Large gaps in point-coupled periodic systems of manifolds

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Abstract

We study a free quantum motion on periodically structured manifolds composed of elementary two-dimensional "cells" connected either by linear segments or through points where the two cells touch. The general theory is illustrated with numerous examples in which the elementary components are spherical surfaces arranged into chains in a straight or zigzag way, or two-dimensional square-lattice "carpets". We show that the spectra of such systems have an infinite number of gaps and that the latter dominate the spectrum at high energies.

1 Introduction

The spectral behaviour of periodic systems is of a great importance. Having typically a band structure, such spectra differ by the number and structure of the gaps. For usual Schrödinger operators the number of gaps is generically infinite in the one-dimensional situation and finite in higher dimensions.

Moreover, the gap widths decrease as the energy tends to infinity, the rate of decay being tied to the regularity of the potential.

In case of a singular periodic interaction the gaps may not close. A canonical example is the Kronig-Penney (KP) model, i.e. a chain of δ-potentials where the gaps are asymptotically constant [AGH]. Even more singular couplings like generalized point interactions may exhibit gaps which are growing at the same rate as the bands [EGr], or even grow while the band widths are asymptotically constant. A typical example of such a behaviour is a modification of the KP model with a chain of the so-called δ'-interactions [AGH]. This behaviour is not restricted to one dimension; similar results can be derived e.g. for lattice graphs with appropriate boundary conditions coupling the wave functions at the vertices [Ex, EGa].

Large gaps has interesting physical consequences. For instance, the corresponding Wannier-Stark problem in which we add a linear background potential to a periodic chain of δ'-interactions has counterintuitive properties: the absolutely continuous spectrum of the corresponding Hamiltonian is empty [AEL], and in fact, the spectrum is known to be pure point for "most values" of the potential slope [ADE]. These results can be explained by observing that tilted gaps represent classically forbidden regions and that their large widths prevent the particle of propagating over long distances.

On the other hand, the physical meaning of the δ'-coupling remained unclear for a long time. Recently it has been demonstrated that this interaction can be approximated in the norm resolvent sense by a family of Schrödinger operators – see [ENZ] where also a bibliography to the problem is given – but previous studies brought some interesting non-potential approximations. An interesting example is given by a "bubble scattering" in which two halflines are attached to the surface of a sphere – see [Ki] and also [ETV, Br]. Such a system typically exhibits numerous resonances but the background transmission probability dominates and vanishes at the limit of large energies. This observation is of importance because systems of a mixed dimensionality are not just a mathematicians toy, but they can model real objects such as a fullerene molecule coupled to a pair of nanotubes [Ka].[1]

The aim of the present paper is to study systems with components of different dimension in the periodic setting. We intend to demonstrate that the structure of the configuration space in this case is reflected in the gap

[1] Another model for such systems could be that of manifolds connected smoothly by thin tubes. Existence of gaps in this setting was demonstrated recently by Post [Po].

behaviour. After describing a general method to couple periodic systems of spheres, either joining them by line segments or directly through points where they touch, we will discuss in Sections 3-5 a number of examples. The results, summarized in Proposition 5.1, show that in all the considered cases the number of gaps are infinite and the gap-to-band width ratio increases with the band index. The estimated growth is slower than in the case of the δ'-interaction, and it is slower for a two-dimensional lattice than for a linear chain, but it is still powerlike for spheres joined by linear segments, thus confirming our conjecture that the effect is related to the change in dimensionality the particle must undergo. Even for a tighter coupling, however, where the spheres are coupled directly through contact points, the gap-to-band ratio is still logarithmically increasing.

2 General theory

2.1 Building blocks of the Hamiltonian

Suppose that X_0 is a two-dimensional Riemann manifold. By H_0 we denote a Schrödinger operator,

$$H_0 = |g|^{-1/2}(-i\partial_j - A_j)|g|^{1/2}g^{jk}(-i\partial_k - A_k) + V \,,$$

on $L^2(X_0, |g|^{1/2}\mathrm{d}x)$ with smooth vector and scalar potentials. The formalism we are going to describe extends easily to the case $\dim X_0 = 3$ but we will limit ourselves here to referring to [BG2] for guidelines concerning such a generalization. The metric structure of X_0 is fixed and we will employ the shorthand notation $L^2(X_0)$ for simplicity in the following. Let further X_j, $j = 1, \ldots, n$, be a finite or semiinfinite line segment which can be identified with the interval $[0, d_j)$, $0 < d_j < \infty$. No external potentials are supposed to act on the particle on X_j, i.e. we consider the free operators $H_j = -\mathrm{d}^2/\mathrm{d}x^2$ on $L^2(X_j)$ with Neumann's condition at the endpoints (the "right" endpoint $x = d_j$ requires a boundary condition only if $d_j < \infty$) as the building blocks of the system Hamiltonian.

As we have said above we consider systems with configuration space consisting of infinite number of copies of a manifold which are connected either by isolated points common for the pair of neighbouring copies, or by line segments connecting such points. We will concentrate on the latter case which is more complicated. The former one can be regarded as the limiting situation where the length of the connecting segments tends to zero, and the corresponding modification of the formalism is easy.

A building block of our model is thus a "hedgehog manifold" obtained by attaching each segment X_j to X_0 at a point $q_j \in X_0$, or more exactly, by identifying the point $0 \in X_j$ with $q_j \in X_0$; we suppose that all the connection points q_j are mutually different. The topological space constructed in this way will be denoted as $\hat{X}$; it can be endowed with a natural measure which restricts to the Riemannian measure on X_0 and to the Lebesgue measure on each $X_j\,,\; j = 1, \ldots, n$. This yields the identification

$$L^2(\hat{X}) = L^2(X_0) \oplus L^2(X_1) \oplus \cdots L^2(X_n)$$

for the Hilbert state space of the system.

By S_0 we denote the restriction of the operator H_0 defined above to the family of functions

$$\{\, f \in \mathcal{D}(H_0) \,:\, f(q_1) = \cdots = f(q_n) = 0 \,\}\,,$$

which obviously makes sense as long as $\dim X_0 \leq 3$. In a similar way we use the symbol S_j, $j = 1, \ldots, n\,,$ for the restriction of H_j to the set $\{f \in \mathcal{D}(H_j) :\, f(0) = 0\}$. The Schrödinger operators we consider are *by definition* self-adjoint extensions of the symmetric operator $S = S_0 \oplus S_1 \oplus \cdots \oplus S_n$; their construction is a standard matter discussed in numerous papers starting with [EŠ1]. The most efficient way to describe them is based on a bijective correspondence with the Lagrangian planes in $\mathcal{G} \times \mathcal{G}$, where $\mathcal{G} = \mathbb{C}^{2n}$. To describe it, we introduce the boundary-value operators

$$\Gamma^1,\, \Gamma^2 :\; \mathcal{D}(S^*) \to \mathcal{G}\,,$$

by

$$\begin{aligned} \Gamma^1(f) &:= (a(f_0, q_1), \ldots, a(f_0, q_n), -f_1'(0), \ldots, -f_n'(0))\,, \\ \Gamma^2(f) &:= (b(f_0, q_1), \ldots, b(f_0, q_n), f_1(0), \ldots, f_n(0))\,. \end{aligned} \tag{2.1}$$

Here $a(f_0, q_j) =: a_j(f_0)$ and $b(f_0, q_j) =: b_j(f_0)$ are the leading-term coefficients of the asymptotics of f_0 in the vicinity of the point q_j as determined in [BG1, BG2], or the generalized boundary values $2\pi(\dim X_0 - 1)L_0$ and L_1, respectively, in the terminology of [EŠ1, EŠ2].

Let Λ be a Lagrangian plane in $\mathcal{G} \times \mathcal{G}$, i.e. $\Lambda^{\perp} = \Lambda$ with respect to the skew-Hermitean product $[x|y] := \langle x_1|y_2\rangle - \langle x_2|y_1\rangle$ in $\mathcal{G} \times \mathcal{G}$. Then any restriction of the adjoint operator S^* to a family of functions from $\mathcal{D}(S^*)$ specified by the boundary condition $(\Gamma^1 f, \Gamma^2 f) \in \Lambda$ is a self-adjoint operator which we denote H^Λ. Recall that a Lagrangian plane is, in general, the graph of a self-adjoint operator $L : \mathcal{G} \to \mathcal{G}$ so that the above boundary condition can be rewritten as $\Gamma^2 f = L(\Gamma^1 f)$. To avoid problems with the invertibility of L one can view Λ also as the graph of a "multivalued" operator in $\mathcal{G}$, in other words, one may describe it through a relation $Lx = My$, $(x, y) \in \mathcal{G} \times \mathcal{G}$, where $L, M : \mathcal{G} \to \mathcal{G}$ are linear operators satisfying the conditions [KS]:

(i) $LM^* = ML^*$,
(ii) $\mathrm{rank}(L, -M) = n$.

2.2 The resolvent

We are concerned with spectral properties of the said self-adjoint extensions, which are as usual defined from the resolvent. The latter is expressed here by Krein's formula [AGH, App. A]: If we denote by H^0 the decoupled operator $H_0 \oplus H_1 \oplus \cdots H_n$, then we have

$$(H^\Lambda - z)^{-1} = (H^0 - z)^{-1} - \gamma(z)[Q(z) - \Lambda]^{-1}\gamma^*(z) \tag{2.2}$$

for any z in the resolvent set, in particular for $z \notin \mathbb{C} \setminus \mathbb{R}$, where the operator $\gamma(z) : \mathcal{G} \to \mathcal{H}$ is given by the formula

$$\gamma(z) := \left(\Gamma^1 \restriction \mathcal{N}_z\right)^{-1}, \quad \mathcal{N}_z = \mathrm{Ker}\,(S^* - z)\,,$$

and $Q(z) : \mathcal{G} \to \mathcal{G}$ is defined as

$$Q(z) := \Gamma^2 \gamma(z)\,.$$

Then the inverse $[Q(z) - \Lambda]^{-1}$ exists for all non-real z. To find an explicit expression for the Green function of the operator H^Λ from (2.2) we need to know the Green function G_0 of H^0.

Notice first that it is easy to find the Green function G_j of H_j: one has

$$G_j(x, x'; z) = \frac{\cosh\left[-\sqrt{-z}(d_j - |x - x'|)\right] + \cosh\left[-\sqrt{-z}(d_j - (x + x')\right]}{2\sqrt{-z}\,\sinh\left[-\sqrt{-z}d_j\right]}\,. \tag{2.3}$$

Using the natural decomposition $\mathcal{G} = \mathbb{C}^{2n} = \mathbb{C}^n \times \mathbb{C}^n$ we write the matrix representation of the operator $[Q(z) - \Lambda]^{-1}$ in block form,

$$[Q(z) - \Lambda]^{-1} = \begin{bmatrix} T(z) & W(z) \\ U(z) & V(z) \end{bmatrix} . \tag{2.4}$$

Since $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots \mathcal{H}_n$, the Green function of the operator H^Λ can be represented as a matrix of integral kernels of operators acting from $\mathcal{H}_k$ to $\mathcal{H}_j$,

$$G^\Lambda(x, x'; z) = \left(G^\Lambda_{jk}(x_j, x'_k; z)\right)_{0 \le j,k \le n} \quad \text{with} \quad x_j \in X_j,\ x'_k \in X_k . \tag{2.5}$$

Let $(\xi_1, \ldots, \xi_n, \eta_1, \ldots, \eta_n) \in \mathcal{G} = \mathbb{C}^n \times \mathbb{C}^n$, then a direct calculation yields

$$\begin{aligned} &\gamma(z)(\xi_1, \ldots, \xi_n, \eta_1, \ldots, \eta_n) \\ &\quad = \left(\sum_{j=1}^n G_0(\cdot, q_j; z)\xi_j,\ G_1(\cdot, 0; z)\eta_1, \ldots, G_n(\cdot, 0; z)\eta_n \right) . \end{aligned}$$

This implies the adjoint operator action,

$$\gamma^*(\bar z)(f_0, f_1, \ldots, f_n) = (\xi_1, \ldots, \xi_n, \eta_1, \ldots, \eta_n) ,$$

where

$$\xi_j = \int_{X_0} G_0(q_j, x; z) f_0(x)\, |g(x)|^{1/2}\, \mathrm{d}x , \quad \eta_j = \int_{X_j} G_j(0, x; z) f_j(x)\, \mathrm{d}x .$$

The matrix $Q(z)$ then has block-diagonal form

$$Q(z) = \begin{bmatrix} Q^{11}(z) & 0 \\ 0 & Q^{22}(z) \end{bmatrix} ,$$

here $Q^{11}(z)$ coincides with the Q-matrix Q_0 for the pair (S_0, H_0). Recall that the Q-function in the Krein formula always corresponds to a pair of a self-adjoint operators and fixed symmetric restriction. In the present case it has the form

$$Q_0^{jk}(z) = G_0^{\mathrm{ren}}(q_j, q_k; z) , \tag{2.6}$$

where G_0^{ren} is the renormalized Green's function obtained from G_0 by subtracting the diagonal singularity,

$$G_0^{\mathrm{ren}}(x_0, x'_0; z) = \begin{cases} G_0(x_0, x'_0; z) , & \text{if } x_0 \ne x'_0; \\ \displaystyle\lim_{y_0 \to x_0} \left[G_0(x_0, y_0; z) + \frac{1}{2\pi} \ln \rho(x_0, y_0) \right] , & \text{if } x_0 = x'_0. \end{cases}$$

Here $\rho(x_0, y_0)$ denotes the geodesic distance on X_0. On the other hand, the matrix $Q^{22}(z)$ is diagonal,

$$Q^{22}_{jk}(z) = \delta_{jk} G_j(0, 0; z) \, .$$

Using the above formulae we can write the matrix element kernels in (2.5) more explicitly,

$$G_{jk}(x_j, x'_k; z) = \delta_{jk} G_j(x_j, x'_j; z) - K_{jk}(x_j, x'_k; z) \, ,$$

where

$$\begin{aligned}
K_{00}(x_0, x'_0; z) &= \sum_{j,k=1}^{n} t_{jk}(z) G_0(x_0, q_j; z) G_0(q_k, x'_0; z) \, , \\
K_{0k}(x_0, x'_k; z) &= G_k(0, x'_k; z) \sum_{j=1}^{n} w_{jk}(z) G_0(x_0, q_j; z) \, , \quad k > 0 \, , \\
K_{j0}(x_j, x'_0; z) &= G_j(x_j, 0, ; z) \sum_{k=1}^{n} u_{jk}(z) G_0(q_k, x'_0; z) \, , \quad j > 0 \, , \\
K_{jk}(x_j, x'_k; z) &= v_{jk}(z) G_j(x_j, 0, ; z) G_k(0, x'_k; z) \, , \quad j, k > 0 \, ;
\end{aligned}$$

the coefficients refering to the block representation (2.4), $(t_{jk}(z)) = T(z)$, etc., can be in principle computed explicitly.

2.3 Coupling hedgehog manifolds

In the next step we are going to glue together the building blocks considered so far. To begin with, we consider such a manifold $\hat{X}$ and select some number of finite segments of lengths $d_1, \dots, d_s$, $1 \le s \le n$. At the same time, we fix a finite number of distinct points $p_1, \dots, p_m \in X_0$ such that $\{p_1, \dots, p_n\} \cap \{q_1, \dots, q_n\} = \emptyset$. We fix a Hamiltonian H^Λ on $\hat{X}$ and consider its restriction $\tilde{S}$ to the set of functions

$$\left\{ f \in \mathcal{D}(H^\Lambda) \, : \, f(p_1) = \dots = f(p_m) = f(d_1) = \dots = f(d_s) = 0 \right\} .$$

Let us find the $\mathcal{Q}$-matrix of the pair $(\tilde{S}, H^\Lambda)$ which is a $(m+s) \times (m+s)$ matrix $\tilde{Q}(z)$ with block structure,

$$\tilde{Q}(z) = \begin{bmatrix} \tilde{Q}^{11}(z) & \tilde{Q}^{12}(z) \\ \tilde{Q}^{21}(z) & \tilde{Q}^{22}(z) \end{bmatrix} .$$

Using the formula for the Green function of H^Λ we can write the elements of the above matrix as

$$\begin{aligned}
\tilde{Q}^{11}_{jk}(z) &= \delta_{jk} G_0^{\mathrm{ren}}(p_j,p_j;z) + (1-\delta_{jk}) G_0(p_j,p_k;z) \\
&\quad - K_{00}(p_j,p_k;z)\,, \qquad 1 \le j,k \le m\,, \\
\tilde{Q}^{12}_{jk}(z) &= -K_{0k}(p_j,d_k;z)\,, \qquad 1 \le j \le m\,,\ 1 \le k \le s\,, \\
\tilde{Q}^{21}_{jk}(z) &= -K_{j0}(d_j,p_k;z)\,, \qquad 1 \le j \le s\,,\ 1 \le k \le m\,, \\
\tilde{Q}^{22}_{jk}(z) &= \delta_{jk} G_j(d_j,d_j;z) - K_{jk}(d_j,d_k;z)\,, \quad 1 \le j,k \le s\,.
\end{aligned} \tag{2.7}$$

Recall that G_0^{ren} denotes the renormalized Green's function; we drop of course the superscript whenever the two arguments are different.

The coupling will be realized through conditions relating the generalized boundary values. We will not strive for at most generality, however, because formulae encompassing manifolds with arbitrary n, m would be rather cumbersome. We will instead discuss in some detail properties of a quantum particle living on chained manifolds of different dimensions, i.e. the case $m = n = 1$; later on we will extend the argument to a particular situation with $m = n = 2$.

Consider, therefore, a manifold X_0 on which a pair of mutually different points p, q is selected. At q, a segment of a length d is attached, while p is a "socket" to which another "tailed" manifold can be coupled. In analogy with (2.6) we introduce the matrix

$$Q_0(z) = \begin{bmatrix} G_0^{\mathrm{ren}}(q,q;z) & G_0(p,q;z) \\ G_0(q,p;z) & G_0^{\mathrm{ren}}(p,p;z) \end{bmatrix}, \tag{2.8}$$

and similarly, the segment will be characterized by

$$Q_1(z) = \begin{bmatrix} G_1(0,0;z) & G_1(0,d;z) \\ G_1(d,0;z) & G_1(d,d;z) \end{bmatrix}. \tag{2.9}$$

Using (2.3) we find

$$Q_1^{jk}(z) = \frac{\delta_{jk}}{\sqrt{-z}} \coth\left(\sqrt{-z}d\right) + \frac{1-\delta_{jk}}{\sqrt{-z}\sinh\left(\sqrt{-z}d\right)}\,,$$

or

$$Q_1^{jk}(z) = \frac{\delta_{jk}}{k}\cot(kd) + \frac{1-\delta_{jk}}{k\sin(kd)} \tag{2.10}$$

in the usual momentum notation, $k := i\sqrt{-z}$ for $z \in \mathbb{C} \setminus \mathbb{R}_+$.

The operator H^Λ on $\hat{X}$ is specified by the boundary conditions at the point q identified with the left endpoint of the segment, $0 \in [0, d)$. In general, these conditions can be given in the form,

$$\begin{aligned} b(f_0, q) &= \alpha f_1'(0) + \beta a(f_0, q) , \\ f_1(0) &= \gamma f_1'(0) - \bar{\alpha} a(f_0, q) , \end{aligned} \tag{2.11}$$

with β, $\gamma \in \mathbb{R}$ and $\alpha \in \mathbb{C}$; we suppose $\alpha \neq 0$ such that the manifold X_0 and the segment are coupled in a nontrivial way. For the sake of simplicity we will restrict ourselves to the case where $\beta = \gamma = 0$, i.e.

$$b(f_0, q) = \alpha f_1'(0) , \quad f_1(0) = -\bar{\alpha} a(f_0, q) . \tag{2.12}$$

This can be regarded as a "minimal" coupling between the two configuration-space components, because in the "switched-off state", $\alpha = 0$, the manifold Hamiltonian contains no point interaction at the point q and the segment part satisfies the Dirichlet condition at $x_1 = 0$. Notice, however, that there are other natural choices such as

$$\alpha = \sqrt{\frac{2\rho}{\pi}} , \quad \beta = -\pi(1 + \ln\sqrt{\rho}) , \quad \gamma = 2\rho ,$$

which describes the particle passing through the junction at a low energy if the segment models a thin tube of radius ρ – cf. [EŠ2].

The boundary condition (2.12) can be cast into the form given in Sec. 2.1 if we choose M as the 2×2 unit matrix and

$$L := \begin{bmatrix} 0 & \alpha \\ \bar{\alpha} & 0 \end{bmatrix} . \tag{2.13}$$

The Q-matrix entering Krein's formula for the operator H^Λ can be expressed in terms of the matrices (2.8) and (2.9) as

$$Q(z) = \begin{bmatrix} Q_0^{11} & 0 \\ 0 & Q_1^{11} \end{bmatrix} . \tag{2.14}$$

¿From (2.13) and (2.14) we find

$$[Q(z) - \Lambda]^{-1} = \frac{1}{Q_0^{11}(z) Q_1^{11}(z) - |\alpha|^2} \begin{bmatrix} Q_1^{11}(z) & -\alpha \\ -\bar{\alpha} & Q_0^{11}(z) \end{bmatrix} ,$$

and therefore

$$\begin{aligned}
G^{\Lambda}_{00}(x_0,x_0';z) &= G_0(x_0,x_0';z) - \frac{Q_1^{11}(z)}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\, G_0(x_0,q;z)G_0(q,x_0';z),\\
G^{\Lambda}_{01}(x_0,x_1';z) &= \frac{\alpha}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\, G_0(x_0,q;z)G_1(0,x_1';z)\,,\\
G^{\Lambda}_{10}(x_1,x_0';z) &= \frac{\bar{\alpha}}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\, G_1(x_1,0;z)G_0(q,x_0';z)\,,\\
G^{\Lambda}_{11}(x_1,x_1';z) &= G_1(x_1,x_1';z) - \frac{Q_0^{11}(z)}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\, G_1(x_1,0;z)G_1(0,x_1';z)\,.
\end{aligned}$$

Thus we can calculate the matrix elements (2.7) (the indices j,k are trivial in the present example and we will drop them):

$$\begin{aligned}
\tilde{Q}^{11}(z) &= \tilde{Q}_0^{22}(z) - \frac{Q_1^{11}(z)Q_0^{12}(z)Q_0^{21}(z)}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\,,\\
\tilde{Q}^{12}(z) &= \frac{\alpha Q_1^{12}(z)Q_0^{21}(z)}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\,,\\
\tilde{Q}^{21}(z) &= \frac{\bar{\alpha} Q_0^{12}(z)Q_1^{21}(z)}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\,,\\
\tilde{Q}^{22}(z) &= \tilde{Q}_1^{22}(z) - \frac{Q_0^{11}(z)Q_1^{12}(z)Q_1^{21}(z)}{Q_0^{11}(z)Q_1^{11}(z)-|\alpha|^2}\,.
\end{aligned} \tag{2.15}$$

These formulae can be made even more explicit by plugging in (2.10).

2.4 Point-coupled manifolds

In the same way one can treat the limiting situation when the lengths of the connecting segment shrink to zero. Then only the boundary conditions have be modified. Consider the simplest case when X_0 and X_1 are coupled by identifying the points $p_j \in X_j,\ j = 0,1$. The generalized boundary values (2.1) are then replaced by

$$\begin{aligned}
\Gamma^1(f_0,f_1) &:= (a(f_0,p_0), a(f_1,p_1))\ ,\\
\Gamma^2(f_0,f_1) &:= (b(f_0,p_0), b(f_1,p_1))\ .
\end{aligned}$$

Such a coupling was first discussed in [EŠ3] in the situation where X_0 and X_1 are two planes. The four-parameter set of all possible self-adjoint extensions was described there and the result adapts easily to more general manifolds. For the sake of simplicity, however, we will again restrict our attention to the "minimal" coupling given by the conditions

$$b(f_0, p_0) = \alpha a(f_1, p_1)\,, \quad b(f_1, p_1) = \bar{\alpha} a(f_0, p_0) \tag{2.16}$$

with a complex parameter α, decoupled manifolds corresponding to $\alpha = 0$.

3 Infinite necklaces

3.1 General periodic case

As an illustration of how to couple "hedgehog" manifolds, we are now going to analyze now the simplest nontrivial case i.e. when the building blocks discussed above are chained into an infinite "necklace". To define the Hamiltonian we have to specify the boundary conditions coupling the outer endpoint of the segment of the first building block, starting at q, to the point p of the second one. The boundary-value operators $\tilde{\Gamma}^1$ and $\tilde{\Gamma}^2$ for the operator $\tilde{S}$ are of the form

$$\begin{aligned} \Gamma^1(f_0, f_1) &:= (a(f_0, p), f_1'(d))\,, \\ \Gamma^2(f_0, f_1) &:= (b(f_0, p), f_1(d))\,. \end{aligned}$$

Notice the positive sign of $f_1'(d)$ in comparison with (2.1) which reflects the orientation of the segment $[0, d]$.

Consider now a countable family of identical copies of the manifold $\hat{X}$, i.e. $\hat{X}_M = \hat{X}$ for all $m \in \mathbb{Z}$ and set $\hat{Z} := \bigcup_{m\in\mathbb{Z}} \hat{X}_m$. The state Hilbert space of this necklace is

$$L^2(\hat{Z}) = \bigoplus_{m=-\infty}^{\infty} L^2(\hat{X}_m)\,.$$

Schrödinger operators on the necklace will be identified with self-adjoint extensions of the symmetric operator $\hat{S} := \bigoplus_{m\in\mathbb{Z}} \tilde{S}_m$, where $\tilde{S}_m := \tilde{S}$ for any $m \in \mathbb{Z}$. Obviously, the boundary-value space of $\hat{S}$ is of the form

$$\hat{\mathcal{G}} = \bigoplus_{m=-\infty}^{\infty} \tilde{\mathcal{G}}_m \qquad \text{with} \quad \tilde{\mathcal{G}}_m = \mathbb{C}^2 \quad \text{forall} \quad m$$

and

$$\hat{\Gamma}^j = \bigoplus_{m=-\infty}^{\infty} \tilde{\Gamma}^j_m \qquad \text{with} \quad \tilde{\Gamma}^j_m = \tilde{\Gamma}^j \quad \text{forall} \quad m \quad \text{and} \quad j = 1, 2\,.$$

Of course, the operator $\hat{S}$ has infinite deficiency indices, and therefore plenty of self-adjoint extensions. We restrict our attention to those which are local in the sense that exactly the point d of $\hat{X}_m$ is coupled with the point p of $\hat{X}_{m+1}$. Moreover, we will consider the situation when the coupling d to p and q to 0 is *minimal* in the sense described above. Consequently, for an element $g = \{g_m\} \in \hat{\mathcal{G}}$ with $g_m = (f_{0,m}, f_{1,m})$ we impose boundary conditions analogous to (2.12):

$$b(f_{0,m}, p) = \alpha f'_{1,m-1}(0)\,, \quad f_{1,m}(0) = -\bar{\alpha} a(f_{0,m+1}, p)\,;$$

this can be written concisely as

$$\hat{\Gamma}^2 g = L \hat{\Gamma}^1 g\,, \tag{3.1}$$

where L is an operator in $\hat{\mathcal{G}}$ given by a matrix $L = (L_{mn})_{m,n\in\mathbb{Z}}$, where $L_{mn} = 0$ if $|m-n| \neq 1$ and

$$L_{m,m+1} = \begin{bmatrix} 0 & \alpha \\ 0 & 0 \end{bmatrix}, \quad L_{m+1,m} = \begin{bmatrix} 0 & 0 \\ \bar{\alpha} & 0 \end{bmatrix}.$$

We then infer that the self-adjoint operator H^L specified by the boundary conditions (3.1) has the following resolvent

$$(\hat{H}^L - z)^{-1} = (\hat{H}^0 - z)^{-1} - \hat{\gamma}(z)[\hat{Q}(z) - L]^{-1} \hat{\gamma}^*(z)\,,$$

where $\hat{Q}(z) = \{\delta_{mn} \tilde{Q}(z)\}$. In this way, the dispersion relation for $\hat{H}^L$ can be obtained by introducing the quasimomentum $\theta \in [0, 2\pi)$ and performing the Fourier transformation of the operator $\hat{Q}(z) - L$. Thus result is an operator in the space $L^2((0, 2\pi)) \otimes \mathcal{G}$ with kernel

$$P(\theta, z) := \sum_{m=-\infty}^{\infty} \left(\hat{Q}_{m0}(z) - L_{m0} \right) \mathrm{e}^{im\theta} = \tilde{Q}(z) - \begin{bmatrix} 0 & \alpha\, \mathrm{e}^{i\theta} \\ \bar{\alpha}\, \mathrm{e}^{-i\theta} & 0 \end{bmatrix}.$$

The dispersion relation is of the form $\det P(\theta, z) = 0$, or

$$\det \begin{vmatrix} \tilde{Q}_{11}(z) & \tilde{Q}_{12}(z) - \alpha\, \mathrm{e}^{i\theta} \\ \tilde{Q}_{21}(z) - \bar{\alpha}\, \mathrm{e}^{-i\theta} & \tilde{Q}_{22}(z) \end{vmatrix} = 0\,,$$

which is equivalent to

$$\det \tilde{Q}(z) - \left(\tilde{Q}_{12}(z)\bar{\alpha}\, \mathrm{e}^{-i\theta} + \tilde{Q}_{21}(z)\alpha\, \mathrm{e}^{i\theta}\right) - |\alpha|^2 = 0\,. \tag{3.2}$$

As in similar situations, we have isospectrality with respect to the coupling-constant phase: put $\varphi = \arg\alpha$, i.e. $\alpha = |\alpha|\mathrm{e}^{i\varphi}$, then the last condition can be written as

$$\det \tilde{Q}(z) - |\alpha| \left(\tilde{Q}_{12}(z)\, \mathrm{e}^{-i(\theta+\varphi)} + \tilde{Q}_{21}(z)\, \mathrm{e}^{i(\theta+\varphi)}\right) - |\alpha|^2 = 0\,,$$

which shows that without loss of generality we may restrict ourselves to the case $\alpha \geq 0$; this we shall assume in the following. Using the fact that $\tilde{Q}_{21}^*(z) = \tilde{Q}_{12}(z)$ holds for real z, the condition (3.2) can be rewritten as

$$\det \tilde{Q}(z) - |\alpha|^2 = 2\alpha \left(\operatorname{Re} \tilde{Q}_{12}(z) \cos\theta + \operatorname{Im} \tilde{Q}_{12}(z) \sin\theta\right)\,. \tag{3.3}$$

Hence a necessary condition for $z \in \operatorname{spec}(\hat{H})$ is

$$\frac{|\det \tilde{Q}(z) - |\alpha|^2|}{2\alpha|\tilde{Q}_{12}(z)|} \leq 1\,. \tag{3.4}$$

If $\tilde{Q}_{12}(z) = \tilde{Q}_{21}(z)$, which is true in particular if H^0 is a real operator (i.e. commutes with the complex conjugation), the relation (3.3) simplifies to

$$\cos\theta = \frac{\det \tilde{Q}(z) - |\alpha|^2}{2\alpha \tilde{Q}_{12}(z)}\,, \tag{3.5}$$

and the condition (3.4) becomes necessary and sufficient. If H^0 is real, the condition (3.5) can be made more explicit: using (2.15) and the fact that $Q_j^{11} = Q_j^{22}$ holds for $j = 1, 2$, we find after a short computation

$$\cos\theta = \frac{\det Q_0(z) \det Q_1(z) - 2\alpha^2 Q_0^{11}(z) Q_1^{11}(z) + \alpha^4}{2\alpha^2 Q_0^{12}(z) Q_1^{12}(z)}\,.$$

Furthermore, using (2.10) we get

$$\cos\theta = \frac{\det Q_0(k^2) \sin(kd) - 2\alpha^2 k\, \cos(kd)\, Q_0^{11}(k^2) - \alpha^4 k^2 \sin(kd)}{2\alpha^2 k\, Q_0^{12}(k^2)}\,. \tag{3.6}$$

3.2 Spherical beads

Since our aim is to present solvable examples, we study next the situation when the elementary building-block manifold X_0 is a two-dimensional sphere $\mathbb{S}^2$ of a fixed radius $a > 0$. We parametrize it by spherical coordinates,

$$\begin{aligned} x &= a \cos\vartheta \cos\varphi\,, \\ y &= a \cos\vartheta \sin\varphi\,, \\ z &= a \sin\vartheta\,, \end{aligned}$$

with $\vartheta \in [-\pi/2, \pi/2]$, $\varphi \in [0, 2\pi)$. We will assume that there are no external fields, so the starting operator for construction of the Hamiltonian is the Laplace-Beltrami operator Δ_{LB} on $\mathbb{S}^2$. Its Green's function is an integral operator with the kernel

$$G_0(x, y; z) = -\frac{1}{4\cos(\pi t)}\,\mathcal{P}_{-\frac{1}{2}+t}\left(-\cos\left(\frac{\rho(x,y)}{a}\right)\right)\,, \tag{3.7}$$

where $\mathcal{P}_\lambda$ is the Legendre function, $\rho(x, y)$ is the geodetic distance on the sphere, and

$$t \equiv t(z) := \frac{1}{2}\sqrt{1 + 4a^2 z}\,.$$

This allows us to express the renormalized Green's function, i.e. we find

$$Q_0^{jj}(z) = -\frac{1}{2\pi}\left[\psi\left(\frac{1}{2} + t\right) - \frac{\pi}{2}\tan(\pi t) - \ln 2a + C_E\right]\,, \tag{3.8}$$

(see e.g. [BE, Tab. 3.9.2]), where C_E is Euler's number and ψ the digamma function. We use again the conventional notation $z = k^2$ for the energy parameter; if there is no danger of misunderstanding we will often supposes the dependence of various quantities on k.

3.3 Loose necklaces

We shall next consider two particular segment-connected periodic chains:

Example I: Suppose that the connecting segments are attached at antipodal points as sketched in Fig. 1 so that the geodesic distance of the junctions is πa. We will denote the segment connecting the spheres $\mathbb{S}^2_n$ and $\mathbb{S}^2_{n+1}$ as I_n, with the endpoints $0^{(n)} \equiv p_1^{(n)} \in \mathbb{S}^2_n$ and $d^{(n)} \equiv p_3^{(n+1)} \in \mathbb{S}^2_{n+1}$. The lower-index numeration is somewhat arbitrary and serves just to having a common

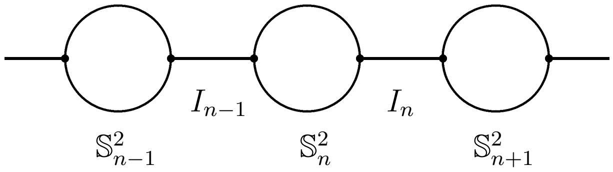

Figure 1: A loose straight necklace

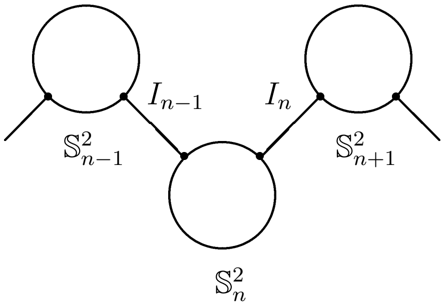

Figure 2: A loose zigzag necklace

notation for the present configuration and that considered below.

Example II: Alternatively, assume that the junction points are chosen on one pole and on the equator point, as sketched in Fig. 2, such that their geodesic distance is $\pi a/2$. The segment I_n now connects the points $0^{(n)} \equiv p_1^{(n)} \in \mathbb{S}^2_n$ and $d^{(n)} \equiv p_2^{(n+1)} \in \mathbb{S}^2_{n+1}$.

While the diagonal part (3.8) of the matrix Q_0 does not depend on the way we arrange the spheres, the off-diagonal parts differ and now become

$$Q_0^{i,i\pm 1} = -\frac{1}{8\sqrt{\pi}} \frac{\Gamma\left(\frac{1}{4}+\frac{t}{2}\right)}{\Gamma\left(\frac{3}{4}+\frac{t}{2}\right)} \frac{1}{\cos\pi\left(\frac{1}{4}+\frac{t}{2}\right)}\,, \tag{3.9}$$

$$Q_0^{i,i\pm 2} = Q_0^{21}(k^2) = -\frac{1}{4\cos(\pi t)}\,, \tag{3.10}$$

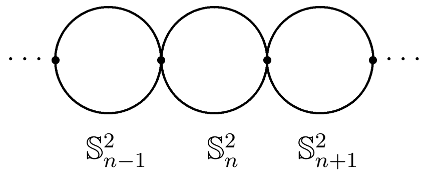

Figure 3: A tight straight necklace

for the zigzag and straight case, respectively, with the notation we have adopted. In the same way, the dispersion relation (3.6) becomes

$$Q_0^{11}Q_0^{11} - Q_0^{1j}Q_0^{1j} - 2\alpha^2 k\,\cot(kd)\,Q_0^{11} - 2\alpha^2 k\,\frac{Q_0^{1j}}{\sin(kd)}\,\cos\theta - \alpha^4 k^2 = 0 \quad (3.11)$$

with $j = 2, 3$ in Examples II and I, respectively. Let us remark that the condition with $j = 2$ is valid whenever all the Q_0^{12} are the same. Hence the spectrum does not change when we rotate an arbitrary semi-infinite part of the chain around the axis given by the appropriate connecting segment, such that, geometrically speaking, the zigzag chain need not be periodic.

3.4 Tight necklaces

In a similar way, one can treat periodic sphere chains which are connected through points where they touch (i.e. shrinking the line segments to zero), with the boundary conditions (3.1) replaced by (2.16) at each junction. We shall consider again two particular situations analogous to the periodic chains discussed above:

Example III: Suppose that the junctions are situated at antipodal points as sketched in Fig. 3, being obtained by identifying the points $p_1^{(n)} \in \mathbb{S}^2_n$ and $p_3^{(n+1)} \in \mathbb{S}^2_{n+1}$.

Example IV: The tight zigzag chain in Fig. 4 is obtained by identifying the points $p_1^{(n)} \in \mathbb{S}^2_n$ and $p_2^{(n+1)} \in \mathbb{S}^2_{n+1}$.

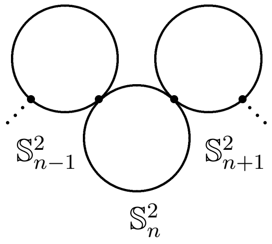

Figure 4: A tight zigzag necklace

The dispersion relation now reads

$$Q_0^{11}Q_0^{11} - Q_0^{1j}Q_0^{1j} - 2\alpha\, Q_0^{1j}\, \cos\theta + \alpha^2 = 0 \tag{3.12}$$

with $j = 2, 3$ corresponding to the Examples IV and III, respectively.

4 Square bead carpets

So far we have considered only "manifolds" with a linear structure. Having in mind essential differences between spectra of periodic Schrödinger operators in different dimensions to detect, it is useful to also to look systems which are periodic in more than one direction; we will do this again by first analyzing simple examples. This time we arrange our spherical "beads" into a square lattice, coupling them either by line segments or directly through touching points.

Example V: Suppose that the connecting segments are attached at four equally spaced points at the sphere equator as sketched in Fig. 5, where the labeling of the junctions and segments is indicated. With the notation introduced in Fig.5 the boundary conditions defining the Hamiltonian read

$$\begin{aligned}
b\left(f_0^{(n,m)}, p_1^{(n,m)}\right) &= -\alpha\left(f_1^{(n+\frac{1}{2},m)}\right)'\left(0^{(n+\frac{1}{2},m)}\right)\,, \\
f_1^{(n+\frac{1}{2},m)}\left(0^{(n+\frac{1}{2},m)}\right) &= \bar{\alpha}a\left(f_0^{(n,m)}, p_1^{(n,m)}\right)\,, \\
b\left(f_0^{(n,m)}, p_3^{(n,m)}\right) &= -\alpha\left(f_1^{(n-\frac{1}{2},m)}\right)'\left(d^{(n-\frac{1}{2},m)}\right)\,,
\end{aligned}$$

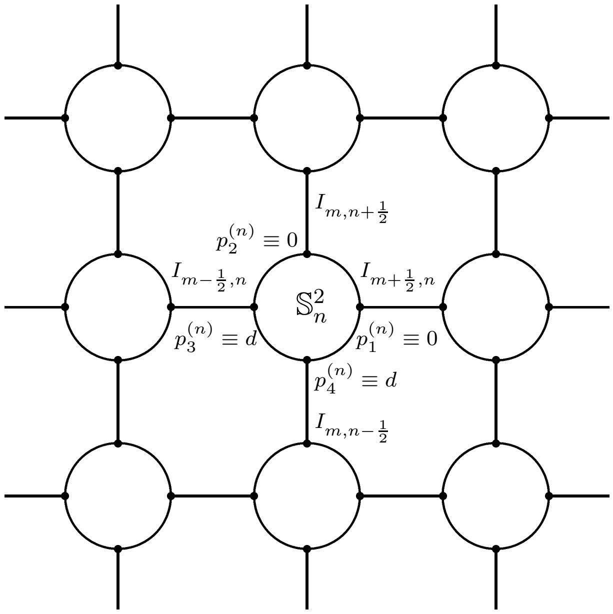

Figure 5: A loose square bead carpet

$$
\begin{aligned}
f_1^{(n-\frac{1}{2},m)}\left(d^{(n-\frac{1}{2},m)}\right) &= \bar{\alpha} a\left(f_0^{(n,m)}, p_3^{(n,m)}\right) , \\
b\left(f_0^{(n,m)}, p_2^{(n,m)}\right) &= -\alpha\left(f_1^{(n,m+\frac{1}{2})}\right)'\left(0^{(n,m+\frac{1}{2})}\right) , \\
f_1^{(n,m+\frac{1}{2})}\left(0^{(n,m+\frac{1}{2})}\right) &= \bar{\alpha} a\left(f_0^{(n,m)}, p_2^{(n,m)}\right) , \\
b\left(f_0^{(n,m)}, p_4^{(n,m)}\right) &= -\alpha\left(f_1^{(n,m-\frac{1}{2})}\right)'\left(0^{(n,m-\frac{1}{2})}\right) , \\
f_1^{(n,m-\frac{1}{2})}\left(0^{(n,m-\frac{1}{2})}\right) &= \bar{\alpha} a\left(f_0^{(n,m)}, p_4^{(n,m)}\right) .
\end{aligned}
$$

The dispersion relation is derived as in the previous section, but it becomes rather cumbersome. It is useful to introduce the following notation:

$$
\begin{aligned}
\Delta &:= \frac{1}{k^2}\left(Q_0^{12}Q_0^{12} - Q_0^{11}Q_0^{11}\right) + \frac{2\alpha^2}{k\sin(kd)}\left(Q_0^{11}\cos(kd) + Q_0^{12}\right) + \alpha^4 , \\
a_j &:= Q_0^{1,j+1}\Delta + \left(\frac{Q_0^{1,j+1}}{k^2} - (-1)^j\frac{\alpha^2}{k\sin(kd)}\right)\left(Q_0^{12}Q_0^{12} + Q_0^{13}Q_0^{13}\right) \\
&\quad + 2\, Q_0^{12}Q_0^{13}\left(\frac{Q_0^{1,2-j}}{k^2} + (-1)^j\frac{\alpha^2}{k\sin(kd)}\right) , \; j = 0, 1 , \\
b_0 &:= \frac{1}{k^2\sin^2(kd)}\left[\frac{Q_0^{11}Q_0^{11} - Q_0^{12}Q_0^{12}}{k\sin(kd)}\cos(kd) + \alpha^2 Q_0^{11}\right] - \frac{\Delta\cos(kd)}{k\sin(kd)} , \\
b_1 &:= \frac{1}{k^2\sin^2(kd)}\left[\frac{Q_0^{11}Q_0^{11} - Q_0^{12}Q_0^{12}}{k\sin(kd)} - \alpha^2 Q_0^{11}\right] , \\
c_j &:= \frac{\alpha}{k\sin(kd)}\left[\alpha^2 Q_0^{1,4-j} + \frac{Q_0^{1,4-j}Q_0^{11}\cos(kd)}{k\sin(kd)}\right.
\end{aligned}
$$

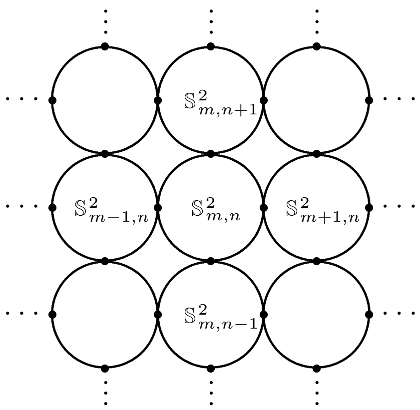

Figure 6: A tight square bead carpet

$$- \left.\frac{Q_0^{1,j+1}Q_0^{11} + Q_0^{1,4-j}Q_0^{12}\cos(kd)}{k\sin(kd)}\right] , \; j = 1, 2\,.$$

Using this notation, we can write the spectral condition as

$$\begin{aligned}
&(a_0^2 - a_1^2)(b_0^2 - b_1^2) + (c_1^2 - c_2^2)^2 - 2[(c_1 + c_2)^2(a_0b_0 + a_1b_1) \\
&\quad -2c_1c_2(a_0 + a_1)(b_0 + b_1)] \\
&\quad +2\alpha\Delta\left[(a_0b_0 + a_1b_1 - c_1^2)c_1 + a_0b_1 + a_1b_0 - c_1c_2)c_2\right](\cos\theta_1 + \cos\theta_2) \\
&\quad +2\alpha^2\Delta^2\left[(c_1^2 - c_2^2)\cos(\theta_1 + \theta_2) + (c_1^2 - a_1b_1)\cos(\theta_1 - \theta_2) + c_1^2 - a_0b_0\right] \\
&\quad -2\alpha^3\Delta^3c_1(\cos\theta_1 + \cos\theta_2) + \alpha^4\Delta^4 = 0\,. \qquad (4.1)
\end{aligned}$$

where θ_1, θ_2 are the quasimomentum components.

Example VI: This arises from Example V by shrinking the connecting segments to zero, as indicated in Fig. 6 where the labeling of the junctions is the same as in the previous example. After a straightforward calculation we find that the spectral condition now takes the form

$$\begin{aligned}
&(Q_0^{11}Q_0^{11} - Q_0^{13}Q_0^{13})^2 - 4Q_0^{12}Q_0^{12}(Q_0^{11} - Q_0^{13})^2 + 2\alpha[Q_0^{13}Q_0^{13}Q_0^{13} \\
&\quad -Q_0^{11}Q_0^{11}Q_0^{13} + 2Q_0^{11}Q_0^{12}Q_0^{12} - 2Q_0^{12}Q_0^{12}Q_0^{13}](\cos\theta_1 + \cos\theta_2) \\
&\quad +2\alpha^2\left[Q_0^{13}Q_0^{13} - Q_0^{11}Q_0^{11} + 2(Q_0^{13}Q_0^{13} - Q_0^{12}Q_0^{12})\right]\cos\theta_1\cos\theta_2 \\
&\quad -2\alpha^3Q_0^{13}(\cos\theta_1 + \cos\theta_2) + \alpha^4 = 0\,. \qquad (4.2)
\end{aligned}$$

5 Gap dominance at large energies

As customary in periodic systems the spectrum of the above described operators (which we denote by $H_{\mathrm{I}}, \dots, H_{\mathrm{VI}}$ according to the example number) has band structure. To see how the gap width and the band width are related at high energies, consider first the points

$$k'_n := \frac{\pi n}{d}\,, \quad k''_n := \frac{\sqrt{n(n+1)}}{a}\,, \quad n = 1, 2, \dots\,, \tag{5.1}$$

for which $\sin(dk'_n) = \cos(dk'_n) = \cos\pi\left(\frac{1}{4} + \frac{1}{2}t(k''_{2n})\right) = 0$, such that the functions Q_0^{ij} and Q_1^{ij} have poles. Thus it is natural to look for spectral bands in the vicinity of these points. We fix $\epsilon > 0$ and denote by $J'_n = [k'_n - \delta'_n, k'_n + \delta'_n]$ the maximal closed neighbourhood of the point k'_n in which the inequality

$$|\sin(kd)| \le k^{-\epsilon}$$

is satisfied; in the same way the intervals $J''_n = [k''_n - \delta''_n, k''_n + \tilde{\delta}''_n]$ and $J'''_n = [k''_{2n} - \delta'''_n, k'_{2n} + \tilde{\delta}'''_n]$ correspond to the inequalities

$$|\cos(kd)| \le k^{-\epsilon} \quad \text{and} \quad \left|\cos\pi\left(\frac{1}{4} + \frac{t}{2}\right)\right| \le k^{-\epsilon}\,, \tag{5.2}$$

respectively. It is clear that all the $\delta'_n, \dots, \tilde{\delta}'''_n$ are strictly positive, and it is not difficult to check that

$$\delta'_n \sim d^{-1}(k'_n)^{-\epsilon}\,, \quad \delta''_n, \tilde{\delta}''_n \sim 2(\pi a)^{-1}(k'_n)^{-\epsilon}\,, \quad \delta'''_n, \tilde{\delta}'''_n \sim 4(\pi a)^{-1}(k'_{2n})^{-\epsilon}$$

as $n \to \infty$. Our aim is to show that for a sufficiently high energy the spectral gaps contain the complement of the above intervals. More specifically, define

$$\Omega_K := [K, \infty) \setminus \bigcup_{n=1}^{\infty} (J'_n \cup J''_n \cup J'''_n)$$

for a fixed $K > 0$.In this set, we have $(\sin(kd))^{-1} = \mathcal{O}(k^{\epsilon})$ as $k \to \infty$, and similarly

$$Q_0^{11} = \mathcal{O}(k^{\epsilon})\,, \quad Q_0^{12} = \mathcal{O}(k^{\epsilon-1})\,, \quad Q_0^{13} = \mathcal{O}(k^{\epsilon})\,,$$

where the first relation was derived using the asymptotic relation

$$\frac{\Gamma\left(\frac{1}{4} + \frac{t}{2}\right)}{\Gamma\left(\frac{3}{4} + \frac{t}{2}\right)} = \frac{2}{t}\left(1 + \mathcal{O}(t^{-2})\right)\,,$$

which follows from the Stirling formula. These relations show that the left-hand-side of (3.11) behaves in Ω_K as

$$-\alpha^4 k^2 + \mathcal{O}(k^{1+2\epsilon})$$

for $k \to \infty$, and therefore it diverges uniformly in θ as long as $0 < \epsilon < \frac{1}{2}$. Consequently, there is $K > 0$ such that

$$\mathrm{spec} H_{\mathrm{I}} \cap \Omega_K = \mathrm{spec} H_{\mathrm{I}} \cap \Omega_K = \emptyset\,.$$

Let us pass to the relation (4.1). Notice first that $\Delta \to \alpha^4$ as $k \to \infty$ in Ω_K. Furthermore, for $0 < \epsilon < \frac{1}{2}$ we have

$$a_0 = \mathcal{O}(k^{\epsilon})\,,\; a_1 = \mathcal{O}(k^{2\epsilon-1})\,,\; b_j = \mathcal{O}(k^{\epsilon-1})\,,\; c_1 = \mathcal{O}(k^{2\epsilon-1})\,,\; c_2 = \mathcal{O}(k^{4\epsilon-1})\,.$$

Consequently for $\epsilon < \frac{1}{4}$, the left-hand side of the spectral condition tends to $\alpha^8 \neq 0$, which implies

$$\mathrm{spec}(H_{\mathrm{V}}) \cap \Omega_K = \emptyset$$

for K large enough.

The tight necklaces and carpets exhibit a different behaviour. Now we replace the intervals J''_n, J'''_n defined by (5.2) by $\hat{J}''_n = [k''_n - \eta''_n, k''_n - \tilde{\eta}''_n]$ and $\hat{J}'''_n = [k''_{2n} - \eta'''_n, k_{2n} - \tilde{\eta}'''_n]$ given in a similar way by

$$|\cos(kd)| \le (\ln k)^{-\epsilon} \quad \text{and} \quad \left|\cos\pi\left(\frac{1}{4} + \frac{t}{2}\right)\right| \le (\ln k)^{-\epsilon}\,. \tag{5.3}$$

It is straightforward to check that

$$\eta''_n, \tilde{\eta}''_n \sim 2(\pi a)^{-1}(\ln k'_n)^{-\epsilon}\,, \quad \eta'''_n, \tilde{\eta}'''_n \sim 4(\pi a)^{-1}(\ln k'_{2n})^{-\epsilon}\,.$$

Consider the set $\hat{\Omega}_K := [K, \infty) \setminus \bigcup_{n=1}^{\infty}(\hat{J}''_n \cup \hat{J}'''_n)$ with a fixed $K > 1$. If $k \to \infty$ in this set, the following estimates hold:

$$Q_0^{11} = A\, \ln k + \mathcal{O}((\ln k)^{\epsilon})\,, \quad Q_0^{12} = \mathcal{O}(k^{-1}(\ln k)^{\epsilon})\,, \quad Q_0^{13} = \mathcal{O}((\ln k)^{\epsilon})\,,$$

with $A \neq 0$. These relations show that the left-hand side of (3.12) diverges for $\epsilon < 1$ like $(\ln k)^2$, uniformly in θ as $k \to \infty$ within $\hat{\Omega}_K$. By the same token, the left-hand side of (4.2) diverges for $\epsilon < 1$ like $(\ln k)^4$, uniformly in θ_1, θ_2. We infer that there is a $K > 1$ such that

$$\mathrm{spec} H_{\mathrm{III}} \cap \hat{\Omega}_K = \mathrm{spec} H_{\mathrm{IV}} \cap \hat{\Omega}_K = \mathrm{spec} H_{\mathrm{VI}} \cap \hat{\Omega}_K = \emptyset\,.$$

Now it is easy to estimate the band and gap widths. The points $E'_n = (k'_n)^2$ and $E''_n = (k''_n)^2$ around which the bands concentrate are asymptotically like $c'n^2$ and $c''n^2$, respectively, by (5.1). The widths of the excluded intervals behave, in the case of a loose connection, as

$$|J'_n|\,,\ |J'_n|\,,\ |J'_n| \sim \text{const}\, n^{1-\epsilon}\,.$$

Hence the total length B_n of the bands contained in the union of the intervals J'_n, J''_n, and J'''_n is of order $B_n \lesssim \text{const}\, n^{1-\epsilon}$, and the total length L_n of the adjacent gaps is $L_n \gtrsim \text{const}\,(n - n^{1-\epsilon}) \approx \text{const}\, n$. In the case of a tight connection the band length is estimated instead by $B_n \lesssim \text{const}\, n(\ln n)^{-\epsilon}$ which still gives gap length increasing linearly with n. We sum up our discussion with the following result:

Proposition 5.1 *For loosely connected necklaces and carpets the band-to-gap ratio satisfies the bound*

$$\frac{B_n}{L_n} \lesssim \text{const}\, n^{-\epsilon}$$

as $n \to \infty$, *with a positive* $\epsilon < \frac{1}{2}$ *in Examples I and II, and* $\epsilon < \frac{1}{4}$ *in Example V. On the other hand, for the tightly connected necklaces and carpets in Examples III, IV, and VI, we have*

$$\frac{B_n}{L_n} \lesssim \text{const}\,(\ln n)^{-\epsilon}$$

as $n \to \infty$, *with any positive* $\epsilon < 1$.

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