Contact interactions on graph superlattices

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We consider a quantum mechanical particle living on a graph and discuss the behaviour of its wavefunction at graph vertices. In addition to the standard (or δ type) boundary conditions with continuous wavefunctions, we investigate two types of a singular coupling which are analogous to the δ' interaction and its symmetrized version for particle on a line. We show that these couplings can be used to model graph superlattices in which point junctions are replaced by complicated geometric scatterers. We also discuss the band spectra for rectangular lattices with the mentioned couplings. We show that they roughly correspond to their Kronig–Penney analogues: the δ' lattices have bands whose widths are asymptotically bounded and do not approach zero, while the δ lattice *gap* widths are bounded. However, if the lattice–spacing ratio is an irrational number badly approximable by rationals, and the δ coupling constant is small enough, the δ lattice has *no gaps* above the threshold of the spectrum. On the other hand, infinitely many gaps emerge above a critical value of the coupling constant; for almost all ratios this value is zero.

1 Introduction

The problem of describing a quantum particle living on a graph is not new in quantum mechanics; it appeared for the first time in early fifties in connection with the free–electron model of organic molecules [26]. Writing down a Hamiltonian of such a particle requires to check that the coupling between the wavefunctions at branching point of the graph defines a self–adjoint operator, or in physical terms, that the probability flow is preserved there. This is conventionally achieved by demanding that the wavefunctions are continuous at the junctions and satisfy the conditions

$$\sum_j f_j'(x_m) \;=\; c_m f(x_m)\,, \tag{1.1}$$

where m is the vertex number, the sum runs over all links entering this vertex, $f(x_m)$ is the common value of the functions f_j there, and c_m is a real parameter.

In recent years the interest to quantum mechanics on graphs has been revived — see, *e.g.*, [1, 5, 6, 8, 9, 16, 19, 20] and references therein — in particular, as a reaction to the rapid progress of fabrication techniques which allow us nowadays to produce plenty of graph–like structures of a pure semiconductor material, for which graph Hamiltonians represent a natural model. This posed anew the question about physical plausibility of the boundary conditions (1.1).

This problem has two basic aspects. The first of them concerns the derivation of graph models from a more realistic description, in which the configuration space consists of a system of coupled tubes. This is still not the true system in which the tubes are complicated many–body objects, but the crystallic structure of the semiconductor material makes it a reasonable approximation.

Replacing a tube system by a graph of the same geometry, say, by the tube axes, means a substantial simplification. The reason is that one cannot *assume* that the wavefunction in a tube is independent of the radial a azimuthal coordinates as the authors of [19] naively suggest. The tube Laplacian is specified by appropriate boundary conditions, so there is a fully concrete system of transverse eigenfunctions; most frequently the tube boundary is assumed to be Dirichlet in which case none of these eigenfunctions is constant. The graph approximation is generally expected to work in situation where the tubes under consideration are thin enough so that the transverse–mode eigenstates are well separated in energy and their geometrically induced coupling coming from bending and branching is weak.

The one–mode approximation for a single bent tube can be justified [12, 13] but the problem is in no case a simple one. The case of a branched tube is even harder because a typical branching region is self–similar with respect to changes of the tube widths, so there is no natural parameter to switch off the intermode coupling. In general, we know neither the condition under which the graph approximation works for a branched tube, nor the boundary conditions which should model a particular branching geometry. However, we are not going to discuss these problems in the present paper, apart from some comments given in the concluding section.

The second aspect concerns intrinsic properties of the graph Hamiltonians: one may ask what is the family of admissible operators and which place is occupied in this class by those referring to the conditions (1.1). This problem was solved in [16] where we showed how a general graph Hamiltonian can be constructed using the von Neumann theory of self–adjoint extensions. However, the operator family obtained in this way is large: even if we exclude nonlocal interactions, *i.e.*, we forbid particle hopping between different branching points, each vertex of the graph is associated with n^2 real parameters, where n is the number of links entering the junction.

Motivated by this we discussed in [16] in detail several subfamilies of such operators. The simplest situation occurs if the domain of a graph Hamiltonian is required to consists of functions which are continuous at each vertex. Then we arrive back at the situation we started with, namely at the conditions (1.1) in which every junction is characterized by a single parameter. Contrary to the claim made in [19], however, this parameter is a real number and not a function of energy.

The above discussion shows that until derived within a squeezing–tube approximation, the wavefunction continuity is just an assumption which we may or may not adopt. If we decide to drop it, the next more general class of graph Hamiltonians consists of those which are *locally* permutation invariant at each vertex; we have shown in [16] that any junction is then described by a *pair* of real parameters in such a way that

$$f_j(x_m) \,=\, A_m f_j'(x_m) \,+\, B_m \sum_{k\neq j} f_k'(x_m)\,, \quad j \,=\, 1,\dots,n_m\,, \tag{1.2}$$

where the indices have the same meaning as above; this condition reduces to (1.1) for $A_m = B_m =: c_m^{-1}$. At the same time, a junction can be described also by two one–parameter families of boundary conditions, which represent singular limits of (1.2) when $A_m, B_m \to \pm\infty$ while

$$C_m \,:=\, B_m - A_m \quad \text{or} \quad D_m \,:= n_m[A_m + (n_m-1)B_m] \tag{1.3}$$

is kept preserved; they are described by the boundary conditions (2.5) and (2.6) below, respectively.

Although these couplings and their scattering properties were discussed in detail in [16], their meaning remained somewhat obscurred. Our aim in this paper is to show that they represent in a sense a counterpart to the coupling given by (1.1), and that they generalize naturally the concept of δ' interaction which has attracted attention recently in connection with spectral properties of Wannier–Stark systems [6, 7, 23]. This will be done in the next section; we are also going to show there that the relation between δ' and geometric scatterers discovered in [6] extends to vertices of any number of links.

After that we shall discuss the spectra of periodic rectangular lattices in which each junction is described by one of the couplings mentioned above. For the sake of simplicity, we restrict ourselves to the planar case, however, the results have a straightforward extension to higher dimensions. We shall demonstrate, in particular, that the δ lattice spectrum depends substantially on the ratio θ of the rectangle sides. It can even happen that there are no gaps above the threshold of the spectrum; this is the case if θ is badly approximable by rationals and the coupling is "weak" enough. On the other hand, infinitely many gaps exist for almost all θ but the gap pattern, as well as the band pattern for a δ_s' lattice, is again irregular for an irrational θ. A summary of the results has been given in [14].

2 δ' and δ'_s interactions

Throughout this section we will consider a single branching, hence we may drop the index denoting the junction. For simplicity we will deal with the graph Γ_n consisting of n halflines whose endpoints are connected at a single point; as explained in [16], the boundary conditions describing the coupling are local and may be used for any n–link vertex.

The state Hilbert space for a spinless particle having Γ_n as the configuration space is $\mathcal{H} := \bigoplus_{j=1}^n L^2(0,\infty)$ and the free Hamiltonian acts at $f \equiv \{f_j\}$ as $Hf = \{-f_j''\}$; its domain consists of all functions whose components are $H^{2,2}$ on the halflines and satisfy appropriate boundary conditions at the connection point which relate the boundary values $f_j(0+)$ and $f_j'(0+)$, $j = 1,\dots,n$. For the sake of brevity we shall drop the arguments as long as a single connection point is concerned.

2.1 A warm–up: singular interactions on line

Consider first the case of Γ_2 which is naturally isomorphic a line with a single point interaction. In general, there is a four–parameter family of such interactions — *cf.* [2, 10, 11, 15, 29]. The best known among them are the δ interactions for which the wavefunction is continuous at the point supporting the interaction, while its derivative has a jump proportional to the function value [3, Sec.I.3]. Another important class are the δ' interactions where the roles of the functions and derivatives are reversed: the wavefunctions now satisfy the conditions

$$f_+' = f_-' := f' , \qquad f_+ - f_- = \beta f' , \qquad \beta \in I\!R . \tag{2.1}$$

The name is somewhat misleading because in distinction to δ , the δ' interaction *cannot* be approximated by Schrödinger operators with scaled potentials [3, 30]. Instead, one can use approximations by families of rank–one operators [30] or velocity–dependent potentials [10]. Another way to understand the δ' interactions has been suggested in [6]: replacing the line by a "spiked–onion" graph, *i.e.*, cutting it into two halflines and joining the loose ends by N links of length ℓ , one can reproduce the high–energy scattering behaviour of the δ' interaction *up to a phase factor* in the limit when $N \to \infty$, $\ell \to 0$ and $\beta := N\ell$ is kept preserved.

In the two–parameter family of space–reversal invariant interactions there is another subset with a similar property which may be regarded as a *symmetrized version* of the δ' interaction; it is characterized by the boundary conditions

$$f_+' + f_-' = 0 , \qquad f_+ + f_- = Df_+' , \qquad D \in I\!R . \tag{2.2}$$

It is easy to check that it has a bound state of energy $-4D^{-2}$ provided $D < 0$ and the reflection and transmission amplitudes for a plane wave of momentum k are

$$r(k) \;=\; \frac{-ikD}{2-ikD} , \qquad t(k) \;=\; \frac{-2}{2-ikD} , \tag{2.3}$$

which up to signs coincides with both the δ' result (for $\beta = D$) and the high–energy behaviour of the limiting geometric scatterer.

2.2 Vertices with n links

Let us look now how the above results extend to a quantum motion on Γ_n with $n \geq 3$. The coupling with continuous wavefunctions is a natural analogue of the δ interaction, so we shall use for it the same name. The boundary conditions (1.1) can be rewritten as

$$f_1 = \cdots = f_n =: f\,, \qquad \sum_{j=1}^{n} f'_j \,=\, cf\,. \tag{2.4}$$

The first of the two classes mentioned in the introduction is for a given $C \in I\!R$ characterized by the relations

$$\sum_{j=1}^{n} f'_j \,=\, 0 \qquad \text{and} \qquad f_j - f_k + C(f'_j - f'_k) \,=\, 0\,, \quad j,k = 1,\dots,n\,; \tag{2.5}$$

it is clear that just n among these conditions are independent. For $n = 2$ this coincides with the requirements (2.1) if we put $\beta = -2C$; recall that both links are now positive real halflines so one of the derivatives has to change sign. In view of this analogy *we shall refer to the coupling (2.5) as to* δ'. It is sufficient to consider $C \neq 0$, because otherwise the conditions (2.5) reduce to (2.4) for $c = 0$. On the other hand, the second exceptional class is given by

$$f'_1 = \cdots = f'_n =: f'\,, \qquad \sum_{j=1}^{n} f_j \,=\, Df' \tag{2.6}$$

with $D \in I\!R$. In the two–link case this correspond to the condition (2.2), hence we shall speak about the δ'_s *coupling.*

To justify the claim represented by the relation (1.3), let us solve (1.2) with respect to the derivatives. This yields

$$f'_j \,=\, \frac{\mathcal{D}_{n-2}}{(A-B)\mathcal{D}_{n-1}}\, f_j \,-\, \frac{B}{(A-B)\mathcal{D}_{n-1}} \sum_{k\neq j} f_k\,, \tag{2.7}$$

where $\mathcal{D}_m := A + mB$. In the first limit of (1.3) we arrive then at

$$Cf'_j \,=\, \frac{1-n}{n}\, f_j \,+\, \frac{1}{n} \sum_{k\neq j} f_k\,,$$

which is equivalent to (2.5), while the other limit gives

$$f'_j \,=\, \frac{1}{D} \sum_{k=1}^{n} f_k\,, \qquad j = 1,\dots,n\,,$$

i.e., the condition (2.6).

Each of the three operators on Γ_n described above can exhibit bound states with eigenfunctions localized around the junction — this happens *iff* the corresponding parameter, c, $-C$ or D, respectively, is negative (we keep the notation of [16]; it would be more natural in the present context to change the sign of C). Since any solution to the free Schrödinger equation is of the form $\{\alpha_j\, e^{-\kappa x_j}\}$, it is sufficient to substitute to the boundary conditions (2.4)–(2.6) to check that the corresponding eigenvalues are

$$\epsilon(c) \,=\, -\left(\frac{c}{n}\right)^2, \quad \epsilon(C) \,=\, -\,C^{-2} \qquad \text{and} \qquad \epsilon(D) \,=\, -\left(\frac{n}{D}\right)^2$$

in the three cases; the δ and δ'_s eigenvalues are simple, while the δ' bound state has multiplicity $n-1$. Also the scattering properties of these junctions are easily found — see [16].

2.3 Geometric–scatterer junctions

Now we want to show that the "spiked–onion" argument mentioned in Section 2.1 can be naturally extended to δ' and δ'_s couplings on Γ_n, $n\ge 3$. Let us replace the latter by the graph $\Gamma_n(N,\ell)$ sketched on Figure 1: every pair of halfline endpoints is connected by N links of length ℓ; the corresponding variables will run through the interval $[-\ell/2,\ell/2]$. We shall assume that the coupling at each graph node is given by the condition (2.4) with the same parameter c.

Using the permutation symmetry of the Hamiltonian, we can write a general scattering–solution Ansatz in the following form:

(i) $e^{-ikx}+r\,e^{ikx}$ at a chosen external link (halfline),

(ii) $t\,e^{ikx}$ at the other $n-1$ halflines,

(iii) $\alpha\, e^{ikx}+\beta\, e^{-ikx}$ at the $2N$ connecting links coupled to the "incident" halfline,

(iv) $\delta\,\cos kx$ at the remaining $N\left[\binom{n}{2}-2\right]$ connecting links.

The condition (2.4) now yields the following system of equations

$$\begin{aligned} 1+r &= \alpha\bar\eta+\beta\eta \\ t \,=\, \alpha\eta+\beta\bar\eta &= \delta\cos\frac{k\ell}{2} \\ r-1+N(n-1)(\alpha\bar\eta-\beta\eta) &= \gamma(1+r) \\ t-N(\alpha\eta-\beta\bar\eta)-iN(n-2)\delta\,\sin\frac{k\ell}{2} &= \gamma t\,, \end{aligned} \tag{2.8}$$

where we have denoted

$$\eta \,:=\, e^{ik\ell/2}\,, \qquad \gamma \,:=\, \frac{c}{ik}\,.$$

The first three equations coming from the continuity requirement are solved by

$$\alpha = \frac{i}{2}\,\frac{\bar\eta(1+r)-\eta t}{\sin k\ell}\,, \qquad \beta = \frac{i}{2}\,\frac{\bar\eta t-\eta(1+r)}{\sin k\ell}\,, \qquad \delta = \frac{t}{\cos\frac{k\ell}{2}}\,.$$

Next we substitute these values into the remaining two of the equations (2.8) and use the identity

$$\cot 2x-(n-2)\tan x = (n-1)\cot 2x-(n-2)\csc 2x\;;$$

introducing

$$P \equiv P(k) := 1-\gamma+iN(n-1)\cot k\ell\,, \qquad Q\equiv Q(k) := \frac{iN}{\sin k\ell}\,,$$

we can rewrite the resulting system as

$$rP-(n-1)Qt = \bar P\,, \qquad -rQ+t[P-(n-2)Q] = Q\,.$$

Since $\mathrm{Re}\,P=1$, the sought reflection and transmission amplitudes are given by

$$\begin{aligned} r(k) &= \frac{|P|^2-(n-2)\bar PQ+(n-1)Q^2}{P^2-(n-2)PQ+(n-1)Q^2}\,,\\ t(k) &= \frac{2Q}{P^2-(n-2)PQ+(n-1)Q^2}\,. \end{aligned} \tag{2.9}$$

It is straightforward to check the identity

$$|P^2-(n-2)PQ+(n-1)Q^2|^2-||P|^2-(n-2)\bar PQ+(n-1)Q^2|^2 = 4(n-1)|Q|^2\,,$$

so the S–matrix is unitary,

$$|r(k)|^2+(n-1)|t(k)|^2 = 1\,. \tag{2.10}$$

Consider now the limit of increasingly complicated scatterers; in other words, we put $\ell := \frac{\tau}{N}$ and let $N\to\infty$. The expressions (2.9) then can be for large N rewritten as

$$\begin{aligned} r(k) &= \frac{n-2-\frac{nc}{ik}-\binom{n}{2}ik\tau}{-n+\frac{nc}{ik}+\binom{n}{2}ik\tau}+\mathcal{O}(N^{-1})\,,\\ t(k) &= \frac{-2}{-n+\frac{nc}{ik}+\binom{n}{2}ik\tau}+\mathcal{O}(N^{-1})\,, \end{aligned} \tag{2.11}$$

from where the limits immediately follow. At large energies, in particular, the terms containing c can be neglected and the amplitudes (2.11) behave as

$$r(k)\approx\frac{n-2-\binom{n}{2}ik\tau}{-n+\binom{n}{2}ik\tau}\,, \qquad t(k)\approx\frac{-2}{-n+\binom{n}{2}ik\tau}\;; \tag{2.12}$$

if $c = 0$, of course, the right sides give the expressions of the limiting amplitudes for any k.

Let us now compare this result to the S–matrices corresponding to our two singular couplings which have been computed in [16]. In the δ' case the reflection and transmission amplitudes are

$$r(k) = \frac{2 - n + inkC}{n + inkC}, \qquad t(k) = \frac{2}{n + inkC}; \tag{2.13}$$

choosing $\tau := -\frac{2C}{n-1}$, we get at high energies the same $t(k)$, while the reflection amplitude differs by the phase factor $-2\arg(n - 2 + inkC)$ which goes to π as $k \to \infty$. As for the δ'_s coupling, we have

$$r(k) = \frac{n - 2 - ikD}{n - ikD}, \qquad t(k) = \frac{-2}{n - ikD}, \tag{2.14}$$

so one has to put $\tau := \frac{2D}{n(n-1)}$ to recover the S–matrix elements (2.12) up to a sign, which is switched for all of them.

Hence both the singular couplings reproduce the high–energy behaviour of the limiting geometric scatterer up to a phase factor. They are the only ones with this property in the class (1.2). To see this, consider the reflection amplitude corresponding to (1.2). Leaving aside the case $A = B$ corresponding to (2.4) when we have $\lim_{k\to\infty} r(k) = \frac{2-n}{n}$, its high–energy behaviour is

$$r(k) = \frac{n - 2 + ik\left(1 - \frac{A}{B}\right)\mathcal{D}_{n-1}}{-n + 2\left(1 - \frac{A}{B}\right) + ik\left(1 - \frac{A}{B}\right)\mathcal{D}_{n-1}} + \mathcal{O}(k^{-2}),$$

which certainly differs from (2.12) by more than a phase factor. On the other hand, all these couplings (with exception of the case $A = B$) represent the effective *Neumann* decoupling at high energies, $\lim_{k\to\infty} r(k) = 1$, while the geometric scatterer mimicks rather the *Dirichlet* decoupling, $\lim_{k\to\infty} r(k) = -1$.

3 Lattices with a singular coupling

Consider now the case which has attracted some attention recently [5, 19] as a model of quantum–wire superlattices. We shall assume that the graph in question is a rectangular lattice with the spacings ℓ_1, ℓ_2 in the x and y direction, respectively (*cf.* Figure 2). In addition, we suppose that each graph vertex is endowed with *the same* coupling of one of the above described types. We restrict ourselves to the planar situation just for the sake of simplicity; the band conditions obtained below and the method of their solution have a straightforward extension to higher dimensions.

3.1 The Bloch analysis

To find the band spectrum of such a lattice, we start from a natural Ansatz for the Bloch solutions: we choose

$$\begin{aligned} f_m(x) &= e^{im\theta_2\ell_2}\left(a_n e^{ikx}+b_n e^{-ikx}\right) \qquad \dots \qquad x\in(n\ell_1,(n+1)\ell_1) \\ g_n(y) &= e^{in\theta_1\ell_1}\left(c_m e^{iky}+d_m e^{-iky}\right) \qquad \dots \qquad y\in(m\ell_2,(m+1)\ell_2) \end{aligned} \tag{3.1}$$

The coefficients on neighbouring links are related by

$$\begin{aligned} a_{n+1}\xi\, e^{ikx}+b_{n+1}\bar\xi\, e^{-ikx} &= \sigma(a_n e^{ikx}+b_n e^{-ikx})\,, \\ c_{m+1}\eta\, e^{iky}+d_{m+1}\bar\eta\, e^{-iky} &= \tau(b_m e^{iky}+d_m e^{-iky})\,, \end{aligned} \tag{3.2}$$

where we have denoted for the sake of brevity

$$\sigma := e^{i\theta_1\ell_1}\,,\quad \tau := e^{i\theta_2\ell_2}\,,\quad \xi := e^{ik\ell_1}\,,\quad \eta := e^{ik\ell_2}\,;$$

this conditions allow us to compute easily the needed boundary values.

Let us begin with the δ coupling, where the relations (2.4) now read

$$\begin{aligned} f_m(n\ell_1+0) = f_m(n\ell_1-0) = g_n(m\ell_2+0) = g_n(n\ell_2-0) &=: F_{mn}\,, \\ f'_m(n\ell_1+0)-f'_m(n\ell_1-0)+g'_n(m\ell_2+0)-g'_n(n\ell_2-0) &= cF_{mn}\,. \end{aligned} \tag{3.3}$$

Substituting the boundary values, we get a homogeneous system a four independent equations for the coefficients, which has a solution provided

$$-2ik\bar\tau(\eta-\bar\eta)[1-\bar\sigma(\xi+\bar\xi)+\bar\sigma^2]+c\bar\sigma\bar\tau(\xi-\bar\xi)(\eta-\bar\eta)-2ik\bar\sigma(\xi-\bar\xi)[1-\bar\tau(\eta+\bar\eta)+\bar\tau^2] = 0\,.$$

Returning to the original quantities, we can cast it into the form

$$\frac{\cos\theta_1\ell_1-\cos k\ell_1}{\sin k\ell_1}+\frac{\cos\theta_2\ell_2-\cos k\ell_2}{\sin k\ell_2}-\frac{c}{2k} = 0\,; \tag{3.4}$$

this is the result obtained in [19], and in [5] for the particular case $c=0$.

If we assume instead that the lattice links are coupled by the δ'_s interaction, the requirement (3.3) is replaced by

$$\begin{aligned} f'_m(n\ell_1+0) = -f'_m(n\ell_1-0) = g'_n(m\ell_2+0) = -g'_n(n\ell_2-0) &=: G_{mn}\,, \\ f_m(n\ell_1+0)+f_m(n\ell_1-0)+g_n(m\ell_2+0)+g_n(n\ell_2-0) &= DG_{mn}\,; \end{aligned} \tag{3.5}$$

solving it in the same way we arrive at the condition

$$\frac{\cos\theta_1\ell_1+\cos k\ell_1}{\sin k\ell_1}+\frac{\cos\theta_2\ell_2+\cos k\ell_2}{\sin k\ell_2}-\frac{Dk}{2} = 0\,. \tag{3.6}$$

Finally, in the δ' case the coupling conditions read

$$\begin{aligned}
f'_m(n\ell_1{+}0) - f'_m(n\ell_1{-}0) + g'_n(m\ell_2{+}0) - g'_n(m\ell_2{-}0) &= 0\,, \\
f_m(n\ell_1{+}0) - g_n(m\ell_2{+}0) + C(f'_m(n\ell_1{+}0) - g'_n(m\ell_2{+}0)) &= 0\,, \\
g_n(m\ell_2{+}0) - f_m(n\ell_1{-}0) + C(g'_n(m\ell_2{+}0) + f'_m(n\ell_1{-}0)) &= 0\,, \\
f_m(n\ell_1{-}0) - g_n(m\ell_2{-}0) + C(-f'_m(n\ell_1{-}0) + g'_n(m\ell_2{-}0)) &= 0\,.
\end{aligned} \tag{3.7}$$

The solvability condition is now slightly more complicated; it can be written as

$$\sum_{j=1}^{2} \frac{\cos\theta_j\ell_j - \mathrm{Re}\,((1{-}ikC)e^{ik\ell_j})}{\mathrm{Im}\,((1{+}ikC)^{-2}e^{ik\ell_j})} = 0\,. \tag{3.8}$$

At high energies, however, this relation simplifies: up to $\mathcal{O}(k^{-1})$ terms it acquires the form

$$\frac{\cos\theta_1\ell_1 - \cos k\ell_1}{\sin k\ell_1} + \frac{\cos\theta_2\ell_2 - \cos k\ell_2}{\sin k\ell_2} - 2Ck = 0\,. \tag{3.9}$$

For a single junction considered in Section 2.3, a δ'_s coupling with the parameter D has, up to a phase factor, the same asymptotic behaviour as δ' for $C = -D/n$. Using this substitution for $n = 4$ we arrive at the relation (3.6) with the parameters $\theta_j\ell_j$ replaced by $\theta_j\ell_j + \pi$. Hence the band spectra of the δ' and δ'_s lattices behave alike at high energies; we shall discuss below only the second case which is simpler.

3.2 δ lattice spectra

The condition (3.4) yields no restriction on k if $c = 0$ as the authors of [5] pointed out; the spectrum covers the interval $[0,\infty)$ and in the isotropic case, $\ell_1 = \ell_2$, one can write the energy $\epsilon(k^2) := k^2$ in terms of the Bloch parameters (quasimomentum components) θ_1, θ_2 explicitly.

This is no longer true if the coupling constant is nonzero. Nevertheless, one can say a lot about the spectrum determined by (3.4). To solve this condition, let us rewrite it as

$$\frac{c}{2k} = F(k; v_1, v_2) := \sum_{j=1}^{2} \frac{v_j - \cos k\ell_j}{\sin k\ell_j}\,, \tag{3.10}$$

where $v_j := \cos\theta_j\ell_j$. Since these parameters run through the interval $[-1,1]$, we find easily

$$\begin{aligned}
-\cot\frac{k\ell_j}{2} \le \frac{v_j - \cos k\ell_j}{\sin k\ell_j} \le \tan\frac{k\ell_j}{2} \qquad &\ldots \qquad \sin k\ell_j > 0\,, \\
\tan\frac{k\ell_j}{2} \le \frac{v_j - \cos k\ell_j}{\sin k\ell_j} \le -\cot\frac{k\ell_j}{2} \qquad &\ldots \qquad \sin k\ell_j > 0\,.
\end{aligned}$$

¿From here we obtain the extremum values of $F(k;\cdot,\cdot)$ for a fixed k:

$$\begin{aligned} F_+(k) &:= \max_{v_j\in[-1,1]} F(k;v_1,v_2) \;=\; \sum_{j=1}^{2} \tan\left(\frac{k\ell_j}{2} - \frac{\pi}{2}\left[\frac{k\ell_j}{\pi}\right]\right), \\ F_-(k) &:= \min_{v_j\in[-1,1]} F(k;v_1,v_2) \;=\; -\sum_{j=1}^{2} \cot\left(\frac{k\ell_j}{2} - \frac{\pi}{2}\left[\frac{k\ell_j}{\pi}\right]\right), \end{aligned} \tag{3.11}$$

where the symbol $[\cdot]$ denotes the integer part; at the singular points the value is understood as the limit from the right or left, respectively. By definition we have $\pm F_\pm(k) \ge 0$, hence the *gap* condition can be expressed as

$$\pm\frac{c}{2k} > \pm F_\pm(k) \tag{3.12}$$

for $\pm c > 0$, respectively. This applies to positive enegies, on the negative halfline one compares instead $\frac{c}{2\kappa}$, where $\kappa := -ik$, with the extremum values

$$F_+(\kappa) := -\sum_{j=1}^{2} \tanh\left(\frac{\kappa\ell_j}{2}\right), \qquad F_-(\kappa) := -\sum_{j=1}^{2} \coth\left(\frac{\kappa\ell_j}{2}\right); \tag{3.13}$$

since both of them are negative, there is obviously no negative spectrum for $c \ge 0$. Notice that the band condition for a one–dimensional array of δ interactions can be rewritten in the same form with a single term on the right sides of the relations (3.11) and (3.13); it is easy to reproduce from here the spectrum of the Kronig–Penney model [3, Sec.III.2].

Let us collect first some simple properties of the spectrum which follow directly from the condition (3.12) and its negative–energy counterpart. We introduce

$$\ell := \sqrt{\ell_1\ell_2}, \qquad \theta := \frac{\ell_2}{\ell_1} \qquad \text{and} \qquad L := \max(\ell_1,\ell_2), \tag{3.14}$$

so

$$\ell_1 = \ell\theta^{-1/2}, \qquad \ell_2 = \ell\theta^{1/2}, \qquad \min(\ell_1^{-1},\ell_2^{-1}) = L^{-1},$$

and denote by $\sigma(\ell,\theta,c)$ the spectrum of the corresponding δ lattice Hamiltonian.

Proposition 3.1 *(a) The spectrum has a band structure,* $\sigma(\ell,\theta,c) = \bigcup_{r=1}^{N}[\alpha_r,\beta_r]$ *for some* $N \ge 1$*, where* $\alpha_r < \beta_r < \alpha_{r+1}$.

(b) $\sigma(\ell,\theta,0) = [0,\infty)$.

(c) If $c > 0$*, each* β_r *is of the form* $\left(\frac{\pi n}{\lambda}\right)^2$ *for* $\lambda = \ell_1$ *or* ℓ_2*, and some* $n \in \mathbb{Z}$. *Similarly,* $\alpha_r = \left(\frac{\pi m}{\lambda}\right)^2$ *with* $m \in \mathbb{Z}$ *for* $c < 0$ *and* $r \ge 2$.

(d) $\pm\alpha_1 > 0$ *holds iff* $\pm c > 0$.

(e) For $c < -4\ell^{-1}(\theta^{1/2}+\theta^{-1/2})$ *,* $\beta_1 < 0$ *and* $\alpha_2 = \left(\frac{\pi}{L}\right)^2$ *.*

(f) $\sigma(\ell,\theta,c') \cap I\!\!R_+ \subset \sigma(\ell,\theta,c) \cap I\!\!R_+$ *holds for* $|c'| > |c|$ *.*

(g) Each gap is contained in the intersection of a pair of gaps of the Kronig–Penney model with the coupling constant c *and spacings* ℓ_1 *and* ℓ_2 *.*

(h) All gaps above the threshold are finite. If there is an infinite number of them, their widths are asymptotically bounded,

$$\alpha_{r+1} - \beta_r \;<\; 2|c|(\ell_1+\ell_2)^{-1} + \mathcal{O}(r^{-1})\,. \tag{3.15}$$

The property (g) allows us to localize spectral gaps by those of the Kronig–Penney model. By negation, it illustrates that transport properties of the lattice are better than a combination of its x and y projections. If a given energy is contained in a band in one of the directions, then by (3.4) it is trivially also in a band of the lattice Hamiltonian. The converse is not true, of course: the condition may be satisfied even if none of the factors can be annulated separately. Of course, different solutions correspond to different quasimomenta and different directions in which the particle is able to "dribble" through the lattice.

However, the most interesting property of the spectrum is its irregular dependence on θ coming from the existence of competing periods in (3.11). To formulate the results, we have to recall some notions from the number theory [21, 27]. Irrational numbers can be classified with respect to how "fast" they can be approximated by rationals. In particular, such a number is called *badly approximable* if there is a $\delta > 0$ such that

$$\left|\theta \,-\, \frac{p}{q}\right| \,>\, \frac{\delta}{q^2}\,. \tag{3.16}$$

This is a non–empty subset in the family of all Diophantine numbers; for instance, it contains all algebraic numbers of degree 2 , *i.e.*, irrational solutions of a quadratic equation with rational coefficients. On the other hand, the Lebesgue measure of this set is zero.

One can also write θ as a continued fraction $[a_0, a_1, \dots]$ with integer coefficients; such a representation is unique and provides a natural way to gauge the approximation properties. The faster the a_n's grow, the better is θ approximated by the truncated fractions; the worst irrational from this point of view is the golden mean $\frac{1}{2}(1+\sqrt{5}) = [1,1,1,\dots]$. A counterpart to badly approximable numbers is the class of irrationals with an unbounded sequence of coefficients,

$$\limsup_{n\to\infty} a_n \,=\, \infty\,,$$

which has the following property: there are sequences $\{m_r\}_{r=1}^{\infty}$, $\{n_r\}_{r=1}^{\infty}$ of pairwise relatively prime integers such that

$$\lim_{r\to\infty} n_r^2 \left|\theta \,-\, \frac{m_r}{n_r}\right| \,=\, 0\,. \tag{3.17}$$

These numbers, which may be called *Last admissible* [22], have full Lebesgue measure. It is sometimes convenient to express these approximations using number–theory symbols: the fractional part $\{x\} := x - [x]$, and $\|x\| := \min(\{x\}, 1-\{x\})$. Since the number in question may be indexed, to distiguish the fractional part from a sequence, we shall always specify the range of indices in the latter case.

Theorem 3.2 *(a) If θ is rational, $\sigma(\ell, \theta, c)$ has infinitely many gaps for any nonzero coupling constant c.*

(b) For badly a approximable θ there is $c_0 > 0$ such that for $|c| < c_0$ the spectrum has no gaps above the threshold, $\beta_1 = \infty$.

(c) $\sigma(\ell, \theta, c)$ has infinitely many gaps for any θ provided $|c|L > 5^{-1/2}\pi^2$.

(d) If θ is Last admissible, there are infinitely many gaps for any $c \neq 0$.

Proof: We shall suppose that $c > 0$; the argument for a negative coupling constant is analogous. If $\theta = \frac{p}{q}$, the function F_+ has infinitely many zeros in $\mathbb{R}_+$ without accumulation points, so (a) follows. On the other hand, $F_+(k) > 0$ for any $k > 0$ if θ is irrational, hence we have to investigate local minima of this function. They occur at $k_n := \frac{\pi n}{\ell_1}$ and $\tilde{k}_m := \frac{\pi m}{\ell_2}$ with $n, m \in \mathbb{Z}_+$, and the corresponding values are

$$F_+(k_n) = \tan\left(\frac{\pi}{2}\{n\theta\}\right), \qquad F_+(\tilde{k}_m) = \tan\left(\frac{\pi}{2}\{m\theta^{-1}\}\right).$$

If θ is badly approximable, the condition (3.16) yields

$$F_+(k_n) > \frac{\pi}{2}\{n\theta\} \geq \frac{\pi}{2}\|n\theta\| > \frac{\pi\delta}{2n}.$$

Since θ^{-1} is also badly approximable, we get $F_+(\tilde{k}_m) > \frac{\pi\delta}{2m}$; if different constants correspond to θ, θ^{-1}, we call δ the smaller of the two. This implies that for c small enough

$$F_+(k_n) > \frac{c}{2k_n}, \qquad F_+(\tilde{k}_m) > \frac{c}{2\tilde{k}_m},$$

holds for all $n, m \in \mathbb{Z}_+$, *i.e.*, the assertion (b).

By the Hurwitz extension of Dirichlet's theorem [27, Sec.II.1] one can find to any irrational θ sequences $\{n_r\}_{r=1}^{\infty}$, $\{m_r\}_{r=1}^{\infty}$ in such a way that $|n_r\theta - m_r| < 5^{-1/2}n_r^{-1}$. Moreover, these approximations can be constructed explicitly in terms of truncated continued fractions [21, Chap.10]. Choosing the truncations of even lengths (without the integer part), we obtain a sequence $\{\frac{m_r}{n_r}\}_{r=1}^{\infty}$ approaching θ from below. In that case $\{n_r\theta\} \to 0$, and we get the estimate

$$F_+(k_{n_r}) < \frac{\pi}{2}(1+\varepsilon)\{n_r\theta\} < \frac{\pi(1+\varepsilon)}{2\sqrt{5}\, n_r}$$

for any $\varepsilon > 0$ and r large enough. In the same way one can approximate θ^{-1}. By (3.12) we find that there are infinitely many gaps if $c > 5^{-1/2}\pi^2 L^{-1}(1+\varepsilon)$ for any $\varepsilon > 0$, *i.e.*, the assertion (c).

Let finally θ be a Last admissible number. Without loss of generality we may suppose that

$$\limsup_{n\to\infty} a_{2n} = \infty$$

holds for its continued–fraction representation; otherwise we use instead

$$\theta^{-1} = \begin{cases} [0, a_0, a_1, \dots] & \dots \quad a_0 \neq 0 \\ \\ [a_1, a_2, a_3, \dots] & \dots \quad a_0 = 0 \end{cases}$$

By (3.17) there is a sequence $\{n_r\}_{r=1}^{\infty}$ such that $n_r\{n_r\theta\} \to 0+$. This means that for all large enough r we have

$$n_r F_+(k_{n_r}) = n_r \tan\left(\frac{\pi}{2}\{n_r\theta\}\right) < \pi n_r \{n_r\theta\} \to 0 .$$

Hence $k_{n_r} F_+(k_{n_r}) \to 0$ too, so there are infinitely many values of k accumulating at infinity for which $kF_+(k) < \frac{c}{2}$. ∎

Remark 3.3 The critical value of $\pi^2/\sqrt{5} = 4.414\dots$ in the part (c) cannot be pushed down — *cf.* [27, Sec.II.1]. The bound is saturated for the golden mean, $\theta = \frac{1}{2}(1+\sqrt{5})$, and moreover, there are *no* gaps if $|c|L$ is below the critical value in this case.

3.3 δ'_s lattice spectra

Let us turn to lattices with a δ'_s coupling. The relation (3.6) can be rewritten as

$$\frac{Dk}{2} = -F(k; -v_1, -v_2) , \tag{3.18}$$

so the *bands* are now determined by the inequalities

$$\mp F_{\mp}(k) \geq \pm \frac{Dk}{2} , \qquad \pm D > 0 . \tag{3.19}$$

This concerns positive energies; on the negative halfline we have instead the condition

$$F_+(\kappa) \geq \frac{D\kappa}{2} \geq F_-(\kappa) \tag{3.20}$$

with $F_\pm(\kappa)$ given by (3.13); the change in sign is due to the fact that k is now in numerator on the left side of (3.18). Replacing $F_\pm(k)$ by similar expressions containing a single term, we obtain in this way the band spectrum of the one–dimensional array of δ'_s interactions.

Remark 3.4 Notice that the latter coincides with that of the δ' array of the same parameters [3, Sec.III.3], because the corresponding transfer matrices differ just by sign; in higher dimensions the relation between δ' and δ'_s is not that simple.

We shall use again the definitions (3.14) and employ the symbol $\sigma(\ell,\theta,D)$ for the spectrum of the δ'_s lattice Hamiltonian. The conditions (3.19) and (3.20) have the following easy consequences:

Proposition 3.5 *(a) The spectrum has a band structure. For any nonzero D the number of gaps is infinite, $\sigma(\ell,\theta,D)=\bigcup_{r=1}^{\infty}[\alpha_r,\beta_r]$ with $\alpha_r<\beta_r<\alpha_{r+1}$.*

(b) $\sigma(\ell,\theta,0)=[0,\infty)$.

(c) If $D>0$, each α_r equals $\left(\frac{\pi n}{\lambda}\right)^2$ for $\lambda=\ell_1$ or ℓ_2, and some $n\in\mathbb{Z}$. On the other hand, $\beta_r=\left(\frac{\pi m}{\lambda}\right)^2$ with $m\in\mathbb{Z}$ for $D<0$ and $r\ge 2$.

(d) $\alpha_1=0$ for $D\ge 0$, while $\alpha_1<0$ if $D<0$.

(e) For $-\ell_1-\ell_2<D<0$ we have $\beta_1<0$ and $\alpha_2=0$.

(f) $\sigma(\ell,\theta,D')\cap\mathbb{R}_+\subset\sigma(\ell,\theta,D)\cap\mathbb{R}_+$ holds for $|D'|>|D|$.

(g) Each gap is contained in the intersection of a pair of δ' Kronig–Penney gaps — see Remark 3.4 — with the coupling constant D and spacings ℓ_1 and ℓ_2.

In distinction to the δ lattice there are therefore always infinitely many gaps for $D\ne 0$. As in the Kronig–Penney case and its δ' analogue, the roles of bands and gaps are, roughly speaking, reversed. Comparing to the part (h) of Proposition 3.1, however, the asymptotics of band widths is slightly more complicated.

It is clear that if a band $[\alpha_r,\beta_r]$ with $r\gg 1$ is well separated from the rest of the spectrum, its width has the same leading term as in the Kronig–Penney situation,

$$\beta_r-\alpha_r\;=\;\frac{8}{D\ell_j}\;+\;\mathcal{O}(r^{-1})\,, \tag{3.21}$$

where ℓ_j is the length to which this band corresponds by Proposition 3.1c. If θ is rational and the points k_n and $\tilde{k}_m$ coincide, we get in the same way

$$\beta_r-\alpha_r\;=\;\frac{8}{D}\,(\ell_1^{-1}+\ell_2^{-1})+\,\mathcal{O}(r^{-1})\,. \tag{3.22}$$

It may happen, however, that k_n and $\tilde{k}_m$ are not identical but close to each other, so that they still produce a single band. It is obvious from (3.19) that this leads to an enhancement of the band width above the value given by (3.22). The effect is most profound just before the band splits. Suppose, *e.g.*, that $D>0$ and $\tilde{k}_m>k_n$ with $\delta:=\tilde{k}_m-k_n\approx 8/D\ell_1$. The band width in the momentum variable is then $\delta+\eta$ up to error terms, where η solves the equation

$$\eta^2-\delta\theta^{-1}\eta-\delta^2\theta^{-1}\;=\;0\,.$$

The enhancement due to band conspiracy is therefore

$$\frac{\delta+\eta}{\delta(1+\theta^{-1})} \,=\, g(\theta) \,:=\, \frac{2\theta+1+\sqrt{1+4\theta}}{2(\theta+1)}\,. \tag{3.23}$$

The same can be done if the order of $k_n,\, \tilde{k}_m$ is reversed; in combination with (3.21) and (3.22) this yields the following estimates on the band width,

$$\frac{8}{DL} \,+\, \mathcal{O}(r^{-1}) \,<\, \beta_r-\alpha_r \,<\, \frac{8}{D}\,(\ell_1^{-1}\!+\!\ell_2^{-1})\,e(\theta) \,+\, \mathcal{O}(r^{-1})\,, \tag{3.24}$$

where

$$e(\theta) \,:=\, \max\{g(\theta), g(\theta^{-1})\}\,.$$

It is easy to see that $e(\theta)>1$ with $\lim_{\theta\to 0} e(\theta) = \lim_{\theta\to\infty} e(\theta) = 1$. For $\theta=1$ we have $e(\theta) = \frac14\,(3\!+\!\sqrt{5}) = 1.309\ldots$, but the strongest conspiracy occurs if the lattice spacing is close to two to one, and the wider of the conspiring bands is below the other one (above for $D<0$), because the right side of (3.24) reaches its maximum at $g(2)=\frac43$. The value $\theta=2$ itself is, of course, integer so there is no enhancement. Summing this discussion, we have

Proposition 3.6 *The band widths of a δ'_s lattice with $D\ne 0$ satisfy the asymptotic bounds (3.24), where $e(\theta)<\frac43$.*

4 Conclusions

We have said in the introduction that a choice of the coupling at graph nodes in a realistic model should follow from a suitable "zero–diameter" limit of a tube system of the same topology. To illustrate some problems which may arise, recall that a cross–type region in the plane with the Dirichlet boundary exhibits a bound state [28]. Moreover, using the Dirichlet bracketing [25, Sec.XIII.15] in combination with the results of [4], one can check easily that *any* branched (star–shaped) system of infinitely long tubes with the Dirichlet boundary has at least one bound state [17]; sometimes the number of bound states may be even large,*e.g.*, for systems of a narrow–fork form as can be seen from [4]. This conclusion extends to situations where the connecting–region boundary is "rounded" (no squeezing allowed) and the tubes involved are only *asymptotically* straight [12, 17, 18].

The existence of a single bound state could be preserved in the zero–diameter limit provided the corresponding "coupling constant" is chosen with a proper sign as we have pointed out in Section 2.2. However, the couplings discussed here cannot accomodate multiple bound states. Using the more general boundary conditions (1.2) does not help: it is easy to see that such a coupling has at most *two* bound states, $\epsilon_j=-\kappa_j^2$ with

$$\kappa_1 \,:=\, -\,\frac{1}{A-B}\,, \qquad \kappa_2 \,:=\, -\,\frac{1}{A+(n-1)B}\,; \tag{4.1}$$

this happens if the denominators are negative. In general therefore a zero–diameter limit should be expected to work in an energy interval around the continuous spectrum threshold which is kept fixed, or at most it remains small with respect to the intermode distances when the junction region is scaled.

The analysis of both a single junction and a rectangular lattice shows the exceptional role of the "free" operators, *i.e.*, those having the δ coupling with $c=0$ (which is the same as δ' with $C=0$), or δ'_s coupling with $D=0$. Their S–matrix elements, band profile on a lattice, and other properties are, of course, nontrivial due the branching; however, they are the simplest possible. For instance, the reflection and transmission amplitudes through an n wire junction are

$$r = \pm\,\frac{2-n}{n}\,, \qquad t = \pm\,\frac{2}{n} \tag{4.2}$$

for the "free" δ and δ'_s coupling, respectively, independently of energy. Numerical calculations of transport properties through Y–junctions [24] suggest that at least for some systems of n coupled straight tubes, this might be the correct low–energy scattering limit.

On the other hand, a junction of finite–width tubes can have various geometries; in fact, an experimentalist would hardly guarantee that three joined quantum wires have a perfect Y shape. Moreover, if the connection region supports a potential, albeit a weak one, the low–energy scattering properties would be substantially altered. Hence the "non–free" boundary conditions are also of physical interest; one can even conceive easily a tube system in which junction parameters are tuned by application of an external field.

Up to now we had in mind mostly simple junctions. Replacing them by regions of a nontrivial topology we arrive at a situation to which the considerations of Section 2.3 might be regarded as a simplified picture. Since we have shown there that the δ' and δ'_s couplings are, at least within a fixed interval of "intermediate" energies, modelled by complicated enough geometric scatterers, also the conditions (2.5) and (2.6) are likely to have something in common with the real world. Moreover, we have seen that the coupling constant of the limiting ideal scatterer is nonzero and it is fully determined by the geometrical properties of its approximants.

In this respect, a comment is due. Without giving any details, the authors of [19] suggested that such "composed" junctions can be described by the boundary conditions (1.1) with the "renormalized" parameter dependent on energy. This does not contradict our conclusions. For instance, in the simplest case $n=2$ the corresponding reflection and transmission amplitudes, which differ just by the sign from (2.3), may be written formally as the corresponding δ scattering quantities provided we choose $c(k) := -Dk^2$. Hence if one wants to describe a "composed" junction by means of a "dressed" coupling constant — which anyhow makes sense only when a prescription to compute the latter is given — it may happen that it differs substantially from the "bare" coupling.

With this we leave this subject and turn to latice Hamiltonians of Section 3. In addition to their possible use as models of quantum wire superlattices, they represent an interesting mathematical object, and the observed dependence of the spectra on number–theoretical properties of the parameter θ raises many questions. One would like to know, for example, how the band and gap patterns do actually look, what are their fractal properties with respect to θ, or what is the measure of the spectrum relative to a suitable measure on $I\!R$. We intend to return to these problems in a later publication.

The results of Sections 3.2 and 3.3 show that despite there are "less" gaps in two dimensions, and despite the behaviour of bands and gaps is in general irregular — for an irrational θ they exhibit asymptotically a "squared quasiperiodic" distribution — it coincides roughly with that of the Kronig–Penney analogues to our lattices, namely that for the δ coupling the bands dominate at high energies, while the converse is true for the δ'_s. In analogy with the one–dimensional case [6, 7, 23] , one can therefore make a conjecture concerning the situation when a δ'_s lattice with $D \neq 0$ is placed into an electric field. The heuristic tilted–band picture suggests the existence of localization; the spectrum will remain continuous, of course, but an unrestricted propagation may be possible only in the direction *perpendicular* to the electric field. In the δ lattice case, where we have for the one–dimensional situation a guess but no rigorous result, the problem is even more exciting; the results of the present paper show that at least for some values of the lattice parameters there is no localization.

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Figure captions

Figure 1. Scattering on $\Gamma_n(N,\ell)$ with $n=3$ and $N=2$.

Figure 2. A rectangular latice.