get the δ-interaction with the "coupling constant" α, while $\alpha = \gamma = 0$ yields the δ'-interaction of strength β. The family (2.1) describes almost all self-adjoint extensions of $H_0 \upharpoonright \mathcal{D}$, with the exception of the four-point set in the parameter space referring to the situations where the Dirichlet or Neumann conditions are imposed from *both* sides of the point $x = 0$ (see also Remark 2.4a below). The other family of boundary condition we shall use is

$$f'(0+) = af(0+) + cf(0-)\,, \qquad -f'(0-) = \bar c f(0+) + bf(0-) \tag{2.2}$$

with $a, b \in \mathbb{R}$ and $c \in \mathbb{C}$; its advantage is that it allows to describe in a simple way the subset of the parameter space where the conditions decouple and the two halflines become independent.

Proposition 2.1 *Any of the above boundary conditions define a self-adjoint extension to $H_0 \upharpoonright \mathcal{D}$. The conditions (2.1) decouple separating the motion of the left and the right halflines* iff $c = 0$, *which is further equivalent to*

$$\det \mathcal{A} = 4 \quad \text{and} \quad \mathrm{Im}\,\gamma = 0\,. \tag{2.3}$$

The correspondence between the boundary conditions is given by the relations

$$\begin{pmatrix} a & c \\ \bar c & b \end{pmatrix} = \frac{1}{4\beta} \begin{pmatrix} 4 + \det \mathcal{A} + 4\mathrm{Re}\,\gamma & -4 + \det \mathcal{A} - 4i\mathrm{Im}\,\gamma \\ -4 + \det \mathcal{A} + 4i\mathrm{Im}\,\gamma & 4 + \det \mathcal{A} - 4\mathrm{Re}\,\gamma \end{pmatrix}, \tag{2.4}$$

$$\begin{pmatrix} \alpha & \gamma \\ -\bar\gamma & \beta \end{pmatrix} = \frac{4}{a + b - 2\mathrm{Re}\,c} \begin{pmatrix} ab - |c|^2 & \frac12(a-b) - i\mathrm{Im}\,c \\ -\frac12(a-b) - i\mathrm{Im}\,c & 1 \end{pmatrix}, \tag{2.5}$$

where $\det \mathcal{A} = \alpha\beta + |\gamma|^2 = 4\,\frac{a+b+2\mathrm{Re}\,c}{a+b-2\mathrm{Re}\,c}$, *provided the denominators are non-zero.*

Remarks 2.2 *(a)* The conditions (2.2) are in fact a particular case (for $E = 0$) of those used in [10]. More exactly, they are related by the natural isomorphism $U : Uf = \left(\begin{smallmatrix} f_+ \\ f_- \end{smallmatrix}\right)$ between $L^2(\mathbb{R})$ and $L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+)$, where $f_\pm(x) := f(\pm x) \upharpoonright \mathbb{R}^+$; the opposite sign of the derivative in the second condition is due to the change of the orientation of the negative halfline.

(b) This shows, at the same time, that the GPI on line is unitarily equivalent to the non-trivial (*i.e.*, s-wave) part of a "two-channel" point interaction in $\mathbb{R}^3$; in the decoupled case we have in each channel just the point interaction of the strength $\alpha/4\pi$ and $\beta/4\pi$, respectively.

(c) It is clear from (2.4) that the conditions (2.2) make no sense if $\beta = 0$. In this case one can use a reformulation, namely

$$f(0+) = Af'(0+) - Cf'(0-)\,, \qquad f'(0-) = \bar C f(0+) - Bf(0-) \tag{2.6}$$

with $A, B \in \mathbb{R}$ and $C \in \mathbb{C}$, where

$$\begin{pmatrix} A & -C \\ \bar{C} & -B \end{pmatrix} = \frac{1}{ab+|c|^2} \begin{pmatrix} b & -c \\ \bar{c} & -a \end{pmatrix}, \quad \begin{pmatrix} a & c \\ \bar{c} & b \end{pmatrix} = \frac{1}{AB-|C|^2} \begin{pmatrix} B & -C \\ -\bar{C} & A \end{pmatrix}$$

provided again the denominators are non-zero. The conditions (2.6) decouple clearly *iff* $C = 0$.

Let us further comment on relations between (2.1), (2.2) and the other known parametrizations of self-adjoint extensions of the operator $H_0 \upharpoonright \mathcal{D}$:

(i) an "almost general" set of boundary conditions

$$f(0+) = \omega \tilde{a} f(0-) + \omega \tilde{b} f'(0-)\,, \quad f'(0+) = \omega \tilde{c} f(0-) + \omega \tilde{d} f'(0-)\,, \tag{2.7}$$

where $|\omega| = 1$ and $\tilde{a}, \tilde{b}, \tilde{c}, \tilde{d}$ are real numbers such that $\tilde{a}\tilde{d} - \tilde{b}\tilde{c} = 1$, have been used in [9, 12, 16, 19], sometimes without the factor ω which can be removed by a unitary transformation – *cf.* Remark 2.4a below. They are related to (2.1), (2.2) by

$$a = \frac{\tilde{d}}{\tilde{b}}\,, \quad b = \frac{\tilde{a}}{\tilde{b}}\,, \quad c = -\frac{\omega}{\tilde{b}} \tag{2.8}$$

and

$$\alpha = \frac{4\tilde{c}}{\tilde{a} + \tilde{d} + 2\mathrm{Re}\,\omega}\,, \quad \beta = \frac{4\tilde{b}}{\tilde{a} + \tilde{d} + 2\mathrm{Re}\,\omega}\,, \quad \gamma = 2\,\frac{\tilde{d} - \tilde{a} + 2i\mathrm{Im}\,\omega}{\tilde{a} + \tilde{d} + 2\mathrm{Re}\,\omega}\,. \tag{2.9}$$

This covers the δ and δ'-interactions (for $\omega = 1$, $\tilde{a} = \tilde{d}$, $\tilde{b} = 0$ with $\alpha := \tilde{c}$, and $\omega = 1$, $\tilde{a} = \tilde{d}$, $\tilde{c} = 0$ with $\beta := \tilde{b}$, respectively), while the decoupled case is not included,

(ii) in [8], the boundary conditions (2.2) have been used, however, the parameters have been written in the form

$$a = \rho_c + \beta_c \quad b = \rho_c + \alpha_c\,, \quad c = -\rho_c\, e^{-i\theta_c} \tag{2.10}$$

with $\alpha_c, \beta_c \in \mathbb{R}$, $\rho_c \ge 0$ and $\theta_c \in [0, 2\pi)$. The relation to (2.1) is

$$\begin{aligned} \alpha &= 4\,\frac{\alpha_c\beta_c + \rho_c(\alpha_c + \beta_c)}{\alpha_c + \beta_c + 4\rho_c \cos^2\left(\frac{1}{2}\theta_c\right)}\,, \quad \beta = \frac{4}{\alpha_c + \beta_c + 4\rho_c \cos^2\left(\frac{1}{2}\theta_c\right)} \\ \gamma &= 2\,\frac{\beta_c - \alpha_c - 2i\rho_c \sin\theta_c}{\alpha_c + \beta_c + 4\rho_c \cos^2\left(\frac{1}{2}\theta_c\right)}\,. \end{aligned} \tag{2.11}$$

The corresponding boundary conditions again do not cover the case $\beta = 0$ including the δ-interaction. On the other hand, δ' corresponds to $\alpha_c = \beta_c = \theta_c = 0$ and the coupling constant $\beta := \rho_c^{-1}$, and the decoupled case to $\rho_c = 0$, *(iii)* the following two-parameter family was studied in [19]

$$f(0+) = -\gamma_s f(0-) - \delta_s f'(0-)\,, \quad f'(0+) = -\beta_s f(0-) - \alpha_s f'(0-)\,, \quad (2.12)$$

where the parameters involved are real numbers such that $\alpha_s + \gamma_s = -2$ and $\alpha_s\gamma_s - \beta_s\delta_s = 1$. The parameters of (2.1) and (2.2) are then given by

$$\alpha_s = \frac{(\gamma_s+1)^2}{\delta_s}\,, \quad \beta = -\delta_s\,, \quad \gamma = \gamma_s + 1 \quad (2.13)$$

and

$$a = -\frac{\gamma_s+2}{\delta_s}\,, \quad b = \frac{\gamma_s}{\delta_s}\,, \quad c = \frac{1}{\delta_s}\,. \quad (2.14)$$

This yields the δ'-interaction with $\gamma_s = -1$ and $\beta := -\delta_s$, while neither δ nor the decoupled case make sense here,

(iv) the three-parameter family

$$f(0+) = e^{-z} f(0-)\,, \quad rf(0+) + f'(0-) = e^{\bar z}(rf(0-) + f'(0-)) \quad (2.15)$$

has been used in [9]; it is disjoint with the previous one with the exception of the free case. We have

$$\alpha = \frac{4r(e^{2\mathrm{Re}\,z} - 1)}{|1+e^z|^2}\,, \quad \beta = 0\,, \quad \gamma = 2\,\frac{e^{\bar z} - 1}{e^{\bar z} + 1}\,. \quad (2.16)$$

Hence this parametrization is suitable for the extensions with $\beta = 0$ which are covered neither by (2.2) nor by (2.12). We can, of course, use the modification of Remark 2.2c for which the parameters are

$$A = \frac{1}{r(e^{2\mathrm{Re}\,z} - 1)}\,, \quad B = \frac{e^{2\mathrm{Re}\,z}}{r(e^{2\mathrm{Re}\,z} - 1)}\,, \quad C = \frac{e^{\bar z}}{r(e^{2\mathrm{Re}\,z} - 1)}\,. \quad (2.17)$$

It should be stressed that the Chernoff-Hughes parametrization does *not* cover the "pure" δ-interaction either, with the exception of the free case ($\alpha = 0$). The particular choice $r = 0$ and $z \in \mathbb{R}$ has been considered in [16]; it corresponds to the "off-diagonal" interaction with $\alpha = \beta = 0$ and $\gamma \in \mathbb{R}$.

Remark 2.3 There has been some confusion concerning the GPI's in recent physical literature. Apart from a nonsensical proposal critized by the authors of [2] in [3], there is a note [13] aiming at correction of the same mistake. The author has arrived at the just mentioned "off-diagonal" conditions together with the standard δ-interaction ones, however, he proposed also a generalization to "higher derivatives of the δ function", failing to realize that such conditions cannot yield a self-adjoint operator for the (second-order) Schrödinger equation.

Remarks 2.4 *(a)* The relations (2.15) show that the boundary conditions (2.1) and (2.7) have a "hidden degeneracy", namely the zero values of all coefficients describe together with the free Hamiltonian H_0 also the one-parameter family of extensions which are unitarily equivalent to H_0 by the operators U_ω : $(U_\omega f)(x) = (\Theta(-x) + \omega\Theta(x))f(x)$; they could be dubbed "quasifree".

(b) Since the time-reversal operator is represented by complex conjugation on $L^2(\mathbb{R})$, the extensions *invariant w.r.t. the time reversal* are those with real coefficients in the corresponding boundary conditions, *i.e.*, γ, c, $C \in \mathbb{R}$ in (2.1), (2.2) and (2.6), respectively; this includes both δ and δ'-interactions, as well as the decoupled case. For the other boundary conditions mentioned, this requires $\omega = \pm 1$ for (2.7) where, of course, the sign can be absorbed into the coefficients; $\theta_c = 0, \pi$ for the parametrization (2.10) and $z \in \mathbb{R}$ for (2.15); the extensions given by (2.12) are time-reversal invariant.

(c) Notice also that the operator U_ω of *(a)* produces in general one-parameter families of unitarily equivalent (and therefore isospectral) extensions corresponding to fixed a, b and $|c|$; among each family, just the operators with $c = \pm|c|$ are time-reversal invariant.

(d) In the same way, one can ask about extensions *invariant w.r.t. the space reflection.* Since the boundary values satisfy $(Rf)(0\pm) = f(0\mp)$ and $(Rf)'(0\pm) = -f'(0\mp)$ for $R:\ (Rf)(x) = f(-x)$, we see that this requires $\gamma = 0$; hence every space-reflection invariant extension is at the same time invariant w.r.t. the time reversal. In the other parametrizations mentioned, the condition is equivalent to $a = b$ and $c \in \mathbb{R}$ for (2.2), or $\alpha_c = \beta_c$, $\theta_c = 0, \pi$ for (2.10), and to $\tilde{a} = \tilde{d}$, $\omega = \pm 1$ for (2.7). No extension given by (2.12) is space-reflection invariant, while the class specified by (2.15) has a trivial – quasifree in the sense of *(a)* – intersection with the space-reflection invariant extensions. In particular, the δ and δ'-interactions are space reflection invariant; for the decoupled case this is true *iff* $a = b$.

2.2 The resolvent

For the sake of brevity, we shall use the symbol $\mathcal{A}$ for a general point in the parameter space referring to the appropriate choice of the coefficients described above; the corresponding self-adjoint extension of $H_0 \upharpoonright \mathcal{D}$ will be denoted $H_{\mathcal{A}}$.

To analyse spectral properties of these operators, we need to know the corresponding resolvent. It is, of course, an integral operator, so we have to find the corresponding kernel. We denote conventionally $k := \sqrt{z}$ with the cut along the positive real axis.

Proposition 2.5 *The resolvent kernel of* $H_{\mathcal{A}}$ *for* $\mathcal{A} := \left(\begin{smallmatrix} \alpha & \gamma \\ -\bar{\gamma} & \beta \end{smallmatrix}\right)$ *is*

$$G_{\mathcal{A}}(x, x'; k) \;=\; \frac{1}{k}\,\left(\Theta(x)\Theta(x')e^{ikx_>}\sin kx_< \;-\; \Theta(-x)\Theta(-x')e^{ikx_<}\sin kx_>\right)$$

$$
\begin{aligned}
&+\frac{\beta}{2}\,F_{\mathcal{A}}(k)^{-1}\,\{\Theta(x)\Theta(x')\,(4+\det\mathcal{A}-4\mathrm{Re}\,\gamma-4ik\beta)e^{ik(x+x')}\\
&+\Theta(-x)\Theta(-x')\,(4+\det\mathcal{A}+4\mathrm{Re}\,\gamma-4ik\beta)e^{-ik(x+x')}\\
&+\Theta(x)\Theta(-x')\,(4-\det\mathcal{A}+4\mathrm{Im}\,\gamma)e^{ik(x-x')}\\
&+\Theta(-x)\Theta(x')\,(4-\det\mathcal{A}-4\mathrm{Im}\,\gamma)e^{-ik(x-x')}\}\,,
\end{aligned}
\tag{2.18}
$$

where $F_{\mathcal{A}}(k) := (\alpha\beta+|\gamma|^2-2ik\beta)(2-ik\beta)-|\gamma|^2$ *, the symbols* $x_>, x_<$ *mean the maximum and minimum of* $x,\, x'$ *, respectively, and* Θ *is the Heaviside function. In the parametrization (2.2), it expresses as*

$$
\begin{aligned}
G_{\mathcal{A}}(x,x';k) \;=\; &\frac{1}{k}\,\left(\Theta(x)\Theta(x')e^{ikx_>}\sin kx_< \;-\; \Theta(-x)\Theta(-x')e^{ikx_<}\sin kx_>\right)\\
&+D_{\mathcal{A}}(k)^{-1}\,\{\Theta(x)\Theta(x')\,(b-ik)e^{ik(x+x')}+\;\Theta(-x)\Theta(-x')\,(a-ik)e^{-ik(x+x')}\\
&-\Theta(x)\Theta(-x')\,c\,e^{ik(x-x')}-\;\Theta(-x)\Theta(x')\,\bar c\,e^{-ik(x-x')}\}
\end{aligned}
\tag{2.19}
$$

with $D_{\mathcal{A}} := (a-ik)(b-ik)-|c|^2$ *.*

Proof: Using the Krein-formula argument from Proposition 2.1 of [10] together with the unitary equivalence of Remark 2.2a, we obtain the latter formula; the former then follows from (2.4). ∎

In the particular case of δ-interaction, $\mathcal{A}=\left(\begin{smallmatrix}\alpha & 0\\ 0 & 0\end{smallmatrix}\right)$, one can use fact that $\frac{\beta}{2}\,F_{\mathcal{A}}(k)^{-1}\to\frac14\,(\alpha-2ik)^{-1}$ as $\beta,\gamma\to 0$ together with the identity

$$
\frac{1}{\alpha-2ik} \;=\; \frac{i}{2k} \;-\; \frac{2k\alpha}{2k+i\alpha}\,\left(\frac{i}{2k}\right)^2
$$

to check that the resolvent kernel reduces to the standard expression

$$
G_\alpha(x,x';k) \;=\; \frac{i}{2k}\,e^{ik|x-x'|} \;-\; \frac{2k\alpha}{2k+i\alpha}\,\left(\frac{i}{2k}\right)^2\,e^{ik|x|}e^{ik|x'|}
$$

(*cf.* [2], Chap.I.3). On the other hand, using the identities

$$
-\,\frac{i}{2k}\;+\;\frac{i+k\beta}{k(2-ik\beta)} \;=\; -\,\left(\frac{i}{2\pi}\right)^2\,\frac{2\beta k^2}{2-ik\beta} \;=\; \frac{i}{2k}\;-\;\frac{i}{k(2-ik\beta)}\,,
$$

we check easily that for $\alpha=\gamma=0$ we arrive back at the standard δ'-expression

$$
G_\beta(x,x';k) \;=\; \frac{i}{2k}\,e^{ik|x-x'|}\;-\;\frac{2\beta k^2}{2-ik\beta}\,\tilde G(x)\tilde G(x')\,,
$$

where $\tilde G(x) := \frac{i}{2k}\,e^{ikx}\mathrm{sgn}\,x$ (*cf.* [2], Chap.I.4). A similar simplification can be obtained in the decoupled case which is not surprising, of course, because the formula (2.19) was constructed starting from the decoupled resolvent [10, Proposition 2.1].

2.3 Spectral properties

Since the GPI under consideration represents a finite-rank perturbation to (the resolvent of) H_0, the essential spectrum is preserved, $\sigma_{ess}(H_{\mathcal{A}}) = \mathbb{R}^+$. Moreover, using the explicit form of the resolvent given above, it is easy to check that there is no singularly continuous spectrum (*cf.* [18, Thm.XIII.9]), so $\sigma_{ac}(H_{\mathcal{A}}) = \mathbb{R}^+$ and the only non-trivial effect the perturbation may produce are eigenvalues of $H_{\mathcal{A}}$ without accumulation points (at most two in $(-\infty, 0)$).

We know from [10] that if a potential is added to the GPI, the resolvent kernel may have a singularity at a general point of the complex k-plane. In the present case, however, the singularities are confined to the imaginary axis only, hence it is useful to the quantity

$$\kappa := -ik\,.$$

The spectral condition $D_{\mathcal{A}}(k) = 0$ is then solved by $k_\pm$ corresponding to

$$\kappa_\pm = -\frac{1}{2}(a+b) \mp \frac{1}{2}\sqrt{(a-b)^2 + 4|c|^2}\,, \tag{2.20}$$

or

$$\kappa_\pm = \frac{1}{4\beta}\left\{ -(4+\det\mathcal{A}) \pm \sqrt{(4-\det\mathcal{A})^2 + 16|\gamma|^2} \right\}. \tag{2.21}$$

These singularities produce an eigenvalue provided the corresponding root κ is positive, otherwise we have a zero-energy resonance (for $\kappa = 0$) or an antibound state, *i.e.*, a resonance hidden deeply on the second sheet of the complex energy surface, for $\kappa < 0$.

Proposition 2.6 *The operator $H_{\mathcal{A}}$ has at most two eigenvalues which are given by the formula*

$$\epsilon_\pm := -\kappa_\pm^2 = -\frac{1}{2}(a^2 + b^2 + 2|c|^2) \pm \sqrt{\frac{1}{4}(a^2 - b^2)^2 + (a+b)^2|c|^2} \tag{2.22}$$

provided the corresponding root $\kappa_\pm$ is positive, or

$$\epsilon_\pm = -\frac{8(2+|\gamma|^2) + (\det\mathcal{A})^2}{8\beta^2} \pm \frac{4+\det\mathcal{A}}{16\beta^2}\sqrt{(4-\det\mathcal{A})^2 + 16|\gamma|^2}\,. \tag{2.23}$$

The corresponding eigenfunction are $f_\pm := f_\kappa$ for $\kappa = \kappa_\pm$, where

$$f_\kappa(x) := \mu\Theta(x)\, e^{-\kappa x} + \nu\Theta(-x)\, e^{\kappa x} \tag{2.24}$$

with the coefficients

$$\mu_\pm := \sqrt{\frac{2\kappa_\pm(b+\kappa_\pm)}{a+b+2\kappa_\pm}}\,, \qquad \nu_\pm := -\frac{\bar{c}}{|c|}\sqrt{\frac{2\kappa_\pm(a+\kappa_\pm)}{a+b+2\kappa_\pm}}\,. \tag{2.25}$$

Proof: The relations (2.22) and (2.23) are obtained by an elementary algebra. Since f_κ is the only square integrable solution to $f''+\kappa^2 f = 0$, it is sufficient to substitute it into the boundary conditions to get (2.25). ∎

Let us further mention some particular cases:

(i) if $ab < 0$, *i.e.*, $4|\mathrm{Re}\,\gamma| > |4+\det\mathcal{A}|$, there is always one bound state and one antibound state,

(ii) if both the decoupled operators on the halflines refer to a repulsive interaction, $a,b > 0$, it is still possible to have a bound state, *i.e.*, an eigenvalue of $H_{\mathcal{A}}$; this *"binding by conspiracy"* occurs *iff* $a \neq b$ and the coupling is strong enough, $|c| > \frac{1}{2}\left|\frac{a+b}{a-b}\right|$,

(iii) *two different eigenvalues* exist provided both a,b are negative, non-equal and the coupling of the halflines is weak enough,

$$|c| < \frac{1}{2}\left|\frac{a+b}{a-b}\right| . \tag{2.26}$$

In the parametrization (2.1), these conditions acquire a rather non-transparent form

$$\begin{aligned}(4+\det\mathcal{A})\mathrm{sgn}\,\beta &> \mathrm{Re}\,\gamma \geq 0\,, \\ \beta^2(4+\det\mathcal{A})^2 &> 4|\mathrm{Re}\,\gamma|^2\left((4-\det\mathcal{A})^2+16|\mathrm{Im}\,\gamma|^2\right)\end{aligned}$$

(iv) the *eigenvalue crossing* occurs *iff* $a=b$ and $c=0$. This, in turn, is clear also in the parametrization of (2.1): the condition $\det\mathcal{A}=4$ and $\gamma=0$ comprises of the decoupling requirement plus $\mathrm{Re}\,\gamma=0$, *i.e.*, $a=b$,

(v) the *δ-interaction* does not fit well into this scheme because of the lack of the parametrization (2.2). Using the modification of Remark 2.2c, we can rewrite the spectral condition as

$$(1-ikA)(1-ikB)+k^2|C|^2=0\,.$$

For $A=B=C=\alpha^{-1}$ it has the only solution $\kappa=-\alpha/2$ which yields a bound state for $\alpha<0$. One can also use the parametrization (2.1): putting $\gamma=0$ we get

$$\kappa_\pm := \frac{-4-\alpha\beta\pm|4-\alpha\beta|}{4\beta} = \begin{cases} -\frac{\alpha}{2} \\ -\frac{2}{\beta}\end{cases} \tag{2.27}$$

for all non-zero β, and only the upper solution survives the limit $\beta\to 0$,

(vi) the *δ'-interaction*, on the other hand, corresponds to $a=b=-c=\beta^{-1}$. The resolvent has again a simple pole: the spectral condition $D_{\mathcal{A}}(k)=0$ is solved by $\kappa=-2/\beta$ and $\kappa=0$, where the former solution yields a bound state for $\beta<0$, while the latter corresponds to no pole because of the vanishing residuum. We see also that only the lower solution in (2.27) is preserved in the limit $\alpha=0$.

2.4 Scattering

Using the observation made at the beginning of the preceding subsection and the Birman-Kuroda theorem [18, Thm.XI.9], one can check easily that the wave operators $\Omega_\pm(H_0, H_{\mathcal{A}})$ exist and are asymptotically complete. It is also straightforward to find that the on-shell scattering matrix is

$$S(k) = \begin{pmatrix} t(k) & r(k) \\ -\bar{r}(k) & \bar{t}(k) \end{pmatrix} \tag{2.28}$$

with

$$\begin{aligned} r(k) &= -\frac{(a-ik)(b+ik)-|c|^2}{(a-ik)(b-ik)-|c|^2} = 2\,\frac{-\det\mathcal{A}+(\gamma-ik\beta)(\bar{\gamma}-ik\beta)}{(2-ik\beta)(\det\mathcal{A}-2ik\beta)-2|\gamma|^2}\,, \\ t(k) &= \frac{2ikc}{(a-ik)(b-ik)-|c|^2} = -\,ik\beta\,\frac{4-\det\mathcal{A}+4i\mathrm{Im}\,\gamma}{(2-ik\beta)(\det\mathcal{A}-2ik\beta)-2|\gamma|^2}\,, \end{aligned}$$

and to check that it is unitary because $|r(k)|^2+|t(k)|^2=1$. It follows from Proposition 2.1 that there is no transmission in the decoupled case, and we easily the standard expressions corresponding to the particular cases of the δ and δ'-interactions [2, Chap. I.3,4].

The *low-* and *high-energy behaviour* of the GPI depends substantially on the parameters. For small k we have

$$\begin{aligned} r(k) &= -1-\frac{ik}{2\alpha}(4+\det\mathcal{A}+4\mathrm{Re}\,\gamma)+\mathcal{O}(k^2)\,, \\ t(k) &= -\frac{ik}{2\alpha}(4-\det\mathcal{A}+4i\mathrm{Im}\,\gamma)+\mathcal{O}(k^2) \end{aligned} \tag{2.29}$$

provided $\alpha\ne 0$; hence we have a full decoupling in the limit $k\to 0$. On the other hand, if $\alpha=0$ we find

$$r(k) = \frac{4\mathrm{Re}\,\gamma-2ik\beta}{4+|\gamma|^2-2ik\beta}\,, \qquad t(k) = \frac{4-|\gamma|^2+4i\mathrm{Im}\,\gamma}{4+|\gamma|^2-2ik\beta}\,,$$

so the GPI is transparent in the low-energy limit *iff* $\mathrm{Re}\,\gamma=0$ (which includes the case of δ'-interaction) while in general both the reflection and transmission amplitudes are non-zero.

At high energies the value of β is important; if it is non-zero then the S-matrix elements behave as

$$\begin{aligned} r(k) &= -1+\frac{i}{2\beta k}(4+\det\mathcal{A}+4\mathrm{Re}\,\gamma)+\mathcal{O}(k^{-2})\,, \\ t(k) &= \frac{i}{2\beta k}(4-\det\mathcal{A}+4i\mathrm{Im}\,\gamma)+\mathcal{O}(k^{-2})\,. \end{aligned} \tag{2.30}$$

Hence if the GPI contains a non-zero "component" of the δ'-interaction, it exhibits a full high-energy decoupling. On the other hand, the limit $\beta \to 0$ yields

$$r(k) \;=\; -\,\frac{2\alpha + 4ik\mathrm{Re}\,\gamma}{2\alpha - ik(4+|\gamma|^2)}\,, \qquad t(k) \;=\; -ik\,\frac{4-|\gamma|^2+4i\mathrm{Im}\,\gamma}{2\alpha - ik(4+|\gamma|^2)}\,, \tag{2.31}$$

so the GPI is transparent in the high-energy limit *iff* $\mathrm{Re}\,\gamma = 0$ (which includes the case of δ-interaction) while in general again neither the reflection nor transmission are suppressed. Notice the remarkable duality between the scattering properties at low and high energies when the roles of α and β are switched.

3 The geometric phase

Let us investigate the phase resulting from a parameter change. For simplicity, consider the case $a=b$ with $c=|c|\,e^{i\xi}$; this corresponds to

$$\mathcal{A} \;=\; \frac{2}{a-|c|\cos\xi}\begin{pmatrix} a^2-|c|^2 & -i|c|\,\sin\xi \\ -i|c|\,\sin\xi & 1 \end{pmatrix}.$$

Then we have $\kappa_\pm = -a \mp |c|$ and the coefficients (2.25) are $\mu_\pm = \sqrt{-a\mp|c|}$ and $\nu_\pm = -\,e^{-i\xi}\sqrt{-a\mp|c|}$ so

$$\begin{aligned} df_{\kappa_\pm}(x) = \Big\{ \frac{1}{2(|c|\pm a)}\, f_{\kappa_\pm}(x) \;\pm\; x\Big[\sqrt{-a\mp|c|}\,\Theta(x)\,e^{(a\pm|c|)x} \\ +\,e^{-i\xi}\sqrt{-a\mp|c|}\,\Theta(-x)\,e^{-(a\pm|c|)x}\Big]\Big\}\,d|c| +\, i\,e^{-i\xi}\sqrt{-a\mp|c|}\,\Theta(-x)\,e^{-(a\pm|c|)x}\,d\xi\,. \end{aligned}$$

As a simple example, consider $|c|$ fixed and let ξ run through $[0,2\pi)$, then we obtain a non-trivial Berry phase,

$$\int_0^{2\pi} i(f_{\kappa_\pm}, df_{\kappa_\pm}) \;=\; \int_0^{2\pi} d\xi\,(-a\mp|c|)\int_{-\infty}^0 e^{-2(a\pm|c|)x}dx \;=\; \frac{1}{2}\int_0^{2\pi} d\xi \;=\; \pi\,,$$

independently of $|c|$.

4 Arrays of generalized point interactions

Consider an equidistant array of GPI's supported by the lattice $\mathcal{L} := \{n\ell\}_{n=-\infty}^{\infty}$ with a spacing $\ell > 0$. Let the boundary conditions at the n-th lattice point be given by $\mathcal{A}_n$; for simplicity, we shall restrict our attention to the case when none of them is separating, *i.e.*, $\det\mathcal{A}_n \ne 4$ or $\mathrm{Im}\,\gamma_n \ne 0$ holds for each n.

We denote the corresponding operator by $H(\{\mathcal{A}_n\},\mathcal{L})$; it acts as the free Hamiltonian outside $\mathcal{L}$, *i.e.*, $(H(\{\mathcal{A}_n\},\mathcal{L})f)(x) = -f''(x)$ for $n\ell < x < (n+1)\ell$ and at the points $x=n\ell$ the functions of $D(H(\{\mathcal{A}_n\},\mathcal{L}))$ satisfy the boundary conditions of the form (2.1) with the coefficients given by $\mathcal{A}_n$.

In particular, if all the $\mathcal{A}_n$ are the same, $\mathcal{A}_n = \mathcal{A}$, we write $H(\{\mathcal{A}_n\},\mathcal{L}) =: H(\mathcal{A},\ell)$. This corresponds to a periodic system and one expects it to have a band-type spectrum.

Theorem 4.1 *The spectrum of $H(\mathcal{A},\ell)$ with a non-separating $\mathcal{A}\neq 0$ is purely absolutely continuous and of the form $\sigma(H(\mathcal{A},\ell))=\bigcup_{m=0}^{\infty}\Delta_m(\mathcal{A},\ell)$, where $\Delta_m(\mathcal{A},\ell)$ are mutually disjoint closed intervals, the lowest of which may be empty.*

(a) If $\beta\neq 0$, the spectral bands $\Delta_m(\mathcal{A},\ell)$ are centered roughly at the values

$$\epsilon_m := \pi^2 m^2 + (-1)^m\,\frac{2(4+\det\mathcal{A})}{\beta\ell} + \mathcal{O}(m^{-1}) \tag{4.1}$$

and their widths are asymptotically constant at high energies,

$$|\Delta_m(\mathcal{A},\ell)| = \frac{2\sqrt{(4-\det\mathcal{A})^2+16|\mathrm{Im}\,\gamma|^2}}{|\beta|\ell} + \mathcal{O}(m^{-1})\,. \tag{4.2}$$

It follows that the width $|\Gamma_m(\mathcal{A},\ell)|$ of the m-th gap is growing linearly up to higher-order terms as $m\to\infty$.

(b) If $\beta=0$ and $\mathrm{Re}\,\gamma\neq 0$, the widths of both bands and gaps are growing,

$$|\Delta_m(\mathcal{A},\ell)| = \frac{4\pi m}{\ell}\,\arcsin\left(\frac{\sqrt{(4-|\gamma|^2)^2+16|\mathrm{Im}\,\gamma|^2}}{4+|\gamma|^2}\right)\left(1+\mathcal{O}(m^{-1})\right), \tag{4.3}$$

$$|\Gamma_m(\mathcal{A},\ell)| = \frac{4\pi m}{\ell}\,\arccos\left(\frac{\sqrt{(4-|\gamma|^2)^2+16|\mathrm{Im}\,\gamma|^2}}{4+|\gamma|^2}\right)\left(1+\mathcal{O}(m^{-1})\right). \tag{4.4}$$

(c) If $\beta=0$ and $\mathrm{Re}\,\gamma=0$, the m-th gap has π^2m^2 as one endpoint and its width is asymptotically constant,

$$|\Gamma_m(\mathcal{A},\ell)| = \frac{8|\alpha|}{(4+|\gamma|^2)\ell} + \mathcal{O}(m^{-1})\,. \tag{4.5}$$

Consequently, the band widths $|\Delta_m(\mathcal{A},\ell)|$ grow linearly up to higher-order terms as $m\to\infty$.

Proof: Following the standard Bloch decomposition we have to find eigenvalues of the GPI Hamiltonian on $L^2(-\ell/2,\ell/2)$ with the boundary conditions

$$f\left(-\frac{\ell}{2}\right) = e^{i\theta} f\left(\frac{\ell}{2}\right), \quad f'\left(-\frac{\ell}{2}\right) = e^{i\theta} f'\left(\frac{\ell}{2}\right). \tag{4.6}$$

In combination with (2.1), it requires the determinant

$$\left|\begin{array}{cccc} \frac{\alpha}{2}+ik\left(1+\frac{\gamma}{2}\right) & \frac{\alpha}{2}-ik\left(1+\frac{\gamma}{2}\right) & \frac{\alpha}{2}-ik\left(1-\frac{\gamma}{2}\right) & \frac{\alpha}{2}+ik\left(1-\frac{\gamma}{2}\right) \\ 1-\frac{\bar\gamma}{2}+ik\beta & 1-\frac{\bar\gamma}{2}-ik\beta & -1-\frac{\bar\gamma}{2}+ik\beta & -1-\frac{\bar\gamma}{2}-ik\beta \\ e^{-ik\ell/2} & e^{ik\ell/2} & -e^{i(\theta+k\ell/2)} & -e^{i(\theta-k\ell/2)} \\ e^{-ik\ell/2} & -e^{ik\ell/2} & -e^{i(\theta+k\ell/2)} & e^{i(\theta-k\ell/2)} \end{array}\right|$$

to be zero, which yields the band condition

$$\mathrm{Re}\,\left((4-\det\mathcal{A}+i\mathrm{Im}\,\gamma)\,e^{i\theta}\right)\;=\;(4+\det\mathcal{A})\cos k\ell\;+\;\frac{2}{k}(\alpha-\beta k^2)\sin k\ell\,. \tag{4.7}$$

For $\beta\neq 0$ the *rhs* is asymptotically dominated by growing oscillations coming from the last term; finding its zeros and expanding around them we prove the assertion *(a)*. If $\beta=0$, we can rewrite the band condition as

$$\mathrm{Re}\,\left(t(\infty)\,e^{i\theta}\right)\;=\;\cos k\ell\;+\;\frac{2\alpha}{k(4+|\gamma|^2)}\sin k\ell\,, \tag{4.8}$$

where $t(\infty):=\lim_{k\to\infty}t(k)$ is given by (2.31). Suppose first that $\mathrm{Re}\,\gamma\neq 0$ (and $\gamma\neq\pm 2$ because the GPI is non-separating by assumption), then $0<|t(\infty)|<1$. The *rhs* is asymptotically dominated by the first term; this yields *(b)*. Finally, for $\mathrm{Re}\,\gamma=0$ we can adapt easily the standard Kronig-Penney argument [2, Chap.III.2] with α replaced by $\alpha(4+|\gamma|^2)^{-1}$. ∎

With the stated motivation in mind, we have concentrated on the infinite number of gaps and their asymptotic behaviour, using a not fully standard band numbering. We shall not discuss other properties such as the bottom of the spectrum, band profiles *etc.*; they can be obtained in the same way as in the particular cases of the δ and δ'-interactions – *cf.* [2, Chaps. III.2,3].

The main conclusion of the theorem is that the high-energy behaviour of the generalized Kronig-Penney model reflects that of the one-center GPI. If there is a non-vanishing "component" of the δ'-interaction in $H_{\mathcal{A}}$ leading to the high-energy decoupling, the corresponding $H(\mathcal{A},\ell)$ has the gap-to-band width ratio growing approximately linearly with the band number.

On the other hand, the case *(c)* exhibits the δ-type behaviour with widening bands and asymptotically constant gaps. A new type of behaviour intermediate between the δ and δ' extremes corresponds to the case *(b)*: here both gaps and bands are widening and the ratio of their width is asymptotically constant.

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