A Dirichlet-to-Neumann map approach to resonance gaps and bands of periodic networks

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Abstract

The spectral structure of the ordinary periodic Schrödinger operator is usually found by analyzing the corresponding transfer matrix. In that approach the exponentials with quasi-momentum in the argument appear as eigenvalues of the transfer matrix for quasi-periodic solutions of the homogeneous Schrödinger equation, and the corresponding Weyl functions appear as coordinates of the associated eigenvectors. That approach, though effective for tight-binding analysis of one-dimensional periodic Schrödinger operators, is inconvenient for spectral analysis on realistic periodic quantum networks with multi-dimensional period, particularly where several leads are attached to each vertex. Further, the transfer-matrix approach cannot be extended to the partial Schrödinger equation. In this paper we propose an alternative approach using the Dirichlet-to-Neumann map is rather than the transfer matrix, and show that this new approach easily generalizes to the case of networks with multi-dimensional period. We apply this approach to realistic quantum networks, obtaining conditions for the existence of resonance gaps or bands.

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1 Introduction: transfer matrix and DN map

The classical approach to Floquet-Bloch (FB) solutions of the periodic Schrödinger operator is based on the transfer matrix constructed in terms of the standard solutions as follows. Consider the Schrödinger equation

$$L(u) \equiv -u'' + q(x)u = \lambda u, \tag{1}$$

with a real, measurable, and essentially bounded periodic potential $q(x) = q(x+1)$. Standard solutions θ, φ, satisfy the initial conditions

$$\begin{aligned}\theta(0,\lambda) = 1, \quad \theta'(0,\lambda) = 0,\\ \varphi(0,\lambda) = 0, \quad \varphi'(0,\lambda) = 1.\end{aligned}$$

Then, the transfer matrix for Cauchy data over one period, $T(\lambda, 1)$, defined by

$$\begin{pmatrix} u(1,\lambda) \\ u'(1,\lambda) \end{pmatrix} = T(\lambda,1) \begin{pmatrix} u(0,\lambda) \\ u'(0,\lambda) \end{pmatrix}, \tag{2}$$

is represented as

$$T(\lambda,1) = \begin{pmatrix} \theta(1,\lambda) & \varphi(1,\lambda) \\ \theta'(1,\lambda) & \varphi'(1,\lambda) \end{pmatrix}.$$

The eigenvalues of T are

$$\Theta_{\pm} = s \pm \sqrt{s^2 - 1}$$

where $s(\lambda) = (\theta(1,\lambda) + \varphi'(1,\lambda))/2$ is defined by the trace of the transfer matrix $T(\lambda, 1)$. Note that we have used the Wronskian property $W(\theta, \varphi) = 1$ as determined by Abel's formula. Hence, the spectrum of the periodic Schrödinger operator in (1) is absolutely-continuous and defined by the condition $-1 \leq s(\lambda) \leq 1$. The eigenvalues written as *quasi-momenta exponentials* $\Theta_{\pm} = \exp\{\pm ip(\lambda)\}$ define the quasi-momentum p, $\Im p \geq 0$. The corresponding eigenvectors $(1,\, m_{\pm})$ define the FB-solutions $\chi_{\pm}(x,\lambda) = \theta(x,\lambda) + m_{\pm}\varphi(x,\lambda)$, which are square-integrable on the right and left semi x-axis, $\mathbb{R}_{\pm}$, respectively, i.e., $\chi_{\pm} \in L_2(\mathbb{R}_{\pm})$ for $\Im p > 0$ (see e.g. [1]).

One can use also the Dirichlet-to-Neumann (DN) map $\Lambda(\lambda)$ for one period, instead of the transfer matrix. In this simple case the DN map is defined as the map from the pair of boundary values $(u(0,\lambda), u(1,\lambda))^{\mathrm{T}}$, of any solution u of (1), to the outward derivatives $(-u'(0,\lambda), u'(1,\lambda))^{\mathrm{T}}$ on the boundary $\{0,\, 1\}$ of the period, i.e.,

$$\Lambda(\lambda) \begin{pmatrix} u(0,\lambda) \\ u(1,\lambda) \end{pmatrix} = \begin{pmatrix} -u'(0,\lambda) \\ u'(1,\lambda) \end{pmatrix}. \tag{3}$$

(For more general definitions see [2, 3, 4].)

The DN map can be written in terms of the standard solutions (of the Cauchy problem) by solving the linear system obtained from substituting the transfer matrix relation (2) into (3), giving the formula

$$\Lambda(\lambda) = \begin{pmatrix} \dfrac{\theta(1,\lambda)}{\varphi(1,\lambda)} & -\dfrac{1}{\varphi(1,\lambda)} \\ -\dfrac{1}{\varphi(1,\lambda)} & \dfrac{\varphi'(1,\lambda)}{\varphi(1,\lambda)} \end{pmatrix}. \tag{4}$$

One can see that the DN map is represented by a symmetric matrix function that is real on the real λ-axis, and has simple poles at the eigenvalues of the Dirichlet problem on one period. Other properties of the DN map may be easily derived from (4) and the general properties of the standard solutions θ and φ.

Analogs of the standard solutions, and hence generalizations of (4), do not exist in multi-dimensional geometries, or even on branching graphs. Nevertheless, in these more general cases the DN map can be conveniently calculated in terms of canonical solutions of the associated boundary-value problem on one period. In the remaining part of this section we demonstrate that approach by deriving some spectral results for the one-dimensional periodic Schrödinger operator, without recourse to the standard solutions or the transfer matrix.

In the one-dimensional case one can introduce a pair of solutions $\varphi_0 (= \varphi)$ and φ_1 of equation (1) which satisfy the initial conditions, at distinct boundary points,

$$\begin{aligned} \varphi_0(0,\lambda) = 0, \quad \varphi_0'(0,\lambda) = 1, \\ \varphi_1(1,\lambda) = 0, \quad \varphi_1'(1,\lambda) = 1. \end{aligned}$$

The DN map can be represented in terms of these solutions as

$$\Lambda(\lambda) = \begin{pmatrix} -\dfrac{\varphi_1'(0,\lambda)}{\varphi_1(0,\lambda)} & -\dfrac{1}{\varphi_0(1,\lambda)} \\ \dfrac{1}{\varphi_1(0,\lambda)} & \dfrac{\varphi_0'(1,\lambda)}{\varphi_0(1,\lambda)} \end{pmatrix}. \tag{5}$$

Symmetry of the matrix in (5) follows from reciprocity. It follows from general properties of the DN map that the matrix in (5) is a meromorphic function of the spectral parameter λ, has negative imaginary part in the upper half-plane $\Im\lambda > 0$, is real hermitian on the real λ-axis, and has simple poles at the eigenvalues λ_l of the operator L defined on $L_2(0,1)$ with zero boundary conditions on $\{0,\ 1\}$. Denote by Φ_l the associated real normalized eigenfunctions, and by $\vec{\Phi}_l' = \left(-\Phi_l'(0), \Phi_l'(1)\right)^{\mathrm{T}}$ the corresponding vector of outward derivatives on the boundary of the period. The DN map can then be represented by an absolutely and uniformly convergent series. For instance (see [3]), assuming that $\lambda_l \neq 0$, we obtain

$$\Lambda(\lambda) = \Lambda(0) - \lambda \sum_{l=1}^{\infty} \frac{\begin{pmatrix} \Phi_l'(0)\,\Phi_l'(0) & -\Phi_l'(0)\,\Phi_l'(1) \\ -\Phi_l'(0)\,\Phi_l'(1) & \Phi_l'(1)\,\Phi_l'(1) \end{pmatrix}}{\lambda_l(\lambda_l - \lambda)} = \Lambda(0) - \lambda \sum_{l=1}^{\infty} \frac{|\vec{\Phi}_l'|^2\, P_l}{\lambda_l(\lambda_l - \lambda)}. \tag{6}$$

Here P_l is denotes the orthogonal projection onto the one-dimensional subspace spanned by $\vec{\Phi}_l'$, and $|\vec{\Phi}_l'|^2 = |\Phi_l'(0)|^2 + |\Phi_l'(1)|^2$.

The approach to spectral analysis on quantum graphs based on the DN map is more practical than approaches based on the local Cauchy problem, because representations (5), (6) allow one to take into account the geometry (topology) of the graph before developing any analytical machinery (see [5, 6]). Nevertheless, in the next section we continue to develop the DN map version of the classical stylized problem of spectral analysis in one dimension, to reveal resonance effects.

2 Spectral structure of the 1-D periodic Schrödinger operator via the DN map

Representations (4), (5), (6) of the DN map are convenient general tools for studying spectral properties of the Schrödinger operator on a finite interval, or in the periodic case. In particular, on a given interval Δ of the spectral parameter we may replace the DN map by a rational matrix-function with a finite number of simple poles on real axis, since under certain assumptions we may include only the finite number of terms of the spectral series (6) with poles in the interval. In that case, the derivation of resonance formulae is reduced to the solution of algebraic equations. We proceed now under the assumption that this approximation may be used for the DN map. Then the solution u of the periodic Schrödinger equation (1) which fulfills the quasi-periodic boundary conditions at the ends of the interval $(0,1)$,

$$\begin{aligned} u_1 &= \Theta_\pm u_0 \\ u_1' &= \Theta_\pm u_0' \end{aligned}$$

can be extended as a bounded quasi-periodic functions u_+ on the semi-axis $\mathbb{R}_+ = (0, \infty)$ and u_- on $\mathbb{R}_- = (-\infty, 0)$ if and only if $|\Theta_\pm| \leq 1$, respectively. Then the ratio $\mu_-(0,\lambda) = u_-'(0,\lambda)/u_-(0,\lambda)$ coincides with the Weyl function of the operator L in $L_2(\mathbb{R}_+)$ with homogeneous Dirichlet condition $u(0) = 0$. Similarly $\mu_+(0,\lambda) = u_+'(0,\lambda)/u_+(0,\lambda)$ serves as a Weyl function of L in $L_2(\mathbb{R}_-)$. In particular the quasi-momentum exponential $\Theta = \exp\{ip\}$ and the Weyl-function μ can be found from the boundary condition (3) from the DN map since

$$\Lambda \begin{pmatrix} u_0 \\ \Theta u_0 \end{pmatrix} = \mu \begin{pmatrix} -u_0 \\ \Theta u_0 \end{pmatrix},$$

or

$$\Lambda \begin{pmatrix} 1 \\ \Theta \end{pmatrix} = \mu \begin{pmatrix} -1 \\ \Theta \end{pmatrix}. \tag{7}$$

This gives us the equations

$$\left.\begin{array}{l} \det \left[\Lambda + \mu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] = 0, \\ \Lambda_{00} + \Lambda_{01}\Theta + \mu = 0, \\ \Lambda_{10} + \Lambda_{11}\Theta - \mu\Theta = 0. \end{array}\right\} \tag{8}$$

Equations (8) give formulae for Θ and μ, which reveal the resonance phenomena in the structure of the periodic Schrödinger operator. Denoting the rational approximations to the matrix elements of the DN map by b_{st}, i.e.,

$$\Lambda(\lambda) = B = \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix},$$

we obtain the eigenvalues $\mu_\pm$ as zeroes of the second degree polynomial

$$\mu_\pm = \frac{b_{11} - b_{00}}{2} \pm \sqrt{\left(\frac{b_{11} - b_{00}}{2}\right)^2 + \det B},$$

and the corresponding quasi-momentum exponentials as solutions of linear equations. For instance, if $b_{01}(\lambda) \neq 0$, we can use the second equation in (8) to give explicitly that

$$\Theta_\pm = -\frac{b_{00} + \mu_\pm}{b_{01}} = -\frac{1}{b_{01}} \left(\frac{b_{11} + b_{00}}{2} \pm \sqrt{\left(\frac{b_{11} - b_{00}}{2}\right)^2 + \det B} \right). \tag{9}$$

We choose the branch of the square root such that the quasi-momentum exponential Θ_+ is a contracting function, i.e. $|\Theta_+(\lambda)| < 1$, on the upper half-plane $\Im\lambda > 0$. (Actually the quasi-momentum exponential is contracting on the complement of the absolutely-continuous spectrum of the periodic Schrödinger operator, i.e. the positive half-axis.) Then the complementary exponential Θ_- is defined by the equation

$$\Theta_-\Theta_+ = \frac{1}{b_{01}^2}\left[\left(\frac{b_{11}+b_{00}}{2}\right)^2 - \left(\frac{b_{11}-b_{00}}{2}\right)^2 - \det B\right] = 1.$$

We summarize the calculations above, in the following statement.

Theorem 2.1 *a) The absolutely continuous spectrum of the periodic Schrödinger operator L on $L_2(\mathbb{R})$ coincides with the closure σ of the set of points on the real axis $\{\lambda\}$ where the eigenvalues μ of the spectral problem (7) have non-zero imaginary parts, that is,*

$$\left(\frac{\Lambda_{00}-\Lambda_{11}}{2}\right)^2 + \det\Lambda < 0,$$

while the boundary points of the spectrum are defined by the zeroes of the equation

$$\left(\frac{\Lambda_{00}-\Lambda_{11}}{2}\right)^2 + \det\Lambda = 0. \tag{10}$$

b) If the DN map Λ is approximated by a rational function B, then the approximate positions of the boundary points of the absolutely-continuous spectrum are defined by the equation

$$\left(\frac{b_{00}-b_{11}}{2}\right)^2 + \det B = 0$$

involving the approximating function B.

Proof of the statement a) is obtained by summarizing the previous calculations. The second statement follows from the matrix version of Rouche's theorem [7].

Remark. Equation (10) reveals the resonance structure of the spectrum of the periodic Schrödinger operator: *the real points λ where*

$$\left(\frac{\Lambda_{00}(\lambda)+\Lambda_{11}(\lambda)}{2}\right)^2 > \Lambda_{01}(\lambda)\Lambda_{10}(\lambda)$$

belong to the complement of the spectrum. In particular, assume that the Schrödinger operator on the period with zero boundary conditions has a simple eigenvalue λ_1 with the eigenvector Φ_1. Then this eigenvalue sits on the boundary of the absolutely continuous spectrum of the periodic problem, on the right or left end of the spectral band respectively, depending whether

$$\left(\Phi_1'(1)+\Phi_1'(0)\right)^2 - \Phi_1'(0)\Phi_1'(0) > 0$$

or

$$\left(\Phi_1'(1)+\Phi_1'(0)\right)^2 - \Phi_1'(0)\Phi_1'(0) < 0.$$

The proof of the statement is obtained by using the rational approximation of the DN map at the isolated simple eigenvalue. Note that the classical description of end-points of the spectral bands of the periodic operator as eigenvalues of the periodic and anti-periodic problem may be also derived from (9).

3 Periodic quantum graph with resonance nodes

In this section we continue the study in [9] that explored a solvable model of a periodic quantum graph with resonance vertices supplied with Hamiltonian A of inner degrees of freedom. Here we focus on studying the influence of the resonance properties of the vertex part on the spectral structure of the Schrödinger operator on the graph. Similar studies can be found in [8] that considered the tight-binding problem for the one-dimensional periodic Schrödinger operator, while in [5, 6] the quantum waveguide and graph with the general structure of the vertex part were considered based on the DN map approach.

In [9] the study of the periodic chain with resonance nodes was reduced to the periodic spectral problem with the energy-dependent boundary conditions

$$-u''(x) = \lambda u(x), x \neq n, \text{ and } u'(n+0) - u'(n-0) - \left(\gamma_{00} - \frac{|\gamma_{01}|^2 M(\lambda)}{\gamma_{11} M(\lambda) + 1} \right) u(n) = 0, \tag{11}$$

where $M(\lambda) = \langle \frac{I+\lambda A}{A-\lambda I} e, e\rangle$ is the Weyl function of the inner Hamiltonian at the node $x = n$ for all integer n, e is the deficiency vector of the inner Hamiltonian and $\gamma_{st} = \{\Gamma\}_{st}$ are the boundary parameters defined by the hermitian matrix Γ of boundary conditions at the nodes. It was shown in [9] that in case $\gamma_{11} = 0$ the spectral structure of the corresponding operator L is essentially defined by both the geometry of the graph (the length of the period) and by the spectral structure of the inner Hamiltonian. Roughly speaking, the absolutely continuous spectrum of the spectral problem with inner Hamiltonian is obtained by a minor perturbation of the absolutely-continuous spectrum of the auxiliary spectral problem with "deaf and dumb" nodes, i.e. with inner Hamiltonian disconnected if $\gamma_{01} = \bar{\gamma}_{10} = 0$, to give

$$-u''(x) = \lambda u(x), x \neq n, \text{ and } u'(n+0) - u'(n-0) - \gamma_{00} u(n) = 0. \tag{12}$$

In particular, if the eigenvalue α of the inner Hamiltonian sits on the spectral gap of the above "deaf and dumb" problem (12) , then the "decorated" spectral problem (11) with inner Hamiltonian attached via non-trivial ($\gamma_{01} = \bar{\gamma}_{10} \neq 0$) boundary condition, then the spectral problem (11) with resonance nodes has a "new" spectral band centred at the point α, size proportional to $|\gamma_{01}|^2$. Conversely, if the eigenvalue of the inner Hamiltonian sits inside some spectral band of the "deaf and dumb" problem (12), then the decorated spectral problem has a spectral gap near α, with size proportional to $|\gamma_{01}|^2$. This observation was also described in [10] and re-discovered later in a more general setting in [11], where the term "decoration" was also suggested.

Our aim is to explore the creation of resonance gaps or bands for Schrödinger operator on the one-dimensional graph with n-dimensional rectangular period $\Omega = \cup_s \{-d_s - a_s < x_s < d_s + a_s\}$. We assume that the potential q is supported by the n-star $\Omega_0 = \cup_s \{-a_s < x_s < a_s\}$ and extended by zero onto the "sleeves", i.e. remaining part of the period $\omega = \Omega \backslash \Omega_0 = \cup_s \{\omega_s^- \cup \omega_s^+\}$, where $\omega_s^- = -d_s - a_s < x_s < -a_s$, $\omega_s^+ = a_s < x_s < a_s + d_s$. We assume that at the node $x_s = 0$, $s = 1, 2, \ldots, n$, some self-adjoint boundary conditions are imposed. Consider the operator L^Θ with quasi-periodic boundary conditions on the boundary $\partial\Omega = \Gamma$ of the period, and auxiliary operators L_0, L_K^Θ, L_0^Θ, which are defined as follows.

The operator L_0 is defined on the star Ω_0 by the differential expression on $L_2(\Omega_0)$

$$-u'' + q(x)u = L_0 u, \;\; x \neq 0, \tag{13}$$

with some self-adjoint boundary condition at the node $x_s = 0$, $s = 1, 2, \dots n$ and zero boundary condition at the boundary $\Gamma_0 = \cup_s \gamma_s$ of the star Ω_0. Here γ_s are two-points sets $\{-a_s,\; a_s\}$. The operator L_0 is self-adjoint and has a purely discrete spectrum with quadratic asymptotics at infinity, i.e. $\lambda_l = O(l^2)$ as $\lambda \to \infty$. The corresponding Green's function, Poisson kernel and DN map can be constructed from standard solutions of the second-order differential homogeneous equation $-u'' + q(x)u = \lambda u$, (see e.g. [6]). It is important now that the corresponding DN map can be represented by the absolutely convergent spectral series on the complement of the spectrum

$$\Lambda_0 = \sum_l \frac{\vec{\Psi}_l \rangle \langle \vec{\Psi}_l}{\lambda - \lambda_l}, \tag{14}$$

where $\vec{\Psi}_l$ is a $2n$-vector obtained via restriction onto the boundary Γ_0 of the star of the outward derivatives of the normalized eigenfunction $\Psi_l(x)$ of the L_0. Later we will formulate conditions for forming resonance gaps in terms of the structural characteristics of the DN map.

Let K be a hermitian $2n \times 2n$-matrix. Consider a family of unitary exponentials $\Theta = \{\Theta_s\} = \left\{e^{ip_s}\right\}$, $-\pi < p_s < \pi$. The corresponding operator L_K^Θ on the "sleeves" (the complement ω of the star in the period) is defined on $L_2(\omega)$ by the differential expression

$$-u'' = L^\Theta u \tag{15}$$

with zero potential and K boundary condition on the border $\Gamma_0 = \bar{\omega} \cap \overline{\Omega}_0$ of the star Ω_0

$$(\vec{u}' - K\vec{u})\Big|_{\Gamma_0} = 0. \tag{16}$$

Here prime denotes the derivative in the outward direction with respect to ω. In addition, we impose the quasi-periodic boundary conditions on the boundary $\Gamma = \cup_s \{(-a_s - d_s),\, (a_s + d_s)\}$ of the period

$$u(a_s + d_s) = \Theta_s\, u(-a_s - d_s), \;\; u'(a_s + d_s) = \Theta_s\, u'(-a_s - d_s), \tag{17}$$

where prime denotes the derivative in the positive direction. The operator L_K^Θ is self-adjoint and has a discrete spectrum with quadratic asymptotics $\lambda_l^\Theta = O(l^2)$ as $l \to \infty$.

It is convenient to calculate the spectrum of L_K^Θ in terms of the DN map of the operator L_0^Θ which has the Dirichlet boundary condition $K^{-1} = 0$ on the boundary Γ_0 of the star. The helpful idea of introduceing the operator L_0^Θ was first used in [5] and later developed in [6]. The operator L_0^Θ is represented as an orthogonal sum of simple addenda $L_0^\Theta = \sum_{s=1}^n l_s$, with operators l_s defined on "sleeves" as $-u''$ in $L_2(\omega_s^-) \oplus L_2(\omega_s^+)$ with zero boundary condition at the boundary of the star and the quasi-periodic boundary condition (17) at the boundary of the period. The operator L_0^Θ is also self-adjoint and has a discrete spectrum with quadratic asymptotics.

The DN map Λ_0^Θ of the operator L_0^Θ is represented by a diagonal matrix made up of the DN maps of the one-dimensional operators l_s (see [5], [6])

$$\Lambda_s^{\Theta_s} = \frac{k}{\sin 2kd_s}\begin{pmatrix} \cos 2kd_s & -\overline{\Theta}_s \\ -\Theta_s & \cos 2kd_s \end{pmatrix} \tag{18}$$

with $k^2 = \lambda$. The DN map transfers the 2-vector $\{u_s(-a_s),\ u_s(a_s)\}^{\mathrm{T}}$ of boundary data at γ_s into the vector $\{u_s'(-a_s),\ u_s'(a_s)\}^{\mathrm{T}}$ of the exterior derivatives with respect to $\omega_s^{\mp}$ of the solution of the equation $-u'' = \lambda u$ with the quasi-periodic boundary conditions (17).

The DN map of the operator L_0^Θ is also represented by the absolutely convergent spectral series like (14). For instance

$$\Lambda_0^\Theta = \sum_{s=1}^{n} \sum_{l} \frac{\vec{\Psi}_l^s\rangle\, \langle\vec{\Psi}_l^s}{\lambda - \lambda_l^s},$$

where $\vec{\Psi}_l^s$ is the 2-vector consisting of the exterior derivatives (with respect to $\omega_s^{\mp}$) at $-a_s$ and a_s of the corresponding normalized eigenfunction with $\lambda_l^s = \lambda_l^s(\Theta_s)$.

The operator L^Θ is defined on the period $\Omega = \omega\cup\Gamma_0\cup\Omega_0$ by proper differential expressions either (13) on the star Ω_0 or (15) on the complement ω, with smooth matching on Γ_0, the previous boundary condition at the origin and the quasi-periodic boundary condition (17) at the boundary of the period. This operator is also self-adjoint, with discrete spectrum which has quadratic asymptotics.

The eigenvalues of L_K^Θ are found from the matching conditions at the boundary of the star, as suggested in [5], [6].

Lemma 3.1 *The spectrum of the operator L_K^Θ is defined in terms of the Dirichlet-to-Neumann map of the auxiliary operator L_0^Θ as vector-zeroes $\{\lambda\}$ of the equation*

$$\left[\Lambda_0^\Theta + K\right] e = 0. \tag{19}$$

The operators L^Θ, L_K^Θ, L_0^Θ may serve as a tool for investigation of the periodic problem on the infinite lattice of non-overlapping periods $\mathbf{\Omega} = \cup_{\mathbf{m}} [\Omega + 2\langle \mathbf{m},\ \mathbf{a}+\mathbf{d}\rangle]$, where $\mathbf{a}, \mathbf{d}$ are vectors with coordinates a_s, d_s, and $\mathbf{m}$ are vector-integers $\mathbf{m} = (m_1,\ m_2,\ m_3,\ \dots,\ m_n)$. The periodic operator $\mathcal{L}$ on $L_2(\mathbf{\Omega})$ is defined by proper differential expressions on the Sobolev class $W_2^2(\mathbf{\Omega})$ (with appropriate matching at the common boundaries of periods), and the operators $\mathcal{L}_K$, $\mathcal{L}_0$ are defined in a similar way on the periodic lattice of non-overlapping sleeves $\omega_{\text{per}} = \cup_{\mathbf{m}} [\omega + 2\langle \mathbf{m},\ \mathbf{a}+\mathbf{d}\rangle]$, where $\mathbf{a}, \mathbf{d}$ with appropriate matching (17) at the common boundaries of periods and boundary conditions (16) at $\mathbf{\Gamma_0} = \cup_{\mathbf{m}} [\Gamma_0 + 2\langle \mathbf{m},\ \mathbf{a}+\mathbf{d}\rangle]$. Here $\mathbf{a}, \mathbf{d}$ with the hermitian matrix K or zero boundary condition $K^{-1} = 0$ respectively.

The operators $\mathcal{L}_K$, $\mathcal{L}_0$ play roles of operators with "deaf and dumb nodes" similar to the construction for the one-dimensional lattice described at the beginning of this section. Spectral bands of $\mathcal{L}_K$ are obtained as joining of all vector zeroes $\lambda_l^s(\Theta)$ defined by the dispersion curve (19) with $\Theta = \{e^{i\,p_s}\}$, $-\pi < p_s < \pi$. The root vectors $e_l^s(\Theta)$ are normalized. Note that all zeros are real, and the operator $\left[\Lambda_0^\Theta + K\right]$ in $E = \mathbf{C}^{2n}$ is hermitian on real λ-axis and is invertible on the orthogonal complement $E \ominus \left\{ e_l^s(\Theta) \right\}$, if $\lambda_l^s(\Theta)$ is not a multiple point sitting on different branches of spectrum. For multiple points the inverse operator is defined on the orthogonal complement of the complete kernel $\bigvee e_l^s(\Theta)$ of the crossing branches of the dispersion curve (19).

Define the operator with resonance nodes $\mathcal{L}$ on the rectangular lattice formed of periods Ω as periodic Schrödinger operator on functions which satisfy the above standard boundary conditions at the centres of stars and appropriate matching conditions at the boundaries of them. The spectral analysis of the operator $\mathcal{L}$ is reduced in standard way, see for instant [1], to the spectral analysis of the corresponding auxiliary operator $\mathcal{L}^\Theta$ on the period Ω with quasi-periodic boundary conditions. The elements from the domain of $\mathcal{L}^\Theta$ fulfill just conventional matching conditions on the boundaries of the lattice of the stars $\mathbf{\Gamma}_0 = \partial\,\mathbf{\Omega}_0$, $\mathbf{\Omega}_0 = \cup_{\mathbf{m}} [\Omega_0 + 2\langle \mathbf{m},\, \mathbf{a} + \mathbf{d} \rangle]$. The eigenfunctions of the absolutely continuous spectrum of $\mathcal{L}$ (the FB-solutions of the equation $\mathcal{L}\, u = \lambda\, u$) are obtained via quasi-periodic continuation of eigenfunction of the auxiliary operator $\mathcal{L}^\Theta$ on the whole lattice.

Now we are prepared to consider the problem of forming the resonance gap. Assume that the simple eigenvalue λ_1 of the operator L_0 is revealed as a pole of the corresponding DN map. Note then

$$\Lambda_0(\lambda) = |\vec{\Psi}_1|^2 \, \frac{P_1}{\lambda - \lambda_1} + Q_1(\lambda), \tag{20}$$

with the residue defined by the one-dimensional projection P_1 onto the vector $\vec{\Psi}_1 = \left\{ \dots, -\psi_1'(-a_s),\, \psi_1'(a_s), \dots \right\}$ of the outward derivatives of the associated normalized eigenfunction ψ_1 at the boundary $\Gamma_0 = \partial\Omega_0$ of the star. Assume that it coincides with the eigenvalue $\lambda^\Theta = \lambda_1^\Theta$ of the operator L_K^Θ, i.e.

$$\left[\Lambda_0^\Theta(\lambda) + K \right] e_1(\Theta) = 0$$

for some $\Theta = \Theta_1$. Denote by $P_1^\perp$ the complementary projection of P_1, $P_1^\perp + P_1 = I$ and by P_1^Θ, $P_1^{\perp,\Theta}$ the orthogonal projections onto the one-dimensional null-space $\{e_1(\Theta)\}$ of the operator-function $\left[\Lambda_0^\Theta(\lambda) + K \right]$.

Theorem 3.2 *If the simple eigenvalue λ_1 of the operator L_0 sits on the absolutely continuous spectrum of the operator $\mathcal{L}_K$, and the operator*

$$\mathcal{K}^\Theta = P_1^\perp \left[Q_1 - K + P^{\perp,\Theta} \left(\Lambda_0^\Theta + K \right) P^{\perp,\Theta} \right] P_1^\perp \tag{21}$$

is invertible for each value of quasi-momentum where $\lambda^\Theta = \lambda$, then the point λ_1 is a regular point of the operator $\mathcal{L}$.

Proof Assuming that the point λ_1 belongs to the spectrum of the operator $\mathcal{L}^\Theta$ we should have a non-zero vector $e(\Theta)$ that satisfies the equation $\left[\Lambda_0^\Theta(\lambda_1) + \Lambda_0(\lambda_1) \right] e(\Theta) = 0$. Then $P_1\, e(\Theta) = 0$. Hence, due to the decomposition (20)

$$\left[Q_1 - K + P^{\perp,\Theta} \left(\Lambda_0^\Theta + K \right) P^{\perp,\Theta} \right] e(\Theta) = 0,$$

since P^{Θ} reduces to $\left(\Lambda_0^{\Theta} + K\right)$ and $P^{\Theta}\left(\Lambda^{\Theta} + K\right)P^{\Theta} = 0$. Since $e(\Theta) = P_1^{\perp}\, e(\Theta)$, we can re-write the previous equation as

$$P_1^{\perp}\left[Q_1 - K + P^{\perp,\Theta}\left(\Lambda_0^{\Theta} + K\right)P^{\perp,\Theta}\right]P_1^{\perp} e(\Theta) := \mathcal{K}^{\Theta}(\lambda_1)\, e(\Theta) = 0,$$

which means that the operator $\mathcal{K}^{\Theta}(\lambda_1)$ has a (non-trivial) null space. Conversely, the condition of the theorem requires invertibility of $\mathcal{K}^{\Theta}(\lambda_1)$. This finishes the proof for given value p, $\Theta = e^{ip}$, of the quasi-momentum, $p = p_1$. In case that $\lambda = \lambda_1$ is a multiple point, $\lambda_1 = \lambda^{\Theta_1} = \lambda^{\Theta_2} = \dots$, and the above condition is fulfilled for all of the Θ's, then λ_1 is a regular point of the operator $\mathcal{L}$.
Corollary. If λ_1 is a multiple point of the absolutely-continuous spectrum of the operator $\mathcal{L}_K$ with the multiplicity ν_1, but the condition (21) is fulfilled only for ν_1' values of the quasi-momentum, $\nu_1' < \nu_1$, then the multiplicity of the continuous spectrum of $\mathcal{L}$ at this point is not greater than $\nu_1 - \nu_1'$.
Remark If λ_1 is a multiple eigenvalue of the operator L_0 the multiplicity of the eigenvalue coincides with the dimension of the subspace of the corresponding vectors of derivatives $\Psi_{1,l}$ of the corresponding orthogonal normalized system of eigenfunctions. This permits to extend the above theorem and the Corollary to the case of multiple eigenvalues.

The above statement gives a condition of forming of spectral gaps. One can formulate a similar condition for resonance spectral bands.

Theorem 3.3 *Assume that λ_1 is a simple eigenvalue of the operator L_0, so that the DN map of L_0 admits the decomposition (20). If λ_1 is a regular point of the operator $\mathcal{L}_K$ with $K = Q_1(\lambda_1)$, and there exists a (small) disc D_1 centered at λ_1, such that on the corresponding circle $\Sigma_1 = \partial D_1$ the condition*

$$\sup_{\lambda \in \Sigma_1} \frac{\left|\langle \Psi_1,\, \left[\Lambda_0^{\Theta} + K\right]^{-1} \Psi_1\rangle\right|}{|\lambda - \lambda_1|} < 1 \tag{22}$$

is fulfilled. Then there are points of the absolutely continuous spectrum of the operator $\mathcal{L}$ inside D_1.

Proof It will suffice to prove that there exists a solution e of the equation $\left[\Lambda_0 + \Lambda_0^{\Theta}\right] e = 0$. Representing the DN map of the operator L_0 in form (20) and assuming that λ_1 is a regular point of the operator $\mathcal{L}_K$, $K = Q_1(\lambda_1)$ and hence the operator $\Lambda_0^{\theta} + K$ is invertible for any $\Theta = e^{ip}$, $-\pi < p < \pi$. Then we can re-write the equation for e in the following form

$$\frac{\left[\Lambda_0^{\Theta} + K\right]^{-1} \Psi_1\rangle\, \langle \Psi_1,\, e\rangle}{\lambda - \lambda_1} + e = 0.$$

This equation is reduced to the scalar equation

$$\frac{\langle \Psi_1,\, \left[\Lambda_0^{\Theta} + K\right]^{-1} \Psi_1\rangle}{\lambda - \lambda_1} + 1 = 0.$$

According to Rouché theorem this equation has, under the above condition (22) a single root $\hat{\lambda}_1(\theta)$ at some point inside Σ_1. This root is real and depends continuously on λ_1, Θ due to the continuity of $\Lambda_0^\Theta(\lambda), Q_1(\lambda)$. Hence there is a spectral band of the operator $\mathcal{L}$ overlapping with $D_1 = \text{Int } \Sigma_1$.

It is known that a quantum network may be modelled by a quantum graph with proper boundary conditions at the vertices. (See e.g. [12, 13] for quantum networks with finite leads and [4] for networks with infinite leads.) In [4] the quantum network with straight leads is represented in the form of the star-shaped graph with one-dimensional Schrödinger operator on it and the resonance vertex. The scattering matrix of the model inherits essential features of the scattering matrix of the network. The geometric machinery of recovering of conditions of resonance forming of spectral gaps and bands developed in this section may be extended, based on [4], to realistic quantum networks.

4 Resonance gaps for the periodic Schrödinger operator

In this section we sketch an approach to studying the spectral properties of the multi-dimensional Schrödinger operator based on the DN map (see [5] for details). This approach allows one, in particular, to observe the creation of the resonance bands and gaps in a similar way to the previous section.

Consider the periodic Schrödinger equation with the rectangular period $\Omega = \{-d_s - a_s < x_s < d_s + a_s,\ s = 1, 2, \ldots, n\}$. Assume that the real measurable locally bounded potential q is supported by the strictly inner parallelepiped $\Omega_0 = \{-a_s < x_s < a_s\}$. We obtain the periodic potential on the whole space R^n via periodic continuation of q: $q(x + 2\langle \mathbf{m}, \mathbf{a} + \mathbf{b}\rangle) = q(x)$, $x \in \Omega$. The spectral analysis of the corresponding periodic Schrödinger operator

$$-\triangle u + q(x)u = \mathcal{L}u$$

is reduced (cf. [1]) to the analysis of the regular Schrödinger operator L^Θ on the period with quasi-periodic boundary conditions on the boundary

$$\Gamma = \partial\Omega = \cup_s \{x_s = \pm(d_s + a_s),\ (d_t + a_t) \le x_t \le (d_t + a_t),\ t \ne s\}$$

defined by unitary operators Θ_s, $s = 1, 2, \ldots, n$, acting on spaces of square-integrable functions on the faces of the period. An example is

$$u(-a_s) = \Theta_s u(a_s), \quad -\frac{\partial u}{\partial n}(-a_s) = \Theta_s \frac{\partial u}{\partial n}(a_s), \tag{23}$$

where n is the outward normal. Together with the operator L^Θ we consider the operators defined by the same differential expressions $-\triangle$ and $-\triangle + q$ on $\Omega \backslash \Omega_0$ and on Ω_0 respectively, with quasi-periodic boundary condition (23) on $\partial\Omega = \Gamma$ and some self-adjoint boundary condition with a hermitian operator K on $\partial\Omega_0 = \Gamma_0$ for the operator $-\triangle = L_K^\Theta$ on $L_2(\Omega \backslash \Omega_0)$. That is,

$$\left(\frac{\partial u}{\partial n} - Ku\right)\bigg|_{\Gamma_0} = 0,$$

and the zero boundary condition on Γ_0 for the operator $-\triangle + q(x) = L_0$ on $L_2(\Omega_0)$. Both operators are self-adjoint and have discrete spectra. We assume that the Green's functions of both operators G_K^Θ, G_0 and the corresponding DN maps (with $K^{-1} = 0$ on the "inner" boundary $\Gamma_0 = \partial\Omega_0$) are constructed, and the DN maps Λ^Θ, Λ_0 are represented by properly altered spectral series, [3], for instance

$$\Lambda^\Theta(\lambda) = \Lambda^\Theta_{-1} - (\lambda+1)\, P^+_{-1} P_{-1} + (\lambda+1) \sum_l \frac{\frac{\partial\Psi_l}{\partial n}\rangle\,\langle\frac{\partial\Psi_l}{\partial n}}{\lambda_l(\lambda-\lambda_l)},$$

for $L^\Theta_K := L^\Theta_\infty$ if $K^{-1} = 0$. The similar representation is valid for Λ_0. The eigenvalues of L^Θ are found from the matching conditions at the boundary, as suggested in [5], [6].

Theorem 4.1 *The spectrum of the operator L^Θ is defined as the set of all vector-zeroes of the operator-valued function*

$$\left[\Lambda^\Theta_\infty + \Lambda_0\right] e = 0.$$

The proof follows from the straightforward matching on the boundary Γ_0 of the inner parallelepiped Ω_0. Unfortunately we do not have now an explicit formula for Λ^Θ_∞. Nevertheless, one can calculate the eigenvalues and eigenfunctions of the operators L^Θ_∞, L_0 and substitute the DN maps by the corresponding rational functions based on above spectral series. This gives a practical method of recovering of the spectral structure of the periodic operator $\mathcal{L}$, and, in particular, permits us to obtain conditions for the creation of resonance gaps and bands.

4.1 Space of vector functions

In this section we revisit the analysis of section 2 for the one-dimensional Schrödinger operator L on vector-valued functions taking values in the finite-dimensional space E, $\dim E = n$. We introduce also the two copies $E^\pm$ of the space E associated with the boundary points $\pm a$ of the period, and the orthogonal sum $E^- \oplus E^+ = \mathbf{E}$. Elements from E and $\mathbf{E}$ are denoted by e and $\mathbf{e}$ respectively. Assume that we already know the DN map of the operator L on the period and can represent it in form of the polar decomposition near the simple "resonance" eigenvalue λ_r of the Dirichlet problem for L on the period. The corresponding normalized eigenfunction will be denoted by φ_r, and its boundary values and the boundary values of its derivative in the outward direction at the boundary points $\pm a$ of the period will be denoted by $\varphi_r^\pm$, $\phi_r^\pm$, respectively. We will use also the vector $\phi_r = \left(\phi_r^-, \phi_r^+\right) \in E^- \oplus E^+$, and denote by $\mathbf{P}_r$ an orthogonal projection in $\mathbf{E} = E^- \oplus E^+$ onto the one-dimensional subspace spanned by ϕ_r, $\| \phi_r \| = \alpha_r$. Then the DN map of the operator L on the period can be represented near the resonance eigenvalue as the combination of the polar term near λ_r and the smooth part

$$\Lambda(\lambda) = \frac{\alpha_r^2 \mathbf{P}_r}{\lambda - \lambda_r} + Q_r(\lambda) : \mathbf{E} \to \mathbf{E}. \tag{24}$$

If necessary, additional polar terms may be transferred from Q into the polar group. Our aim now is to reveal the spectral structure of the problem with the quasi-periodic boundary conditions on the boundary of the period

$$\varphi(a) = \Theta\varphi(-a), \qquad (25)$$
$$\phi(a) = -\Theta\phi(-a),$$

with a unitary operator Θ acting from E^- into E^+. Without loss of generality one can assume that we choose the basis consisting of eigenvectors of the operator Θ in E. Then the operator Θ is represented by the diagonal matrix $\mathrm{diag}\left\{e^{ip_s/a}\right\}$, $-\pi < p_s < \pi,\ s = 1, 2, \dots n$. The minus in front of $\phi(a)$ appears because in quasi-periodic conditions (25) we reverse the outward direction of the derivative at $-a$ into the positive direction. Substitution of (24) into (25) gives the following dispersion equation connecting the eigenvalues λ^Θ of the quasi-periodic problem with the quasi-momentum exponential Θ. Assume that the DN map acts on $\mathbf{E}$ as

$$\Lambda(\lambda)\begin{pmatrix}\varphi(-a)\\ \Theta\varphi(-a)\end{pmatrix} = \begin{pmatrix}-\phi(-a)\\ \Theta\phi(-a)\end{pmatrix}.$$

Introduce the linear operator $\mu_+ : E^- \to E^-$ transforming the boundary data $\varphi(a)$ of the quasi-periodic solution into the boundary data of the corresponding derivative in the positive direction $\phi(-a)$, that is, $\phi(-a) = -\mu_+\varphi(-a)$. Then the dispersion equation takes the form

$$\Lambda(\lambda)\begin{pmatrix}\varphi(-a)\\ \Theta\varphi(-a)\end{pmatrix} = \mu_+\begin{pmatrix}-\varphi(-a)\\ \Theta\varphi(-a)\end{pmatrix}. \qquad (26)$$

Now we denote $\varphi(-a) = \nu$ and eliminate μ_+, based on the matrix representation of the DN map with respect to the orthogonal decomposition $\mathbf{E} = E^- \oplus E^+$

$$\Lambda = \begin{pmatrix}\Lambda_{--} & \Lambda_{-+}\\ \Lambda_{+-} & \Lambda_{++}\end{pmatrix},$$

$$\Lambda_{+-}\nu + \Lambda_{++}\Theta\nu + \Theta\Lambda_{--}\nu + \Theta\Lambda_{-+}\Theta\nu = 0. \qquad (27)$$

Identifying the spaces $E^- = E^+ = E$ we can see from equation (27) that the eigenvalues of the quasi-periodic problem are found as zero eigenvalues of the hermitian matrix

$$\Theta^{-1/2}\Lambda_{+-}\Theta^{-1/2} + \Theta^{-1/2}\Lambda_{++}\Theta^{1/2} + \Theta^{1/2}\Lambda_{--}\Theta^{-1/2} + \Theta^{1/2}\Lambda_{-+}\Theta^{1/2} := \mathbf{\Lambda}^\Theta$$

$$\det\mathbf{\Lambda}^\Theta = 0. \qquad (28)$$

The corresponding eigenvectors are obtained via $\Theta^{-1/2}\nu = \Theta^{-1/2}\varphi(-a)$. Notice that Λ is a sum of the one-dimensional polar term and a smooth part Q. Then the matrix $\mathbf{\Lambda}^\Theta$ can be represented as a sum of the one-dimensional term associated with the resonance eigenvalue

$$\mathbf{\Lambda}^\Theta_{res} = \frac{\Theta^{-1/2}\phi_+\rangle\langle\phi_-\Theta^{-1/2} + \Theta^{-1/2}\phi_+\rangle\langle\phi_+\Theta^{1/2} + \Theta^{1/2}\phi_-\rangle\langle\phi_-\Theta^{-1/2} + \Theta^{1/2}\phi_-\rangle\langle\phi_+\Theta^{1/2}}{\lambda - \lambda_r},$$

and the term associated with the smooth (at λ_r) part Q

$$\mathbf{\Lambda}^\Theta_Q = \frac{\Theta^{-1/2}Q_{+-}\langle\Theta^{-1/2} + \Theta^{-1/2}Q_{++}\Theta^{1/2} + \Theta^{1/2}Q_{--}\Theta^{-1/2} + \Theta^{1/2}Q_-\Theta^{1/2}}{\lambda - \lambda_r}.$$

The following conditional result is almost obvious now.

Theorem 4.2 *Assume that there are two operators L_r, L_Q such that the DN maps on the corresponding Dirichlet problems on the period coincide with $\Lambda(\lambda)$ and $Q(\lambda)$, respectively, and the numerator of the resonance part is non-zero for a given value Θ. Then one the following alternatives is true.*
Either the spectral point λ belongs to the discrete spectrum of the operator L_Q, but does not belong to the discrete spectrum of the operator L_r,
or,
the spectral point λ_r belongs to the discrete spectrum of the operator L_r, and it does not belong to the discrete spectrum of the operator L_Q.

The proof follows from the previous observation.

In the one-dimensional case dim $E = 1$ the dispersion equation (27) becomes scalar with $\Theta = e^{ip}$, $\Lambda_{+-} = |\Lambda_{+-}|e^{-ip_0} = \bar{\Lambda}_{+-}$. We have

$$\cos(p - p_0) = -\frac{\Lambda_{--} + \Lambda_{++}}{|\Lambda_{+-}|}.$$

Therefore, the band-spectrum of the corresponding periodic problem is described by the condition

$$|\Lambda_{--} + \Lambda_{++}| \leq |\Lambda_{+-}|. \tag{29}$$

Characteristic details of spectrum of the periodic problem like forming bands or gaps can be revealed now via observing contribution from the smooth and resonance parts in (29).

4.2 Multi-dimensional periodic Schrödinger operator

Now based on section 4.1 we attempt to formulate spectral results for the multi-dimensional periodic Schrödinger operator. Assuming that the period is just a cube $\Omega = \{-a \leq x_s \leq a,\ s = 1, 2, \ldots n\}$, we represent the boundary of the cube as a sum of positive and negative squares $\Gamma_s^{\pm} = \Omega \cap \{x_s = \pm a\}$. Introduce the corresponding spaces of scalar square-integrable functions $E_s^{\pm} = L_2(\Gamma_s^{\pm})$ and the corresponding orthogonal sums $E^{\pm} = \sum_s \oplus E_s^{\pm}$. The quasi-periodic conditions on the boundary can be defined by diagonal unitary exponent $\Theta = \mathrm{diag}\left\{e^{ip_s/a}\right\}$. We denote by L the Schrödinger operator on the period with zero boundary conditions on the boundary. The DN map of L will be denoted by Λ. In the presence of resonance eigenvalues it admits the representation (24). The quasi-periodic boundary conditions are imposed on vectors

$$\varphi^{\pm} = \left(\varphi|_{\Gamma_1^{\pm}}, \varphi|_{\Gamma_2^{\pm}}, \ldots, \varphi|_{\Gamma_n^{\pm}}\right)$$

of the boundary values of elements and the vectors of the corresponding normal derivatives in the outgoing direction

$$\phi^{\pm} = \left(\frac{\partial\varphi}{\partial n}|_{\Gamma_1^{\pm}}, \frac{\partial\varphi}{\partial n}|_{\Gamma_2^{\pm}}, \ldots, \frac{\partial\varphi}{\partial n}|_{\Gamma_n^{\pm}}\right)$$

Then the role of the condition (25) is played now by

$$\varphi^{+} = \Theta\varphi^{-},$$
$$\phi^{+} = -\Theta\phi^{-},$$

and the dispersion equation is represented in the form

$$\Lambda(\lambda)\begin{pmatrix} \varphi^{-} \\ \Theta\varphi^{-} \end{pmatrix} = \begin{pmatrix} -\phi^{-} \\ \Theta\phi^{-} \end{pmatrix}. \tag{30}$$

For the quasi-periodic solutions of the periodic Schrödinger equation we can introduce the linear operator μ_{+} transforming the vector φ^{-} into $-\phi^{-}$. Then the dispersion equation (30) may be written as

$$\Lambda(\lambda)\begin{pmatrix} \varphi^{-} \\ \Theta\varphi^{-} \end{pmatrix} = \mu_{+}\begin{pmatrix} -\varphi^{-} \\ \Theta\varphi^{-} \end{pmatrix}. \tag{31}$$

Further we denote the vector φ^{-} by ν and eliminate μ_{+} as in (26). This gives an analog of equation (27), which may beeliminatedispereq2 transformed to the following more convenient form

$$\Theta^{-1/2}\Lambda_{+-}\Theta^{-1/2} + \Theta^{-1/2}\Lambda_{++}\Theta^{1/2} + \Theta^{1/2}\Lambda_{--}\Theta^{-1/2} + \Theta^{1/2}\Lambda_{-+}\Theta^{1/2} := \mathbf{\Lambda}^{\Theta},$$
$$\mathbf{\Lambda}^{\Theta} e = 0. \tag{32}$$

The only difference of the multi-dimensional problem from the one-dimensional problem is the infinite dimension of $E^{\pm}$. *One can believe* that for Schrödinger operator with a trigonometric polynomial potential a reasonably good description of spectrum of the periodic operator for low energies can be obtained via substituting the space E_{N} of finite linear combinations of exponentials which satisfy quasi-periodic boundary conditions instead of the infinite-dimensional spaces $E^{\pm}$. Then the remaining calculations should be the same, as in the one-dimensional case. We plan to organize a computer experiment to reveal numerically the conditions for resonance gaps and bands, based on analysis of the finite-dimensional version of the equation (32)

$$\det \mathbf{\Lambda}^{\Theta}_{N} = 0,$$

with

$$\mathbf{\Lambda}^{\Theta}_{N} := P_{N}\mathbf{\Lambda}^{\Theta}P_{N}, \;\; P_{N} := P_{E_N}.$$

5 Numerical examples

In this section we will consider some numerical examples for the Schrödinger operator on the one-dimensional graph with 2-dimensional rectangular period Ω as discussed in section 3. We assume that $q = 0$ everywhere and the δ-type boundary conditions are imposed at the node $x_{s} = 0$, $s = 1, 2$, (see [14]), i.e.,

$$\left.\begin{aligned} u(0) := u_{1}(-0) = u_{1}(+0) = u_{2}(-0) = u_{2}(+0), \\ u_{1}'(-0) + u_{1}'(+0) + u_{2}'(-0) + u_{2}'(+0) = tu(0), \end{aligned}\right\} \tag{33}$$

where the prime denotes the derivative in the outer direction with respect to the node at the origin, and t is a real number.

The approach, which has been developed in section 3, consists of the following steps. Firstly, the Dirichlet-to-Neumann map $\Lambda_0(\lambda)$, a 4×4-matrix function, for the operator L_0 should be calculated. Secondly, one has to choose a simple eigenvalue s_0 of the operator L_0, which is at the same time a pole of Λ_0; that is the formulae (20) are fulfilled with $\lambda_1 = s_0$. To go on to the next point the operator K, a self-adjoint 4×4-matrix, are required, which is defined by equation (20) as

$$K := Q_1(s_0) \tag{34}$$

Further, spectral (Fermi) surfaces are considered in a neighbourhood of the point s_0 for two periodical problems, the initial one with the operator $\mathcal{L}$ and the auxiliary problem with the operator $\mathcal{L}_K$ where boundary conditions generated by the matrix K. Pictures of Fermi surfaces for different energies similar to others can be found in [15]. Finally, Theorem 3.2 claims that if the point s_0 lies on the spectrum of the operator $\mathcal{L}_K$ then it may belong to a gap of the operator $\mathcal{L}$, and it certainly happens when the matrix in (21) is invertible.

1. In our example the operator L_0 is defined on the cross $\{-1 < x_1 < 1, x_2 = 0\} \cup \{x_1 = 0, -\pi/5 < x_2 < \pi/5\}$ with conditions (33) at the origin and $t = 15$. Then the matrix function $\Lambda_0(\lambda)$ has the following representation

$$\Lambda_0(\lambda) = \Lambda_e(\lambda)/d(\lambda),$$

where Λ_e is an entire matrix function on the complex plane $\mathbf{C}$ and

$$d(\lambda) := \sin(\pi\sqrt{\lambda}/5)\sin(\sqrt{\lambda})\Big(15\sin(\pi\sqrt{\lambda}/5))\sin(\sqrt{\lambda})$$
$$+2\sin(\pi\sqrt{\lambda}/5))\cos(\sqrt{\lambda})\sqrt{\lambda} + 2\cos(\pi\sqrt{\lambda}/5)\sin(\sqrt{\lambda})\sqrt{\lambda}\Big). \tag{35}$$

2. On the second step let us consider four of the first eigenvalues of the operator L_0, i.e. poles of the matrix $\Lambda_0(\lambda)$ or roots of the denominator (35). They are

$$s_1 := 7.654855816,\ s_2 := 9.869604404,\ s_3 := 18.58533237,\ s_4 := 25.$$

It has to be noticed that

1) s_1, s_2, and s_3 are poles of the matrix entry $(\Lambda_0)_{11}$,
2) s_1, s_3, and s_4 are poles of $(\Lambda_0)_{33}$,
3) they are simple poles

3. On this step the matrix K for each pole $\lambda_1 = s_n$ in (34) has been calculated.

$$K_1 = \begin{pmatrix} -2.977118629 & 4.054789217 & 0.4785883266 & 0.4785883266 \\ 4.054789217 & -2.977118629 & 0.4785883266 & 0.4785883266 \\ 0.4785883266 & 0.4785883266 & -0.6717778349 & -0.2036856816 \\ 0.4785883266 & 0.4785883266 & -0.2036856816 & -0.6717778349 \end{pmatrix}$$

$$K_2 = \begin{pmatrix} 3.830084912 & 2.330084908 & 1.707684776 & 1.707684776 \\ 2.330084908 & 3.830084912 & 1.707684776 & 1.707684776 \\ 1.707684776 & 1.707684776 & -1.339830153 & -0.000000000 \\ 1.707684776 & 1.707684776 & 0.000000000 & -1.339830153 \end{pmatrix}$$

$$K_3 = \begin{pmatrix} 1.174324748 & -0.6550685566 & -0.4945512075 & -0.4945512075 \\ -0.6550685566 & 1.174324748 & -0.4945512075 & -0.4945512075 \\ -0.4945512075 & -0.4945512075 & -4.004026312 & 5.325367110 \\ -0.4945512075 & -0.4945512075 & 5.325367110 & -4.004026312 \end{pmatrix}$$

$$K_4 = \begin{pmatrix} -1.479064584 & 0.000000000 & -2.607088030 & -2.607088030 \\ 0.000000000 & -1.479064584 & -2.607088030 & -2.607088030 \\ -2.607088030 & -2.607088030 & 4.204129781 & 1.816805625 \\ -2.607088030 & -2.607088030 & 1.816805625 & 4.204129781 \end{pmatrix}$$

4. Now we are ready to compare spectra of the periodic operators $\mathcal{L}$ and $\mathcal{L}_{_K}$ in a neighbourhood of each point s_n, $n = 1, 2, 3, 4$. We choose $d_1 = d_2 = 1$ and put $z = lambda$ $\Theta_{_1} = \cos x + i \sin x$ and $\Theta_{_2} = \cos y + i \sin y$. To calculate the spectrum of the operator $\mathcal{L}_{_K}$ we need the Dirichlet-to-Neumann map $L_p := \Lambda^{\Theta}_{_0}$ of the operator $L^{\Theta}_{_0}$, which is obtained as a diagonal matrix combined of DN maps (18) of the one-dimensional operators $l_{_s}$ (see [6]). Then the known dispersion equation ([14]) will be used for the operator $\mathcal{L}$. Thus we have the DN map of the operator $L^{\Theta}_{_0}$

$$L_p := \frac{\sqrt{z}}{\sin(2\sqrt{z})} \begin{pmatrix} \cos(2\sqrt{z}) & -\cos x + i \sin x & 0 & 0 \\ -\cos x - i \sin x & \cos(2\sqrt{z}) & 0 & 0 \\ 0 & 0 & \cos(2\sqrt{z}) & -\cos y + i \sin y \\ 0 & 0 & -\cos y - i \sin y & \cos(2\sqrt{z}) \end{pmatrix}$$

and the dispersion equation for the operator $\mathcal{L}$

$$\frac{\cos x - \cos(2\sqrt{z})}{\sin(2\sqrt{z})} + \frac{\cos(y) - \cos(2(\pi/5+1))\sqrt{z}}{\sin(2(\pi/5+1)\sqrt{z})} = \frac{15}{2\sqrt{z}} \tag{36}$$

On the figures 1-4 below the spectra of the operators $\mathcal{L}_{K_j}$ on the left and $\mathcal{L}$ on the right are shown in a neighborhood of one of the points s_j, $j = 1,\ 2,\ 3,\ 4$.

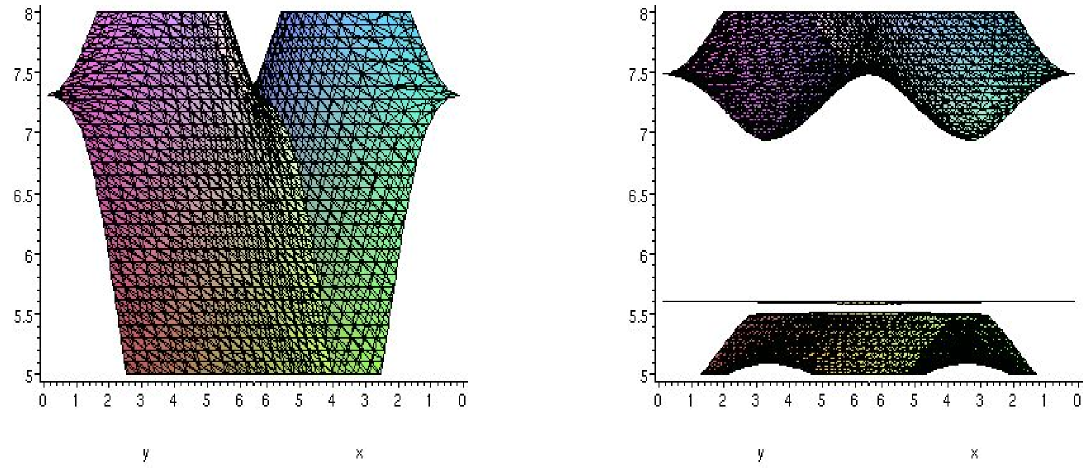

Figure 1: $s_1 = 7.65$

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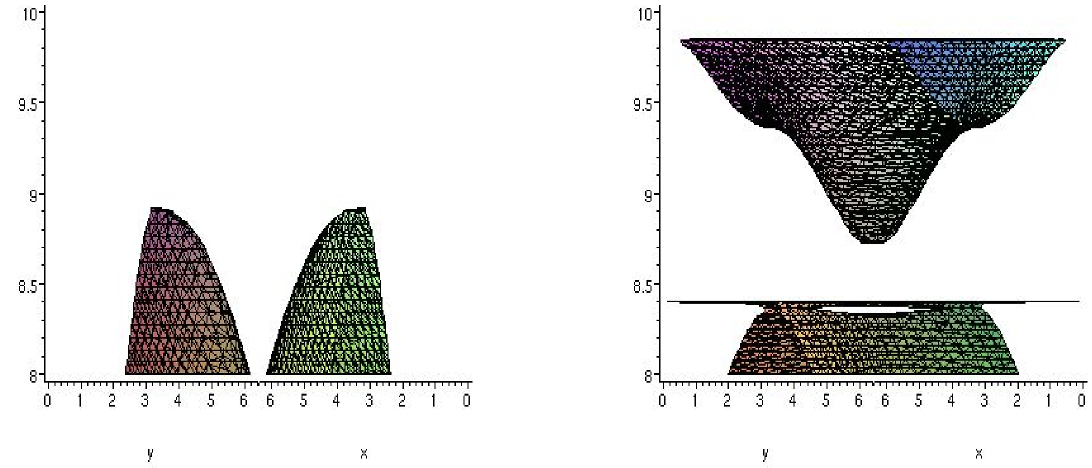

Figure 2: $s_2 = 9.87$

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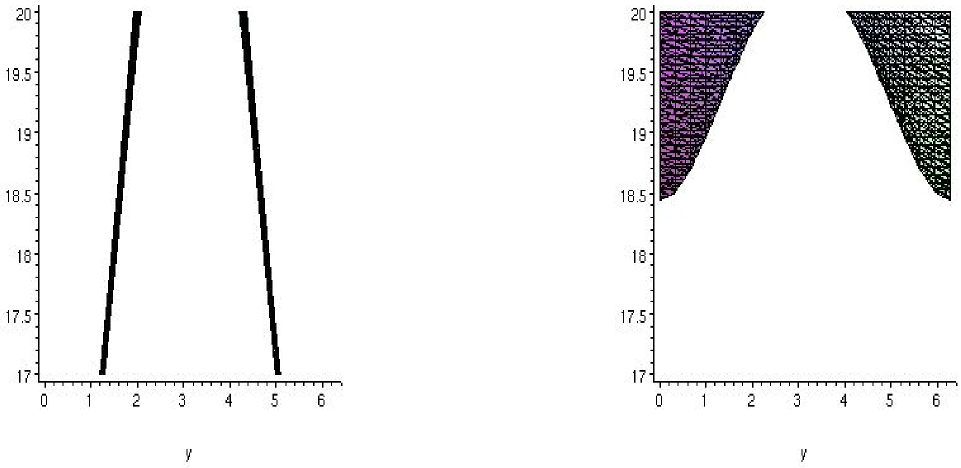

Figure 3: $s_3 = 9.87$

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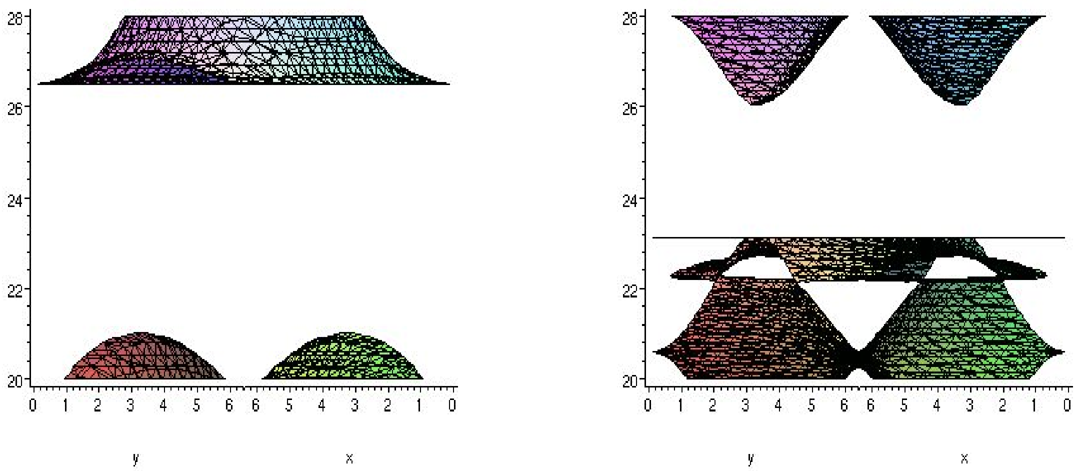

Figure 4: $s_4 = 25$

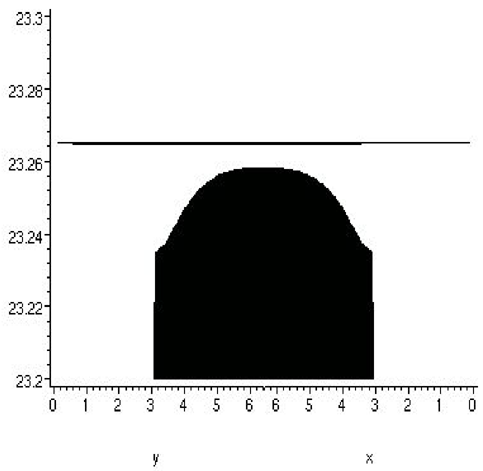

Figure 5: $s_4 = 25$