Dirichlet-to-Neumann map machinery for resonance gaps and bands of periodic Networks

C. Fox [1], V. Oleinik [2] and B. Pavlov [1,2]

[1]Department of Mathematics, University of Auckland, Private Bag 92019, Auckland, New Zealand;
[2] V.A. Fock Institute for Physics, St. Petersburg University, 198505, Petrodvorets, St.Petersburg, Russia.

Abstract

Usually spectral structure of the ordinary periodic Schrödinger operator is revealed based on analysis of the corresponding transfer-matrix. In this approach the quasi-momentum exponentials appear as eigenvalues of the transfer-matrix which correspond to quasi-periodic solutions of the homogeneous Schrödinger equation, and the corresponding Weyl functions are obtained as coordinates of the appropriate eigenvectors. This 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, where several leads are attached to each vertex, and can't be extended to partial Schrödinger equation. We propose an alternative approach where the Dirichlet-to-Neumann map is used instead of the transfer matrix. We apply this approach to obtain, for realistic quantum networks, conditions of existence of resonance gaps or bands.

PACS numbers: 73.63.Hs,73.23.Ad,85.35.-p,85.35.Be
Keywords: Periodic Schrödinger operator, Floquet-Bloch solutions, Dirichlet-to-Neumann map.

1 Introduction: transfer matrix and DN-map

The classical approach to description of Floquet-Bloch (FB) solutions of the periodic Schrödinger operator is based on the transfer-matrix constructed of the standard solutions θ, φ of the homogeneous Schrödinger equation

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

with a real measurable essentially bounded periodic potential $q(x) = q(x+1)$ and special initial conditions

$$\begin{array}{ll} \theta(0,\lambda) = 1, & \theta'(0,\lambda) = 0, \\ \varphi(0,\lambda) = 0, & \varphi'(0,\lambda) = 1. \end{array} \tag{2}$$

The corresponding transfer-matrix on the period is presented as

$$T(\lambda, 1) = \begin{pmatrix} \theta(1,\lambda) & \varphi(1,\lambda) \\ \theta'(1,\lambda) & \varphi'(1,\lambda) \end{pmatrix} \tag{3}$$

It has eigenvalues presented as quasi-momentum exponentials $\Theta_{\pm} = \exp\{\pm i p(\lambda)\}$ which define the quasi-momentum p, $\Im p \geq 0$. The corresponding eigen-vectors $\left(1,\, m_{\pm}\right)$ define the FB-solutions $\chi_{\pm}(x,\lambda) = \theta(x,\lambda) + m_{\pm}\varphi(x,\lambda)$ which are square-integrable on the right or left semi-axis $R_{\pm}$ of x-axis respectively : $\chi_{\pm} \in L_2(R_{\pm})$ for complex values of the quasi-momentum p, $\Im p > 0$, see for instance [1]. Note that in this classical approach the quasi-momenta exponentials appear as eigenvalues of the transfer-matrix :

$$\Theta_{\pm} = s \pm \sqrt{s^2 - 1} \tag{4}$$

where $s(\lambda) = (\theta(1,\lambda) + \varphi'(1,\lambda))/2$ is defined by the trace of the transfer-matrix $T(\lambda,1)$ on the period. The absolutely-continuous spectrum of the corresponding periodic Schrödinger operator is defined by the condition $-1 \leq s(\lambda) \leq 1$.

One can use also the Dirichlet-to-Neumann map (DN-map) $\Lambda(\lambda)$ on the period instead of the transfer-matrix. In our simplest case (see more general definitions in [2, 3, 4]) DN-map is defined as a map of the pair of the boundary values $(u(0,\lambda),\, u(1,\lambda)) = (u_0,\, u_1)$ of any solution u of the homogeneous Schrödinger equation (1) into the derivatives of it $\left(-u_0',\, u_1'\right)$ in outgoing direction at the boundary $\{0,\, 1\}$ of the period:

$$\Lambda(\lambda)\begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \begin{pmatrix} -u_0' \\ u_1' \end{pmatrix}. \tag{5}$$

The DN-map can be calculated as a solution of the linear system obtained via substitution into (5) the connection between Cauchy data

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

defined by the transfer-matrix. This gives the following formula for DN-map:

$$\Lambda(\lambda) = \begin{pmatrix} \frac{\theta(1,\lambda)}{\varphi(1,\lambda)} & -\frac{1}{\varphi(1,\lambda)} \\ -\frac{1}{\varphi(1,\lambda)} & \frac{\varphi'(1,\lambda)}{\varphi(1,\lambda)} \end{pmatrix}. \tag{6}$$

The above formula for DN-map was derived based on standard solutions of Cauchy problem. One can see that the DN-map is a symmetric matrix function, and it is real on the real axis λ and has simple poles at the eigenvalues of the Dirichlet problem on the period. Other properties of the DN-map may be easily derived from the general properties of the standard solutions θ and φ.

Analogs of these solutions do not exist in multi-dimensional case or even on branching graphs. Nevertheless the DN-map can be conveniently calculated in more general cases too, based on standard solutions of relevant boundary problems on the period. In the remaining part of this section we derive some spectral results for the one-dimensional periodic Schrödinger operator without use of the standard solutions or the transfer-matrix.

In one-dimensional case one can introduce a pair of solutions $\varphi_0 := \varphi$ and φ_1 of the equation (1) which fulfills the initial conditions at $x = 1$:

$$\begin{array}{ll} \varphi_0(0,\lambda) = 0, & \varphi_0'(0,\lambda) = 1 \\ \varphi_1(1,\lambda) = 0 & \varphi_1'(1,\lambda) = 1, \end{array}. \tag{7}$$

The DN-map can be presented in terms of these solutions as

$$\Lambda(\lambda) = \begin{pmatrix} -\frac{\varphi_1'(0,\lambda)}{\varphi_1(0,\lambda)} & -\frac{1}{\varphi_0(1,\lambda)} \\ \frac{1}{\varphi_1(0,\lambda)} & \frac{\varphi_0'(1,\lambda)}{\varphi_0(1,\lambda)} \end{pmatrix}. \quad (8)$$

The matrix (8) is symmetric due to the Wronskian property $W(\varphi_0, \varphi_1)$ =Const. It follows from general properties of DN-map that the matrix (8) is meromorphic function of the spectral parameter λ which has a negative imaginary part in the upper half-plane $\Im\lambda > 0$, is real hermitian on the real axis of λ and has simple poles at the eigenvalues λ_l of the operator L defined in $L_2(0,1)$ by the above differential expression and zero boundary conditions at the ends $x = 0, 1$ of the interval. Denoting by Φ_l the real normalized eigenfunctions of the operator L and by $\vec{\Phi}_l' :\equiv \left(-\Phi_l'(0), \Phi_l'(1)\right)$ the corresponding "boundary vector" combined of the derivatives of the eigenfunction Φ_l in outgoing direction at the boundary of the period, we can represent the DN-map by the absolutely and uniformly convergent series. For instance, assuming that $\lambda_l \neq 0$, we obtain:

$$\Lambda(\lambda) = \Lambda(0) - \lambda \sum_{l=0}^{\infty} \frac{\begin{pmatrix} \Phi_l'(0)\,\Phi_l'(0) & -\Phi_l'(0)\,\Phi_l'(1) \\ -\Phi_l'(0)\,\Phi_l'(1) & \Phi_l'(1)\,\Phi_l'(1) \end{pmatrix}}{\lambda_l(\lambda_l - \lambda)}$$

$$= \Lambda(0) - \lambda \sum_{l=0}^{\infty} \frac{|\vec{\Phi}_l'|^2\, P_l}{\lambda_l(\lambda_l - \lambda)}. \quad (9)$$

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

The approach to spectral analysis on quantum graphs based on DN-map is more practical that one based on local Cauchy problem, because it permits to take into account the geometry (topology) of the graph before developing analytical machinery, see [10, 11]. Nevertheless we present below, in the next section, the DN-version of the classical problem of spectral analysis in 1-d case based on DN-map, to reveal the resonance effects.

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

The above representations (6, 8, 9) of the DN-map are convenient general tools of study of spectral properties of the Schrödinger operator on a finite interval or in periodic case. In particular, on a given interval of the spectral parameter Δ under certain assumptions we can take into account only a finite number of terms of the above spectral series (9) with poles on the interval, thus substituting the DN-map by a rational matrix-function with a finite number of simple poles on real axis. In this case derivation of interesting resonance formulae is reduced just to solution of algebraic equations. We proceed now under assumption that this approximation is used for the DN- map. Then the solution u of the periodic Schrödinger equation (1) which fulfills the quasi-periodic boundary conditions at the end of the interval (0, 1):

$$\begin{aligned} u_1 &= \Theta_\pm u_0 \\ u_1' &= \Theta_\pm u_0' \end{aligned} \tag{10}$$

can be extended as a bounded quasi-periodic function on the semi-axis $R_+ = (0, \infty)$ or $R_- = (-\infty, 0)$ if and only if $|\Theta_\pm| \leq 1$. Then the corresponding ratio $\mu_- = u'_{-,0}/u_{-,0}$ coincides with Weyl function of the corresponding operator in $L_2(R_+)$

$$lu = -u'' + qu,\ u(0) = 0. \tag{11}$$

Similarly $\mu_{+,0} = u'_{+,0}/u_{+,0}$ serves as a Weyl-function of the corresponding operator in $L_2(R_-)$. In particular the quasi-momentum exponential $\Theta = \exp\{ip\}$ and the Weyl-function μ can be found from the above boundary condition (5) based on the DN-map:

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

or

$$\Lambda \begin{pmatrix} 1 \\ \Theta \end{pmatrix} = \mu \begin{pmatrix} -1 \\ \Theta \end{pmatrix}. \tag{12}$$

This gives us the following equations:

$$\begin{aligned} &\det \left[\Lambda + \mu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] = 0, \\ &\Lambda_{00} + \Lambda_{01}\Theta + \mu = 0, \\ &\Lambda_{10} + \Lambda_{11}\Theta - \mu\Theta = 0. \end{aligned} \tag{13}$$

Equations (13) give the formulae for Θ, μ, which reveal the resonance phenomena in the structure of the corresponding periodic Schrödinger operator. Denoting the matrix elements of the DN-map (or the corresponding rational approximations of them) by b_{st}:

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

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 (13):

$$\Theta_\pm = -\frac{b_{00} + \mu_\pm}{b_{01}} = -\frac{1}{b_{01}} \left(\frac{b_{11} + b_{00}}{2} \pm \sqrt{\left(\frac{b_{11} - b_{00}}{2} \right)^2 + \det B} \right). \tag{14}$$

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

$$\Theta_-\Theta_+ = \frac{1}{b_{01}^2}\left[\left(\frac{b_{11}+b_{00}}{2}\right)^2 - \left(\frac{b_{11}-b_{00}}{2}\right)^2 - \det B\right] = \frac{b_{10}}{b_{01}} = 1. \tag{15}$$

Summarizing results of the above calculations, we obtain the following statement:

Theorem 2.1 *The absolutely continuous spectrum of the periodic Schrödinger operator L in $L_2(R)$ coincides with the closure σ of the set of points on the real axis $\{\lambda\}$ where the eigenvalues of the spectral problem (12)*

$$\left[\Lambda + \mu\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]\nu = 0 \tag{16}$$

have a non-trivial imaginary part:

$$\left(\frac{\Lambda_{00}-\Lambda_{11}}{2}\right)^2 + \det\Lambda < 0 \tag{17}$$

and the boundary points of the spectrum are defined by the zeroes of the corresponding equation:

$$\left(\frac{\Lambda_{00}-\Lambda_{11}}{2}\right)^2 + \det\Lambda = 0. \tag{18}$$

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 from the corresponding equation involving the approximating function:

$$\left(\frac{b_{00}-b_{11}}{2}\right)^2 + \det B = 0. \tag{19}$$

Proof of the first statement is obtained via summarizing of the previous calculations. The second statement involving the approximation by rational function is derived based on matrix version of Rouche theorem, see [6].

Corollary The equation (18) reveals the resonance structure of the spectrum of the periodic Schrödinger operator : the real points λ where

$$\left(\frac{\Lambda_{00}(\lambda)+\Lambda_{11}(\lambda)}{2}\right)^2 > \Lambda_{01}(\lambda)\Lambda_{10}(\lambda) \tag{20}$$

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 on the condition

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

or

$$\left(\Phi_1'(1) + \Phi_1'(0)\right)^2 - \Phi_1'(0)\Phi_1'(0) < 0. \tag{21}$$

Proof of the statement is obtained based on 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 (14).

3 Periodic Quantum graph with resonance nodes

In [5] the tight-binding problem for one-dimensional periodic Schrödinger operator is considered. In [7] a solvable model of a periodic quantum graph with resonance vertices supplied with Hamiltonian A of inner degrees of freedom was explored. In [10, 11] the quantum waveguide and graph with the general structure of the vertex part were considered based on DN-map approach. In this section we focus on study of influence of the resonance properties of the vertex part on the spectral structure of the Schrödinger operator on the graph, continuing actually the study presented in [7].

In [7] the study of the periodic chain with resonance nodes was reduced to the periodic spectral problem with energy-dependent boundary conditions :

$$-u'' = \lambda u,\ [u'] - \left(\gamma_{00} - \frac{|\gamma_{01}|^2 M(\lambda)}{\gamma_{11} M(\lambda) + 1}\right) u\Big|_{x=n} = 0, \tag{22}$$

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 $x = n$, 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 [7] 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 minor perturbation of the absolutely-continuous spectrum of the auxiliary spectral problem with “ deaf and dumb” nodes (with inner Hamiltonian disconnected $\gamma_{01} = \bar\gamma_{10} = 0$):

$$-u'' = \lambda u,\ [u'] - \gamma_{00} u\Big|_{x=n} = 0. \tag{23}$$

In particular, if the eigenvalue α of the inner Hamiltonian sits on the spectral gap of the above “deaf and dumb” problem (23) , then the “decorated” spectral problem (22) with inner Hamiltonian attached via non-trivial ($\gamma_{01} = \bar\gamma_{10} \neq 0$) boundary condition, then the spectral problem (22) with resonance nodes has a “new” spectral band centered at the point α, size proportional to $|\gamma_{01}|^2$. Vice versa, if the eigenvalue of the inner Hamiltonian sits inside some spectral band of the "deaf and dumb" problem (23), then the decorated spectral problem has a spectral gap near α, size proportional to $|\gamma_{01}|^2$. This observation was described also in [8] and later in more general situation re-discovered in [9], where the convenient term "decoration" was also suggested.

Our aim is: to explore creation of resonance gaps or bands for Schrödinger operator on the one-dimensional graph with n-dimensional rectangular period Ω. 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"- remaining part of the period : $\omega = \Omega\backslash\Omega_0 = \cup_s \left\{\omega_s^- \cup \omega_s^+\right\}$, 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, and consider below 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.

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

$$-u'' + q(x)u = L_0 u \tag{24}$$

and by some self-adjoint boundary condition at the node $x_s = 0$, $s = 1, 2, \ldots n$ and zero boundary condition at the boundary of the star $\Gamma_0 = \cup_s \gamma_s$, where γ_s are two-points sets $\{-a_s,\ a_s\}$. The operator L_0 is self-adjoint and has purely discrete spectrum with quadratic asymptotics at infinity $\lambda_l = O(l^2)$. The corresponding Green function, Poisson kernel and Dirichlet-to-Neumann map can be constructed of standard solutions of second-order differential homogeneous equation $-u'' + q(x)u = \lambda u$, see for instance ([11]). It is important now that the corresponding Dirichlet-to-Neumann map can be presented by the absolutely convergent spectral series on the complement of the spectrum:

$$\Lambda_0 = \sum_l \frac{\vec{\Psi}_l\rangle\,\langle\vec{\Psi}_l}{\lambda - \lambda_l}, \tag{25}$$

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

Consider a family of unitary exponentials $\Theta = \{\Theta_s\} = \left\{e^{ip_s}\right\}$, $-\pi < p_s < \pi$ and the corresponding operator L_K^Θ on the "sleeves" - the complement ω of the star in the period - defined in $L_2(\omega)$ by the differential expression

$$-u'' = L^\Theta u \tag{26}$$

with zero potential and zero boundary condition on the border of the star Γ_0 defined by the hermitian matrix K

$$(\vec{u}' - K\vec{u})\Big|_{\Gamma_0} = 0, \tag{27}$$

where the prime denotes the derivative in the outer direction with respect to ω. We impose also the quasi-periodic boundary conditions on the boundary $\Gamma = \cup_s \{(-a_s - d_s),\ (a_s + d_s)\}$ of the period:

$$u(a_s + d_s) = \Theta_s\, u(-a_s - d_s),\ \ u'(a_s + d_s) = \Theta_s\, u'(-a_s - d_s), \tag{28}$$

where the derivative in positive direction is denoted by prime. The Operator L_K^Θ is self-adjoint and has discrete spectrum with quadratic asymptotics $\lambda_l^\Theta = O(l^2)$. It is convenient to calculate the spectrum of the operator L_K^Θ in terms of DN-map of the corresponding operator L_0^Θ which corresponds to the Dirichlet boundary condition $K^{-1} = 0$ on the boundary Γ_0 of the star. The helpful idea to introduce the operator L_0^Θ was used first in the paper [10] and later developed in [11]. The operator L_0^Θ is presented 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 (28) at the boundary of the period. The Operator L_K^Θ is also self-adjoint and has discrete spectrum with quadratic asymptotics.

The Dirichlet-to-Neumann map Λ_0^Θ of the operator L_0^Θ is obtained as diagonal matrix combined of DN-maps of the one-dimensional operators l_s (see [11]):

$$\Lambda_s^{\Theta_s} = \frac{k}{\sin 2kd_s} \begin{pmatrix} \cos 2kd_s & -\overline{\Theta}_s \\ -\Theta_s & \cos 2kd_s \end{pmatrix}. \tag{29}$$

The DN-map transfers the 2-vector $\{u_s(-a_s),\ u_s(a_s)\}$ of boundary data at γ_s into the vector $\left\{u_s'(-a_s),\ u_s'(a_s)\right\}$ of the corresponding derivatives (in outside direction with respect to ω_s) of the solution of the equation $-u'' = \lambda u$ submitted to the above quasi-periodic boundary conditions (28).

The Dirichlet-to-Neumann map of the operator L_0^Θ is also presented by the absolutely convergent spectral series like (25), for instance

$$\Lambda_0^\Theta = \sum_{s=1}^n \sum_l \frac{\vec{\Psi}_l^s\rangle\,\langle\vec{\Psi}_l^s}{\lambda - \lambda_l^s}, \tag{30}$$

where $\vec{\Psi}_l^s$ is 2-vector combined of the outside derivatives (with respect to $\omega_\pm^s$) of the corresponding normalized eigenfunctions at $-a_s$, a_s respectively, and $\lambda_l^s = \lambda_l^s(\Theta_s)$.

The operator L^Θ is defined on the period Ω by proper differential expressions on the cross and on the complement, with smooth matching on Γ_0, the previous boundary condition at the origin and the quasi-periodic boundary condition (28) at the boundary of the period. This operator is self-adjoint too 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 [10], [11]:

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:*

$$\left[\Lambda_0^\Theta + K\right] e = 0. \tag{31}$$

The operators L^Θ, L_K^Θ, L_0^Θ may serve a tool for investigation of the corresponding 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 $\mathbf{m} = (m_1, m_2, m_3, \ldots, m_n)$. The periodic operator $\mathcal{L}$ in $L_2(\mathbf{\Omega})$ 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 $\omega = \cup_{\mathbf{m}} [\omega + 2\langle \mathbf{m}, \mathbf{a} + \mathbf{d}\rangle]$, where $\mathbf{a}, \mathbf{d}$ with appropriate matching at the common boundaries of periods and boundary conditions (27) at $\mathbf{\Gamma_0} = \cup_{\mathbf{m}} [\Gamma_0 + 2\langle \mathbf{m}, \mathbf{a} + \mathbf{d}\rangle]$, where $\mathbf{a}, \mathbf{d}$ 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 ones constructed on the one-dimensional lattice described in the beginning of actual section. Spectral bands of $\mathcal{L}_K$ are obtained as joining of all vector zeroes $\lambda_l^s(\Theta)$ defined by the above dispersion curve (31) with $\Theta = \{e^{ip_s}\}$, $-\pi < p_s < \pi$. 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 axis λ and 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 (31).

Define the operator with resonance nodes L on the rectangular lattice formed of periods Ω as periodic Schrödinger operator on functions which satisfy the above standard boundary conditions at the centers 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 $\mathbf{\Gamma}_0 = \partial\,\mathbf{\Omega}_0$. The eigenfunctions of the absolutely continuous spectrum of $\mathcal{L}$ (the FB-solutions of the equation $\mathcal{L}\chi_p = \lambda\,\chi_p$) are obtained via quasi-periodic continuation of eigenfunction of the auxiliary operator L^Θ on the whole lattice.

Now we are prepared to consider the problem of forming of 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, see :

$$\Lambda_0(\lambda) = |\vec{\Psi}_1|^2\,\frac{P_1}{\lambda - \lambda_1} + Q_1(\lambda), \tag{32}$$

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 outside derivatives of the corresponding 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

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

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*

$$\mathcal{K}^\Theta = P_1^\perp\left[Q_1 - K + P^{\perp,\Theta}\left(\Lambda_0^\Theta + K\right)P^{\perp,\Theta}\right]P_1^\perp \tag{33}$$

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 $e(\Theta)$ which fulfills 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 (32):

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

since P^{Θ} reduces $\left(\Lambda_0^{\Theta} + K\right)$ 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. Vice versa, 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 if $\lambda = \lambda_1$ is a multiple point, $\lambda_1 = \lambda^{\Theta_1} = \lambda^{\Theta_2} = \ldots$, and the above condition is fulfilled for all of them, then λ_1 is a regular point of the operator $\mathcal{L}$. End of the proof

Corollary. If the 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 (33) 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 that $\nu_1 - \nu_1'$.

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 (32). If* λ_1 *is a regular point of the operator* $\mathcal{L}_K$ *with* $K = Q_1(\lambda_1)$, *and there exist a (small) disc* D_1 *centered at* λ_1, *such that on the corresponding circle* $\Sigma_1 = \partial D_1$ *the condition*

$$\sup_{\lambda\in\Sigma_1} \frac{\left|\langle\Psi_1,\, \left[\Lambda_0^{\Theta} + K\right]^{-1} \Psi_1\rangle\right|}{|\lambda - \lambda_1|} < 1 \tag{34}$$

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

Proof It suffice to prove that there exists a solution e of the equation $\left[\Lambda_0 + \Lambda_0^{\Theta}\right] e = 0$. Presenting the DN-map of the operator L_0 in form (32) 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

$$\frac{\langle \Psi_1, \left[\Lambda_0^\theta + K\right]^{-1} \Psi_1 \rangle}{\lambda - \lambda_1} + 1 = 0. \tag{35}$$

According to Rouche theorem this equation has, under the above condition (34) 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 continuity of $\Lambda_0^\Theta(\lambda), Q_1(\lambda)$. Hence there is a spectral band of the operator $\mathcal{L}$ overlapping with $D_1 = \text{Int } \Sigma_1$. End of the proof.

It is known that a quantum network may be modeled by the Quantum graph with proper boundary conditions at the vertices, see for instance [12, 13] for quantum networks with finite leads and [4] for network with infinite leads. In [4] the quantum network with straight leads is presented in 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. We postpone description of this material to the following publication.

4 Resonance gaps for periodic Schrödinger operator

In this section we sketch an approach to study of spectral properties of the multi-dimensional Schrödinger operator based on DN-map (see [10] for details). This approach permits, in particular, to observe creation of the resonance bands and gaps similarly to the material of the previous section.

Consider the periodic Schrödinger equation with the rectangular period $\Omega = \{-d_s - a_s < x_s < d_s + a_s,\ s = 1, 2, \dots n\}$. 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: $q(x + 2\langle \mathbf{m}, \mathbf{a} + \mathbf{b}\rangle) = q(x)$, $x \in \Omega$. Spectral analysis of the corresponding periodic Schrödinger operator

$$-\triangle u + q(x)u = \mathcal{L}u \tag{36}$$

is reduced, see [1], to analysis of the corresponding regular Schrödinger operator L^Θ on the period with the quasi-periodic boundary conditions on the boundary

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

defined by unitary operators Θ_s, $s = 1, 2, \dots, n$, acting in spaces of square-integrable functions on the faces of the period, for instance :

$$u(-a_s) = \Theta_s u(a_s),\ -\frac{\partial u}{\partial n}(-a_s) = \Theta_s \frac{\partial u}{\partial n}(a_s), \tag{37}$$

where n is the outer normal on the face. 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 (37) on $\partial\Omega = \Gamma$ and some self-adjoint boundary condition with an hermitian operator K on $\partial\Omega_0 = \Gamma_0$ - for $-\triangle = L_K^\Theta$ in $L_2(\Omega\backslash\Omega_0)$:

$$\left(\frac{\partial u}{\partial n} - Ku\right)\Big|_{\Gamma_0} = 0, \tag{38}$$

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

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

for $L_K^\Theta := L_\infty^\Theta$ with $K^{-1} = 0$. Similar representation is valid for Λ_0. The eigenvalues of L^Θ are found from the matching conditions at the boundary, as suggested in [10], [11]:

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

$$\left[\Lambda_\infty^\Theta + \Lambda_0\right] e = 0.$$

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 of 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 to obtain conditions of creation of the resonance gaps and bands. We postpone the discussion to the following publication.

4.1 Space of vector functions

In this section we revisit the above analysis (see section 2) of the one-dimensional Schrödinger operator L on vector- functions taking values in the finite-dimensional space E, dim $E = n$. We introduce also 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 ($\mathbf{E}$) are denoted by e, ν ($\mathbf{e}$, ν with proper indices. Assume that we already know the DN-map of the operator L on the period and can present 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 outside 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 presented near the resonance eigenvalue as the combination of the polar term near λ_r and the smooth part:

$$\Lambda(\lambda) = \frac{\alpha_r^2 \mathbf{P}_r}{\lambda - \lambda_r} + Q_r(\lambda) : \mathbf{E} \to \mathbf{E}. \tag{39}$$

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:

$$\begin{aligned} \varphi(a) &= \Theta\varphi(-a), \\ \phi(a) &= -\Theta\phi(-a), \end{aligned} \tag{40}$$

with an unitary operator Θ acting from E^- into E^+. Without loss of generality one can assume that we choose the basis of eigen-vectors of the operator Θ in E. Then the operator Θ is presented by the diagonal matrix diag$\left\{e^{ip_s/a}\right\}$, $-\pi < p_s < \pi$, $s = 1, 2, \ldots n$. The minus in front of $\phi(a)$ appears because in quasi-periodic conditions (40) we revert the outside direction of the derivative at $-a$ into the positive direction. Substitution of (39) into (40) gives the following dispersion equation connecting the eigenvalues λ^Θ of the quasi-periodic problem with the quasi-momentum exponential Θ. Assuming that the DN-map act in $\mathbf{E}$ as:

$$\Lambda(\lambda)\begin{pmatrix} \varphi(-a) \\ \Theta\varphi(-a) \end{pmatrix} = \begin{pmatrix} -\phi(-a) \\ \Theta\phi(-a) \end{pmatrix}. \tag{41}$$

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 $\phi(-a)$: $\phi(-a) = -\mu_+\varphi(-a)$. Then the dispersion equation takes the form

$$\Lambda(\lambda)\begin{pmatrix} \varphi(-a) \\ \Theta\varphi(-a) \end{pmatrix} = \mu_+\begin{pmatrix} -\varphi(-a) \\ \Theta\varphi(-a) \end{pmatrix}. \tag{42}$$

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

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

$$\Lambda_{+-}\nu + \Lambda_{++}\Theta\nu + \Theta\Lambda_{--}\nu + \Theta\Lambda_{-+}\Theta\nu = 0. \tag{43}$$

Identifying the spaces $E^- = E^+ = E$ we can see from the equation (43) that the eigenvalues of the quasi-periodic problem are found as zero eigenvalues of the hermitian matrix

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

$$\det\mathbf{\Lambda}^\Theta = 0. \tag{44}$$

The corresponding eigenvectors are $\Theta^{-1/2}\nu = \Theta^{-1/2}\varphi(-a)$. 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 presented as a sum of the one-dimensional term associated with the resonance eigenvalue:

$$\mathbf{\Lambda}^\Theta_{res} =$$

$$\frac{\Theta^{-1/2}\phi_+\rangle\langle\phi_-\Theta^{-1/2} + \Theta^{-1/2}\phi_+\rangle\langle\phi_+\Theta^{1/2} + \Theta^{1/2}\phi_-\rangle\langle\phi_-\Theta^{-1/2} + \Theta^{1/2}\phi_-\rangle\langle\phi_+\Theta^{1/2}}{\lambda - \lambda_r}, \tag{45}$$

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

$$\mathbf{\Lambda}_Q^{\Theta} =$$

$$\frac{\Theta^{-1/2} Q_{+-} \langle \Theta^{-1/2} + \Theta^{-1/2} Q_{++} \Theta^{1/2} + \Theta^{1/2} Q_{--} \Theta^{-1/2} + \Theta^{1/2} Q_{-} \Theta^{1/2}}{\lambda - \lambda_r}. \tag{46}$$

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 given value Θ. Then the following alternative is true:*

Either the spectral point λ belongs to discrete spectrum of the operator of the operator L_Q, but does not belong to the discrete spectrum of the operator L_r,

or, vice versa,

The spectral point λ_r belongs to the discrete spectrum of the operator L_r, then it does not belong to the discrete spectrum of the operator L_Q.

$\widehat{\text{P}}$roof follows from the previous observation (44)

In one-dimensional case dim $E = 1$ this condition may be re-written in more constructive form, because the dispersion equation (43) becomes scalar with $\Theta = e^{ip}$, $\Lambda_{+-} = |\Lambda_{+-}| e^{-ip_0} = \bar{\Lambda}_{+-}$:

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

The band-spectrum of the corresponding periodic problem is described then by the condition:

$$|\Lambda_{--} + \Lambda_{++}| \leq |\Lambda_{+-}|. \tag{47}$$

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 part in (47).

4.2 Multi-dimensional periodic Schrödinger operator

Now based on section 4.1 we attempt to formulate the spectral program for the multi-dimensional periodic Schrödinger operator. Assuming that the period if just a cube $\Omega = \{-a \leq x_s \leq a,\, s = 1, 2, \dots n\}$, we present 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-interable 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 $\Theta = \text{diag}\left\{ e^{ip_s/a} \right\}$. 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 presence of the resonance eigenvalue it admits the representation (39). The quasi-periodic boundary conditions are imposed on vectors

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

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

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

Then the role of the condition (40) is played now by

$$\begin{aligned} \varphi^{+} &= \Theta \varphi^{-}, \\ \phi^{+} &= -\Theta \phi^{-}, \end{aligned} \tag{48}$$

and the dispersion equation is presented in form

$$\Lambda(\lambda) \begin{pmatrix} \varphi^{-} \\ \Theta \varphi^{-} \end{pmatrix} = \begin{pmatrix} -\phi^{-} \\ \Theta \phi^{-} \end{pmatrix}. \tag{49}$$

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 (49) may be transformed to

$$\Lambda(\lambda) \begin{pmatrix} \varphi^{-} \\ \Theta \varphi^{-} \end{pmatrix} = \mu_+ \begin{pmatrix} -\varphi^{-} \\ \Theta \varphi^{-} \end{pmatrix}. \tag{50}$$

Further we denote the vector φ^- by ν and eliminate μ_+ as above. This gives an analog of the equation (43), which may be transformed to more convenient form as before:

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

$$\mathbf{\Lambda}^{\Theta} e = 0. \tag{51}$$

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 potential presented by trigonometric polynomial a reasonably good description of spectrum of the periodic operator for low energies is obtain via substitution the infinite-dimensional spaces $E^{\pm}$ by the space E_N of finite linear combinations of exponentials which satisfy quasi-periodic boundary conditions. Then the remaining algebra is the same, as in one-dimensional case. We plan to organize a computer experiment to reveal numerically the conditions for resonance gaps and bands, based on analysis of finite-dimensional version of the equation (51)

$$\det \mathbf{\Lambda}_N^{\Theta} = 0.$$

with

$$\mathbf{\Lambda}_N^{\Theta} := P_N \mathbf{\Lambda}^{\Theta} P_N, \quad P_N := P_{E_N}.$$

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 from the 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]). The latter means that

$$\begin{cases} u(0) := u_1(-0) = u_1(+0) = u_2(-0) = u_2(+0), \\ \\ u_1'(-0) + u_1'(+0) + u_2'(-0) + u_2'(+0) = tu(0), \end{cases} \tag{52}$$

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 (32) 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 (32) as

$$K := Q_1(s_0) \tag{53}$$

Further, spectral (Fermi) surfaces of two periodical problems - the initial one with the operator $\mathcal{L}$ and the problem with boundary conditions generated by the matrix K (the operator $\mathcal{L}_K$) - are considered in a neighbourhood of the point s_0. Pictures of Fermi surfaces for different energies similar to others one can find 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 (33) is invertible. To solve this explicit problem we will use Maple package.

1. In our example the operator L_0 is defined on the cross $\{-a_1 < x_1 < a_1,\ x_2 = 0\} \cup \{x_1 = 0,\ -a_2 < x_2 < a_2\}$ with conditions (52) at the origin. We put $a_1 = 1$, $a_2 = \pi/5$ and $t = 15$ and calculate the matrix function $\Lambda_0(\lambda)$.

An ansatz of the solution in the general case with constant potentials on each interval and different lengths of intervals looks like:

$y := (x, n) -> u[n] * cos((x - (-1)^n * a[n]) * r[n]) + b[n] * sin((x - (-1)^n * a[n]) * r[n])$:

The derivative of the solution y(x,n):

$dy := D[1](y)$:

The value of the exterior derivative at the origin:

$dy0 := n -> (-1)^n * dy(0, n)$:

The value of the exterior derivative at the boundary point:

$dya := n -> (-1)^n * dy((-1)^n * a[n], n)$:

The delta boundary conditions at the origin:

$eq1 := \{y(0,2) - y(0,1), y(0,3) - y(0,1), y(0,4) - y(0,1),$
$dy0(1) + dy0(2) + dy0(3) + dy0(4) = t * y(0,1)\}$:

The solution of the system (eq1):

$bs := solve(eq1, \{b[1], b[2], b[3], b[4]\})$:

$b := n- > subs(bs, b[n])$:
The common denominator:
$d1 := denom(b(1))$:
Verification:
$d1 - denom(b(2)) : d1 - denom(b(3)) : d1 - denom(b(4))$:
Numerators of derivative of the solution at the end points:
$num := n- > subs(b[n] = b(n), dya(n)) * d1$:
DN-map (without the denominator) consists of the following elements:
$f := (i, j)- > coeff(num(i), u[j])$:
The DN-map in the general case:
$f1 := (i, j)- > coeff(num(i), u[j])/d1$:
$Lambda[0, g] := matrix(4, 4, f1)$:
To get a numerical example we put $a_1 = a_2 = 1$, $a_3 = a_4 = \pi/5$, $r_1 = r_2 = r_3 = r_4 = \sqrt{\lambda}$ and $t = 15$. Then the denominator of the matrix $\Lambda_0(\lambda)$ is
$d1sl := factor(subs(r[1] = sqrt(lambda), r[2] = sqrt(lambda),$
$r[3] = sqrt(lambda), r[4] = sqrt(lambda), a[1] = 1, a[2] = 1,$
$a[3] = Pi/5, a[4] = Pi/5, t = 15, d1));$

$$d1sl := \sin(\pi\sqrt{\lambda}/5)\sin(\sqrt{\lambda})\Big(15\sin(\pi\sqrt{\lambda}/5))\sin(\sqrt{\lambda})$$
$$+2\sin(\pi\sqrt{\lambda}/5))\cos(\sqrt{\lambda})\sqrt{\lambda} + 2\cos(\pi\sqrt{\lambda}/5)\sin(\sqrt{\lambda})\sqrt{\lambda}\Big) \tag{54}$$

$fl := (i, j)- > subs(t = 15, a[1] = 1, a[2] = 1, a[3] = Pi/5,$
$a[4] = Pi/5, r[1] = sqrt(lambda), r[2] = sqrt(lambda), r[3] = sqrt(lambda),$
$r[4] = sqrt(lambda), f(i, j))/(subs(r = sqrt(lambda),$
$l1 = 1, l2 = Pi/5, t = 15, d1sl))$:
$Lambda[0] := matrix(4, 4, fl)$:

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 (54). They are:
$s[1] := (fsolve(subs(sqrt(lambda) = x, d1sl), x, 0.1..3))^2;$
$s[2] := (fsolve(subs(sqrt(lambda) = x, d1sl), x, 3..3.5))^2;$
$s[3] := (fsolve(subs(sqrt(lambda) = x, d1sl), x = 3.5..4.5))^2;$
$s[4] := (fsolve(subs(sqrt(lambda) = x, d1sl), x = 4.5..5.5))^2;$

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

It has to be noticed that the points s_1, s_2, and s_3 are poles of the matrix entry $(\Lambda_0)_{11}$, but s_1, s_3, and s_4 of $(\Lambda_0)_{33}$. Indeed:
$evalf(subs(lambda = s[1], numer(factor(Lambda[0][1, 1]))));$
$evalf(subs(lambda = s[1], denom(factor(Lambda[0][1, 1]))));$

$$-7.547597859;\ 0.2562941348\,10^{-9}$$

$evalf(subs(lambda = s[2], numer(factor(Lambda[0][1, 1]))));$
$evalf(subs(lambda = s[2], denom(factor(Lambda[0][1, 1]))));$

$$9.078454376;\ \ 0.2370799640\,10^{-8}$$

$evalf(subs(lambda = s[3], numer(factor(Lambda[0][1, 1]))));$
$evalf(subs(lambda = s[3], denom(factor(Lambda[0][1, 1]))));$

$$-7.796082583,\ \ -0.2577531355\,10^{-7}$$

$evalf(subs(lambda = s[4], numer(factor(Lambda[0][1, 1]))));$
$evalf(subs(lambda = s[4], denom(factor(Lambda[0][1, 1]))));$

$$13.60052780;\ \ -9.195357651$$

$evalf(subs(lambda = s[1], numer(factor(Lambda[0][3, 3]))));$
$evalf(subs(lambda = s[1], denom(factor(Lambda[0][3, 3]))));$

$$-2.802706642;\ \ 0.6901917721\,10^{-9}$$

$evalf(subs(lambda = s[2], numer(factor(Lambda[0][3, 3]))));$
$evalf(subs(lambda = s[2], denom(factor(Lambda[0][3, 3]))));$

$$7.122852563;\ \ -5.316235449$$

$evalf(subs(lambda = s[3], numer(factor(Lambda[0][3, 3]))));$
$evalf(subs(lambda = s[3], denom(factor(Lambda[0][3, 3]))));$

$$17.10867022;\ \ 0.1174530036\,10^{-7}$$

$evalf(subs(lambda = s[4], numer(factor(Lambda[0][3, 3]))));$
$evalf(subs(lambda = s[4], denom(factor(Lambda[0][3, 3]))));$

$$-23.97310689;\ \ -0.3933572215\,10^{-8}$$

The poles $s_1 - s_4$ are simple because derivatives w of the denominator (54) do not equal to zero at them.
$Dl := diff(d1sl, lambda);$
$w1 := evalf(subs(lambda = s[1], Dl)); w2 := evalf(subs(lambda = s[2], Dl));$
$w3 := evalf(subs(lambda = s[3], Dl)); w4 := evalf(subs(lambda = s[4], Dl));$

$w1 = -1.184089395;\ \ w2 = 0.8461051510;\ \ w3 = -0.7685726386;\ \ w4 = 0.5777613611$

3. The matrix K for each pole $\lambda_1 = s_n$ in (53) is calculated by the following way:
$ks1 := (i, j)- > coeff(convert(series(fk(i, j) * (lambda$
$-s[1])/w1 - subs(lambda = s[1], fk(i, j)) * (d1sl)/w1^2,$
$lambda = s[1], 3), polynom), lambda - s[1], 2) :$

$K[1] := matrix(4,4,ks1);$

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

$ks2 := (i,j)-> coeff(convert(series(fk(i,j)*(lambda$
$-s[2])/w2 - subs(lambda = s[2], fk(i,j))*(d1sl)/w2^2,$
$lambda = s[2], 3), polynom), lambda - s[2], 2):$
$K[2] := matrix(4,4,ks2);$

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

$ks3 := (i,j)-> coeff(convert(series(fk(i,j)*(lambda$
$-s[3])/w3 - subs(lambda = s[3], fk(i,j))*(d1sl)/w3^2,$
$lambda = s[3], 3), polynom), lambda - s[3], 2):$
$K[3] := matrix(4,4,ks3);$

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

$ks4 := (i,j)-> coeff(convert(series(fk(i,j)*(lambda$
$-s[4])/w4 - subs(lambda = s[4], fk(i,j))*(d1sl)/w4^2,$
$lambda = s[4], 3), polynom), lambda - s[4], 2):$
$K[4] := matrix(4,4,ks4);$

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

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 $Lp := \Lambda_0^\Theta$ of the operator L_0^Θ, which is obtained as a diagonal matrix combined of DN-maps (29) of the one-dimensional operators l_s (see [11]). Then the known dispersion equation ([14]) will be used for the operator $\mathcal{L}$.
Dirichlet-to-Neumann map $Lp := \Lambda_0^\Theta$:

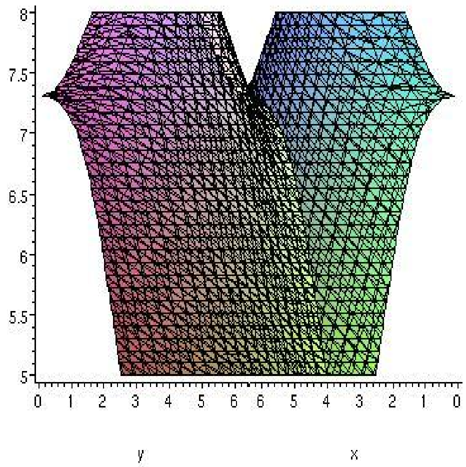
$g := sqrt(z)/sin(2*sqrt(z)):$
$Lp := matrix([[cos(2*sqrt(z))*g, (-cos(x) + I*sin(x))*g, 0, 0],$

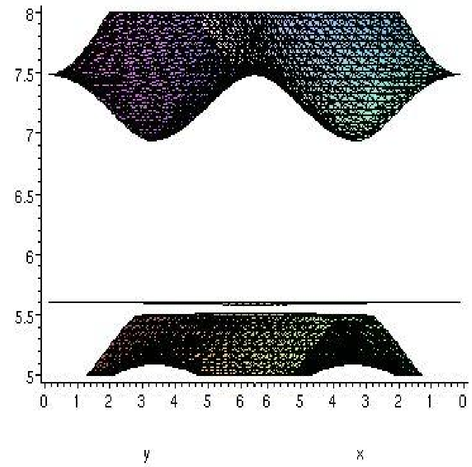
$[(-cos(x) - I * sin(x)) * g, cos(2 * sqrt(z)) * g, 0, 0],$
$[0, 0, cos(2 * sqrt(z)) * g, (-cos(y) + I * sin(y)) * g],$
$[0, 0, (-cos(y) - I * sin(y)) * g, cos(2 * sqrt(z)) * g]]);$

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

Dispersion equation for the operator $\mathcal{L}$:
$dpe := (cos(x) - cos(2 * sqrt(z)))/sin(2 * sqrt(z))$
$+(cos(y) - cos(2 * (Pi/5 + 1) * sqrt(z)))/sin(2 * (Pi/5 + 1) * sqrt(z)))$
$-15/2/sqrt(z) = 0;$

$$\frac{\cos x - \cos(2\sqrt{z})}{\sin(2\sqrt{z})} + \frac{\cos(y) - \cos(2(\pi/5+1))\sqrt{z}}{\sin(2(\pi/5+1)\sqrt{z})} = \frac{15}{2\sqrt{z}} \tag{55}$$





Fugure 1: $s_1 = 7.65$

4.1 Pole s_1.

The spectrum of the operator $\mathcal{L}_{K_1}$ in a neighbourhood of the point s_1 (Fig.1, left).

$lpk1 := (i,j) -> evalf((Lp[i,j] + K[1][i,j])):$

$LpK1 := matrix(4,4,lpk1):$

$F1 := subs(I = 0, simplify(det(LpK1))):$

$implicitplot3d(F1, x = 0..2*Pi, y = 0..2*Pi, z = 5..8, grid = [20,20,30]);$

The spectrum of the operator $\mathcal{L}$ in a neighbourhood of the point s_1 (Fig.1, right).

$implicitplot3d(dpe, x = 0..2*Pi, y = 0..2*Pi, z = 5..8, grid = [30,30,50]);$

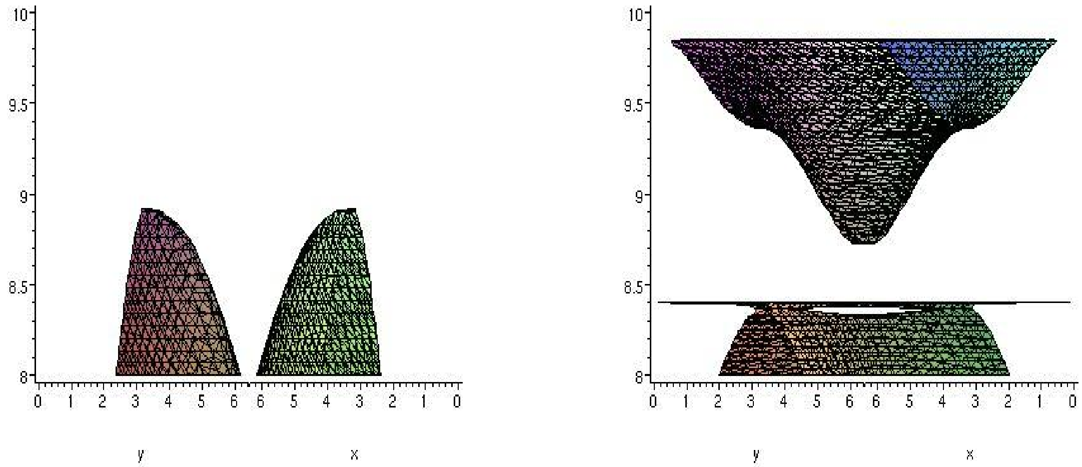


Figure 2: $s_2 = 9.87$

4.2 Pole s_2.

The spectrum of the operator $\mathcal{L}_{K_2}$ in a neighbourhood of the point s_2 (Fig.2, left).

$lpk2 := (i, j)- > evalf((Lp[i, j] + K[2][i, j])) :$

$LpK2 := matrix(4, 4, lpk2) :$

$F2 := subs(I = 0, simplify(det(LpK2))) :$

$implicitplot3d(F2, x = 0..2 * Pi, y = 0..2 * Pi, z = 8..10, grid = [30, 30, 30]);$

The spectrum of the operator $\mathcal{L}$ in a neighbourhood of the point s_1 (Fig.2, right).

$implicitplot3d(dpe, x = 0..2 * Pi, y = 0..2 * Pi, z = 8..10, grid = [20, 20, 50]);$

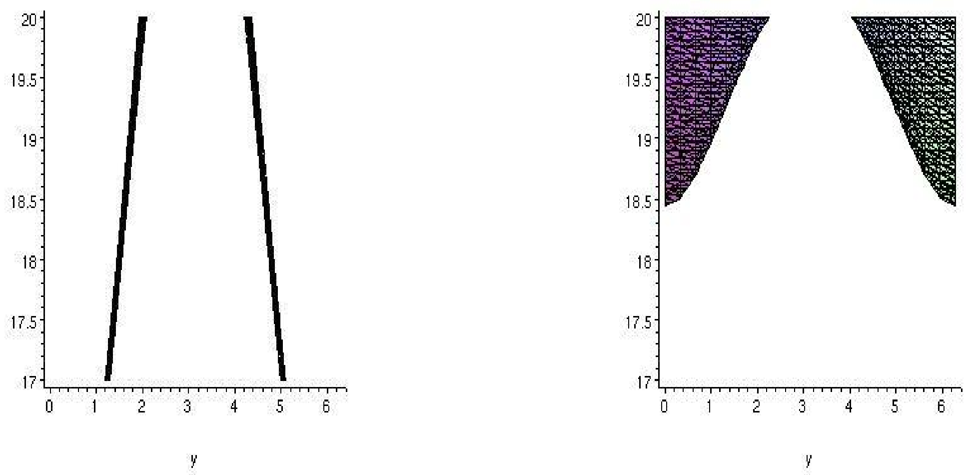


Figure 3: $s_3 = 18.58$

4.3 Pole s_3.
The spectrum of the operator $\mathcal{L}_{K_3}$ in a neighbourhood of the point s_3 (Fig.3, left).

$lpk3 := (i,j)->evalf((Lp[i,j] + K[3][i,j]))$:

$LpK3 := matrix(4,4,lpk3)$:

$F3 := subs(I = 0, simplify(det(LpK3)))$:

$implicitplot3d(F3, x = 0..2*Pi, y = 0..2*Pi, z = 17..20, grid = [20,20,150])$;

The spectrum of the operator $\mathcal{L}$ in a neighbourhood of the point s_3 (Fig.3, right).

$implicitplot3d(dpe, x = 0..2*Pi, y = 0..2*Pi, z = 17..20, grid = [20,20,50])$;

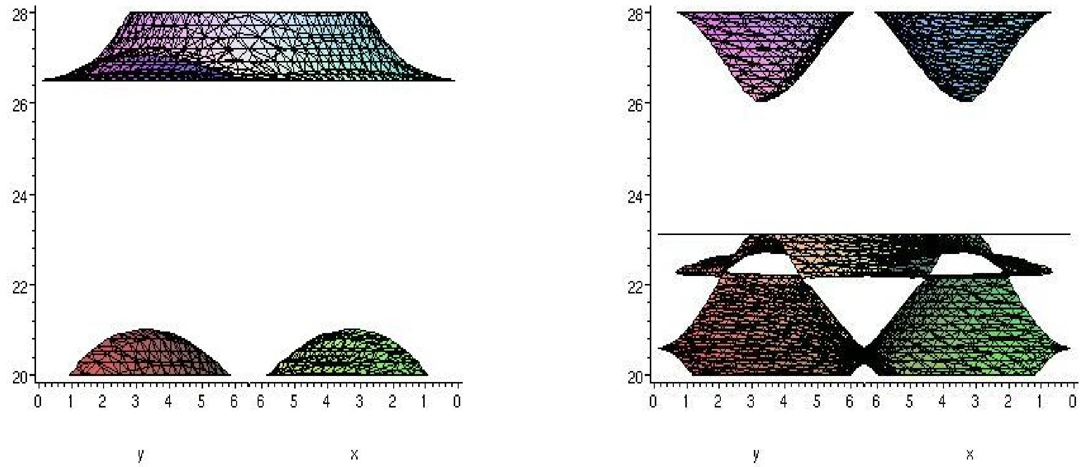


Figure 4: $s_4 = 25$

4.4 Pole s_4.

The spectrum of the operator $\mathcal{L}_{K_4}$ in a neighbourhood of the point s_4 (Fig.4, left).

$lpk4 := (i,j)-> evalf((Lp[i,j] + K[4][i,j])):$

$LpK4 := matrix(4,4,lpk4):$

$F4 := subs(I = 0, simplify(det(LpK4))):$

$implicitplot3d(F4, x = 0..2 * Pi, y = 0..2 * Pi, z = 20..28, grid = [20, 20, 30]);$

The spectrum of the operator $\mathcal{L}$ in a neighbourhood of the point s_1 (Fig.4, right; Fig.5).

$implicitplot3d(dpe, x = 0..2 * Pi, y = 0..2 * Pi, z = 20..28, grid = [20, 20, 50]);$

$implicitplot3d(dpe, x = 0..2 * Pi, y = 0..2 * Pi, z = 23.2..23.3, grid = [20, 20, 250]);$

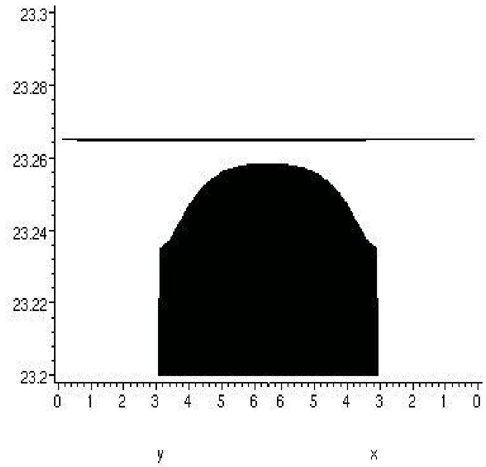


Figure 5: $s_4 = 25$

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