Point interactions in a tube

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Abstract. We discuss discuss spectral and scattering properties of a particle confined to a straight Dirichlet tube in $\mathbb{R}^3$ with a family of point interactions.

Point interactions belong to the list of problems to which Sergio Albeverio made a significant contribution. This topic combines a practical importance as a source of numerous solvable models with an aesthetic appeal as the monograph [**1**] witnesses. At the same time it is far to be closed; despite the extensive and thorough character of the mentioned treatise new questions still arise.

One of them concerns point interactions in tubular regions which represent a natural model for a "quantum wire" with impurities. The simplest situation when the tube is a straight planar strip was investigated in [**4**]; we refer to this paper for a detailed motivation and bibliography. In the present paper we present a brief discussion of a straight tube in $\mathbb{R}^3$ with a family of point interactions.

1. The one-center case

Let $\Omega := \mathbb{R}\times M$ where $M\subset\mathbb{R}^2$ is a closed compact set; we suppose that it is pathwise connected and ∂M has the segment property [**5**]. The free Hamiltonian is the corresponding Dirichlet Laplacian, $H_0=-\Delta_D^\Omega$ with the domain $W_0^{2,2}(\Omega)$. It can be expressed by means of the one-dimensional Laplacian and $-\Delta_D^M$. The last named operator has a purely discrete spectrum; we denote by χ_n, ν_n its eigenfuctions and eigenvalues, respectively. For any $z\in\mathbb{C}\setminus[\nu_0,\infty)$ the free resolvent is an integral operator with the kernel

$$(1.1)\quad G_0(\vec x_1,\vec x_2;z)\,\equiv\,(H_0-z)^{-1}(\vec x_1,\vec x_2)\,=\,\frac{i}{2}\sum_{n=0}^{\infty}\frac{e^{ik_n(z)|x_1-x_2|}}{k_n(z)}\,\chi_n(\vec y_1)\chi_n(\vec y_2)\,,$$

where $\vec x_j=(x_j,\vec y_j)$ and $k_n(z):=\sqrt{z-\nu_n}$, which is defined and smooth except at $\vec x_1=\vec x_2$. It is a multivalued function of z with cuts $[\nu_n,\infty)$, $n=0,1,\dots$.

Suppose now that a point interaction is situated at $\vec a=(a,\vec b)\in M^o$. We define it as in [**1**], i.e. as a self-adjoint extension of the operator $-\Delta_D^\Omega\upharpoonright C_0^\infty(\Omega\setminus\{\vec a\})$. We employ generalized boundary values

$$(1.2)\qquad L_0(\psi,\vec a)\,:=\,\lim_{\vec x\to\vec a}\psi(\vec x)|\vec x-\vec a|\,,\qquad L_1(\psi,\vec a)\,:=\,\lim_{\vec x\to\vec a}\left[\psi(\vec x)-\frac{L_0(\psi,\vec a)}{|\vec x-\vec a|}\right]\,;$$

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then the extension in question is specified by the boundary condition

$$L_1(\psi,\vec a) + 4\pi\alpha L_0(\psi,\vec a) \,=\, 0 \tag{1.3}$$

for a given $\alpha\in\mathbb{R}$. We shall denote it $H(\alpha,\vec a)$; the case $\alpha=\infty$, i.e. $L_0(\psi,\vec a)=0$, corresponds to the free Hamiltonian H_0.

The resolvent of $H(\alpha,\vec a)$ is obtained by Krein's formula. Mimicking the argument of [**4**] we get

$$(H(\alpha,\vec a)-z)^{-1}(\vec x_1,\vec x_2) \,=\, G_0(\vec x_1,\vec x_2;z) + \frac{G_0(\vec x_1,\vec a;z)G_0(\vec a,\vec x_2;z)}{\alpha-\xi(\vec a;z)}\,, \tag{1.4}$$

where $\xi(\vec a;z)$ is the regularized Green's function at $\vec a$,

$$\xi(\vec a;z) \,=\, \lim_{u\to 0}\left[\frac{i}{2}\sum_{n=0}^{\infty}\frac{e^{ik_n u}}{k_n}|\chi_n(\vec b)|^2 - \frac{1}{4\pi u}\right]. \tag{1.5}$$

The existence of the limit follows from the kernel behaviour at the singularity [**7**]. However, we also need a prescription how to compute it and this differs from the two-dimensional case. We use semiclassical properties of the above series terms [**5**]. The transverse eigenvalues behave as $\nu_n\approx 4\pi|M|^{-1}n$ for $n\to\infty$ so $k_n = 2i\sqrt{\pi}|M|^{-1/2}\sqrt{n}+\mathcal{O}(1)$. On the other hand, the probability densities $|\chi_n|^2$ are rapidly oscillating functions. Since M supports no potential the mean value of these oscillations equals the constant $|M|^{-1}$; assuming that $|\chi_n(\vec b)|^2$ oscillates around this value as $n\to\infty$ we can assess the divergence rate of the first series. Next we use the identity

$$\frac{1}{4\pi u} \,=\, \beta\int_0^\infty \frac{e^{-\gamma u\sqrt{s}}}{\sqrt{s}}\,ds$$

with $\gamma := 2\sqrt{\pi}|M|^{-1/2}$ and $\beta^{-1} := 4\sqrt{\pi|M|}$ and write the r.h.s. as a sum of the integrals over $(n,n+1)$ obtaining

$$\xi(\vec a;z) \,=\, \lim_{u\to 0}\left[\sum_{n=0}^{\infty}\frac{e^{-\kappa_n u}}{2\kappa_n}|\chi_n(\vec b)|^2 + \frac{e^{-\gamma u\sqrt{n+1}}-e^{-\gamma u\sqrt{n}}}{4\pi u}\right],$$

where $\kappa_n(z) := -ik_n(z) = \sqrt{\nu_n - z}$. In combination with the preceding argument, it is easy to check that the summand has a uniform bound of order $o(n^{-3/2})$. Hence the limit can be interchanged with the sum and

$$\xi(\vec a;z) \,=\, \sum_{n=0}^{\infty}\left[\frac{|\chi_n(\vec b)|^2}{2\kappa_n(z)} + \frac{\sqrt{n}-\sqrt{n+1}}{2\sqrt{\pi|M|}}\right]. \tag{1.6}$$

REMARKS 1.1. (i) We do not give here details of the oscillation argument. Notice that the conclusions made below can be obtained even without it, up to an additive renormalization of the coupling constant, since by the Weyl formula and the uniform boundedness of the χ_n's the difference $\xi(\vec a;z)-\xi(\vec a;z_0)$ is given by a convergent series.
(ii) The scaling behaviour for $\Omega^\sigma = \mathbb{R}\times M^\sigma$ with $M^\sigma := \sigma M$, $\sigma>0$ is more complicated than in the two-dimensional case. We have $\xi(\vec{a^\sigma};z\sigma^{-2}) = \sigma^{-1}\xi(\vec a;z)$, so the singularities of the resolvent kernel are related by

$$\epsilon^\sigma(\alpha^\sigma,\vec{a^\sigma}) \,=\, \sigma^{-2}\epsilon(\alpha,\vec a)\,, \quad \alpha^\sigma := \sigma^{-1}\alpha\,. \tag{1.7}$$

PROPOSITION 1.2. *The operator $H(\alpha,\vec{a})$ has for any $\alpha\in\mathbb{R}$ a single eigenvalue $\epsilon(\alpha,\vec{a})\in(-\infty,\nu_0)$. The corresponding eigenfunction is*

$$\psi(\vec{x};\alpha,\vec{a}) \;=\; \sum_{n=0}^{\infty}\frac{e^{-\kappa_n(\epsilon)|x-a|}}{2\kappa_n(\epsilon)}\chi_n(\vec{y})\chi_n(\vec{b})\,. \tag{1.8}$$

The function $\epsilon(\cdot,\vec{a})$ is strictly increasing and behaves as

$$\epsilon(\alpha,\vec{a}) \;=\; \nu_0-\left(\frac{|\chi_0(\vec{b})|^2}{2\alpha}\right)^2+\mathcal{O}(\alpha^{-3})\,, \tag{1.9}$$

in the limit of weak coupling, $\alpha\to+\infty$. Moreover, there are no eigenvalues embedded in $\sigma_c(H(\alpha,\vec{a}))=[\nu_0,\infty)$.

PROOF: Due to (1.6), $\xi(\vec{a};\cdot)$ is strictly increasing with $\mathrm{Ran}\,\xi=\mathbb{R}$ and $\xi(\vec{a};z)=\frac{1}{2}|\chi_0(\vec{b})|^2(\nu_0-z)^{-1/2}+\mathcal{O}(1)$ as $z\to\nu_0-$. The non-normalized eigenfunction (1.8) is given by the residue term in (1.4). To check the absence of embedded eigenvalues we have to show that $\xi(\vec{a};z)=\alpha$ has no solutions on $[\nu_0,\infty)$. Away of the thresholds, this follows from

$$\mathrm{Im}\,\xi(\vec{a};z) \;=\; \sum_{\{n:\,\nu_n<z\}}\frac{|\chi_n(\vec{b})|^2}{2\sqrt{\nu_n-z}}>0\,. \tag{1.10}$$

If $|\chi_n(\vec{b})|^2\neq 0$, the resolvent kernel has a finite limit as z approaches ν_n, otherwise it has the same singularity as $G_0(\vec{x}_1,\vec{a};\cdot)$ there, so in neither case it has a pole. ∎

Mimicking the argument of [**4**] we also get

PROPOSITION 1.3. *The on-shell S-matrix at energy $z=k^2$ is a $2N_{\mathrm{open}}\times 2N_{\mathrm{open}}$ unitary matrix with elementary blocks*

$$S_{nm} \;=\; \sqrt{\frac{k_m}{k_n}}\begin{pmatrix} t_{nm} & r_{nm}\\ \tilde{r}_{nm} & \tilde{t}_{nm}\end{pmatrix}\,,\qquad n,m=1,\dots,N_{\mathrm{open}}\,, \tag{1.11}$$

where $N_{\mathrm{open}}:=\mathrm{card}\{\nu_n:\ \nu_n<z\}$, the tilded quantities are obtained by switching sign of the longitudinal component of $\vec{a}$, $a\mapsto -a$, and

$$r_{nm}e^{-ik_m a} \;=\; (t_{nm}-\delta_{nm})e^{ik_m a} \;=\; \frac{i}{2k_m}\,\frac{e^{ik_n a}}{\alpha-\xi(\vec{a};z)}\,\chi_n(\vec{b})\chi_m(\vec{b})\,. \tag{1.12}$$

2. Finite number of perturbations

Denote $\vec{a}:=\{a_1,\dots a_N\}$, where $\vec{a}_j=(a_j,\vec{b}_j)$, and $\alpha:=\{\alpha_1,\dots,\alpha_N\}$, $j=1,\dots,N$. The Hamiltonian $(H(\alpha,\vec{a})$ with N point interactions is defined as the self-adjoint extension of the operator $-\Delta_D^M\restriction C_0^\infty(\Omega\setminus\{\vec{a}\})$ specified by the boundary conditions

$$L_1(\psi,\vec{a}_j)+4\pi\alpha_j L_0(\psi,\vec{a}_j) \;=\; 0\,,\quad j=1,\dots,N\,. \tag{2.1}$$

The resolvent is again found by means of the Krein formula:

(2.2)

$$(H(\alpha,\vec{a})-z)^{-1}(\vec{x}_1,\vec{x}_2) \;=\; G_0(\vec{x}_1,\vec{x}_2;z)+\sum_{j,k=1}^{N}\lambda_{jk}(\alpha,\vec{a};z)G_0(\vec{x}_1,\vec{a};z)G_0(\vec{a},\vec{x}_2;z)\,,$$

where $\lambda(\alpha,\vec{a};z)=\Lambda(\alpha,\vec{a};z)^{-1}$ with

$$\Lambda_{jj}=\alpha_j-\xi(\vec{a}_j;z)\,,\qquad \Lambda_{jk}=-G_0(\vec{a}_j,\vec{a}_k;z)\quad\text{for}\quad j\neq k\,, \tag{2.3}$$

where $\xi(\vec a_j;z)$ is given by (1.5), (1.6). With these prerequisites we can derive spectral properties of our point-interaction Hamiltonian.

THEOREM 2.1. *(a) The spectrum of $H(\alpha,\vec a)$ consists for any $\alpha\in\mathbb{R}^N$ of the absolutely continuous part $[\nu_0,\infty)$ and eigenvalues $\epsilon_1<\epsilon_2\le\cdots\le\epsilon_m<\nu_0$ with $1\le m\le N$, given by the condition*

$$\det\Lambda(\alpha,\vec a,z)\;=\;0\,. \tag{2.4}$$

The corresponding eigenfunctions are $\psi(\vec x)=\sum_{j=1}^N d_jG_0(\vec x,\vec a_j;z)$, where $d\in\mathbb{R}^N$ solves $\sum_{m=1}^N\Lambda(z)_{jm}d_m=0$. The ground-state eigenfunction is positive.
(b) $z>\nu_0$ cannot be an eigenvalue corresponding to an eigenvector from the subspace $\bigoplus_{\{n:\,\nu_n<z\}}L^2(\mathbb{R})\otimes\{\chi_n\}$. On the other hand, $H(\alpha,\vec a)$ can have embedded eigenvalues if the family $\{\Omega,\,\vec a,\,\alpha\}$ has a suitable symmetry.
(c) In the weak coupling limit, $|A|:=\min_{1\le j\le N}\alpha_j\to\infty$, there is a single eigenvalue which behaves as

$$\epsilon(\alpha,\vec a)\;=\;\nu_0-\left(\frac{\left(\sum_{j=1}^N\chi_0(\vec b_j)\right)^2}{2\sum_{j=1}^N\alpha_j\chi_0(\vec b_j)}\right)^2+\mathcal{O}\left(|A|^{-3}\right)\,. \tag{2.5}$$

PROOF: (a) A finite-rank perturbation in the resolvent preserves $\sigma_{ac}(H_0)=[\nu_0,\infty)$. The discrete spectrum is determined by poles of the resolvent coming from the coefficients λ_{jk} in (2.2). This yields (2.4); the eigenfunctions are obtained in the same way as in [**1, 4**]. The next question concerns the existence of solutions to (2.4). If $z\to-\infty$ the matrix can be written as $\xi(\vec a;z)\tilde\Lambda(\alpha,\vec a,z)$, where $\tilde\Lambda\to-I$, hence all eigenvalues of $\Lambda(\alpha,\vec a,z)$ tend to $+\infty$. On the other hand, for $z\to\nu_0-$ we have

$$\Lambda(\alpha,\vec a,z)\;=\;-\,\frac{1}{2\sqrt{\nu_0-z}}\,M_1\,+\mathcal{O}(1)\,,$$

where $M_1:=(\chi_0(\vec b_j)\chi_0(\vec b_m))_{j,m=1}^N$. This matrix has, in particular, an eigenvector $(\chi_0(\vec b_1),\dots,\chi_0(\vec b_N))$ corresponding to the *positive* eigenvalue $\sum_{j=1}^N\chi_0(\vec b_j)^2$, and therefore at least one of the eigenvalues of $\Lambda(\alpha,\vec a,z)$ tends to $-\infty$ as $z\to\nu_0-$. Using the continuity we see that there is an eigenvalue which crosses zero, i.e. $H(\alpha,\vec a)$ has at least one eigenvalue. By a straightforward differentiation we find

$$\frac{d}{dz}\,\Lambda(z)_{jm}\;=\;-\sum_{n=0}^\infty\frac{e^{-|a_j-a_m|\sqrt{\nu_n-z}}}{4(\nu_n-z)^{3/2}}\,\left(1+|a_j-a_m|\sqrt{\nu_n-z}\right)\,\chi_0(\vec b_j)\chi_0(\vec b_m)\,.$$

The matrix function $\Lambda(\cdot)$ is monotonous if for any $c\in\mathbb{C}^N$ the quantity $\frac{d}{dz}(c,\Lambda(z)c)$ has a definite sign (is non-positive in our case). This is true provided the function $f:\,f(x)=e^{-\kappa|x|}(1+\kappa|x|)$ is of positive type for any $\kappa>0$, which follows from the identity

$$(1+\kappa|x|)\,e^{-\kappa|x|}\;=\;\frac{2\kappa^3}{\pi}\int_{\mathbb{R}}\frac{e^{ipx}}{(p^2+\kappa^2)^2}\,dp$$

and Bochner's theorem [**5**, Sec.IX.2]. In fact, since the measure in the last integral is pointwise positive, $\frac{d}{dz}\,\Lambda(z)$ is even strictly positive; it means that all the eigenvalues of $\Lambda(\alpha,\vec a;z)$ are decreasing functions of z and $H(\alpha,\vec a)$ has at most N eigenvalues.

To check that the ground state is non-degenerate, we have to demonstrate that the lowest eigenvalue of $\Lambda(z)$ is simple for any $z\in(-\infty,\nu_0)$, which is equivalent to the claim that the matrix semigroup $\{\, e^{-t\Lambda(z)} \,:\, t \ge 0 \,\}$ is positivity preserving [**5**, Sec.XIII.12]. The last property is ensured if all the non-diagonal elements of $\Lambda(z)$ are negative; we have $\Lambda(z)_{jm} = -G_0(\vec a_j, \vec a_m; z)$ by (2.3) so the desired result follows from the positivity of the free-resolvent kernel. The coefficients may be therefore chosen of the same sign for the ground state; in fact, as strictly positive because $d_{j_0} = 0$ would mean that the eigenfunction is smooth at $\vec x = \vec a_{j_0}$ so the corresponding interaction is absent, $\alpha_{j_0} = \infty$.

(b) Suppose now that $H\varphi = z\varphi$ for some $z > \nu_0$. We adapt again the argument from [**1**, Sec.II.1] and pick an arbitrary $z' \in \rho(H)$; then there is a vector $\psi_0 \in D(H_0)$ which allows us to write

$$\varphi \,=\, \psi_0 + \sum_{j=1}^{N} d_j G_0(\cdot, \vec a_j; z')\,. \tag{2.6}$$

Furthermore, we expand ψ_0 as a series, $\psi_0(\vec x) = \sum_{n=0}^{\infty} g_n(x)\chi_n(\vec y)$ with the coefficients $g_n \in L^2(\mathbb{R})$. Using the identity $(H_0 - z)\psi_0 = (z - z')\sum_{j=1}^{N} d_j G_0(\cdot, \vec a_j; z')$ and the fact that $\{\chi_n\}$ is an orthonormal basis in $L^2(M)$, we obtain a system of equations; by the Fourier-Plancherel operator it is transformed into

$$(p^2 - z + \nu_n)\hat g_n(p) \,=\, \frac{z - z'}{2\pi} \sum_{j=1}^{N} d_j \chi_n(\vec b_j)\, \frac{e^{-ipa_j}}{p^2 - z' + \nu_n}\,. \tag{2.7}$$

If $g_n \in L^2$ the same has to be true for $\hat g_n$; this is impossible if $z > \nu_n$ and the r.h.s. of (2.7) is nonzero at $\pm p_n$, where $p_n := \sqrt{\nu_n - z}$, since $\hat g_n^2$ would have then a non-integrable singularity. If $N > 1$, it might happen that the r.h.s. of (2.7) is not zero identically. However, if the a_j are mutually different, $\sum_{j=1}^{N} d_j \chi_n(\vec b_j)\, e^{\mp ipa_j} = 0$ implies $d_j = 0$ by linear independence. On the other hand, if some of them coincide we find $\sum_j d_j \chi_n(\vec b_j) = 0$ where the index runs through the values with the same longitudinal coordinate a_j, and therefore $\hat g_n = 0$ again.

The condition $\nu_n < z$ in the above argument is crucial; the operator $H(\alpha, \vec a)$ can have embedded eigenvalues with eigenfunctions in the orthogonal complement of the mentioned subspace if $N > 1$. Examples can be constructed as in [**4**] (or other similar systems – cf.[**3**]) using M with a symmetry: one has to choose a family of weak enough point interactions with the same symmetry.

(c) We denote $A := \mathrm{diag}(\alpha_1, \dots, \alpha_N)$, and use the decomposition

$$\Lambda(z) \,=\, \left(A - \tilde\Gamma(z)\right) \left[I - \left(A - \tilde\Gamma(z)\right)^{-1} \frac{M_1}{2\sqrt{\nu_0 - z}} \right],$$

where $\tilde\Gamma(z)$ is a remainder independent of α, whose norm is bounded as $z \to \nu_0-$, and M_1 is the matrix defined above. The first factor is regular for $|A|$ large enough. Since M_1 is rank one we have to solve the equation

$$\eta \sum_{j,k=1}^{N} \chi_0(\vec b_j)\alpha_j \left(I - \tilde\Gamma(z)A^{-1}\right)_{jk} \chi_0(\vec b_k) - \sum_{j=1}^{N} \chi_0(\vec b_j)^2 \,=\, 0$$

with $\eta := 2\sqrt{\nu_0 - z}$; then (2.5) follows by the implicit-function theorem. ∎

REMARKS 2.2. (i) We get also the weak-coupling asymptotics for the eigenfunction:

$$\psi(x;\alpha,\vec{a}) \;\approx\; \chi_0(\vec{y})\, \frac{2\sum_{j=1}^N \alpha_j \chi_0(\vec{b}_j)^2}{\left(\sum_{j=1}^N \chi_0(\vec{b}_j)^2\right)^2} \sum_{j=1}^N e^{-\sqrt{\nu_0-\epsilon}|x-a_j|}\chi_0(\vec{b}_j)^2$$

$$+ \sum_{n=1}^\infty \chi_n(\vec{b}_j) \sum_{j=1}^N \frac{e^{-\sqrt{\nu_n-\nu_0}|x-a_j|}}{\sqrt{\nu_n-\nu_0}}\, \chi_n(\vec{b}_j)\chi_0(\vec{b}_j)\,.$$

The leading term is a product of $\chi_1(\vec{y})$ with a linear combination of the eigenfunctions of one-dimensional point interactions placed at $a_j,\; j=1,\dots,N$.
(ii) The scattering problem can be treated as in the one-center case. Existence and completeness of wave operators follow from the Kato–Birman theory [**5**]. The reflection and transmission amplitudes from the n-th to the m-th channel are

$$r_{nm}(z) \;=\; \frac{i}{2} \sum_{j,k=1}^N (\Lambda(z)^{-1})_{jk} \frac{\chi_m(\vec{b}_j)\chi_n(\vec{b}_k)}{k_m(z)}\, e^{i(k_m a_j + k_n a_k)}\,,$$

$$t_{nm}(z) \;=\; \delta_{nm} + \frac{i}{2} \sum_{j,k=1}^N (\Lambda(z)^{-1})_{jk} \frac{\chi_m(\vec{b}_j)\chi_n(\vec{b}_k)}{k_m(z)}\, e^{-i(k_m a_j - k_n a_k)} \tag{2.8}$$

and the unitarity condition now reads

$$\sum_{\{m:\,0\le\nu_m<z\}} k_m(t_{nm}\bar{t}_{sm} + r_{nm}\bar{r}_{sm}) \;=\; \delta_{ns}k_n\,,$$

$$\sum_{\{m:\,0\le\nu_m<z\}} k_m\left(\tilde{t}_{nm}\bar{r}_{sm} + \tilde{r}_{nm}\bar{t}_{sm}\right) \;=\; 0\,, \tag{2.9}$$

because S_{nm} is given again by (1.11), where the tilded quantities are obtained by mirror transformation, $a_j \to -a_j$.

3. The periodic case

In the infinite-center case we restrict ourselves to the periodic situation, i.e. we suppose that the set $\{\alpha,\vec{a}\}_{per} = \{[\alpha_j,\vec{a}_j]:\; j=1,2,\dots\}$ in Ω is countably infinite and has a periodic pattern with a period $\ell>0$ and N perturbations in each cell, which we denote again as $\{\alpha,\vec{a}\}$. Following the Floquet-Bloch decomposition, we find the unitary operator $U:\, L^2(\Omega)\to L^2(\mathcal{B},(\ell/2\pi)d\theta; L^2(\hat{\Omega}))$, where

$$\hat{\Omega} \;:=\; [0,\ell)\times M\,, \qquad \mathcal{B} \;:=\; \left[-\frac{\pi}{\ell},\,\frac{\pi}{\ell}\right)\times M\;; \tag{3.1}$$

the x-projections of these sets are the Wigner-Seitz cell of the underlying one-dimensional lattice and the corresponding Brillouin zone, respectively. By means of U, the operator $H(\alpha,\vec{a})$ is unitarily equivalent to

$$U\,H(\{\alpha,\vec{a}\}_{per})\,U^{-1} \;=\; \frac{\ell}{2\pi}\int_{|\theta\ell|\le\pi}^{\oplus} H(\alpha,\vec{a};\theta)\,d\theta\,, \tag{3.2}$$

where $H(\alpha,\vec{a};\theta)$ is the point-interaction Hamiltonian on $L^2(\hat{\Omega})$, i.e. the Laplacian satisfying (2.1) at the points $\vec{a}_j$, Dirichlet b.c. for $x\in[0,\ell)$, $\vec{y}\in\partial M$, and

$$\psi(\ell-,\vec{y}) \;=\; e^{i\theta\ell}\psi(0+,\vec{y})\,, \qquad \frac{\partial\psi}{\partial x}(\ell-,\vec{y}) \;=\; e^{i\theta\ell}\,\frac{\partial\psi}{\partial x}(0+,\vec{y}) \tag{3.3}$$

for $\vec{y} \in M$. The resolvent of $H(\alpha,\vec{a};\theta)$ can be derived by modifying the argument of [**4**, Sec.5]. The "free" eigenvalues

$$\epsilon_{mn}(\theta) := \left(\frac{2\pi m}{\ell} + \theta\right)^2 + \nu_n\,, \quad m \in \mathcal{Z}\,,\; n = 0,2,\dots\,, \tag{3.4}$$

correspond to the eigenfunctions $\eta_m^\theta \otimes \chi_n$, where χ_n are as above and $\eta_m^\theta(x) := \ell^{-1/2}\, e^{i(2\pi m+\theta\ell)x/\ell}$, $m \in \mathcal{Z}$. Moreover, the free resolvent kernel is in analogy with [**4**] obtained by a partial summation of the appropriate double series and equals

$$\begin{aligned} G_0(\vec{x}_1,\vec{x}_2;\theta;z) \;&=\; \sum_{n=0}^{\infty} \frac{\sinh((\ell-|x_1-x_2|)\sqrt{\nu_n-z}) + e^{2i\eta\theta\ell}\sinh(|x_1-x_2|\sqrt{\nu_n-z})}{\cosh(\ell\sqrt{\nu_n-z}) - \cos(\theta\ell)} \\ &\quad \times \frac{\chi_n(\vec{y}_1)\chi_n(\vec{y}_2)}{2\sqrt{\nu_n-z}}\,, \end{aligned} \tag{3.5}$$

where $\eta := \mathrm{sgn}(x_1-x_2)$. The full kernel is then expressed by a formula analogous to (2.2) with

$$\lambda(\alpha,\vec{a},\theta;z) \;=\; \Lambda(\alpha,\vec{a},\theta;z)^{-1}\,, \tag{3.6}$$

where $\Lambda_{jr} = -G_0(\vec{a}_j,\vec{a}_r)$ for $j \ne r$, while the diagonal elements are given by

$$\Lambda_{jj} \;=\; \alpha_j \;-\; \frac{1}{2}\sum_{n=0}^{\infty}\left(\frac{\sinh(\ell\sqrt{\nu_n-z})}{\cosh(\ell\sqrt{\nu_n-z}) - \cos\theta\ell}\,\frac{\chi_n(\vec{y})^2}{\sqrt{\nu_n-z}} \;+\; \frac{\sqrt{n}-\sqrt{n+1}}{\sqrt{\pi|M|}}\right). \tag{3.7}$$

We may also write the last formula as $\Lambda_{jj}(\alpha,\vec{a},\theta;z) = \alpha_j - \xi(\vec{a}_j,\theta;z)$, where the function ξ is for $z \in \mathbb{R}$ more explicitly given by

$$\begin{aligned} \xi(\vec{a}_j,\theta;z) \;&=\; \frac{1}{2}\sum_{\{n:\,\nu_n\le z\}}\left(\frac{\sin(\ell\sqrt{z-\nu_n})}{\cos(\ell\sqrt{z-\nu_n}) - \cos\theta\ell}\,\frac{\chi_n(\vec{b}_j)^2}{\sqrt{z-\nu_n}} \;+\; \frac{\sqrt{n}-\sqrt{n+1}}{\sqrt{\pi|M|}}\right) \\ &\quad +\; \frac{1}{2}\sum_{\{n:\,\nu_n> z\}}\left(\frac{\sinh(\ell\sqrt{\nu_n-z})}{\cosh(\ell\sqrt{\nu_n-z}) - \cos\theta\ell}\,\frac{\chi_n(\vec{b}_j)^2}{\sqrt{\nu_n-z}} \;+\; \frac{\sqrt{n}-\sqrt{n+1}}{\sqrt{\pi|M|}}\right). \end{aligned} \tag{3.8}$$

It is defined everywhere except at

$$\mathcal{E}(\vec{a},\theta) \;:=\; \{\,\epsilon_{mn}(\theta) \in \mathcal{E}(\theta)\;:\;\chi_n(\vec{b}_j) \ne 0\,\}\,, \tag{3.9}$$

where $\mathcal{E}(\theta)$ is the eigenvalue set (3.4). Of course, the r.h.s. of (3.9) makes no sense if $z = \nu_n$ and $\chi_n(\vec{b}_j) \ne 0$, but applying general results on self-adjoint extensions to the one-center case, we can establish *a posteriori* that ξ can be defined there by continuity. Moreover, we find that the function $\xi(\vec{a}_j,\theta;\cdot)$ is monotonously increasing between any pair of neighboring singularities. Then we have the following result.

PROPOSITION 3.1. *For a given $\alpha \in \mathbb{R}^N$ the operator $H(\alpha,\vec{a};\theta)$ has N eigenvalues $\epsilon_{mnj}(\alpha,\vec{a};\theta)$, $j = 1,\dots,N$, in any gap of the set (3.9) determined by*

$$\det\Lambda(\alpha,\vec{a},\theta;z) \;=\; 0\,. \tag{3.10}$$

The corresponding eigenfunctions are $\psi(\vec{x}) = \sum_{j=1}^N d_j G_0(\vec{x},\vec{a}_j,\theta;z)$ where the d_j's are determined by $\Lambda(\alpha,\vec{a},\theta;z)$ as in Theorem 2.1.

The spectrum of the original Hamiltonian $H(\{\alpha,\vec{a}\}_{per})$ consist then of bands,

$$\sigma\left(H(\{\alpha,\vec{a}\}_{per})\right) \;=\; \bigcup_{mnj}\,\{\,\epsilon_{mnj}(\alpha,\vec{a};\theta)\,:\,\theta \in \mathcal{B}\,\}\,. \tag{3.11}$$

One is interested, of course, in its absolute continuity and existence of gaps. We restrict ourselves to the simplest nontrivial situation.

EXAMPLE 3.2. Let $N=1$, i.e. let each cell contain a single point interaction. The condition (3.10) then simplifies to

$$\xi(\vec{a},\theta;z)\,=\,\alpha\,. \tag{3.12}$$

The left hand side is monotonously increasing between its singularities, i.e. the points of $\mathcal{E}(\vec{a},\theta)$. This means that for fixed α, θ there is a sequence $\{\epsilon_r(\alpha,\vec{a},\theta)\}_{r=0}^{\infty}$ arranged in the ascending order; each of them depends, in fact, only on the transverse component $\vec{b}$ of the vector $\vec{a}$. The lowest one satisfies

$$\epsilon_0(\alpha,\vec{a},\theta)\,<\,\nu_0+\theta^2$$

and between each two neighboring points of $\mathcal{E}(\vec{a},\theta)$ there is just one of the other eigenvalues. It is also clear that any of $\epsilon_r(\alpha,\vec{a},\theta)$ is continuous with respect to the parameters and $\epsilon_r(\cdot,\vec{a},\theta)$ is increasing for fixed $\vec{b}$ and θ. Concerning the θ-dependence, the implicit-function theorem tells us that

$$\frac{\partial\epsilon_r(\alpha,\vec{a},\theta)}{\partial\theta}\,=\,-\,\frac{\partial\xi(\vec{a},\theta;z)}{\partial\theta}\left(\frac{\partial\xi(\vec{a},\theta;z)}{\partial z}\right)^{-1}\Bigg|_{(\epsilon_r,\theta)}$$

whenever the denominator is nonzero. Away of the thresholds, $z=\nu_n$, and the points of $\mathcal{E}(\theta)$, a straightforward differentiation shows that $\xi(\vec{a},\cdot;\cdot)$ is analytic in both variables. By (3.8) the numerator is not identically zero; hence the derivative $\partial\epsilon_r(\alpha,\vec{a},\theta)/\partial\theta$ may be zero at some points but never in an interval and *the spectrum of $H(\{\alpha,\vec{a}\}_{per})$ is absolutely continuous* [**5**, Sec.XIII.16].

Let us turn now to the question about the number of gaps. Below $z=\nu_0$ the spectrum may be estimated by means of extrema of the function ξ which yield θ-independent bounds: we have $\xi(\vec{a},\theta;z)\le\xi_+(\vec{a},z)$ where

$$\xi_+(\vec{a},z):=\max_{|\theta\ell|\le\pi}\xi(\vec{a},\theta;z)\,=\,\frac{1}{2}\sum_{n=0}^{\infty}\left(\frac{\chi_0(\vec{b})^2}{\sqrt{\nu_n-z}}\,\coth\left(\frac{\ell}{2}\sqrt{\nu_n-z}\right)\,+\,\frac{\sqrt{n}-\sqrt{n+1}}{\sqrt{\pi|M|}}\right)$$

and a similar formula for the minimum, $\xi_-(\vec{a},z)$, with coth replaced by tanh. Both functions are continuously increasing and tend to $-\infty$ as $z\to-\infty$. On the other hand, $\xi_+(\vec{a},\cdot)$ diverges as $z\to\nu_0-$ while the lower bound $\xi_-(\vec{a},\cdot)$ has a finite limit. This shows, in particular, that the spectral condition (3.12) has no solution for any θ in a left neighborhood of ν_0 provided

$$\begin{aligned}\alpha\,&<\,\xi_-(\vec{a},\nu_0-)\,=\,\frac{\ell}{4}\chi_0(\vec{b})^2-\frac{1}{2\sqrt{\pi|M|}}\\ &+\,\frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{\chi_0(\vec{b})^2}{\sqrt{\nu_n-\nu_0}}\,\tanh\left(\frac{\ell}{2}\sqrt{\nu_n-\nu_0}\right)\,+\,\frac{\sqrt{n}-\sqrt{n+1}}{\sqrt{\pi|M|}}\right)\,;\end{aligned} \tag{3.13}$$

in other words, that a gap exists. The condition (3.13) is satisfied for a strong enough coupling if the point-interaction spacing is kept fixed. On the other hand, inspecting the right-hand-side we see that the gap exists also for any fixed α and the spacing ℓ large enough. In this respect the spectrum is similar to that of a straight polymer in $\mathbb{R}^3$ described in [**1**, Sec.III.1]. However, for our "coated polymer" a much stronger result is valid: we shall show that under a suitable choice of parameters it can have *any finite number* of gaps.

To this end, we consider $z \in (\nu_0+\varepsilon, \nu_1-\varepsilon)$ for a fixed $\varepsilon > 0$ and $\ell \gg \sqrt{|M|}$, and rewrite the right hand side of the relation (3.8) as

$$\xi(\vec{a},\theta;z) \,=\, \xi_0(\vec{a},\theta;z) + \eta(\vec{a},\theta;z)\,,$$

where

$$\xi_0(\vec{a},\theta;z) \,:=\, \frac{\sin(\ell\sqrt{z-\nu_0})}{\cos(\ell\sqrt{z-\nu_0}) - \cos\theta\ell}\, \frac{\chi_0(\vec{b})^2}{2\sqrt{z-\nu_0}}$$

and $\eta(\vec{a},\theta;z)$ is the rest. The latter is monotonously increasing with respect to z and its derivative is bounded everywhere below the second threshold, in particular, in the chosen interval of energies. Moreover, $\eta(\vec{a},\theta;z)$ is bounded from above by

$$\eta_+(\vec{a},z) \,:=\, -\frac{1}{2\sqrt{\pi|M|}} + \frac{1}{2}\sum_{n=1}^{\infty} \left(\frac{\chi_0(\vec{b})^2}{\sqrt{\nu_n-z}} \coth\left(\frac{\ell}{2}\sqrt{\nu_n-z}\right) + \frac{\sqrt{n}-\sqrt{n+1}}{\sqrt{\pi|M|}} \right)$$

and the corresponding minimum, $\eta_-(\vec{a},z)$, is obtained when coth in the last expression is replaced by tanh. These estimates shrink as ℓ becomes large: using the inequality $\coth u - \tanh u < 5\,e^{-2u}$ for $2u \ge 1$, we find

$$\eta_+(\vec{a},z) - \eta_-(\vec{a},z) \,<\, \frac{5}{2}\,\frac{\chi_1(\vec{b})^2}{\sqrt{\nu_1-z}}\, e^{-\ell\sqrt{\nu_1-z}} + \frac{5}{2}\sum_{n=2}^{\infty} \frac{\chi_n(\vec{b})^2}{\sqrt{\nu_n-z}}\, e^{-\ell\sqrt{\nu_n-z}}\,.$$

The series can be estimated by an integral, which yields for a fixed $z \in (\nu_0+\varepsilon, \nu_1-\varepsilon)$ the behavior

$$\eta_+(\vec{a},z) - \eta_-(\vec{a},z) \,=\, \mathcal{O}\left(\sqrt{|M|}\,\ell^{-1}\right)\,. \tag{3.14}$$

On the other hand, the function $g_\theta(u) := \sin u(\cos u - \cos\theta\ell)^{-1}$ is increasing between any two zeros of its denominator. In the intervals, where it is positive, it can be estimated from below by the appropriate branch of $\tan\left(\frac{u}{2}+\pi m\right)$; when it is negative, we have a similar estimate from above with tan replaced by $-\cot$. Hence independently of θ we have either

$$\xi_0(\vec{a},\theta;z) \,\ge\, \frac{\chi_n(\vec{b})^2}{2\sqrt{z-\nu_0}}\, \tan\left(\frac{\pi}{2}\left\{\frac{\ell}{\pi}\sqrt{z-\nu_0}\right\}\right)$$

or

$$\xi_0(\vec{a},\theta;z) \,\le\, -\frac{\chi_n(\vec{b})^2}{2\sqrt{z-\nu_0}}\, \cot\left(\frac{\pi}{2}\left\{\frac{\ell}{\pi}\sqrt{z-\nu_0}\right\}\right)\,,$$

where $\{\cdot\}$ denotes the fractional part. Putting the estimates together we see that the oscillating part dominates, so for sufficiently large $|\alpha|$ there are gaps having $\nu_0 + \left(\frac{\pi m}{\ell}\right)^2$ as one endpoint provided it belongs to $(\nu_0+\varepsilon, \nu_1-\varepsilon)$. In addition, $\tan u + \cot u \ge 2$ which means that the gap between the lower and the upper bound to $\xi(\vec{a},\theta;z)$ never closes within the chosen interval if $\ell/\sqrt{|M|}$ is large enough; we infer that *for any* $\alpha \in \mathbb{R}$ the operator $H(\{\alpha,\vec{a}\}_{per})$ can have *an arbitrary finite number of gaps* in its spectrum provided the spacing of the point-interaction array is large enough.

Conclusions of the example can be extended to a finite number of point perturbations per cell. In a similar way one can treat a toroidal tube supporting point interactions and threaded by a magnetic flux, etc.

A more difficult question concerns the finiteness of the number of open gaps. Recall that the gap number depends strongly on the dimension of a periodic system: for one-dimensional systems it is generically infinite [**5**, Sec.XIII.16], [**1**, Sec.III.2], while for higher dimensions it is finite by the *Bethe-Sommerfeld conjecture*. The latter is known to be true, in particular, for periodic potentials or lattices of point interactions in $\mathbb{R}^3$ – see [**2, 6**]. The tube boundary makes things more complicated, but one still expects that at high energies gaps will close due to overlapping of contributions from different transverse modes. Notice in this connection that in the example we have been looking for gaps in the energy interval where transport is possible in the lowest transverse mode only. Nevertheless, it is not easy to demonstrate that no gaps remain open above a certain energy.

In a similar way, the "mixed dimensionality" of waveguide systems inspires other questions such as existence of a mobility edge in tubes with random point interactions, etc. Generally speaking, solvable models whose genealogy can be traced back to the treatise [**1**] will represent for long a useful laboratory for the spectral theory.

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