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Lattice Kronig-Penney Models

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We discuss periodic Schrödinger operators for a particle on a rectangular lattice of sides ℓ_1, ℓ_2. In addition to the standard (δ-type) coupling with continuous wave functions at lattice nodes, we introduce two other boundary conditions which generalize naturally the one-dimensional δ' interaction and its symmetrized version; both of them can be used as models for geometric scatterers. We show that the band spectrum of these models depends on number-theoretic properties of the parameters. In particular, the δ lattice has no gaps above the threshold if ℓ_2/ℓ_1 is badly approximable by rationals and the coupling constant is small enough.

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In this Letter we discuss Schrödinger equations for a particle whose motion is confined to a rectangular lattice of sides ℓ_1 and ℓ_2 in the plane. We want to make three points. First, we are going to show that, in addition to the standard boundary conditions to couple wave functions at the lattice vertices, there are two other classes which generalize naturally the one-dimensional δ' interaction and its symmetrized version. Second, we demonstrate that these interactions inherit the properties of δ' and represent useful models for the situation when the lattice links are connected via small and complicated geometric scatterers. Finally, we show that the spectra of these lattice Hamiltonians exhibit a dependence on number-theoretic properties of model parameters.

A fresh interest to particle motion on lattices [1] has been motivated by problems of quantum-wire structures. In a broader context of quantum motion on graphs, however, this problem existed four decades ago in connection with the free-electron model of organic molecules [2] and resurfaced recently in different contexts [3–5].

When a quantum Hamiltonian for a graph is constructed, it is essential to ensure that it is self-adjoint, i.e., that the probability current is conserved at the graph vertices. Usually it is achieved by assuming that the wave functions are continuous there and satisfy the condition

$$\sum_j \psi_j'(x_m) = \alpha_m \psi(x_m)\,, \qquad (1)$$

where m is the vertex number, the sum runs over all links entering this vertex, $\psi(x_m)$ is the common value of the functions ψ_j there, and α_m is a real parameter. As long as a single junction is concerned, we drop for brevity the index m and the arguments and write the condition as

$$\psi_1 = \cdots = \psi_n =: \psi\,, \quad \sum_{j=1}^n \psi_j' = \alpha\psi\,, \qquad (2)$$

where n is the number of the connected links. We shall speak about a δ *coupling,* because for $n = 2$ this is nothing but the one-dimensional δ interaction [6].

There are two basic questions about the condition (2). The first is how well a graph can model a more realistic system of branched tubes. It was argued a long time ago [2] that for star-shaped junctions the requirement (2) with $\alpha = 0$ might be the optimal choice, though up to now no strict result exists. At the same time, if the connecting region has a different geometry, supports a potential, or an external field is applied, one expects that other boundary conditions may be more appropriate. However, this problem is difficult, and we are not going to attack it here.

The second question concerns intrinsic properties of graph Hamiltonians: One may ask what are the admissible couplings and which role is played among them by the condition (2). This problem was solved in [4] by means of the von Neumann theory of self-adjoint extensions.

The operator family obtained in this way is large—a local coupling at an n-link junction can be described by n^2 real parameters—so additional restrictions are sought. If the wave functions are demanded to be continuous, we arrive back at the condition (2).

The next, more general, class is couplings which are locally invariant with respect to permutations of the links. They are described by the conditions

$$\psi_j = a\psi_j' + b\sum_{k\neq j}\psi_k', \quad j = 1,\dots,n,$$

where a, b are two real parameters. In addition, one has two singular one-parameter couplings which correspond to the limits $a, b \to \infty$ with $\beta := a - b$ or $\beta_s := n[a + (n-1)b]$ preserved. The corresponding boundary conditions can be given in the explicit form

$$\sum_{j=1}^{n}\psi_j' = 0, \quad \psi_j - \psi_k = \beta(\psi_j' - \psi_k'), \quad j,k = 1,\dots n, \tag{3}$$

and

$$\psi_1' = \cdots = \psi_n' =: \psi', \quad \sum_{j=1}^{n}\psi_j = \beta_s\psi', \tag{4}$$

respectively. We call the first of them δ', because it reduces to the δ' interaction for $n = 2$ [6]. The second one corresponds rather to a symmetrized version of δ' interaction on line, $\psi_+' + \psi_-' = 0$ and $\psi_+ + \psi_- = \beta_s\psi_+'$; hence we shall speak about the δ_s' coupling.

Even in the case $n = 2$ it is not easy to grasp the meaning of the δ' interaction. It *cannot* be obtained as a limit of scaled scalar potentials; one has to use instead nonlocal or velocity dependent interactions [7]. The results are not very illustrative. On the other hand, we have shown in [5] that δ' shares many properties with complicated geometric scatterers. Now we are going to argue that junctions connecting any number of links have the same property.

To this end, we replace a point junction by the graph sketched in Fig. 1: The loose ends of any pair of graph links are connected by N wires of the same length ℓ. We suppose that the wave functions at each vertex of this graph are coupled by the boundary conditions (2) with n replaced by $2N + 1$ and the same α.

The S matrix for such a graph is an $n \times n$ symmetric matrix with the reflection and transmission amplitudes on and off diagonal, respectively. To find it, one has to write the wave functions as combinations of plane waves at each of the $n + N\binom{n}{2}$ graph links, and to demand it satisfy the conditions (2) at each node. Because of the graph symmetry, we arrive at a system of five linear equations. It is straightforward to write them down and to solve them, but it is somewhat lengthy; hence we shall give details elsewhere [8]. The resulting amplitudes are

$$r(k) = \frac{|P|^2 - (n-2)\bar{P}Q + (n-1)Q^2}{P^2 - (n-2)PQ + (n-1)Q^2},$$

$$t(k) = \frac{2Q}{P^2 - (n-2)PQ + (n-1)Q^2},$$

where

$$P := 1 - \frac{\alpha}{ik} + iN(n-1)\cot k\ell, \quad Q := \frac{iN}{\sin k\ell}.$$

One can check directly that the S matrix is unitary,

$$|r(k)|^2 + (n-1)|t(k)|^2 = 1.$$

If we consider increasingly complicated scatterers in which the connecting wires become shorter, i.e., we put $\ell := \tau/N$, the S matrix elements can be expressed as

$$\begin{aligned} r(k) &= \frac{n - 2 - n\alpha/ik - \binom{n}{2}ik\tau}{-n + n\alpha/ik + \binom{n}{2}ik\tau} + \mathcal{O}(N^{-1}), \\ t(k) &= \frac{-2}{-n + n\alpha/ik + \binom{n}{2}ik\tau} + \mathcal{O}(N^{-1}); \end{aligned} \tag{5}$$

the error terms depend on k, but one can make them small in any finite interval of energy by choosing N large enough. It is also clear that the high-energy behavior of the limiting scatterer is independent of α, and we put the latter, therefore, equal to zero.

This result can be compared with the S matrix elements corresponding to our two singular couplings, (3) and (4), which were computed in [4]: they equal

$$r(k) = \frac{2 - n + ink\beta}{n + ink\beta}, \quad t(k) = \frac{2}{n + ink\beta}$$

and

$$r(k) = \frac{n - 2 - ik\beta_s}{n - ik\beta_s}, \quad t(k) = \frac{-2}{n - ik\beta_s},$$

respectively. We can reproduce the corresponding transmission and reflection *probabilities* from (5) with $\alpha = 0$ and N large by choosing $\tau := 2\beta/(n-1)$ and $\tau := 2\beta_s/n(n-1)$ in the two cases. The S matrix elements differ just by a phase factor: They are multiplied by -1 for the δ_s' coupling, while in the δ' case we get the same $t(k)$, and $r(k)$ up to the phase factor $2\arg(n - 2 + ink\beta)$ which goes to π as $k \to \infty$. The difference is important, because

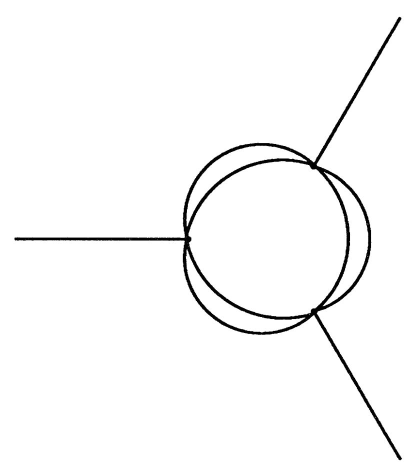

FIG. 1. A geometric-scatterer junction with $n = 3$ and $N = 2$.

the interactions (3) and (4) represent an effective von Neumann decoupling at high energies, $\lim_{k\to\infty} r(k) = 1$, while the geometric scatterer mimics rather the Dirichlet decoupling, $\lim_{k\to\infty} r(k) = -1$.

Let us turn now to our main topic. Consider a rectangular lattice with the node spacings ℓ_1, ℓ_2 in the x and y directions [9], respectively, and suppose that the particle is free at lattice links and the wave functions at each graph lattice vertex are related by the same boundary conditions of one of the above described types with $n = 4$. It is a straightforward if tedious exercise to write the Bloch ansatz for the wave functions and to derive the relation between the energy $E = k^2$ and the quasimomentum components ϑ_j. For a δ lattice this was done in Ref. [1] with the result

$$\frac{\cos\vartheta_1\ell_1 - \cos k\ell_1}{\sin k\ell_1} + \frac{\cos\vartheta_2\ell_2 - \cos k\ell_2}{\sin k\ell_2} - \frac{\alpha}{2k} = 0. \tag{6}$$

In a similar way, one finds that the spectrum of a δ_s' lattice is determined by the condition

$$\frac{\cos\vartheta_1\ell_1 + \cos k\ell_1}{\sin k\ell_1} + \frac{\cos\vartheta_2\ell_2 + \cos k\ell_2}{\sin k\ell_2} - \frac{\beta_s k}{2} = 0, \tag{7}$$

while for a δ' lattice we have

$$\sum_{j=1}^{2} \frac{\cos\vartheta_j\ell_j - \mathrm{Re}[(1 + ik\beta)e^{ik\ell_j}]}{\mathrm{Im}[(1 - ik\beta)^{-2}e^{ik\ell_j}]} = 0.$$

The last relation looks more complicated. For large k, however, it simplifies, up to $\mathcal{O}(k^{-1})$ terms, to the form (7) with $\beta_s = 4\beta$; this means that the spectra of the two lattices have the same high-energy asymptotics.

For simplicity, we shall discuss only the conditions (6) and (7). Though they cannot be solved explicitly with the exception of trivial cases, they provide, nevertheless, useful information about the spectrum. To illustrate that, let us rewrite the first of them in the form

$$\frac{\alpha}{2k} = \sum_{j=1}^{2} \frac{v_j - \cos k\ell_j}{\sin k\ell_j},$$

where the parameters $v_j := \cos\vartheta_j\ell_j$ run through the interval [–1,1]. It is easy to see that, for a fixed k, the maximum of the right side equals

$$F_+(k) := \sum_{j=1}^{2} \tan\left(\frac{k\ell_j}{2} - \frac{\pi}{2}\left[\frac{k\ell_j}{\pi}\right]\right),$$

where the square bracket denotes the integer part, and the minimum $F_-(k)$ is obtained by replacing tan with –cot. Hence the gaps of the δ lattice spectrum on the positive real half line are determined by the condition

$$\pm\alpha/2k > \pm F_\pm(k) \tag{8}$$

for $\pm\alpha > 0$, respectively; for the negative part of the spectrum one has to compare $\alpha/2\kappa$ with the extremum values $iF_\pm(i\kappa)$.

The condition (8) has several simple implications, in particular, as follows: (a) The spectrum has a band structure; it equals $[0,\infty)$ if and only if $\alpha = 0$. (b) If $\alpha > 0$, the upper end of each band is a square of some $k_n := \pi n/\ell_1$ or $\tilde{k}_m := \pi m/\ell_2$, where n, m are integers. Similarly, for $\alpha < 0$ each lower band end, with the exception of the first one, equals k_n^2 or $\tilde{k}_m^2$. (c) The lowest band threshold is positive (negative) for $\pm\alpha > 0$, respectively; if $\alpha < -4(\ell_1^{-1} + \ell_2^{-1})$, the whole first band is negative, and the second one starts at $(\pi/L)^2$, where $L := \max(\ell_1, \ell_2)$. (d) The positive bands shrink with increasing $|\alpha|$. (e) All gaps above the threshold are finite. If there is an infinite number of them, their widths are asymptotically bounded by $2|\alpha|(\ell_1 + \ell_2)^{-1} + \mathcal{O}(r^{-1})$, where r is the gap number.

The most interesting property of the spectrum is its irregular dependence on $\theta := \ell_2/\ell_1$ coming from the existence of competing periods in $F_\pm(k)$. Recall that an irrational number θ is *badly approximable* by rationals if there is a $\delta > 0$ such that $|q\theta - p| > \delta q^{-1}$ holds for all integers [10]. This set is uncountable but of zero measure. Its complement consists of all irrationals whose continued-fraction representation has an unbounded sequence of coefficients. Alternatively, one can say that there are sequences $\{q_r\}$, $\{p_r\}$, of integers such that $q_r|q_r\theta - p_r| \to 0$; we call these numbers *last admissible* [11].

The δ lattice spectrum contains, obviously, infinitely many gaps if θ is rational. For an irrational θ we have the following results:

Theorem.—If θ is badly approximable, there is $\alpha_0 > 0$ such that no gaps exist above the threshold for $|\alpha| < \alpha_0$. On the other hand, the number of gaps is infinite for any θ provided $|\alpha|L > 5^{-1/2}\pi^2$. If θ is last admissible, there are infinitely many gaps for any $\alpha \neq 0$.

The proof is technical and will be, therefore, given elsewhere [8]. However, its idea is simple. For irrational θ the right side of (8) has no zeros, so one has to investigate the sequence of its local minima (for $\alpha > 0$, and maxima otherwise). They occur at the points k_n, $\tilde{k}_m$ with integer n, m; the properties of θ determine how fast this sequence approaches zero. This has to be compared with the sequences $\{\alpha/2k_n\}$ and $\{\alpha/2\tilde{k}_m\}$.

Remark.—The sufficient condition for the existence of infinitely many gaps is saturated for the golden mean, $\theta = \frac{1}{2}(1 + \sqrt{5})$, for which also the critical value $|\alpha_0|\ell$ is $\pi^2(5\theta)^{-1/2} = 3.4699\ldots$; this certainly is not small.

The condition (7) can be solved in a similar way; the spectral bands are now determined by the inequalities

$$\mp F_\mp(k) \geq \pm\beta_s k/2 \tag{9}$$

for $\pm\beta_s > 0$ and $k > 0$, and an analogous relation for the negative part. From here we can make the following conclusions: (a) The spectrum equals $[0,\infty)$ if and only if

$\beta_s = 0$; otherwise, the number of gaps is infinite. (b) If $\beta_s > 0$, the lower end of each band coincides with some k_n^2 or $\tilde{k}_m^2$, where n, m are integers. The same is true for $\beta_s < 0$ and the upper band end, with the exception of the first one. (c) The lowest band threshold is positive (negative) for $\pm\beta_s > 0$, respectively; if $-\ell_1 - \ell_2 < \beta_s < 0$, the whole first band is negative, and the second one starts at zero. (d) The positive bands shrink with increasing $|\beta_s|$.

An analog to the property (*e*) of δ lattices is slightly more complicated. If a band high in the spectrum is well separated, its width Δ_r is the same as in the δ' Kronig-Penney model, $\Delta_r = 8/\beta_s\ell_j + \mathcal{O}(r^{-1})$. If θ is rational and $k_n = \tilde{k}_m$ for some n, m, we have a similar expression with ℓ_j^{-1} replaced by $\ell_1^{-1} + \ell_2^{-1}$. 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. Then the band width is enhanced; the effect is most profound just before the band splits. Using the condition (7), it is straightforward to estimate that the factor of enhancement by conspiracy of bands is, up to error terms, bounded by

$$\max\left\{\frac{2\theta + 1 + \sqrt{1 + 4\theta}}{2(\theta + 1)}, \frac{2\theta^{-1} + 1 + \sqrt{1 + 4\theta^{-1}}}{2(\theta^{-1} + 1)}\right\}.$$

Taking the maximum over θ, we find that the δ_s' lattice bandwidths are asymptotically bounded by

$$\frac{8}{\beta_s L} + \mathcal{O}(r^{-1}) < \Delta_r < \frac{32}{3\beta_s}(\ell_1^{-1} + \ell_2^{-1}) + \mathcal{O}(r^{-1}).$$

The irregular dependence on θ is a new feature coming from the higher dimensionality. On the other hand, the spectra we have discussed above have *roughly* the same behavior as their Kronig-Penney analogs: At high energies the bands dominate in the δ lattice spectrum, while the converse is true for δ' and δ_s'.

If one of the two last lattices is placed into an electric field, the tilted-band picture allows us to conjecture that the conclusions of Refs. [5,12] might extend to higher dimensions. The spectrum now would remain continuous, of course, but an unrestricted propagation would be possible only in the direction *perpendicular* to the field gradient. For a δ lattice, where a phase transition is expected to occur in the one-dimensional situation, and the gaps may close for some irrational θ, the problem is even more exciting.

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