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Cantor and Band Spectra for Periodic Quantum Graphs with Magnetic Fields⋆

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Abstract: We provide an exhaustive spectral analysis of the two-dimensional periodic square graph lattice with a magnetic field. We show that the spectrum consists of the Dirichlet eigenvalues of the edges and of the preimage of the spectrum of a certain discrete operator under the discriminant (Lyapunov function) of a suitable Kronig-Penney Hamiltonian. In particular, between any two Dirichlet eigenvalues the spectrum is a Cantor set for an irrational flux, and is absolutely continuous and has a band structure for a rational flux. The Dirichlet eigenvalues can be isolated or embedded, subject to the choice of parameters. Conditions for both possibilities are given. We show that generically there are infinitely many gaps in the spectrum, and the Bethe-Sommerfeld conjecture fails in this case.

Introduction

The Hamiltonian H of a charged particle in a two-dimensional system subjected to a periodic electric potential and a uniform magnetic field B has a highly non-trivial spectral and topological structure depending on the ratio of the area σ of the elementary cell of the lattice in question and the squared magnetic length $\ell_M^2 = \hbar c/|eB|$ (here e is the electron charge, c is the light velocity, $\hbar$ is the Planck constant). More precisely, denote by θ the number of the magnetic flux quanta through the elementary cell: $\theta = \sigma/2\pi \ell_M^2$. If θ is a rational number, then the spectrum of H has a band structure (i.e. the spectrum is the union of a locally finite family of segments) and for $\theta \neq 0$ each vector bundle of the magnetic Bloch functions corresponding to a completely filled Landau level is non-trivial [33] (for a non-zero integer θ the Chern number of this bundle is exactly the value of the quantized Hall conductance in units $e^2/2\pi \hbar$ [6, 35, 40]). The most likely conjecture is that at irrational values of θ, the spectrum of H has a Cantor

structure. This conjecture was recently proved in the case of the tight-binding model for the magnetic Bloch electron [4, 5, 36]; in this case H is reduced to the Harper operator in the discrete Hilbert space $l^2(\mathbb{Z})$. Due to the Langbein duality [28], the same is true for the Hamiltonian of the nearly-free-electron approximation. As a result of these Cantor properties, the diagram describing the dependence of the spectrum on the flux θ, the so-called Hofstadter butterfly, has a remarkable fractal structure, see e.g. [19, 21, 25].

Little is known for the magnetic Schrödinger operator H in the space $L^2(\mathbb{R}^2)$,

$$ H = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + V(x, y), \tag{1} $$

where $\mathbf{A}$ is the vector potential of B and V is a potential which is periodic with respect to the considered lattice. It is proven in this case, that H has a piece of the Cantor spectrum near the bottom of the spectrum for a restricted class of potentials V [20].

In this connection, the quantum network models (also called the quantum graph models) have attracted considerable interest recently. These models combine some essential features of both discrete and continuous models mentioned above. On the one hand, the Hamiltonian of a magnetic network model has infinitely many magnetic bands of different shape. On the other, the time-independent Schrödinger equation for this Hamiltonian can be reduced to a discrete equation. S. Alexander was the first who performed this reduction [3] in the framework of the percolation approach to the effect of disorder on superconductivity proposed by P. G. de Gennes [11]. A very short and elegant derivation of the Schrödinger equation for a periodic quantum graph with a uniform magnetic field and a constant potential on each edge of the graph is given in [23]. On the mathematical level of rigor the relation between solutions of the Schrödinger equation for H on quantum graphs Γ and those for a Jacoby matrix $J(H)$ on the corresponding combinatorial graphs was established by P. Exner [14]. Nevertheless, the main theorem from [14] is applicable only to finding eigenvalues of H distinct from the Dirichlet eigenvalues on the edges of Γ. As to the points of the continuous spectrum, the main result of [14] allows an exhaustive analysis only in the case when the direct and inverse Schnol-type theorems are known for both H and $J(H)$.

It is worth noting that quantum networks are not only a mathematical tool to get simplified models of various quantum systems, but in many cases experimental devices really have a shape of planar graphs such that the width of the sides is much smaller than the parameters of the dimension of length which characterizes the quantity in question, e.g., much smaller than the magnetic length, the Fermi wave length, the scattering length, etc. [1, 31, 32]. In these cases the quantum graph models are the most adequate ones for simulating spectral, scattering, and transport properties of these devices.

Here we propose an alternative approach to the spectral analysis of quantum graph Hamiltonians based on boundary triples, Dirichlet-to-Neumann maps, and the Krein technique of self-adjoint extensions. Such a machinery works effectively in many other problems connected with explicitly solvable models [2, 34]. In the case of square network lattices with a periodic magnetic field (including a uniform one), an arbitrary L^2-potential on edges and δ-like boundary conditions at the vertices (including the Kirchhoff boundary conditions), we perform an exhaustive spectral analysis of the network Hamiltonian H. It is proved that the spectrum always contains Dirichlet eigenvalues of the edges as infinitely degenerate eigenvalues of H. The rest part of the spectrum is absolutely continuous and has a band structure, if θ is a rational number, and is the union of countably many Cantor sets placed between Dirichlet eigenvalues, otherwise. Moreover, this part is the preimage of the spectrum of the corresponding lattice Hamiltonian

$J(H)$ with respect to a many-sheeted analytic function which is just the discriminant of a generalized Kronig–Penney operator (i.e. the Sturm–Liouville operator with a Kronig–Penney potential). The eigenvalues are isolated if the magnetic flux is non-integer, while for integer magnetic fluxes it depends on the electric potential and on the coupling at the nodes.

1. Magnetic Schrödinger Operator on the Periodic Metric Graph

Consider a planar square graph lattice whose nodes are the points $K_{m,n} := (ml, nl)$, $(m, n) \in \mathbb{Z}^2$, where $l > 0$ is the length of each edge. Two nodes $K_{m,n}$ and $K_{p,q}$ are connected by an edge iff $|m - p| + |n - q| = 1$. We denote the edge between $K_{m,n}$ and $K_{m+1,n}$ by $E_{m,n,r}$ (right), and between $K_{m,n}$ and $K_{m,n+1}$ by $E_{m,n,u}$ (up). Each edge $E_{m,n,r/u}$ will be considered as the segment $[0, l]$ so that 0 is identified in both cases with $K_{m,n}$, and l is identified with $K_{m+1,n}$ for $E_{m,n,r}$ and $K_{m,n+1}$ for $E_{m,n,u}$, respectively. The state space of the lattice is

$$\mathcal{H} = \bigoplus_{(m,n)\in\mathbb{Z}} (\mathcal{H}_{m,n,r} \oplus \mathcal{H}_{m,n,u}), \quad \mathcal{H}_{m,n,r/u} = L^2[0, l].$$

The elements of $\mathcal{H}$ will be denoted as $f = (f_{m,n,r}, f_{m,n,u})$, $f_{m,n,r/u} \in \mathcal{H}_{m,n,r/u}$. On each edge consider the same electric potential $V \in L^2[0, l]$.

We assume that the lattice is subjected to an external magnetic field orthogonal to the plane, $B(x) = (0, 0, b(x))$, $b \in C(\mathbb{R}^2)$, such that the quantity

$$\xi = \frac{1}{2\pi l^2} \int_{F_{m,n}} b(x)dx,$$

where $F_{m,n}$ is the square spanned by $E_{m,n,r}$ and $E_{m,n,u}$, is independent of $m, n \in \mathbb{Z}$. This includes the periodic magnetic field, i.e. the case $b(x_1+l, x_2) = b(x_1, x_2+l) = b(x_1, x_2)$.

The corresponding magnetic vector potential in the symmetric gauge can be written as $A(x_1, x_2, x_3) = (-\pi\xi x_2, \pi\xi x_1, 0) + (A_1(x_1, x_2), A_2(x_1, x_2), 0)$ with

$$\int_{F_{m,n}} \left[\frac{\partial A_2}{\partial x_1}(x_1, x_2) - \frac{\partial A_1}{\partial x_2}(x_1, x_2)\right]dx_1dx_2 \equiv \int_{ml}^{(m+1)l} \left[A_1(t, nl) - A_1(t, (n+1)l)\right]dt$$

$$+ \int_{nl}^{(n+1)l} \left[A_2((m + 1)l, t) - A_2(ml, t)\right]dt = 0 \text{ for all } m, n \in \mathbb{Z}. \tag{2}$$

The presence of the magnetic field leads to non-trivial magnetic potentials on the edges, which are the projections of $A(x)$ on the corresponding directions. The magnetic potentials $A_{m,n,r/u}$ on $E_{m,n,r/u}$ are:

$$A_{m,n,r}(t) = \langle A((ml, nl, 0) + (1, 0, 0)t), (1, 0, 0)\rangle \equiv -\pi\xi nl + A_1(ml + t, nl),$$
$$A_{m,n,u}(t) = \langle A((ml, nl, 0) + (0, 1, 0)t), (0, 1, 0)\rangle \equiv \pi\xi ml + A_2(ml, nl + t).$$

On each of the edges $E_{m,n,r/u}$ we consider the operator

$$L_{m,n,r/u} = \left(-i\frac{d}{dt} - A_{m,n,r/u}\right)^2 + V,$$

with the domain $H^2[0, l]$. The direct sum of these operators over all edges is not self-adjoint, and in order to obtain a self-adjoint operator on the whole lattice it is necessary to introduce boundary conditions at each node. The most general boundary conditions involve a number of parameters and can be found, for example, in [24]. We restrict ourselves by considering the so-called magnetic δ-like interaction at $K_{m,n}$,

$$f_{m,n,r}(0) = \frac{1}{\beta} f_{m,n,u}(0) = f_{m-1,n,r}(l) = \frac{1}{\beta} f_{m,n-1,u}(l) =: f_{m,n},$$

$$\left(\frac{d}{dt} - i A_{m,n,r}\right) f_{m,n,r}(0) + \beta\left(\frac{d}{dt} - i A_{m,n,u}\right) f_{m,n,u}(0)$$

$$-\left(\frac{d}{dt} - i A_{m-1,n,r}\right) f_{m-1,n,r}(l) - \beta\left(\frac{d}{dt} - i A_{m,n-1,u}\right) f_{m,n-1,u}(l) = \alpha f_{m,n}, \tag{3}$$

$$m, n \in \mathbb{Z},$$

where $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R} \setminus \{0\}$. These quantities have the following physical meaning. The parameter $\alpha \neq 0$ is the coupling constant of a δ-like potential at each node. Introducing the parameter β can be treated as considering a more general form of the Hamiltonian H:

$$H = \sum_{jk} \frac{1}{2m_{jk}} \left(p_j - \frac{e}{c} A_j\right) \left(p_k - \frac{e}{c} A_k\right) + V(x, y),$$

where m_{jk} is the effective mass tensor and β is the corresponding anisotropy coefficient (the ratio of the eigenvalues of the symmetric matrix (m_{jk})). In particular, if $\beta = 1$, one obtains H in the form (1); if in addition $\alpha = 0$, we get the magnetic Kirchhoff coupling. This class of boundary conditions covers main couplings used in the physics literature. The self-adjoint operator obtained in this way we denote by L.

2. Gauge Transformations

To study the spectral properties of L it is useful to use the gauge transformation $(f_{m,n,r}, f_{m,n,u}) = (U_{m,n,r}\varphi_{m,n,r}, U_{m,n,u}\varphi_{m,n,u})$ given by

$$f_{m,n,r/u}(t) = \exp\left(i \int_0^t A_{m,n,r/u}(s)\,ds\right)\varphi_{m,n,r/u}(t) =: U_{m,n,r/u}\varphi_{m,n,r/u}(t).$$

There holds $U_{m,n,r/u}^{-1} L_{m,n,r/u} U_{m,n,r/u} = -\dfrac{d^2}{dt^2} + V$, and the boundary conditions (3) for $\varphi = (\varphi_{m,n,r}, \varphi_{m,n,u}) \in U^{-1}(\text{dom } L)$ take the form

$$\widetilde{\varphi}'_{m,n} = \alpha \widetilde{\varphi}_{m,n}, \tag{4a}$$

where

$$\widetilde{\varphi}_{m,n} := \varphi_{m,n,r}(0) = \frac{1}{\beta} \varphi_{m,n,u}(0)$$

$$= \exp\left(-i\pi n\theta + i \int_{(m-1)l}^{ml} A_1(t, nl)dt\right)\varphi_{m-1,n,r}(l)$$

$$= \frac{1}{\beta} \exp\left(i\pi m\theta + i \int_{(n-1)l}^{nl} A_2(ml, t)dt\right)\varphi_{m,n-1,u}(l) \tag{4b}$$

and

$$\widetilde{\varphi}'_{m,n} := \varphi'_{m,n,r}(0) + \beta \varphi'_{m,n,u}(0)$$

$$- \exp\left(-i\pi n\theta + i \int_{(m-1)l}^{ml} A_1(t, nl)dt\right) \varphi'_{m-1,n,r}(l)$$

$$- \beta \exp\left(i\pi m\theta + i \int_{(n-1)l}^{nl} A_2(ml, t)dt\right) \varphi'_{m,n-1,u}(l), \qquad (4c)$$

and $\theta := \xi l^2$ is the number of flux quanta through the elementary cells $F_{m,n}$. Therefore, the operator $\widetilde{L} = U^{-1}LU$ acts on each edge as $\varphi_{m,n,r/u} \mapsto -\varphi''_{m,n,r/u} + V\varphi_{m,n,r/u}$ on functions φ satisfying (4), and its spectrum coincides with the spectrum of L.

To simplify subsequent calculations we apply another gauge transformation,

$$\varphi_{m,n,r/u} = \exp\left(i \int_0^{ml} A_1(t, nl)dt + i \int_0^{nl} A_2(0, t)dt\right) \phi_{m,n,r/u}.$$

Substituting this expression into (4) and using (2) we arrive at an operator acting on each edge as $\phi_{m,n,r/u} \mapsto -\phi''_{m,n,r/u} + V\phi_{m,n,r/u}$ on functions $\phi = (\phi_{m,n,r}, \phi_{m,n,u})$, $\phi_{m,n,r/u} \in H^2[0, l]$, satisfying

$$\phi_{m,n,r}(0) = \frac{1}{\beta} \phi_{m,n,u}(0) = e^{-i\pi n\theta} \phi_{m-1,n,r}(l) = \frac{1}{\beta} e^{i\pi m\theta} \phi_{m,n-1,u}(l) =: \phi_{m,n}, \quad (5a)$$

$$\phi'_{m,n} = \alpha \phi_{m,n}, \qquad m, n, \in \mathbb{Z}, \qquad (5b)$$

where

$$\phi'_{m,n} := \phi'_{m,n,r}(0) + \beta \phi'_{m,n,u}(0) - e^{-i\pi n\theta} \phi'_{m-1,n,r}(l) - \beta e^{i\pi m\theta} \phi'_{m,n-1,u}(l). \qquad (5c)$$

This operator, which we denote by Λ, is unitarily equivalent to the initial magnetic Hamiltonian L. In what follows we work mostly with this new operator.

At this point we emphasize some important circumstances. First, we see that the initial magnetic field must not be necessary periodic to produce a periodic operator on the lattice. Second, for the usual magnetic Schrödinger operators in $L^2(\mathbb{R}^2)$ the spectral analysis for non-zero but periodic magnetic vector potentials (i.e. with the zero flux per cell) essentially differs from that for the Schrödinger operators without magnetic field; even the proof of the absolute continuity of the spectrum is non-trivial [7, 39]. In our case, the operator on the graph with a periodic magnetic vector potential appears to be unitarily equivalent to the operator without magnetic field. Third, for the usual magnetic Schrödinger operators the bottom of the spectrum grows infinitely as the flux becomes infinitely large. In our situation, the spectrum is 1-periodic with respect to the magnetic flux θ, as changing θ by $\theta + 1$ in (5) obviously can be compensated by a unitary transformation. Such periodicity leads to the so-called Aharonov–Bohm oscillations in the corresponding physical quantities.

Remark 1. It is worth noting that Λ is invariant with respect to the so-called magnetic translation group $\mathbb{G}_M$ [41]. In our case this group is generated by the magnetic shift operators τ_r and τ_u,

$$\tau_r \phi_{m,n,r/u}(t) = e^{i\pi n\theta} \phi_{m-1,n,r/u}(t), \quad \tau_u \phi_{m,n,r/u}(t) = e^{-i\pi m\theta} \phi_{m,n-1,r/u}(t).$$

The properties of this group depend drastically on the arithmetic properties of θ [9]. In particular, if θ is irrational, then $\mathbb{G}_M$ has only infinite-dimensional irreducible representations which are trivial on the center of $\mathbb{G}_M$. Therefore, for any irrational θ each point of spec Λ is infinitely degenerate.

Proposition 2. *The operator Λ is semibounded below.*

Proof. Let $\phi \in$ dom Λ. Using the integration by parts and changing suitably the summation order one obtains

$$\langle \phi, \Lambda\phi \rangle = \sum_{m,n} \left(\langle \phi_{m,n,r}, -\phi''_{m,n,r} + V\phi_{m,n,r} \rangle + \langle \phi_{m,n,u}, -\phi''_{m,n,u} + V\phi_{m,n,u} \rangle \right)$$

$$= \sum_{m,n} \left(\overline{\phi_{m,n,r}(0)}\phi'_{m,n,r}(0) - \overline{\phi_{m,n,r}(l)}\phi'_{m,n,r}(l) + \overline{\phi_{m,n,u}(0)}\phi'_{m,n,u}(0) - \overline{\phi_{m,n,u}(l)}\phi'_{m,n,u}(l) \right.$$

$$\left. + \int_0^l \left(|\phi'_{m,n,r}|^2 + V|\phi_{m,n,r}|^2 \right)dx + \int_0^l \left(|\phi'_{m,n,u}|^2 + V|\phi_{m,n,u}|^2 \right)dx \right)$$

$$= \sum_{m,n} \left\{ \int_0^l \left(|\phi'_{m,n,r}|^2 + V|\phi_{m,n,r}|^2 \right)dx + \int_0^l \left(|\phi'_{m,n,u}|^2 + V|\phi_{m,n,u}|^2 \right)dx \right.$$

$$\left. + \overline{\phi_{m,n}} \left(\phi'_{m,n,r}(0) + \beta\phi'_{m,n,u}(0) - e^{-i\pi n\theta}\phi'_{m-1,n,r}(l) - \beta e^{i\pi m\theta}\phi'_{m,n-1,u}(l) \right) \right\}$$

$$= \sum_{m,n} \left\{ \int_0^l \left(|\phi'_{m,n,r}|^2 + V|\phi_{m,n,r}|^2 \right)dx + \int_0^l \left(|\phi'_{m,n,u}|^2 + V|\phi_{m,n,u}|^2 \right)dx + \overline{\phi_{m,n}}\, \phi'_{m,n} \right\}$$

$$= \sum_{m,n} \left\{ \int_0^l \left(|\phi'_{m,n,r}|^2 + V|\phi_{m,n,r}|^2 \right)dx + \int_0^l \left(|\phi'_{m,n,u}|^2 + V|\phi_{m,n,u}|^2 \right)dx + \alpha|\phi_{m,n}|^2 \right\}.$$

Now choose $c \in (0, 1)$ and $C \in \mathbb{R}$ with

$$|\alpha||h(0)|^2 \leq \int_0^l \left(c|h'|^2 + (V + C)|h|^2 \right)dx \quad \text{for all } h \in H^1[0, l]$$

(the existence of such constants follows from the Sobolev inequality), then

$$|\alpha||\phi_{m,n}|^2 \equiv |\alpha||\phi_{m,n,r}(0)|^2 \leq \int_0^l \left(c|\phi'_{m,n,r}|^2 + (V + C)|\phi_{m,n,r}|^2 \right)dx,$$

and

$$\langle \phi, (\Lambda + C)\phi \rangle \geq \sum_{m,n} \int_0^l \left\{ (1 - c)|\phi'_{m,n,r}|^2 + |\phi'_{m,n,u}|^2 + (V + C)|\phi_{m,n,u}|^2 \right\} dx \geq 0.$$

$\square$

3. Boundary Triples

Here we describe briefly the technique of abstract self-adjoint boundary value problems with the help of boundary triples. For more detailed discussion we refer to [12].

Let S be a closed linear operator in a Hilbert space $\mathcal{H}$ with the domain dom S. Assume that there exists an auxiliary Hilbert space $\mathcal{G}$ and two linear maps $\Gamma, \Gamma' : \text{dom } S \to \mathcal{G}$ such that

- for any $f, g \in \text{dom } S$ there holds $\langle f, Sg \rangle - \langle Sf, g \rangle = \langle \Gamma f, \Gamma' g \rangle - \langle \Gamma' f, \Gamma g \rangle$,
- the map $(\Gamma, \Gamma') : \text{dom } S \to \mathcal{G} \oplus \mathcal{G}$ is surjective,
- the set $\ker \Gamma \cap \ker \Gamma'$ is dense in $\mathcal{H}$.

The triple $(\mathcal{G}, \Gamma, \Gamma')$ with the above properties is called a *boundary triple* for S.

Example 3. Let us describe one important example of boundary triple. Let $V \in L^2[0, l]$ be a real-valued function. In $\mathcal{H} = L^2[0, l]$ consider the operator

$$S = -\frac{d^2}{dt^2} + V, \quad \text{dom } S = H^2[0, l], \qquad (6)$$

then one can set

$$\mathcal{G} = \mathbb{C}^2, \quad \Gamma f = \begin{pmatrix} f(0) \\ f(l) \end{pmatrix}, \quad \Gamma' f = \begin{pmatrix} f'(0) \\ -f'(l) \end{pmatrix}. \qquad (7)$$

If an operator S has a boundary triple, then it has self-adjoint restrictions provided S^* is a symmetric operator (see Theorem 3.1.6 in [18]). For example, if T is a self-adjoint operator in $\mathcal{G}$, then the restriction of S to elements f satisfying abstract boundary conditions $\Gamma' f = T\Gamma f$ is a self-adjoint operator in $\mathcal{H}$, which we denote by H_T. Another example is the operator H corresponding to the boundary conditions $\Gamma f = 0$. One can relate the resolvents of H and H_T as well as their spectral properties by the Krein resolvent formula, which is our most important tool in this paper.

Let $z \notin \text{spec } H$. For $g \in \mathcal{G}$ denote by $\gamma(z)g$ the unique solution to the abstract boundary value problem $(S - z)f = 0$ with $\Gamma f = g$ (the solution exists due to the above conditions for Γ and Γ'). Clearly, $\gamma(z)$ is a linear map from $\mathcal{G}$ to $\mathcal{H}$. Denote also by $Q(z)$ the operator on $\mathcal{G}$ given by $Q(z)g = \Gamma'\gamma(z)g$; this map is called the Krein function. The operator-valued functions γ and Q are analytic outside spec H. Moreover, $Q(z)$ is self-adjoint for real z.

Proposition 4. *(A)* (Proposition 2 in [12]) *For $z \notin \text{spec } H \cup \text{spec } H_T$ the operator $Q(z) - T$ acting on $\mathcal{G}$ has a bounded inverse defined everywhere and the Krein resolvent formula holds,*

$$(H - z)^{-1} - (H_T - z)^{-1} = \gamma(z)\big(Q(z) - T\big)^{-1}\gamma^*(\bar{z}).$$

(B) The set spec $H_T \backslash \text{spec } H$ consists exactly of real numbers z such that $0 \in \text{spec}\big(Q(z) - T\big)$.

(C) (Theorem 1 in [16]) *Let $z \in \text{spec } H_T \backslash \text{spec } H$, then z is an eigenvalue of H_T if and only if 0 is an eigenvalue of $Q(z) - T$, and in this case $\gamma(z)$ is an isomorphism of the corresponding eigensubspaces.*

This statement is especially useful if the spectrum of H is a discrete set and the spectrum of H_T is expected to have a positive measure, because one can describe the most part of the spectrum of H_T in terms of $Q(z) - T$.

Example 5. Consider the example given by (6) and (7). The corresponding Krein function $s(z)$ can be obtained as follows. The restriction D of S given by $\Gamma f = 0$ is

$$Df = -f'' + Vf, \quad \mathrm{dom}\, D = \{f \in H^2[0, l] :\ f(0) = f(l) = 0\}. \tag{8}$$

In what follows we denote the eigenvalues of D by μ_k, $k = 0, 1, 2\ldots$, $\mu_0 < \mu_1 < \mu_2 < \ldots$.

Let two functions $u_1, u_2 \in H^2[0, l]$ satisfy

$$u_1, u_2 \in \ker(S - z), \quad \begin{matrix} u_1(0; z) = 0, & u_1'(0; z) = 1, \\ u_2(0; z) = 1, & u_2'(0; z) = 0. \end{matrix} \tag{9}$$

Clearly, for their Wronskian one has $w(z) = u_1'(x; z)u_2(x; z) - u_1(x; z)u_2'(x; z) \equiv 1$. Both u_1, u_2 as well as their derivatives with respect to x are entire functions of z.

Let $z \notin \mathrm{spec}\, D$, then any function f with $-f'' + Vf = zf$ can be written as

$$f(x; z) = \frac{f(l) - f(0)u_2(l; z)}{u_1(l; z)} u_1(x; z) + f(0)u_2(x; z),$$

and the calculation of $f'(0)$ and $-f'(l)$ gives

$$s(z) = \frac{1}{u_1(l; z)} \begin{pmatrix} -u_2(l; z) & \frac{1}{w(z)} \\ w(z) & -u_1'(l; z) \end{pmatrix} \equiv \frac{1}{u_1(l; z)} \begin{pmatrix} -u_2(l; z) & 1 \\ 1 & -u_1'(l; z) \end{pmatrix}. \tag{10}$$

It can be directly seen that $s(z)$ is real and self-adjoint for real z. Clearly, the matrix s has simple poles at μ_k, which are at the same time simple zeros of $u_1(l; z)$. More precisely, by the well-known arguments, see e.g. Eq. (I.4.13) in [29], there holds

$$\left.\frac{\partial u_1(l; z)}{\partial z}\right|_{z=\mu_k} = u_2(l; \mu_k) \int_0^l u_1^2(s, \mu_k)\, ds,$$

and $u_2(l; \mu_k) \neq 0$ due to $u_1'(l; \mu_k)u_2(l; \mu_k) \equiv w(\mu_k) = 1$.

4. Reduction to a Discrete Problem on the Lattice

To describe the spectrum of Λ we use the Krein resolvent formula. Denote by Π the operator acting on each edge as $\phi_{m,n,r/u} \mapsto -\phi_{m,n,r/u}'' + V\phi_{m,n,r/u}$ on functions satisfying only the condition (5a). Clearly, for such functions the expression $\phi_{m,n}'$ given by (5c) makes sense. This operator is not symmetric, as it is a proper extension of the self-adjoint operator Λ.

Proposition 6. *The operator Π is closed and the triple $\left(l^2(\mathbb{Z}^2), \Gamma, \Gamma'\right)$,*

$$\Gamma : \operatorname{dom} \Pi \ni \phi = (\phi_{m,n,r}, \phi_{m,n,u}) \mapsto (\phi_{m,n}) \in l^2(\mathbb{Z}^2),$$

$$\Gamma' : \operatorname{dom} \Pi \ni \phi = (\phi_{m,n,r}, \phi_{m,n,u}) \mapsto (\phi'_{m,n}) \in l^2(\mathbb{Z}^2),$$

is a boundary triple for Π.

Proof. Denote by Ξ the direct sum of operators $-\dfrac{d^2}{dt^2} + V$ with the domain $H^2[0, l]$ over all edges $E_{m,n,r/u}$. Clearly, Ξ is a closed operator, and the functionals

$$g_{m,n,1}(\phi) = \phi_{m,n,r}(0) - \frac{1}{\beta} \phi_{m,n,u}(0),$$

$$g_{m,n,2}(\phi) = \phi_{m,n,r}(0) - e^{-i\pi n\theta} \phi_{m-1,n,r}(l),$$

$$g_{m,n,3}(\phi) = \phi_{m,n,r}(0) - \frac{1}{\beta} e^{i\pi m\theta} \phi_{m,n-1,u}(l)$$

are continuous with respect to the graph norm of Ξ. Therefore, the restriction of Ξ to functions on which all these functionals vanish is a closed operator, and this is exactly Π. For any $\phi \in \operatorname{dom} \Pi$ the inclusions $\Gamma\phi, \Gamma'\phi \in l^2(\mathbb{Z}^2)$ follow from the Sobolev inequality, and both Γ, Γ' are continuous with respect to the graph norm of Π.

Let $\phi, \psi \in \operatorname{dom} \Pi$, then the integration by parts gives

$$\langle \phi, \Pi\psi \rangle - \langle \Pi\phi, \psi \rangle$$

$$\equiv \sum_{m,n\in\mathbb{Z},\, i=r,u} \left(\langle \phi_{m,n,i}, -\psi''_{m,n,i} + V\psi_{m,n,i} \rangle - \langle -\phi''_{m,n,i} + V\phi_{m,n,i}, \psi_{m,n,i} \rangle \right)$$

$$\equiv \sum_{m,n\in\mathbb{Z},\, i=r,u} \left(\langle \phi_{m,n,i}, -\psi''_{m,n,i} \rangle - \langle -\phi''_{m,n,i}, \psi_{m,n,i} \rangle \right)$$

$$= \sum_{m,n\in\mathbb{Z}} \left\{ \overline{\phi_{m,n,r}(0)}\psi'_{m,n,r}(0) + \frac{1}{\beta} \overline{\phi_{m,n,u}(0)}\beta\psi'_{m,n,u}(0) \right.$$

$$- \overline{\phi_{m-1,n,r}(l)}\psi'_{m-1,n,r}(l) - \frac{1}{\beta} \overline{\phi_{m,n-1,u}(l)}\beta\psi'_{m,n-1,u}(l)$$

$$- \overline{\phi'_{m,n,r}(0)}\psi_{m,n,r}(0) - \frac{1}{\beta} \overline{\phi'_{m,n,u}(0)}\beta\psi_{m,n,u}(0)$$

$$\left. + \overline{\phi'_{m-1,n,r}(l)}\psi_{m-1,n,r}(l) + \frac{1}{\beta} \overline{\phi'_{m,n-1,u}(l)}\beta\psi_{m,n-1,u}(l) \right\}$$

$$= \sum_{m,n\in\mathbb{Z}} \left\{ \overline{\phi_{m,n}}\psi'_{m,n,r}(0) + \beta\overline{\phi_{m,n}}\psi'_{m,n,u}(0) \right.$$

$$- \overline{e^{i\pi n\theta}\phi_{m,n}}\psi'_{m-1,n,r}(l) - \beta\overline{e^{-i\pi m\theta}\phi_{m,n}}\psi'_{m,n-1,u}(l)$$

$$- \overline{\phi'_{m,n,r}(0)}\psi_{m,n} - \beta\overline{\phi'_{m,n,u}(0)}\psi_{m,n}$$

$$\left. + \overline{\phi'_{m-1,n,r}(l)}e^{i\pi n\theta}\psi_{m,n} + \beta\overline{\phi'_{m,n-1,u}(l)}e^{-i\pi m\theta}\psi_{m,n} \right\}$$

$$= \sum_{m,n\in\mathbb{Z}} \Big\{ \overline{\phi_{m,n}} \big(\psi'_{m,n,r}(0) + \beta\psi'_{m,n,u}(0)$$

$$- e^{-i\pi n\theta} \psi'_{m-1,n,r}(l) - \beta e^{i\pi m\theta} \psi'_{m,n-1,u}(l) \big) - \big(\overline{\phi'_{m,n,r}(0)} + \beta\overline{\phi'_{m,n,u}(0)}$$

$$- \overline{e^{-i\pi n\theta} \phi'_{m-1,n,r}(l)} - \beta\overline{e^{i\pi m\theta}\phi'_{m,n-1,u}(l)} \big) \psi_{m,n} \Big\}$$

$$= \sum_{m,n\in\mathbb{Z}} \big(\overline{\phi_{m,n}}\psi'_{m,n} - \overline{\phi'_{m,n}}\psi_{m,n} \big) \equiv \langle \Gamma\phi, \Gamma'\psi \rangle - \langle \Gamma'\phi, \Gamma\psi \rangle.$$

Now we verify the surjectivity condition. Choose functions $f_0, f_1 \in H^2[0,l]$, with $f_0(0) = f'_1(0) = 1$, $f'_0(0) = f_1(0) = 0$, $f_k^{(j)}(l) = 0$, $j, k = 0, 1$. Let $g, g' \in l^2(\mathbb{Z}^2)$. For any $p, q \in \mathbb{Z}$ denote

$$h_{p,q,1}(x) = g_{p,q} f_0(x) + \frac{g'_{p,q}}{4} f_1(x),$$

$$h_{p,q,2}(x) = \beta g_{p,q} f_0(x) + \frac{g'_{p,q}}{4\beta} f_1(x),$$

$$h_{p,q,3}(x) = g_{p,q}e^{i\pi q\theta} f_0(l-x) + e^{-i\pi q\theta} \frac{g'_{p,q}}{4} f_1(l-x),$$

$$h_{p,q,4}(x) = \beta g_{p,q}e^{-i\pi q\theta} f_0(l-x) + e^{i\pi p\theta} \frac{g'_{p,q}}{4\beta} f_1(l-x),$$

then $h_{p,q,j} \in H^2[0,l]$, $j = 1, \ldots, 4$, and these functions satisfy

$$h_{p,q,1}(0) = \frac{1}{\beta} h_{p,q,2}(0) = e^{-i\pi q\theta} h_{p,q,3}(l) = \frac{1}{\beta} e^{i\pi p\theta} h_{p,q,4}(l) = g_{p,q},$$

$$h'_{p,q,1}(0) = \beta h'_{p,q,2}(0) = -e^{i\pi q\theta} h'_{p,q,3}(l) = -\beta e^{-i\pi p\theta} h'_{p,q,4}(l) = \frac{g'_{p,q}}{4},$$

$$h_{p,q,1}(l) = h_{p,q,2}(l) = h_{p,q,3}(0) = h_{p,q,4}(0)$$
$$= h'_{p,q,1}(l) = h'_{p,q,2}(l) = h'_{p,q,3}(0) = h'_{p,q,4}(0) = 0.$$

Define $\phi^{(p,q)} = \big(\phi_{m,n,r}^{(p,q)}, \phi_{m,n,u}^{(p,q)} \big) \in \mathcal{H}$ with

$$\phi_{p,q,r}^{(p,q)} = h_{p,q,1}, \quad \phi_{p,q,u}^{(p,q)} = h_{p,q,2}, \quad \phi_{p-1,q,r}^{(p,q)} = h_{p,q,3}, \quad \phi_{p,q-1,u}^{(p,q)} = h_{p,q,4},$$

$$\phi_{m,n,i}^{(p,q)} = 0 \quad \text{for all other } m, n \in \mathbb{Z} \text{ and } i = r, u.$$

Clearly, by construction $\phi^{(p,q)} \in \mathrm{dom}\,\Pi$ and there holds $\big(\Gamma\phi^{(p,q)} \big)_{m,n} \equiv \phi_{m,n}^{(p,q)} = g_{p,q}\delta_{mp}\delta_{nq}$ and $\big(\Gamma'\phi^{(p,q)} \big)_{m,n} \equiv \big(\phi^{(p,q)} \big)'_{m,n} = g'_{p,q}\delta_{mp}\delta_{nq}$, $m, n \in \mathbb{Z}$. It is easy to see that the series $\phi = \sum_{m,n} \phi^{(m,n)}$ converges in the graph norm of Π, hence $\phi \in \mathrm{dom}\,\Pi$. Since $H^2[0,l]$ is continuously imbedded in $C^1[0,l]$, we have $\Gamma\phi = \sum_{m,n} \Gamma\phi^{(m,n)} = g$ and $\Gamma'\phi = \sum_{m,n} \Gamma'\phi^{(m,n)} = g'$. The surjectivity condition is proved.

It remains to note that the set $\ker\,\Gamma \cap \ker\,\Gamma'$ contains the direct sum of $C_0^\infty(0,l)$ over all edges and is obviously dense in $\mathcal{H}$. □

The operator Λ is the restriction of Π to the set of function ϕ satisfying $\Gamma'\phi = \alpha\Gamma\phi$. Consider another self-adjoint extension Π_0 given by $\Gamma\phi = 0$. Clearly, Π_0 is exactly the direct sum of the operators D from (8) over all the edges $E_{m,n,r/u}$. In particular, $\operatorname{spec}\Pi_0 = \operatorname{spec} D$.

Let $z \notin \operatorname{spec} D$, $g \in l^2(\mathbb{Z}^2)$ and ψ_g be the solution of $(\Pi - z)\psi_g = 0$ satisfying the boundary condition $\Gamma\psi_g = g$. Consider the corresponding Krein function $Q(z) : l^2(\mathbb{Z}^2) \ni g \mapsto \Gamma'\psi_g \in l^2(\mathbb{Z}^2)$. Application of Proposition 4 gives the following implicit description of the spectrum of Λ.

Proposition 7. *A number $z \in \mathbb{R} \setminus \operatorname{spec}\Pi_0 \equiv \mathbb{R} \setminus \operatorname{spec} D$ lies in $\operatorname{spec}\Lambda$ iff $0 \in \operatorname{spec}\big[Q(z) - \alpha\big]$. Such z is an eigenvalue of Λ iff 0 is an eigenvalue of $Q(z) - \alpha$.*

Therefore, outside the discrete set $\operatorname{spec}\Pi_0 \equiv \operatorname{spec} D$ we can reduce the spectral problem for Λ to the spectral problem for $Q(z) - \alpha$. Let us calculate $Q(z)$ more explicitly; actually this is our key construction.

Proposition 8. *For $z \notin \operatorname{spec} D$ there holds*

$$Q(z) = (1 + \beta^2)\big(s_{11}(z) + s_{22}(z)\big) + s_{12}(z)M(\theta, \beta), \tag{11}$$

where $M(\theta, \beta)$ is the discrete magnetic Laplacian in $l^2(\mathbb{Z}^2)$,

$$\big(M(\theta, \beta)g\big)_{m,n} = e^{i\pi n\theta}g_{m+1,n} + e^{-i\pi n\theta}g_{m-1,n} + \beta^2\big(e^{-i\pi m\theta}g_{m,n+1} + e^{i\pi m\theta}g_{m,n-1}\big),$$
$$g = (g_{m,n}) \in l^2(\mathbb{Z}^2).$$

Proof. Note that for $\phi = (\phi_{m,n,r}, \phi_{m,n,u})$ in the notation of Proposition 6 there holds

$$\left(\begin{pmatrix}\phi_{m,n,r}(0) \\ \phi_{m,n,r}(l) \\ \phi_{m,n,u}(0) \\ \phi_{m,n,u}(l)\end{pmatrix}\right)_{(m,n)\in\mathbb{Z}^2} = C\Gamma\phi, \quad \Gamma'\phi = B\left(\begin{pmatrix}\phi'_{m,n,r}(0) \\ -\phi'_{m,n,r}(l) \\ \phi'_{m,n,u}(0) \\ -\phi'_{m,n,u}(l)\end{pmatrix}\right)_{(m,n)\in\mathbb{Z}^2}$$

with operators $B : l^2(\mathbb{Z}^2) \otimes \mathbb{C}^4 \to l^2(\mathbb{Z}^2)$ and $C : l^2(\mathbb{Z}^2) \to l^2(\mathbb{Z}^2) \otimes \mathbb{C}^4$ given by

$$B : \left(\begin{pmatrix}h^{(1)}_{m,n} \\ h^{(2)}_{m,n} \\ h^{(3)}_{m,n} \\ h^{(4)}_{m,n}\end{pmatrix}\right) \mapsto \big(h^{(1)}_{m,n} + e^{-i\pi n\theta}h^{(2)}_{m-1,n} + \beta h^{(3)}_{m,n} + \beta e^{i\pi m\theta}h^{(4)}_{m,n-1}\big),$$

and

$$C : (g_{m,n}) \mapsto \left(\begin{pmatrix}g_{m,n} \\ e^{i\pi n\theta}g_{m+1,n} \\ \beta g_{m,n} \\ \beta e^{-i\pi m\theta}g_{m,n+1}\end{pmatrix}\right),$$

cf. (5).

Let $g \in l^2(\mathbb{Z}^2)$. For $z \notin \operatorname{spec} S$, finding the solution ϕ with $(\Pi - z)\phi = 0$ and $\Gamma\phi = g$ reduces to a series of boundary value problems for components of ϕ,

$$\left(-\frac{d^2}{dt^2} + V(t) - z\right)\phi_{m,n,r/u}(t) = 0,$$

$$\left(\begin{pmatrix}\phi_{m,n,r}(0) \\ \phi_{m,n,r}(l) \\ \phi_{m,n,u}(0) \\ \phi_{m,n,u}(l)\end{pmatrix}\right) = Cg,$$

and

$$\begin{pmatrix}\phi'_{m,n,r}(0) \\ -\phi'_{m,n,r}(l) \\ \phi'_{m,n,u}(0) \\ -\phi'_{m,n,u}(l)\end{pmatrix} = \begin{pmatrix}s_{11}(z) & s_{12}(z) & 0 & 0 \\ s_{21}(z) & s_{22}(z) & 0 & 0 \\ 0 & 0 & s_{11}(z) & s_{12}(z) \\ 0 & 0 & s_{21}(z) & s_{22}(z)\end{pmatrix}\begin{pmatrix}\phi_{m,n,r}(0) \\ \phi_{m,n,r}(l) \\ \phi_{m,n,u}(0) \\ \phi_{m,n,u}(l)\end{pmatrix}.$$

For $Q(z)g \equiv \Gamma'\phi$ one has

$$\Gamma'\psi = B\left(\begin{pmatrix}\phi'_{m,n,r}(0) \\ -\phi'_{m,n,r}(l) \\ \phi'_{m,n,u}(0) \\ -\phi'_{m,n,u}(l)\end{pmatrix}\right).$$

Therefore, $Q(z) = BK(z)C$, where $K(z)$ is a linear operator on $l^2(\mathbb{Z}^2) \otimes \mathbb{C}^4$ with the matrix

$$K(z) = \operatorname{diag}\left(\begin{pmatrix}s_{11}(z) & s_{12}(z) & 0 & 0 \\ s_{21}(z) & s_{22}(z) & 0 & 0 \\ 0 & 0 & s_{11}(z) & s_{12}(z) \\ 0 & 0 & s_{21}(z) & s_{22}(z)\end{pmatrix}\right).$$

In other words, for any $g \in l^2(\mathbb{Z}^2)$ one has

$$Cg = \left(\begin{pmatrix}g_{m,n} \\ e^{i\pi n\theta}g_{m+1,n} \\ \beta g_{m,n} \\ \beta e^{-i\pi m\theta}g_{m,n+1}\end{pmatrix}\right),$$

$$K(z)Cg = \left(\begin{pmatrix}s_{11}(z)g_{m,n} + e^{i\pi n\theta}s_{12}(z)g_{m+1,n} \\ s_{21}(z)g_{m,n} + e^{i\pi n\theta}s_{22}(z)g_{m+1,n} \\ \beta\left(s_{11}(z)g_{m,n} + e^{-i\pi m\theta}s_{12}(z)g_{m,n+1}\right) \\ \beta\left(s_{21}(z)g_{m,n} + e^{-i\pi m\theta}s_{22}(z)g_{m,n+1}\right)\end{pmatrix}\right),$$

and, finally,

$$\begin{aligned}\left(Q(z)g\right)_{m,n} &= \left(BK(z)Cg\right)_{m,n} \\ &= (1 + \beta^2)\left(s_{11}(z) + s_{22}(z)\right)g_{m,n} + e^{i\pi n\theta}s_{12}(z)g_{m+1,n} + e^{-i\pi n\theta}s_{21}(z)g_{m-1,n} \\ &+ \beta^2 e^{-i\pi m\theta}s_{12}(z)g_{m,n+1} + \beta^2 e^{i\pi m\theta}s_{21}(z)g_{m,n-1}.\end{aligned} \tag{12}$$

As can be seen from (10), there holds $s_{12}(z) = s_{21}(z)$ and (12) becomes exactly (11). $\qquad\square$

Corollary 9. *A number $z \in \mathbb{R} \setminus \operatorname{spec} D$ lies in the spectrum of L iff*

$$0 \in \operatorname{spec}\left[(1 + \beta^2)\left(s_{11}(z) + s_{22}(z)\right) - \alpha + s_{12}(z)M(\theta, \beta)\right].$$

5. Spectral Analysis

To describe the spectrum of Λ we need some additional information on the Krein matrix $s(z)$ from (10).

Proposition 10. *The matrix $s(z)$ has the following properties:*
(A) $s_{12}(z) \neq 0$ for all $z \notin \operatorname{spec} D$.
(B) For any $\alpha \in \mathbb{R}$ the function

$$\eta(z) = \frac{\alpha}{s_{12}(z)} - (1 + \beta^2) \frac{s_{11}(z) + s_{22}(z)}{s_{12}(z)} \tag{13}$$

can be extended to an entire function.
(C) The function $\dfrac{1}{1 + \beta^2} \eta(z)$ is the discriminant of the (generalized) Sturm-Liouville operator

$$P = -\frac{d^2}{dt^2} + W(t) + W_{\mathrm{KP}}(t), \tag{14}$$

where W is the periodic extension of V, $W(t + nl) = V(t)$, $t \in [0, l)$, $n \in \mathbb{Z}$, and W_{KP} is the Kronig-Penney potential, $W_{\mathrm{KP}}(t) = \dfrac{\alpha}{1 + \beta^2} \sum_{k \in \mathbb{Z}} \delta(t - kl)$; such operators P are also called Kronig-Penney Hamiltonians.
(D) There holds $\eta(\mu_k) \leq -2(1 + \beta^2)$ for even k and $\eta(\mu_k) \geq 2(1 + \beta^2)$ for odd k. (Recall that μ_k are the eigenvalues of D.)
(E) For all real z with $|\eta(z)| < 2(1 + \beta^2)$ there holds $\eta'(z) \neq 0$. The function η has no local minima with $\eta = 2(1 + \beta^2)$ and no local maxima with $\eta = -2(1 + \beta^2)$.

Proof. Recall that $s(z)$ is given by (10) with u_1, u_2 from (9). There holds $s_{12}(z) = \dfrac{1}{u_1(l; z)}$ and $s_{12}(z) \neq 0$ for all $z \notin \operatorname{spec} D$ since $z \mapsto u_1(l; z)$ is an entire function. This proves (A).

Substituting (10) for $z \notin \operatorname{spec} D$ in (13) one arrives at

$$\eta(z) = (1 + \beta^2)\big(u_1'(l; z) + u_2(l; z)\big) + \alpha u_1(l; z)$$

and η obviously has analytic extension to all points of $\operatorname{spec} D$. This proves (B).

To understand the meaning of η look at the operator (14). This operator acts as $f \mapsto -f'' + Wf$ on functions $f \in H^2(\mathbb{R} \setminus l\mathbb{Z})$ satisfying

$$\begin{pmatrix} f'(kl+) \\ f(kl+) \end{pmatrix} = \begin{pmatrix} 1 & \frac{\alpha}{1 + \beta^2} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} f'(kl-) \\ f(kl-) \end{pmatrix}, \quad k \in \mathbb{Z}. \tag{15}$$

Let y_1, y_2 be two solutions of $(P - z)y = 0$ with $y_1(0+; z) = y_2'(0+; z) = 0$ and $y_1'(0+; z) = y_2(0+; z) = 1$. Consider the matrix

$$M(z) = \begin{pmatrix} y_1'(l+; z) & y_2'(l+; z) \\ y_1(l+; z) & y_2(l+; z) \end{pmatrix}.$$

It is well-known that the spectrum of P consists exactly of real z satisfying $\operatorname{tr} M(z) \equiv y_1'(l+; z) + y_2(l+; z) \in [-2, 2]$, see e.g. [15, 22]. The function $\operatorname{tr} M(z)$ is called the discriminant or the Lyapunov function of P and plays an important role in the study of

second order differential operators; if $\alpha = 0$, the study of this function is a classical topic of the theory of ordinary differential equations, see e.g. [10,29].

On the other hand, note that on the interval $(0, l)$ the solutions y_1 and y_2 coincide with u_1 and u_2 from (9), respectively. In particular, $y_{1,2}(l-; z) = u_{1,2}(l; z)$ and $y'_{1,2}(l-; z) = u'_{1,2}(l; z)$ Therefore, taking into account the boundary conditions (15) we can write $M(z)$ in the form

$$M(z) = \begin{pmatrix} \dfrac{\alpha}{1+\beta^2} u_1(l; z) + u'_1(l; z) & \dfrac{\alpha}{1+\beta^2} u_2(l; z) + u'_2(l; z) \\ u_1(l; z) & u_2(l; z) \end{pmatrix},$$

and $\operatorname{tr} M(z) = \dfrac{1}{1+\beta^2} \eta(z)$, which proves (C). The items (D) and (E) describe typical properties of the discriminants of one-dimensional periodic operators.

To prove (D) note that for any k one has $u_1(l, \mu_k) = 0$, and $\eta(\mu_k) = (1 + \beta^2)\big((u'_1(l; \mu_k) + u_2(l; \mu_k)\big)$, i.e. $\dfrac{1}{1+\beta^2} \eta(\mu_k)$ coincides with the value of the discriminant of the classical periodic Sturm–Liouville problem ($\alpha = 0$), for which the requested inequalities are well known, see e.g. Lemma VIII.3.1 in [10].

The first part of (E) is known for much more general potentials, see e.g. Lemma 5.2 in [22]. As for the second part, local maxima with $\eta = -2(1 + \beta^2)$ and local minima with $\eta = 2(1 + \beta^2)$ would be isolated eigenvalues of P, which is impossible, because the spectrum of P is absolutely continuous [30]. □

Therefore, up to the discrete set $\operatorname{spec} D$ the spectrum of Λ is the preimage of $\operatorname{spec} M(\theta, \beta)$ under the entire function η. The operator $M(\theta, \beta)$ is very sensitive to the arithmetic properties of θ and is closely related to the Harper operator, cf. [38]. The nature of the spectrum of $M(\theta, \beta)$ in its dependence on θ is described in the following proposition, which summarizes Theorem 2.7 in [38] (Item A), Theorem 4.2 in [38], Theorem 1.6 in [5] and the main theorem in [4] (Item B), and Theorem 2.1 in [8] (Item C).

Proposition 11. *(A) The operator $M(\theta, \beta)$ has no eigenvalues for all θ and β.*

(B) If θ is irrational, the spectrum of $M(\theta, \beta)$ is a Cantor set. If, in addition, $\beta = 1$, the spectrum has zero Lebesgue measure.
(C) For non-integer θ there holds $\|M(\theta, \beta)\| < 2(1 + \beta^2)$.

The previous discussion gives a description of the spectrum of Λ in $\mathbb{R} \setminus \operatorname{spec} D$. Let us include $\operatorname{spec} D$ into consideration.

Proposition 12. *There holds* $\operatorname{spec} D \subset \operatorname{spec} \Lambda$. *Moreover, each* $\mu_k \in \operatorname{spec} D$ *is an infinitely degenerate eigenvalue of* Λ.

Proof. Consider an eigenvalue μ_k of D and the corresponding eigenfunction f with $f'(0) = 1$ and let $\sigma := f'(l)$.

Let θ be rational. Take $M \in \mathbb{Z}$ such that $\theta M \in 2\mathbb{Z}$. Let $p, q \in \mathbb{Z}$. Denote by ϕ the function from $\mathcal{H}$ whose only non-zero components are

$$\phi_{pM+j,qM,r} = \beta\sigma^j f, \quad \phi_{pM,qM+j,u} = -\sigma^j f,$$
$$\phi_{(p+1)M,qM+j,u} = \sigma^{M+j} f, \quad \phi_{pM+j,(q+1)M,r} = -\beta\sigma^{M+j} f,$$
$$j = 0, \ldots, M - 1.$$

Clearly, $\phi \in \text{dom}\,\Lambda$ and $-\phi''_{m,n,r/u} + (V - \mu_k)\phi_{m,n,r/u} = 0$ for all $m, n \in \mathbb{Z}$. Therefore, ϕ is an eigenfunction of Λ with the eigenvalue μ_k. As p and q are arbitrary, one can construct infinitely many eigenfunctions with non-intersecting supports. Therefore, each μ_k is infinitely degenerate in $\text{spec}\,\Lambda$.

Now let θ be irrational. We use arguments similar to the Schnol-type theorems [27]. For each $n \in \mathbb{Z}$ put $\phi_{-n,n,r} = \beta e^{i\pi n\theta} f$ and $\phi_{-n,n,u} = -e^{i\pi n\theta} f$. The "chain" constructed from these components does not belong to $\mathcal{H}$, but satisfies the boundary conditions (5). Moreover, $-\phi''_{n,-n,r/u} + (V - \mu_k)\phi_{n,-n,r/u} = 0$ for all n, i.e. this chain is a "generalized eigenfunction" of Λ.

Take $\varphi \in C^\infty[0, l]$ with $\varphi(0) = \varphi'(0) = 0$ and $\varphi(l) = \varphi'(l) = 1$. For any $N \in \mathbb{N}$ construct $\psi^{(N)} \in \mathcal{H}$ such that

$$\psi^{(N)}_{-n,n,r/u} = \phi_{-n,n,r/u} \quad \text{if } |n| < N,$$

$$\psi^{(N)}_{-N,N,r} = \varphi\phi_{-N,N,r}, \quad \psi^{(N)}_{N,-N,u} = \varphi\phi_{N,-N,u},$$

$$\psi^{(N)}_{m,n,i} = 0 \quad \text{for all other } m, n \in \mathbb{Z} \text{ and } i = r, u.$$

Clearly, $\psi^{(N)} \in \text{dom}\,\Lambda$ for any N and $\|\psi^{(N)}\| \geq \sqrt{2N}\|f\|$. Moreover, the only two non-zero components of $g^{(N)} = (\Lambda - \mu_k)\psi^{(N)}$ are

$$g^{(N)}_{-N,N,r} = \beta e^{i\pi N\theta}\left(-\varphi'' f - 2\varphi' f' - \varphi f'' + (V - \mu_k)\varphi f\right)$$
$$= -\beta e^{i\pi N\theta}\left(\varphi'' f + 2\varphi' f'\right),$$

and

$$g^{(N)}_{N,-N,u} = -e^{i\pi N\theta}\left(-\varphi'' f - 2\varphi' f' - \varphi f'' + (V - \mu_k)\varphi f\right) = e^{i\pi N\theta}\left(\varphi'' f + 2\varphi' f'\right).$$

Therefore, $\|g^{(N)}\| \equiv \|(\Lambda - \mu_k)\psi^{(N)}\| = \sqrt{1 + \beta^2}\,\|\varphi'' f + 2\varphi' f'\| \equiv C$ and

$$\lim_{N\to\infty} \frac{\|(\Lambda - \mu_k)\psi^{(N)}\|}{\|\psi^{(N)}\|} \leq \lim_{N\to\infty} \frac{C}{\sqrt{2N}\|f\|} = 0,$$

which means that $\mu_k \in \text{spec}\,\Lambda$. Let us show that μ_k is an eigenvalue of Λ. By Proposition 11(C) one has $\|M(\theta, \beta)\| < 2(1 + \beta^2)$. Recall that the spectrum of Λ outside $\text{spec}\,D$ is the preimage of $\text{spec}\,M(\theta, \beta)$ under the function η and, due to Proposition 10(D), does not contain μ_k. As μ_k is an isolated point of the spectrum, it is an eigenvalue of Λ, which is infinitely degenerate according to the arguments given in Remark 1. $\quad\square$

Now we state the main result of the paper.

Theorem 13. *The spectrum of Λ is the union of two sets,*

$$\text{spec}\,\Lambda = \Sigma_0 \cup \Sigma, \quad \Sigma_0 = \text{spec}\,D, \quad \Sigma = \eta^{-1}\big(\text{spec}\,M(\theta, \beta)\big),$$

and has the following properties:

(A) The discrete spectrum is empty and the point spectrum coincides with Σ_0.
(B) The set Σ is non-empty, moreover, the intersection $[\mu_k, \mu_{k+1}] \cap \Sigma$ is non-empty for any k.
(C) For rational θ the singular continuous spectrum of Λ is empty and the absolutely continuous spectrum coincides with Σ and has a band structure.

(D) For irrational θ, the spectrum of Λ is infinitely degenerate. The part Σ is a closed nowhere dense set without isolated points, and $\Sigma \cap (\mu_k, \mu_{k+1})$ is a Cantor set for any $k = 0, 1, 2, \ldots$. If additionally $\beta = 1$, then the spectrum of Λ has no absolutely continuous part and the singular continuous spectrum coincides with Σ.

Proof. Proposition 12 shows that $\Sigma_0 \subset \text{spec}\,\Lambda$. The spectrum of Λ outside spec D is described by Corollary 9 and, in virtue of Proposition 10(B), coincides with Σ.

(A) Propositions 8, 10(B), and 11(A) show the absence of eigenvalues of $Q(z) - \alpha$. By virtue of Proposition 7 the operator Λ has no point spectrum in $\mathbb{R} \setminus \text{spec}\,D$ for any θ. Therefore, due to Proposition 12 the point spectrum coincides with spec D, and all eigenvalues have infinite multiplicity.

(B) The trivial estimate $\|M(\theta, \beta)\| \leq 2(1+\beta^2)$ implies the inclusion spec $M(\theta, \beta) \subset [-2(1 + \beta^2), 2(1 + \beta^2)]$. The assertion follows now from Proposition 10(D).

(C) Let θ be rational. Take $N \in \mathbb{Z}$ with $N\theta \in 2\mathbb{Z}$. The operator Λ appears to be invariant under the shifts $(\phi_{m,n,r}, \phi_{m,n,u}) \mapsto (\phi_{m+kN,n+lN,r}, \phi_{m+kN,n+lN,u})$, $k, l \in \mathbb{Z}$, i.e. is $\mathbb{Z}^2$-periodic and, therefore, the absence of singular spectrum for Λ follows from the standard arguments of the Bloch theory, see e.g. Theorem 11 in [27]. Therefore by (A) Σ coincides with the absolutely continuous spectrum. The spectrum of $M(\theta, \beta)$ consists of finitely many bands, so is $\eta^{-1}(\text{spec}\,M(\theta, \beta))$ between any two Dirichlet eigenvalues.

(D) Now let θ be irrational. The infinite degeneracy of spec Λ follows from the arguments of Remark 1. In view of continuity of η, the set of $z \in \mathbb{R}$ for which $|\eta(z)| < 2(1 + \beta^2)$ is a union of open disjoint intervals I_n. Moreover, due to Proposition 10(D) there is exactly one such interval between any two subsequent eigenvalues of D. Put $J_n = \overline{I_n}$. Note that $\cup J_n$ contains all points z with $|\eta(z)| \leq 2(1 + \beta^2)$. Due to Proposition 10(E), the restriction of η to J_n is a homeomorphism of J_n on the segment $[-2(1 + \beta^2), 2(1 + \beta^2)]$. Therefore, the preimage

$$K_n := \left(\eta|_{J_n}\right)^{-1}\left(\text{spec}\,M(\theta, \beta)\right) \subset J_n$$

is a Cantor set as is true of spec $M(\theta, \beta)$. Moreover, the intersection of any two of sets K_m is empty, which follows from Proposition 11(C) and Proposition 10(D). Therefore, the set $\cup K_n$, which coincides with Σ, is also closed, nowhere dense, and without isolated points.

If $\beta = 1$, then the spectrum of $M(\theta, \beta)$ has zero Lebesgue measure by Proposition 11(B). Since $\left(\eta|_{I_n}\right)^{-1}$ are real-analytic, the sets K_n and hence $\Sigma = \cup K_n$ are also of zero Lebesgue measure. Such a set cannot support absolutely continuous spectrum and does not intersect the point spectrum due to (A), therefore, Σ is the singular continuous spectrum. $\square$

In view of the unitary equivalence between the operators Λ and L, Theorem 13 provides a complete spectral analysis of the magnetic Schrödinger operator on the periodic graph. At the same time, we believe that the operator Λ may be considered as a model of quasiperiodic interaction on quantum graphs and may be useful also outside the problems related to magnetic fields.

We formulate several corollaries in order to answer the following natural questions arising in the case of rational magnetic flux θ:

- Are the eigenvalues of Λ (and of L) isolated or embedded in the continuous spectrum?
- Is the number of gaps in the spectrum finite or infinite? Note that the rank of the lattice defining the magnetic translation group is equal to 2, therefore, one can expect the validity of the Bethe–Sommerfeld conjecture for $\theta = 0$.

We emphasize that these questions are rather non-trivial even for lattices without any potentials; for example, rectangular lattices with δ-boundary conditions at the nodes can have very different properties depending on the coupling constants and the ratio between the edge lengths [13]. We will see that the introduction of scalar potentials on edges provides a mechanism of gap creation similar to the so-called decoration [37].

The case of a non-trivial magnetic field can be treated by a simple norm estimate.

Corollary 14. *If θ is non-integer, then the spectrum of Λ has infinitely many gaps, and all μ_k lie inside the gaps.*

Proof. In this case the set Σ does not contain μ_k due to Propositions 10(D) and 11(D). □

Let us consider now the case without magnetic field in greater details.

Corollary 15. *Let θ be integer.*

(A) *The part Σ of the spectrum of Λ coincides with the spectrum of the Kronig-Penney Hamiltonian P from (14). In particular, if there are inifinitely many gaps in the spectrum of P, then Λ has the same property.*

(B) *If V is a convex smooth function whose derivative does not vanish, then all gaps are open for any α, the spectrum of P and hence also of Λ has infinitely many gaps, and all μ_k are isolated in spec Λ.*

(C) *Let the gap of P near μ_k be closed for $\alpha = 0$. Then μ_k is an embedded eigenvalue of Λ for all α. In particular, μ_k lies on a band edge for $\alpha \neq 0$. For $V = 0$ and $\alpha = 0$ all gaps are closed and all μ_k are embedded into the continuous spectrum.*

Proof. (A) In this case one has spec $M(\theta, \beta) = \left[- 2(1 + \beta^2), 2(1 + \beta^2)\right]$ and the set $\Sigma \equiv \eta^{-1}\left(\left[- 2(1 + \beta^2), 2(1 + \beta^2)\right]\right)$ coincides with the spectrum of P by Proposition 10(C).

(B) Denote $v(z) = u'_1(l; z) + u_2(l; z)$, where u_1 and u_2 are the special solutions from Example 5. Clearly, v is the discriminant of the periodic Sturm-Liouville operator $Q := -\dfrac{d^2}{dt^2} + W$ with W from (14). If $\alpha = 0$, then $P = Q$ and $\eta(z) = (1 + \beta^2)v(z)$ for all z. Let V be smooth convex with $V' \neq 0$ and $\alpha = 0$, then it is proved in [17] (see Lemma 3 and Theorem 2 therein) that all gaps of P are open and that μ_k do not belong to spec $P = \Sigma$, which means that $|v(\mu_k)| > 2$. One has $\eta(\mu_k) = (1 + \beta^2)v(\mu_k) + \alpha u_1(l; \mu_k) = (1 + \beta^2)v(\mu_k)$, and the gap remains open for all $\alpha \neq 0$ as $|\eta(\mu_k)| > 2(1 + \beta^2)$.

(C) The case with $V = 0$ and $\alpha = 0$ is obvious. If the gap near μ_k is closed, then $v(\mu_k) = \pm 2$, $\eta(\mu_k) = \pm 2(1 + \beta^2)$, and $\mu_k \in \Sigma$. Moreover, $v'(\mu_k) = 0$. As $\partial_z u_1(l; \mu_k) \neq 0$ (see Example 5), one has $\eta'(\mu_k) \neq 0$ for $\alpha \neq 0$, which means that $\eta \mp 2(1 + \beta^2)$ changes the sign at μ_k. This means that there is a gap near μ_k. □

6. Concluding Remarks

We hope that the approach presented here can be extended to the analysis of more general periodic magnetic systems, for example, for more complicated combinatorial structures, for nodes and edges with geometric defects or measure potentials, or with the spin-orbital coupling taken into account. Another open question is whether one can deal with more general boundary conditions. Although there are some particular examples for which

the above construction works, we are not able to present a suitable general picture at the moment. We hope to clarify the situation, which actually goes beyond the quantum graph context, in subsequent works.

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