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Quantum Lorentz Gas: Effective Equations and Spectral Analysis

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Abstract—We consider the quantum Lorentz gas (QLG) in the plane. We show that the spectral properties of the quantum Lorentz gas can be obtained from the study of a homogeneous system of one-dimensional integral equations. The qualitative spectral analysis is performed, and the spectrum is shown to have a band structure. The wave functions in the complete configuration space can be constructed in terms of the solutions of the obtained effective equations. We apply the obtained result to a simpler Lorentz gas model including additional symmetry.

Keywords—Quantum Lorentz gas, Spectral analysis.

1. LORENTZ GAS WITH PERIODIC CONFIGURATION OF SCATTERERS AND BOUNDARY VALUE PROBLEM FOR LAPLACIAN

We treat the quantum Lorentz gas (QLG) as a quantum scattering problem in $\mathbf{R}^2$ with eliminated scatterers (disks) of the radius R. We assume that the configuration of scatterers is invariant under the discrete subgroup $\mathcal{G}$ with a compact fundamental domain of the group of all translations of the plane. We consider such subgroup $\mathcal{G}$ for which disks form a hexagonal lattice (see Figure 1) with interdisk distance d.

The Hamiltonian for a particle with mass m is given by the Laplacian

$$H = -\frac{\hbar^2}{2m}\Delta$$

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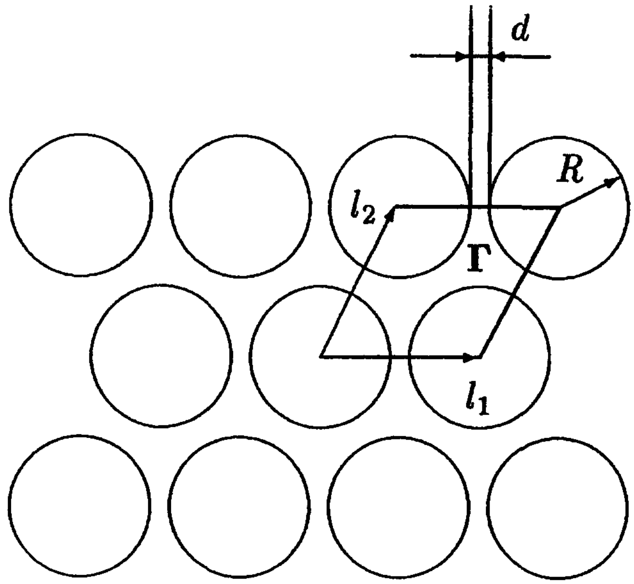

Figure 1. Lorentz billiard and fundamental domain Γ.

acting in the Hilbert space $\mathcal{H} = L^2(\mathbf{R}^2\backslash\widehat{\Omega})$ on the domain

$$D(H) = \left\{\Psi \in \mathcal{H} : \Psi \in W_2^2\left(\mathbf{R}^2\backslash\widehat{\Omega}\right) \text{ and } \Psi|_{\partial\widehat{\Omega}} = 0\right\}.$$

Here, $\widehat{\Omega}$ stands for the union of the disks and $\partial\widehat{\Omega}$ is the union of their boundaries.

The spectral problem for H,

$$H\Psi = z\Psi, \tag{1}$$

is the Schrödinger equation for quantum particles moving in the QLG. Since the fundamental domain Γ is a rhombus (see Figure 1), it covers the plane $\mathbf{R}^2$ and can be treated as a unit lattice cell. Let the two vectors l_1, l_2 be the basic vectors of the correspondent lattice $\mathcal{L}_\Delta$. Due to the Bloch theorem [1], a solution of the original spectral problem (1) can be represented in the quasiperiodic form

$$\Psi(x) = e^{i\langle\theta,x\rangle}u(x), \tag{2}$$

where $u(x)$ is a periodic function with respect to the lattice $\mathcal{L}_\Delta$:

$$u(x + m_1l_1 + m_2l_2) = u(x), \qquad x \in \mathbf{R}^2\backslash\widehat{\Omega}, \quad m_1, m_2 \in \mathbf{Z}, \tag{3}$$

and the quasimomentum vector θ varies in the Brillouin zone $\mathcal{B}_\theta$.

As in solid state physics, the basic vectors b_1, b_2 of the inverse lattice are determined as [1]

$$\langle b_j, l_p\rangle = 2\pi\delta_{jp}, \tag{4}$$

where δ_{jp} is the Kronecker symbol. An arbitrary vector $\theta \in \mathcal{B}_\theta$ can be represented as

$$\theta = \sum_{j=1,2} \gamma_j b_j, \qquad \gamma_j \in [0,1). \tag{5}$$

From equations (4),(5), it follows that

$$\theta_p \equiv \langle\theta, l_p\rangle \in [0, 2\pi), \qquad \text{for all } \theta \in \mathcal{B}_\theta. \tag{6}$$

If we introduce the shift operator T_p with respect to the basic lattice vector l_p, then by formulas (2) and (3), the wave function $\Psi(x)$ in a rhombus $\Gamma_{m_1m_2} = T_1^{m_1}T_2^{m_2}\Gamma$ is given by

$$\Psi(x + m_1l_1 + m_2l_2) = e^{im_1\theta_1}e^{im_2\theta_2}\Psi(x), \qquad x \in \Gamma. \tag{7}$$

Using equation (2), we have the following expression for the partial derivative of $\Psi(x)$ with respect to x_m:

$$\partial_{x_m}\Psi(x) = \left(i\partial_{x_m}\langle\theta,x\rangle u(x) + \partial_{x_m}u(x)\right)e^{i\langle\theta,x\rangle}.$$

As the inner product $\langle\theta,x\rangle$ is a linear function of x, all its partial derivatives $\partial_{x_m}\langle\theta,x\rangle$ do not depend on $x=(x_1,x_2)$. Hence, using equation (3), we have

$$\partial_{x_m}\Psi\left(x+l_p\right) = e^{i\theta_p}\partial_{x_m}\Psi(x).$$

Let ∂_n be the normal derivative operator on the part of the boundary $\partial\Gamma\backslash\partial\widehat{\Omega}$ of the unit cell Γ. Since ∂_n is a linear combination from ∂_{x_m}, it follows by the latter equality that

$$\partial_n\Psi\left(s+l_p\right) = -e^{i\theta_p}\partial_n\Psi(s), \qquad s\in\partial\Gamma\backslash\partial\widehat{\Omega}, \tag{8}$$

where the sign "$-$" is generated by the opposite direction of the external normal n in the points s and $s+l_p$.

Using the properties of Ψ stated above and equations (2), (3), (6), and (8), one can reduce the spectral problem for the QLG with quasiperiodic boundary conditions to the following boundary value problem:

$$-\frac{\hbar^2}{2m}\Delta\psi = z\psi, \tag{9a}$$

$$\psi|_{\partial\Omega_0} = 0, \tag{9b}$$

$$\psi|_{\partial\Omega_{p+2}} = e^{i\theta_p}\psi|_{\partial\Omega_p}, \qquad p=1,2, \tag{9c}$$

$$\partial_n\psi|_{\partial\Omega_{p+2}} = -e^{i\theta_p}\partial_n\psi|_{\partial\Omega_p}, \qquad p=1,2, \tag{9d}$$

where the parts $\partial\Omega_j$ of the boundary $\partial\Omega$ are shown in Figure 2 and quasimomentum components θ_p vary in the interval $\theta_p\in[0,2\pi)$. The boundary value problem (9) determines solutions of the original spectral problem (1) in the subspace with fixed quasimomentum $\theta\in\mathcal{B}_\theta$ determined by its components θ_1, θ_2.

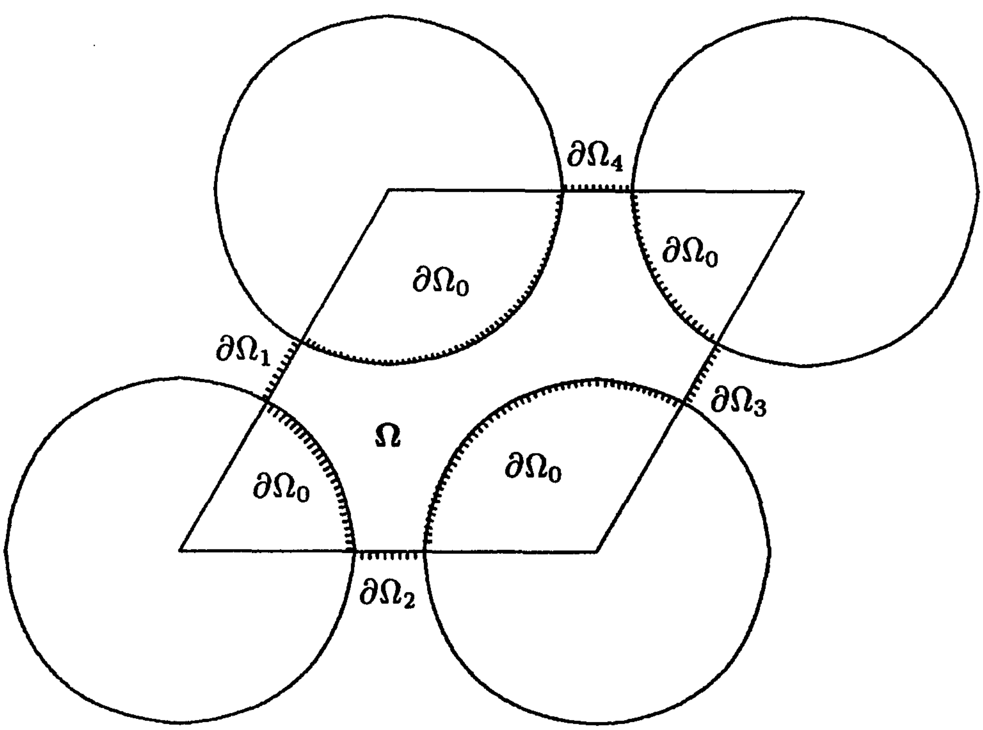

Figure 2. Domain Ω and parts of its boundary $\partial\Omega_p$.

2. FIBERING OF THE HAMILTONIAN AND EFFECTIVE EQUATIONS

In this section, we construct a decomposition of the original Hamiltonian H into a direct integral over the Brillouin zone $\mathcal{B}_\theta$. The spectral problem for the each fiber of the Hamiltonian parametrized by the quasimomentum components θ_1, θ_2 turns out to be equivalent to the boundary value problem (9). That means that one can solve a set of boundary value problems varying the parameters θ_1, θ_2 and in this way obtain the spectrum and eigenfunctions of the original Hamiltonian H. We are going to demonstrate that the spectrum of the QLG problem is continuous and, in the general case, has a band structure, whereas in each fiber, we have a discrete spectrum. The discrete spectrum obtained for the similar system in [2] is related to the fact that only one fiber (fixed by the quasimomentum $\theta = 0$) was considered.

Next, we are going to consider the boundary value problem (9) with some arbitrary fixed parameters θ_1, θ_2. Using the potential theory methods, we construct one-dimensional integral equation for densities on the boundary $\partial\Omega$ in which terms a wave function can be reconstructed. It turns out to be convenient to rewrite this equation in the form of a homogeneous system of five one-dimensional integral equations, which can serve as a base for the numerical investigation of the problem. We are to show that for the finite values of the interdisk distance ($d > 0$), the kernels of those equations are well defined. The eigenvalues of that homogeneous system coincide with the eigenvalues of the boundary value problem (9), and the correspondent eigenfunctions allow us to calculate the wave functions of the original QLG.

Returning to the problem in question, let us mention that the boundary value problem (9) is equivalent to the spectral problem for the operator

$$H_{\theta_1\theta_2} = -\frac{\hbar^2}{2m}\Delta_\Omega$$

in the space $L^2(\Omega)$ with the domain $D_{\theta_1\theta_2}$ determined by the boundary conditions (9b)–(9d) as follows:

$$D_{\theta_1\theta_2} = \left\{\psi \in W_2^2(\Omega) : \text{conditions (9b)–(9d) are valid}\right\}.$$

In terms of the two-parametric family of the operators $H_{\theta_1\theta_2}$, $\theta_p \in [0, 2\pi)$, the original operator H can be represented as the direct integral

$$H = \int_0^{2\pi}\int_0^{2\pi} \oplus H_{\theta_1\theta_2}\, d\theta_1\, d\theta_2. \tag{10}$$

Then the spectrum of the operator H is the union of spectra of the operators $H_{\theta_1\theta_2}$:

$$\sigma(H) = \bigcup_{\theta_1,\theta_2\in[0,2\pi)} \sigma\left(H_{\theta_1\theta_2}\right). \tag{11}$$

The operators $H_{\theta_1\theta_2}$ are determined on the compact domain Ω, thus their spectra are discrete. Varying the parameters $\theta_1, \theta_2 \in [0, 2\pi)$, we obtain in accordance with equation (11) in the general case the band spectrum of the operator H.

Thus, one can restrict the consideration to the spectral analysis of the fibers of the operator H which are the self-adjoint operators $H_{\theta_1\theta_2}$,

$$H_{\theta_1\theta_2}\psi = z\psi, \tag{12}$$

i.e., to the solution of the boundary problem (9). The wave function $\Psi(x)$ of the Hamiltonian H in $\mathbf{R}^2\backslash\widehat{\Omega}$ is reconstructed in terms of the correspondent eigenfunction $\psi(x)$ of the fiber operator $H_{\theta_1\theta_2}$ via equation (7).

It will prove convenient to define the scaled energy λ by

$$\lambda = \frac{2mz}{\hbar^2}.$$

It means that in the classical limit $\hbar \to 0$, we have $\lambda \to \infty$.

Let $G(x, x'; \lambda)$ be the Green function of the Laplacian $-\Delta$ in $\mathbf{R}^2$ which corresponds to the outgoing boundary condition at infinity. It is given by the Hankel function [3]

$$G(x, x', \lambda) = -\frac{i}{4} H_0^{(1)} \left(\sqrt{\lambda}\, |x - x'|\right). \tag{13}$$

We denote the solution of the boundary problem (9) (which is equivalent to the spectral problem (12)) as $\psi(x)$ and use the Green identity:

$$\iint_\Omega [\psi(x')(\Delta + \lambda)G(x, x'; \lambda) - G(x, x'; \lambda)(\Delta + \lambda)\psi(x')]\, d^2x'$$
$$= \int_{\partial\Omega} [\psi(s')\partial_n G(x, s'; \lambda) - G(x, s'; \lambda)\partial\psi(s')]\, ds'.$$

Due to the property of the Green function,

$$(-\Delta - \lambda)G(x, x'; \lambda) = \delta(x - x'),$$

we obtain the following equality valid for any internal point $x \in \Omega$:

$$\psi(x) = \int_{\partial\Omega} [G(x, s'; \lambda)\partial_n \psi(s') - \psi(s')\partial_n G(x, s'; \lambda)]\, ds'. \tag{14}$$

Let us consider a limit $\Omega \ni x \to \partial\Omega$ in the equality (14). For any $d > 0$, the Radon theorem [4] provides the existence of the limit values in the right-hand side of the equality (14). Really the Green function $G(s, s'; \lambda)$, $s, s' \in \partial\Omega$, has a weak singularity $\ln|s - s'|$ in the point $s = s'$, so the correspondent integral converges in the usual sense. The function $\partial_n G(s, s'; \lambda)$ in the vicinity of the point $s = s'$ can be represented as

$$\partial_n G(s, s'; \lambda) = \text{Const} \frac{\cos(n, s - s')}{|s - s'|} (1 + o(1)),$$

where n is the normal vector. Hence, the function $\partial_n G(s, s'; \lambda)$ is singular only in the vicinity of the angle points $s = s' = s_0$ of the boundary $\partial\Omega$ (see Figure 3). Near the angle point $s = s' = s_0$, the function $\cos(n, s - s')$ does not vanish, so we have a singularity of the kernel. It can be calculated [4] that in the vicinity of such points, the limit value of the principal integral does exist and is equal to

$$\lim_{\varepsilon \downarrow 0} \lim_{x \to s_0 \in \partial\Omega} \int_{s_0 - \varepsilon}^{s_0 + \varepsilon} \frac{\cos(n, x - s')}{|x - s'|}\, ds' = \pi - \alpha, \qquad \alpha > 0,$$

where $\alpha > 0$ is the opening of the angle (see Figure 3). Notice, that in our domain Ω in all the angle points s_0, we have $\alpha = \pi/2$.

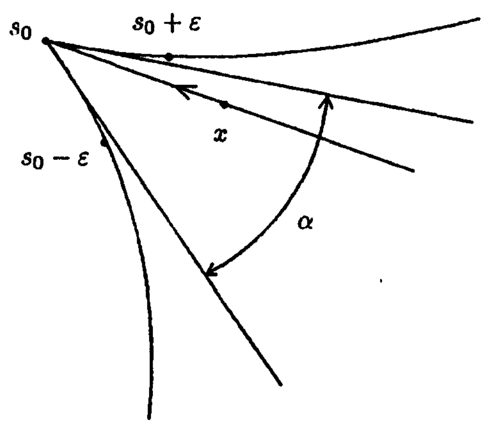

Figure 3. Illustration for the calculation of integral (14) in the vicinity of the angle point $s' = s_0$, $x \to s_0$.

Thus, one can consider the limit $x \to \partial\Omega$ in the equality (14) and obtain the following equation:

$$\psi(s) = \int_{\partial\Omega} [G(s,s';\lambda)\partial_n\psi(s') - \psi(s')\partial_n G(s,s';\lambda)]\, ds', \tag{15}$$

where $s \in \partial\Omega$.

Let us introduce the notations

$$\begin{aligned} \psi_j(s) &= \psi|_{\partial\Omega_j}, && j = 0,1,\ldots,4, \\ \varphi_j(s) &= \partial_n\psi|_{\partial\Omega_j}, && j = 0,1,\ldots,4, \end{aligned}$$

and rewrite the boundary conditions (9c),(9d) in the form

$$\psi_{p+2}(s+l_p) = e^{i\theta_p}\psi_p(s), \qquad p = 1,2, \tag{16a}$$

$$\varphi_{p+2}(s+l_p) = -e^{i\theta_p}\varphi_p(s), \qquad p = 1,2, \tag{16b}$$

respectively.

Now one can rewrite equation (15) as a homogeneous system of integral equations for five independent functions φ_0, φ_1, φ_2, ψ_1, ψ_2. The functions φ_p, ψ_p are determined on $\partial\Omega_p$. Using the boundary conditions (9a) and (16), we rewrite equation (15) as follows:

$$\begin{aligned} &\int_{\partial\Omega_0} G(s,s';\lambda)\varphi_0(s')\, ds' + \sum_{p=1,2}\int_{\partial\Omega_p} \left[G(s,s';\lambda) - e^{i\theta_p}G(s,s'+l_p;\lambda)\right]\varphi_p(s')\, ds' \\ &\quad - \sum_{p=1,2}\int_{\partial\Omega_p} \left[\partial_n G(s,s';\lambda) + e^{i\theta_p}\partial_n G(s,s'+l_p;\lambda)\right]\psi_p(s')\, ds' = w_{\theta_1\theta_2}(s), \end{aligned} \tag{17}$$

where

$$w_{\theta_1\theta_2}(s) = \begin{cases} 0, & s \in \partial\Omega_0, \\ \psi_1(s), & s \in \partial\Omega_1, \\ \psi_2(s), & s \in \partial\Omega_2, \\ e^{i\theta_1}\psi_1(s), & s \in \partial\Omega_3, \\ e^{i\theta_2}\psi_2(s), & s \in \partial\Omega_4. \end{cases}$$

It is convenient to define $l_q = 0$ if $q \le 0$, while l_1, l_2 are the basic lattice vectors. We introduce the integral operators $A_{pq}(\lambda)$ acting from the space $L(\partial\Omega_q)$ (for $q = 0,1,2$) or from $L(\partial\Omega_{q-2})$ (for $q = 3,4$) into the space $L(\partial\Omega_p)$ (for $p = 0,1,2$) or into $L(\partial\Omega_{p-2})$ (for $p = 3,4$). Their kernels are as follows:

$$\begin{aligned} A_{p0}(s,s';\lambda) &= G(s+l_{p-2},s';\lambda), \\ A_{pq}(s,s';\lambda) &= G(s+l_{p-2},s';\lambda) - e^{i\theta_q}G(s+l_{p-2},s'+l_q;\lambda), && q = 1,2, \\ A_{pq}(s,s';\lambda) &= -\partial_n G(s+l_{p-2},s';\lambda) - e^{i\theta_{q-2}}G(s+l_{p-2},s'+l_{q-2};\lambda), && q = 3,4. \end{aligned}$$

Here $s' \in \partial\Omega_q$ for $q = 0,1,2$, $s' \in \partial\Omega_{q-2}$ for $q = 3,4$, and $s \in \partial\Omega_p$ for $p = 0,1,2$, $s \in \partial\Omega_{p-2}$ for $p = 3,4$. We denote as Φ the vector-function

$$\Phi = (\varphi_0,\varphi_1,\varphi_2,\psi_1,\psi_2)^\top.$$

One can see that the following relation is valid:

$$W \equiv \left(0,\psi_1,\psi_2,e^{i\theta_1}\psi_1,e^{i\theta_2}\psi_2\right)^\top = B\Phi, \tag{18}$$

where B stands for the 5×5 matrix

$$B = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & e^{i\theta_1} & 0 \\ 0 & 0 & 0 & 0 & e^{i\theta_2} \end{pmatrix}.$$

Using the relation (18), equation (17) can be rewritten in terms of the matrix B and the operator-valued matrix $A(\lambda) = \{A_{pq}(\lambda)\}_{p,q=0}^{4}$ as the following homogeneous system:

$$(A(\lambda) - B)\,\Phi = 0. \tag{19}$$

Points $z = (\hbar^2/2m)\lambda \in \mathbf{C}$ for which equation (19) has a nontrivial solution Φ coincide with the (discrete) spectrum of the fiber operator $H_{\theta_1\theta_2}$, and the correspondent eigenfunctions $\psi(x)$ can be reconstructed in terms of the vector-function Φ with the help of the equality (14). Thus, equation (19) is an appropriate tool for the spectral analysis of the operator $H_{\theta_1\theta_2}$ and, due to the equality (11), of the original Hamiltonian H. Points $z = (\hbar^2/2m)\lambda \in \sigma(H_{\theta_1\theta_2})$ of the operators $H_{\theta_1\theta_2}$ spectra are unified in the band spectrum of the operator H in accordance with the equality (11).

3. A SIMPLE QUANTUM LORENTZ GAS

The obtained system of effective equations being a possible tool for numerical investigation of the QLG has, however, essential numerical difficulties. Some of them are related to the fact that we have a two-parameter set of boundary value problems. The calculations are simplified if we assume the additional symmetry of the wave function with respect to the rotation by the angle $2\pi/3$. This assumption allows us to obtain the one-parameter set of the effective equations instead of the two-parameter in the general case.

The additional symmetry gives the possibility of considering a curvilinear "triangle" ω being a half of the domain Ω instead of Ω (see Figure 4). In the first step, we are not interested in the wave function inside the curvilinear "triangles" and formally substitute the nodes of the hexagonal graph (see Figure 5) for these triangles. Then we obtain the hexagonal graph where each node is linked with three neighboring nodes. We construct a model link between the neighbouring "triangles" simulated by the nodes of the hexagonal graph. This link, in the most simple and natural way, can be realized as follows. It is convenient to redraw the hexagonal graph into the topologically equivalent graph P shown in Figure 6. That is possible because, in the present step, we consider only the links between the nodes, and the location of the graph on the plane has no significance. We can enumerate the nodes of the graph P by the pairs of integer numbers (m, n), so it can be realized as $\mathbf{Z}^2$. Consider the Hilbert space $l_2(\mathbf{Z}^2)$, $\vec{f} = \{f_{mn}\} \in l_2(\mathbf{Z}^2)$, $f_{mn} \in \mathbf{C}$. The operator F connecting each node with three neighboring nodes is chosen in the form

$$(Ff)_{mn} = f_{m-1,n} + f_{m+1,n} + f_{m,n+\sigma}, \qquad \sigma = (-1)^{m+n}. \tag{20}$$

Obviously, the operator F is self-adjoint, $F = F^*$ in $l_2(\mathbf{Z}^2)$. In order to perform the spectral analysis of the operator F and calculate its wave functions, let us use its Fourier transformation, acting in the Hilbert space $L_2(\mathbf{T}^2)$ on the two-dimensional torus $\mathbf{T}^2$. The element $f \in l_2(\mathbf{Z}^2)$ in this representation turns into

$$f(\xi, \eta) = \sum_{m,n} f_{mn} e^{im\xi} e^{in\eta}. \tag{21}$$

Next, we decompose the space $L_2(\mathbf{T}^2)$ into the orthogonal sum

$$L_2\left(\mathbf{T}^2\right) = L_2^+\left(\mathbf{T}^2\right) \oplus L_2^-\left(\mathbf{T}^2\right),$$

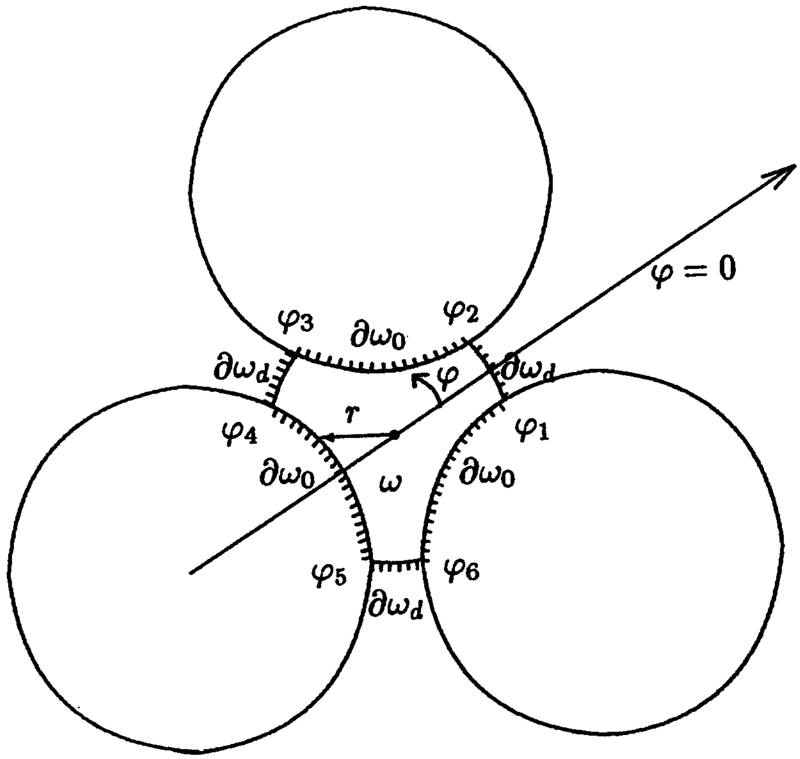

Figure 4. Curvilinear "triangle" ω and parametrization of its boundary $\partial\omega : r = R(\varphi)$.

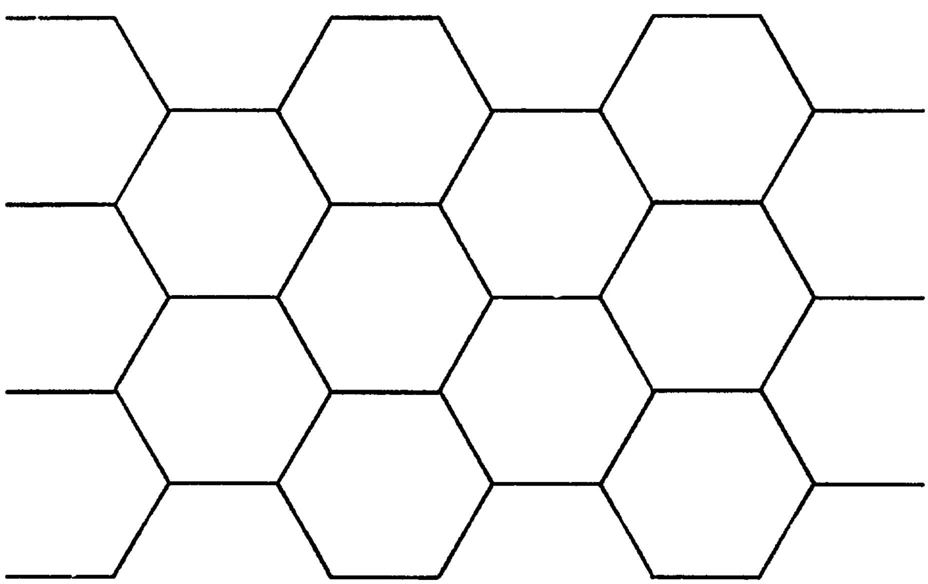

Figure 5. Hexagonal graph. Each node simulates one copy of the "triangle" ω.

where $L_2^+(\mathbf{T}^2)$ consists of the functions $f(\xi,\eta) \in L_2(\mathbf{T}^2)$, where Fourier coefficients $f_{mn} = 0$ if $\sigma = (-1)^{m+n} < 0$. In a similar way for $f(\xi,\eta) \in L_2^-(\mathbf{T}^2)$, the coefficients $f_{mn} = 0$ if $\sigma = (-1)^{m+n} > 0$. Thus, the representation of $\vec{f}$ is given by the vector-function $(f^+(\xi,\eta), f^-(\xi,\eta))^\top$,

$$f^+(\xi,\eta) = \sum_{m,n:\sigma>0} f_{mn} e^{im\xi} e^{in\eta} \in L_2^+\left(\mathbf{T}^2\right),$$

$$f^-(\xi,\eta) = \sum_{m,n:\sigma<0} f_{mn} e^{im\xi} e^{in\eta} \in L_2^-\left(\mathbf{T}^2\right).$$

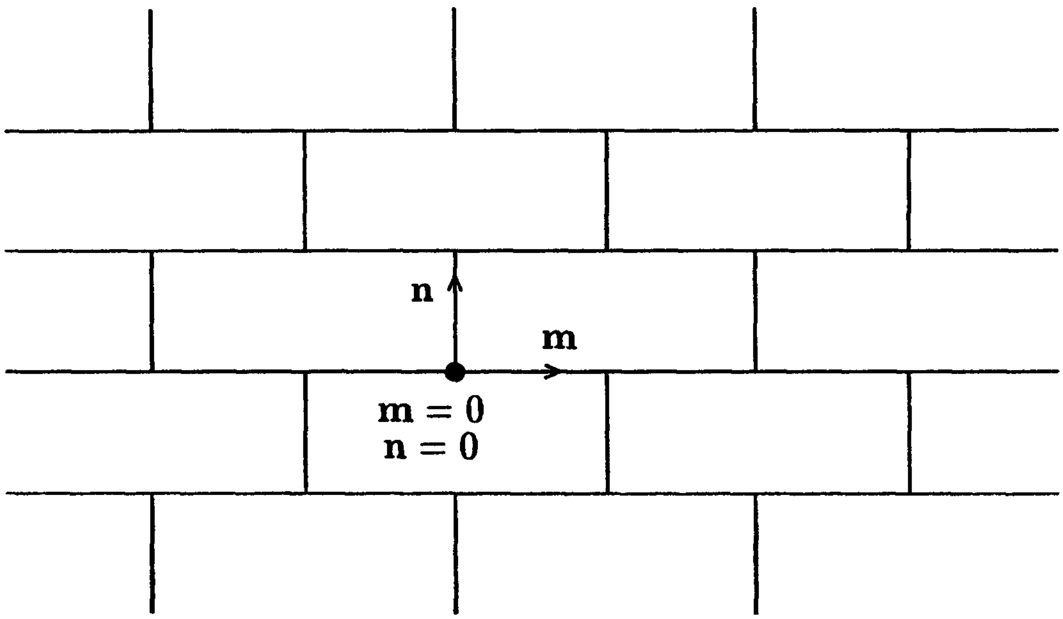

Figure 6. Redrawn hexagonal graph P and parametrization of its nodes.

It can be easily calculated that the representation $\widehat{F}$ of the operator F in the space $L_2^+(\mathbf{T}^2) \oplus L_2^-(\mathbf{T}^2)$ is given by the matrix-operator of multiplication by the matrix-valued function

$$\widehat{F} = \begin{pmatrix} 0 & \overline{\zeta}(\xi,\eta) \\ \zeta(\xi,\eta) & 0 \end{pmatrix}, \tag{22}$$

where the function $\zeta(\xi,\eta)$ is given by the formula

$$\zeta(\xi,\eta) = 2\cos\xi + e^{i\eta}. \tag{23}$$

The spectrum of the operator $\widehat{F}$ coincides with the union of images of the functions $\mu(\xi,\eta) = \pm|\zeta(\xi,\eta)|$, $\xi,\eta \in (-\pi,\pi]$. One can ensure that this is an absolutely continuous spectrum $\sigma(\widehat{F}) = [-3,3]$. The wave functions are parameterized by the points of the torus $Q = (\xi_0,\eta_0) \in \mathbf{T}^2$ and the sign of the point of spectrum $\mu = \pm|\zeta(Q)|$. These wave functions are $(f^+_{(\pm)Q}, f^-_{(\pm)Q})^{\mathrm{T}}$,

$$\begin{aligned} f^+_{(\pm)Q}(\xi,\eta) &= \frac{1}{\sqrt{2}}\delta(\xi-\xi_0)\delta(\eta-\eta_0), \\ f^-_{(\pm)Q}(\xi,\eta) &= \pm\frac{1}{\sqrt{2}}e^{i\psi(Q)}\delta(\xi-\xi_0)\delta(\eta-\eta_0), \end{aligned} \tag{24}$$

where δ stands for delta-function, $\psi(Q) = \arg\zeta(Q)$, and the correspondent spectral point is $\mu_\pm(Q) = \pm|\zeta(Q)|$. Above, the following representation of the complex plane ζ is used (see Figure 7):

$$\zeta = |\mu|e^{i\psi}. \tag{25}$$

Returning back to the representation F in the space $l_2(\mathbf{Z}^2)$, we have

$$\begin{aligned} \sigma(F) &= \sigma\left(\widehat{F}\right) = [-3,3], \\ \left(f_{(\pm)Q}\right)_{mn} &= \frac{1}{2\pi}\iint_{\mathbf{T}^2} d\xi\, d\eta\, f^+_{(\pm)Q}(\xi,\eta)e^{-im\xi}e^{-in\eta} \\ &= \frac{1}{2\sqrt{2}\pi}e^{-im\xi_0}e^{-im\eta_0}, \qquad (-1)^{m+n} > 0, \\ \left(f_{(\pm)Q}\right)_{mn} &= \pm\frac{1}{2\sqrt{2}\pi}e^{i\psi(Q)}e^{-im\xi_0}e^{-im\eta_0}, \qquad (-1)^{m+n} < 0. \end{aligned} \tag{26}$$

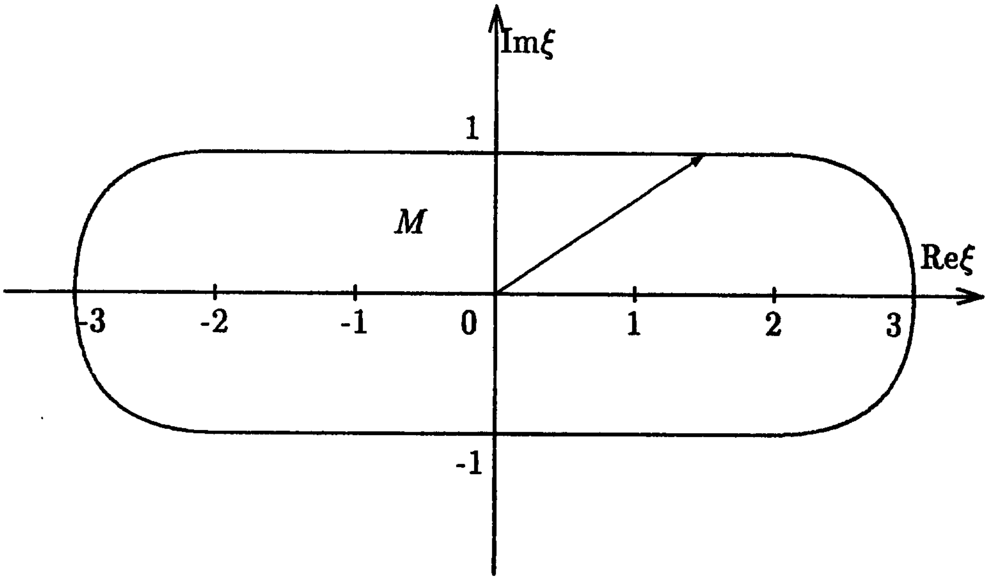

Figure 7. Image M of the torus $\mathbf{T}^2$ on the complex plane ζ, $M = \zeta(\mathbf{T}^2)$.

Every point of the spectrum $\mu \in \sigma(F)$ (except $\mu = \pm 3$) is of infinite-order degeneration. Really, let us consider some point $Q = (\xi_0, \eta_0) \in \mathbf{T}^2$ and the correspondent wave function $\vec{f}_{(\operatorname{sign}\mu)Q} = \{(f_{(\operatorname{sign}\mu)Q})_{mn}\}$. The function $\zeta(Q) = 2\cos\xi_0 + e^{i\eta_0}$ maps the torus $\mathbf{T}^2$ onto the region M on the complex plane ζ (see Figure 7). The inverse mapping $\zeta \to Q(\zeta)$, $\zeta = |\mu|e^{i\psi}$, has four different images $Q_j(|\mu|, \psi) = (\xi_0^j, \eta_0^j)$, $j = 1, \dots, 4$:

$$\begin{aligned} \xi_0^j &= \cos^{-1}\left[\frac{1}{2}\left(|\mu|\cos\psi - \cos\left[\sin^{-1}(|\mu|\sin\psi)\right]\right)\right], \\ \eta_0^j &= \sin^{-1}(|\mu|\sin\psi), \end{aligned} \tag{27}$$

where different indices j correspond to different choices of the function $\sin^{-1} t$, $\cos^{-1} t$ values:

$$\begin{aligned} j = 1 &: \cos^{-1} t \in [0, \pi), & \sin^{-1} t &\in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right), \\ j = 2 &: \cos^{-1} t \in [-\pi, 0), & \sin^{-1} t &\in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right), \\ j = 3 &: \cos^{-1} t \in [0, \pi), & \sin^{-1} t &\in \left[-\pi, -\frac{\pi}{2}\right) \cup \left[\frac{\pi}{2}, \pi\right), \\ j = 4 &: \cos^{-1} t \in [-\pi, 0), & \sin^{-1} t &\in \left[-\pi, -\frac{\pi}{2}\right) \cup \left[\frac{\pi}{2}, \pi\right). \end{aligned} \tag{28}$$

For any j, all the points $(\xi_0^j, \eta_0^j) = Q_j(\zeta) = Q_j(|\mu|, \psi)$ such that $\zeta(Q_j)$ lie on the arcs given by $M \cap \{\zeta : |\zeta| = |\mu|\}$ (see Figure 7) correspond to the same value of the spectral parameter μ or $-\mu$. It means that all the wave functions $\vec{f}_{(\operatorname{sign}\mu)Q_j(|\mu|,\psi)}$ satisfy the equation

$$(F - \mu)\vec{f}_{(\operatorname{sign}\mu)Q_j(|\mu|,\psi)} = 0, \tag{29}$$

for any index $j = 1, \dots, 4$ and any angle $\psi \in \omega(|\mu|) = [-\phi(|\mu|), \phi(|\mu|)] \cup [\pi - \phi(|\mu|), \pi + \phi(|\mu|)]$ (see Figure 7). Hence, all the points $\mu \in (-3, 3)$ are indeed the points of the operator F spectrum of infinite order degeneration.

Thus, the spectral problem for the operator F is completely solved.

Note, that in the above, we have characterized the $(m,n)^{\text{th}}$ node of the hexagonal graph simulating the curvilinear "triangle" by the only complex-valued parameter $f_{mn} \in \mathbf{C}$. That is the consequence of the supposed above symmetry which allows us not to distinguish different "angles" of the "triangle" ω.

Now we consider the total model Hamiltonian acting in the Hilbert space $\mathcal{H}_F = l_2(\mathbf{Z}^2, L_2(\omega))$. We define this Hamiltonian as

$$H_F = \left(-\frac{\hbar^2}{2m}\Delta\right) \otimes I,$$

where I stands for the unit operator in $l_2(\mathbf{Z}^2)$, with the domain

$$D(H_F) = l_2\left(\mathbf{Z}^2, W_2^2(\omega)\right) \cap \{\vec{u}(x) : \vec{u}|_{\partial\omega_0} = 0,\ \vec{u}|_{\partial\omega_d} = F\partial_n \vec{u}|_{\partial\omega_d}\}.$$

Here $\vec{u}(x) = \{u_{mn}(x)\} \in \mathcal{H}_F$, $u_{mn}(x)$ is determined in the $(m,n)^{\text{th}}$ copy of the curvilinear "triangle" ω, ∂_n stands for the (external) normal derivative operator, and $\partial\omega_0$, $\partial\omega_d$ are the parts of the boundary $\partial\omega$ shown in Figure 4. On the boundaries $\partial\omega_0$ of the disks, we have the Dirichlet boundary conditions, and the links of the neighboring curvilinear "triangles" on the splits $\partial\omega_d$ are determined by the operator F described in the previous section.

Let us consider the Hamiltonian H_F in the spectral representation of the operator F. In accordance with equation (26), the wave functions of the operator F are parameterized by the points of the torus $Q \in \mathbf{T}^2$ and by the sign of the correspondent eigenvalue, i.e., the uniformized spectral surface is $\mathbf{T}^2 \oplus \mathbf{T}^2$. These functions form an orthonormal basis in the space $l_2(\mathbf{Z}^2)$. We turn the space $\mathcal{H}_F$ into $\widehat{\mathcal{H}}_F = L_2(\mathbf{T}^2 \oplus \mathbf{T}^2, L_2(\sigma(F)))$ by the representation

$$\vec{u}(x) = \iint_{\mathbf{T}^2} dQ\, \left(u_Q^+(x)\vec{f}_{(+)Q} + u_Q^-(x)\vec{f}_{(-)Q}\right). \tag{30}$$

It is convenient to change variables and turn the integral over the torus $\mathbf{T}^2$ into the integral over four copies of the region M on the complex plane $\zeta(Q)$ (see Figure 7) in accordance with equations (27),(28):

$$dQ_j = J_j^{-1}|\mu| d|\mu|\, d\psi, \qquad j = 1, \ldots, 4.$$

Here J_j stands for the Jacobian

$$\begin{aligned} J_j(|\mu|, \psi) = \begin{vmatrix} \dfrac{\partial \operatorname{Re}\zeta}{\partial \xi_0} & \dfrac{\partial \operatorname{Re}\zeta}{\partial \eta_0} \\ \dfrac{\partial \operatorname{Im}\zeta}{\partial \xi_0} & \dfrac{\partial \operatorname{Im}\zeta}{\partial \eta_0} \end{vmatrix} &= \sin\eta_0^j - 2\sin\xi_0^j \cos\eta_0^j = |\mu|\sin\psi \\ &- 2\sin\left[\cos^{-1}\left(\frac{1}{2}\left(|\mu|\cos\psi - \cos\left[\sin^{-1}(|\mu|\sin\psi)\right]\right)\right)\right]\cos\left[\sin^{-1}(|\mu|\sin\psi)\right], \end{aligned} \tag{31}$$

where the values of the functions $\sin^{-1} t, \cos^{-1} t$ are chosen in accordance with (28). We introduce some more notations:

$$\tau_j(|\mu|, \psi) = |\mu| J_j^{-1}(|\mu|, \psi), \tag{32}$$

$$\vec{f}_\mu^j(\psi) = \vec{f}_{(+)Q_j(|\mu|,\psi)}\Theta(\mu) + \vec{f}_{(-)Q_j(|\mu|,\psi)}\Theta(-\mu), \tag{33}$$

where $\Theta(\mu)$ stands for the step function,

$$\Theta(\mu) = \begin{cases} 1, & \mu \geq 0, \\ 0, & \mu < 0. \end{cases}$$

The spectral decomposition (30) can be rewritten in the form

$$\vec{u}(x) = \int_{-3}^{3} d\mu \sum_{j=1}^{4} \int_{\omega(\mu)} d\psi\, \tau_j(|\mu|, \psi) u_\mu^j(\psi, x) \vec{f}_\mu^j(\psi). \tag{34}$$

The representation (34) is valid for any $\vec{u}(x) \in \mathcal{H}_F$, and the functions

$$u^j_\mu(\psi, x) = \left\langle \vec{u}(x), \vec{f}^j_\mu(\psi) \right\rangle_{l_2(\mathbf{Z}^2)} \tag{35}$$

are the coefficients of this representation.

As $\vec{f}^j_\mu(\psi)$ are the eigenvectors of the operator F,

$$(F - \mu)\vec{f}^j_\mu = 0,$$

the operator H_F can be represented in the form of the direct integral

$$H_F = \int_{-3}^{3} \oplus H_\mu \, d\mu\,(\mu), \tag{36}$$

where H_μ for every μ acts in $L_2(\omega)$,

$$H_\mu = -\frac{\hbar^2}{2m}\Delta,$$

and has the domain

$$D(H_\mu) = W^2_2(\omega) \cap \{u_\mu(x) : u_\mu|_{\partial\omega_0} = 0,\ u_\mu|_{\partial\omega_d} = \mu\, \partial_n u_\mu|_{\partial\omega_d}\}.$$

As H_μ does not depend on index j and angle ψ, the coefficient $u^j_\mu(\psi, x)$ in the representation (34) can be obtained as a combination

$$u^j_\mu(\psi, x) = \sum_{j=1}^{4} \int_{\omega(\mu)} d\psi\, a_j(\psi) u_\mu(x) \tag{37}$$

with arbitrary functions $a_j(\psi)$, which correspond to the infinite-order degeneration of the spectrum $\sigma(F)$.

One can see that the representation (36) is similar to the representation (10) of the original Hamiltonian H, and the role of the fiber operators here is played by the operators H_μ. Hence, as it was done in the previous section, we can consider the set of spectral problems for the operators H_μ and reconstruct the spectrum and the wave functions of the total model Hamiltonian H_F in the terms of their solutions. Notice, that now we have the one-parameter set of the frame operators, which is related to the additional symmetry introduced in our model in this section.

If $\vec{u}(x)$ is the wave function of the operator H_F, $(H_F - z)\vec{u}(x) = 0$, the correspondent functions $u_\mu(x)$ are the solutions of the spectral problems

$$H_\mu u_\mu(x) = z u_\mu(x), \tag{38}$$

and vice versa.

Again the spectrum of the Hamiltonian H_F is the union of the spectra of H_μ,

$$\sigma(H_F) = \bigcup_{\mu \in \sigma(F)} \sigma(H_\mu). \tag{39}$$

Each eigenvalue ε^μ_k of the operator H_μ turns into the spectral band $\{\varepsilon^\mu_k\}_{\mu \in \sigma(F)}$ of the spectrum $\sigma(H_F)$.

In order to perform further analysis, let us consider the spectral problem (38) for the operator H_μ as it was done for the operator $H_{\theta_1\theta_2}$ in the previous section. Using the same method, one can write down the Green identity in the domain ω and using the boundary conditions

$$\begin{aligned} u_\mu|_{\partial\omega_0} &= 0, \\ u_\mu|_{\partial\omega_d} &= \mu\, \partial_n u_\mu|_{\partial\omega_d}, \end{aligned} \tag{40}$$

obtain the following integral equation:

$$u_\mu(s) = \int_{\partial\omega_0} \left[G(s,s',z)\,\partial_n u_\mu(s')\right] ds' + \int_{\partial\omega_d} \left[G(s,s',z) - \mu\partial_n G(s,s',z)\right] \partial_n u_\mu(s')\, ds', \quad (41)$$

which is analogous to equation (15). Following the scheme of the previous section and introducing the correspondent integral operators, one can rewrite equation (41) for the vector-function

$$\Phi_F = \left(\partial_n u_\mu|_{\partial\omega_0}, u_\mu|_{\partial\omega_d}, \partial_n u_\mu|_{\partial\omega_d}\right)^{\mathrm{T}}$$

in a form similar to equation (19). Saving space, we do not present here these calculations, as they are absolutely similar to those in the previous section.

The only result for the model problem we think is useful to show here is the calculation of the normal derivative operator on the boundary $\partial\omega$ of the "triangle" ω. If the boundary $\partial\Omega$ is determined by the function $r = R(\varphi)$ (see Figure 4), then

$$\partial_n = \left[1 + R^{-1}\left(\frac{dR}{d\varphi}\right)^2(\varphi)\right]^{-1/2} \left[\partial_r - R^{-2}\frac{dR}{d\varphi}(\varphi)\partial_\varphi\right].$$

The function $R(\varphi)$ can be easily calculated by geometrical consideration and is given by

$$R(\varphi) = \begin{cases} R_1(\varphi) = (2+d)\cos\varphi - \sqrt{3-(2+d)^2\sin^2\varphi}, & \varphi \in [\varphi_1, \varphi_2], \\ R_2(\varphi) = R_1\left(\varphi - \dfrac{2\pi}{3}\right), & \varphi \in [\varphi_3, \varphi_4], \\ R_3(\varphi) = R_1\left(\varphi + \dfrac{2\pi}{3}\right), & \varphi \in [\varphi_5, \varphi_6], \end{cases}$$

where $\varphi_1 = -\cos^{-1}(1/(d+2)+d/2)$, $\varphi_2 = -\varphi_1$, $\varphi_3 = \varphi_1 + 2\pi/3$, $\varphi_4 = \varphi_2 + 2\pi/3$, $\varphi_5 = \varphi_1 + 4\pi/3$, $\varphi_6 = \varphi_2 + 4\pi/3$ (see Figure 4).

Finally, let us notice that the original QLG problem and the model problem considered in this section have different dimension of the domain of parameters ($\theta \in \mathbf{R}^2$ for QLG and $\mu \in \mathbf{R}^1$ for the model problem), which makes the numerical investigation of the model problem easier. The effective equations in both cases are different only because of the different domain of integration (Ω and ω, respectively).

4. CONCLUSION

The quasiperiodic boundary conditions for the QLG under consideration (i.e., the band spectrum instead of the discrete one in [2,5–9]) bring some difficulties in the direct generalization of methods [2,5–9]. In particular, study of statistics of levels transforms into investigation of spectral density in the bands. Study of the temporal autocorrelation function

$$f_\Psi(t) = |\langle\Psi(0)|\Psi(t)\rangle|^2$$

asymptotical behaviour with respect to t needs the basis property of Bloch waves or wavelets. Also, it is necessary to generalize such physical parameters as Kolmogorov entropy, because the usual definition does not work here. The latter statement is based on the following. If we start from the Sinai's billiard [2,10] and shrink the radius of the disks to zero, one can see that the correspondent classical system given by the limit $R \to 0$ is not chaotic. That is related to the fact that classical trajectories which are influenced by the scatterer are of measure zero. In this sense, the classical system does not "feel" the pointwise scatterer. But it is clear that for the quantum billiard, even for the scatterers of radius $R = 0$, the waves are influenced by the scatterer.

However, before one can generalize the objects standard in the classical billiard theory for the QLG, he should study in detail the spectral structure of the operator H depending on the parameters of the system (in particular, d). A tool for such study can be given by the system of the integral equations constructed in the present paper. However, its numerical investigation (even in the simple model system) faces essential difficulties in the general case (i.e., for the infinite-band spectrum). Hence, it would be useful to single out the "finite-band" case, where the mentioned system of the integral equations can be effectively investigated numerically. At the same time, the "finite-band" property seems to be connected with finite or infinite horizon, or, rigorously speaking, with its quantum analogous.

Contrary to the case of discrete spectrum, we need a definition of quantum chaos different from that given in [2,5–9]. This definition for band spectrum (or in the more general case) can be given in terms of temporal asymptotics of the density operator ρ, whose evolution is determined not by the Schrödinger equation (1), but by the correspondent Liouville equation. One of the possible quantum chaos definitions in these terms was given in [11].

The above-mentioned problems related to the considered QLG will be the subject of our next papers.

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