Magnetic layers with periodic point perturbations

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Abstract

We study spectral properties of a spinless quantum particle confined to an infinite planar layer with hard walls which interacts with a periodic lattice of point perturbations and a homogeneous magnetic field perpendicular to the layer. It is supposed that the lattice cell contains a finite number of impurities and the flux through the cell is rational. Using the Landau-Zak transformation, we convert the problem into investigation of the corresponding fiber operators which is performed by means of Krein's formula. This yields an explicit description of the spectral bands which may be absolutely continuous or degenerate, depending on the parameters of the model.

1 Introduction

The object of the present study is a three-dimensional spinless quantum particle interacting with a homogeneous magnetic field and a periodic point potential. In addition, the particle is confined to a flat layer of a constant width d with Dirichlet boundary conditions, the magnetic field being perpendicular to the layer. The lattice of the point interactions is two-dimensional, not necessarily planar, and both of its generating vectors are, of course, parallel to the boundary planes of the layer.

The problem is clearly motivated by the need of modeling electrons in a semiconductor layer with 'impurities', either natural or artificially created. If they may be supposed to be well localized, one often describes them by point interactions. It is useful because in such a way we get solvable models which make it possible to derive the spectral and scattering properties of a given configuration in a relatively simple way, and at the same time they reproduce the basic features of an actual crystal-lattice layer with some alien atoms and a low-density electron gas. Various systems of this type have been investigated in the literature; we refer to our previous paper [EN] and an earlier study of the two-dimensional analogue [EGŠT] for an extensive bibliography as well as for a discussion of the used approximations.

The said paper [EN] was devoted to investigation of a flat hard-wall layer with a finite number of point interactions, with or without a magnetic field; we analyzed there the spectra, and in the former case also the scattering properties of such systems. The situation is more complicated when the number of point perturbation is infinite. The spectral content of such models is very rich and difficult to treat in the general setting; this is why we restrict our attention here to the particular case specified above in which the periodicity allows us to employ the Bloch-Floquet decomposition, with its specific features due to presence of a homogeneous magnetic field which were first pointed out by J. Zak in his classical papers [Za].

On the other hand, the present work represents a generalization of the results derived in [Ge] for a two-dimensional Schrödinger operator with a periodic point potential and a homogeneous magnetic field perpendicular to the plane. Loosely speaking we 'add' the third dimension in the direction of the magnetic field and allow the positions of the point potentials to 'spread' transversally preserving the periodicity – this is what we meant by a two-dimensional lattice in the first paragraph.

Our basic tool for spectral analysis is the Krein formula which expresses the resolvent perturbation due to the point interactions. It is important that in absence of the impurities the Hamiltonian of the system allows a separation of the plane variables from the transverse one. As a consequence, the free resolvent kernel of the fiber operator (as well as all quantities derived from it such as Bloch eigenfunctions, etc.) can be written by means of explicitly given series. In this sense our model is solvable, the only difference from those in the full space is that there such quantities can be written in terms of elementary or special functions.

In accordance with [Ge] we adopt two more simplifying assumptions: we suppose that the number of point interactions in an elementary cell of the lattice is *finite* and the flux through the cell is *rational*. Especially the second one is important because one naturally expects in analogy with the two-dimensional case that the spectral character can be substantially different for an irrational flux; it is an independent problem of its own interest which we are not going to discuss here. On the other hand, following the setting of the paper [Ge] we study general point perturbations including the situations when the particle can "jump" between different impurity sites within a cell. The reason is that mathematically it does not mean a lot of extra work; physically interesting case is naturally that of point interactions defined by *local* boundary conditions, i.e. with the parameter matrix A appearing in the relation (4.1) being diagonal.

Let us review briefly the contents of the paper. We start in the following section with analyzing the free Hamiltonian. Next, in Section 3, we formulate the Bloch-Floquet theory for the present case; the main result is so-called Landau-Zak transformation which makes it possible to reduce the spectral problem to investigation of suitable fiber operators. This is done by means of Krein's formula in Section 4. The last three sections are devoted to successive analysis of the spectra at three levels of complexity: *(i)* an integer flux (in the units of magnetic-flux quanta) through the elementary cell and a single point interaction in the cell, *(ii)* an integer flux and a finite number of impurities in the elementary cell, *(iii)* and finally, the case of an arbitrary rational flux.

2 Free Hamiltonian

Consider an infinite layer of a fixed width d, i.e. $\Sigma = \mathbb{R}^2 \times [0, d]$. The coordinates we are going to use are $\vec{x} = (x, x_3)$, where $x = (x_1, x_2) \in \mathbb{R}^2$ and $x_3 \in [0, d]$. The layer is placed into a homogeneous magnetic field of intensity $\vec{B} = (0, 0, B)$. We will use the circular gauge, $\vec{A} = \frac{1}{2}B(-x_2, x_1, 0)$, and rational units, $\hbar = c = e = 2m = 1$. A quantum particle confined to the layer is described by the free magnetic Schrödinger operator in $L^2(\Sigma)$,

$$H_0 = (-i\vec{\nabla} - \vec{A})^2, \tag{2.1}$$

with Dirichlet boundary conditions

$$\psi(x, 0) = \psi(x, d) = 0\,, \quad x \in \mathbb{R}^2. \tag{2.2}$$

In the absence of an additional interaction the variable separate, i.e. the operator H_0 can be decomposed into transverse modes,

$$H_0 = \bigoplus_{n=1}^{\infty} h_n \otimes I\,, \quad h_n = \left(-i\frac{\partial}{\partial x_1} + \frac{B}{2}\,x_2\right)^2 + \left(-i\frac{\partial}{\partial x_2} - \frac{B}{2}\,x_1\right)^2 + \left(\frac{\pi n}{d}\right)^2, \tag{2.3}$$

where I is the unit operator in $L^2(0,d)$. The first two terms at the r.h.s., in the following denoted as h, describe a two-dimensional particle in the perpendicular homogeneous field in the circular gauge. The third term represents the energy of the nth transverse mode; the corresponding normalized eigenfunction will be denoted as $\chi_n :\ \chi_n(x_3) = \sqrt{\frac{2}{d}}\,\sin\left(\frac{n\pi x_3}{d}\right)$. The resolvent kernel of the operator h is well known [DMM] to be

$$\begin{aligned} (h-z)^{-1}(x,x') &= \frac{1}{4\pi}\,\exp\left(-i\frac{B}{2}\,x\wedge x' - \frac{|B|}{4}\,|x-x'|^2\right) \\ &\quad \times \Gamma\left(\frac{|B|-z}{2|B|}\right) U\left(\frac{|B|-z}{2|B|}, 1; \frac{|B|}{2}\,|x-x'|^2\right), \end{aligned}$$

where U is the irregular confluent hypergeometric function, Γ is the gamma function and $x\wedge x' := x_1x_2' - x_2x_1'$. For the sake of brevity we denote this kernel as $G_0^{2D}(x,x';z)$. The decomposition (2.3) then yields an explicit form for the resolvent kernel of the operator (2.1), namely

$$\begin{aligned} G_0(\vec{x},\vec{x}';z) &\equiv (H_0-z)^{-1}(x,x_3;x',x_3') \\ &= \sum_{n=1}^{\infty} G_0^{2D}\left(x,x';z-\left(\frac{\pi n}{d}\right)^2\right)\chi_n(x_3)\chi_n(x_3') \\ &= \frac{1}{2\pi d}\,\exp\left(-i\frac{B}{2}\,x\wedge x' - \frac{|B|}{4}\,|x-x'|^2\right) \\ &\times \sum_{n=1}^{\infty} \Gamma\left(\frac{|B|-k_n^2(z)}{2|B|}\right) U\left(\frac{|B|-k_n^2(z)}{2|B|}, 1; \frac{|B|}{2}\,|x-x'|^2\right) \\ &\times\ \sin\left(\frac{n\pi x_3}{d}\right)\sin\left(\frac{n\pi x_3'}{d}\right), \end{aligned} \tag{2.4}$$

where $k_n := \sqrt{z-(\pi n/d)^2}$. Applying Fourier transformation to the transverse part, $\mathcal{M} :\ L^2([0,d]) \mapsto \ell^2(\mathbb{N})$ defined by

$$(\mathcal{M}f)(n) = \int_0^d dy\,\chi_n(y)f(y)\,, \quad n\in\mathbb{N}\,, \tag{2.5}$$

one can rewrite the free resolvent kernel as a matrix with the elements

$$G_0(x,n;x',n';z) = \delta_{nn'} G_0^{2D}\left(x,x';z-\left(\frac{\pi n}{d}\right)^2\right) \tag{2.6}$$

Consequently, the spectrum of the free Hamiltonian consists of Landau levels shifted by the energies of the transverse modes,

$$\sigma\left(H_0\right) = \sigma_{ess}\left(H_0\right) = \left\{|B|(2m+1) + \left(\frac{\pi n}{d}\right)^2 :\ m, n-1 \in \mathbb{N}_0\right\}. \tag{2.7}$$

The energy corresponding to the lth Landau level and nth transverse mode will be denoted as $\varepsilon(l,n) := |B|(2l+1) + (\pi n/d)^2$. If the $|B|$ and $(\pi/d)^2$ are rationally related it may happen that there exist more than one pair of numbers (l_i, n_i) giving the same value, $\varepsilon(l_i, n_i) = z_0$. In such a case we will denote this set of pairs as $J(z_0)$ and the number of these pairs as $|J(z_0)|$.

3 Magnetic translations

Next we consider a lattice $\Gamma = \Lambda + K$, where Λ is a lattice spanned by two independent vectors in $\mathbb{R}^2$, which can be without loss of generality supposed to be $\vec{a} = (a_1, 0, 0)$ and $\vec{b} = (b_1, b_2, 0)$ with $b_2 \neq 0$, and K is a set of $|K|$ points $\vec{\kappa}^i,\ i = 1, \dots, n$, from the elementary cell $\{sa + tb :\ s,t \in [0,1)\} \times (0,d)$ of the (interior of the) layer.

As usual with periodic systems, the first thing to do is to find the appropriate representation of the translation group. In presence of a magnetic field the argument shift must be composed with multiplication by a suitable phase factor. Specifically, the translation by a vector $\vec{v} = (v, 0)$ acts in the state space $L^2(\Sigma)$ of our system as follows,

$$f(\vec{x}) \mapsto \exp(-\pi i \xi\, x \wedge v) f(\vec{x} - \vec{v}), \tag{3.1}$$

where ξ is the number of the flux quanta of the field $\vec{B}$ through the unit area of the plane $\mathbb{R}^2$. Recall that the quantum of magnetic flux is given by $2\pi\hbar c/|e|$, thus with the chosen system of units we have $\xi = B/(2\pi)$. The phase factor at the r.h.s. can be rewritten as $\exp\left(\frac{1}{2}(\vec{B} \times \vec{v}).\vec{x}\right)$. Since $\vec{B} = (0,0,B)$ and we consider translations in the plane, i.e. by a vector $\vec{v} = (v_1, v_2, 0)$, it is obvious that the third coordinate plays a marginal role only in magnetic translations. This allows us to follow closely the procedure used in [Ge] to analyze spectral properties of a particle confined to a plane, i.e. with the third components of the vectors $\vec{v}$ and $\vec{x}$ absent.

Let us briefly summarize needed notions and facts. First we define the group of discrete magnetic translation over the lattice Λ,

$$W(\xi,\Lambda)=\{(\vec{\lambda},\zeta):\ \vec{\lambda}\in\Lambda,\ \zeta=\exp(\pi i\eta n),\ n\in\mathbb{Z}\}\,, \tag{3.2}$$

where $\eta=a_1b_2\xi=a\wedge b\,\xi$ is the number of flux quanta of the field $\vec{B}$ through the elementary cell. In the coordinates relative to the basis $\vec{a}$ and $\vec{b}$ the multiplication in $W(\xi,\Lambda)$ has the form

$$(\vec{\lambda},\zeta)(\vec{\lambda}',\zeta')=\Big(\vec{\lambda}+\vec{\lambda}',\zeta\zeta'\exp(\pi i\eta(\lambda_a\lambda_b'-\lambda_b\lambda_a'))\Big)\,. \tag{3.3}$$

Notice that groups $W(\xi_i,\Lambda_i)$ corresponding to different values of ξ_i and different lattices Λ_i but having the same value of η are isomorphic, hence we will denote the group simply by W_η. Next we define the representation T of the group W_η in the space $L^2(\Sigma)$ as follows

$$(T(\vec{\lambda},\zeta)f)(\vec{x})=\zeta\exp(-\pi i\xi\,x\wedge\lambda)f(\vec{x}-\vec{\lambda})\,. \tag{3.4}$$

Furthermore, replacing $\vec{x}\in\Sigma$ in the last formula by vectors $\vec{\gamma}\in\Gamma$ we get a representation D of W_η in the space $\ell^2(\Gamma)$.

If the flux η is a rational number, then any unitary representation of the group W_η can be uniquely decomposed into orthogonal sum of irreducible representations. Any 'physical' irreducible representations can be parameterized by a point $p=(p_1,p_2)$ from the torus $T^2=[0,1)\times[0,1)$ – see [OT]. If η is an integer, then the group is Abelian and the irreducible representations are one-dimensional, their characters being given by

$$\chi((\vec{\lambda},\zeta);p)=\zeta\exp\Big(-2\pi i(\lambda_ap_1+\lambda_bp_2+(N/2)\lambda_a\lambda_b)\Big)\,. \tag{3.5}$$

For a general rational flux, $\eta=N/M$, the irreducible representations of W_η are generally M-dimensional. In particular, the generators $(\vec{a},1)$ and $(\vec{b},1)$ are in this case given by

$$\begin{aligned}\triangle((\vec{a},1);p) &= \operatorname{diag}\left[e^{-2\pi ip_1},e^{-2\pi i(p_1+\eta)},\dots,e^{-2\pi i(p_1+(M-1)\eta)}\right]\,,\\ \triangle((\vec{b},1);p) &= \begin{bmatrix}0 & I_{M-1}\\ e^{-2\pi ip_2} & 0\end{bmatrix}\,,\end{aligned} \tag{3.6}$$

where zeros in the second line are $(M–1)$-dimensional column and row vectors, respectively. In order to obtain nonequivalent representations, of course, we must restrict here p to the torus $T_\eta^2 = [0, M^{-1}) \times [0, 1)$.

The decomposition into irreducible representations is accomplished by the Landau-Zak transformation $\mathcal{L}_\eta$. Recall that the magnetic translations from W_η does not affect the third coordinate, or in the transverse-modes representation, they do not affect the quantum number n. By a straightforward modification of the two-dimensional formulae [Ge], we define thus $\mathcal{L}_\eta$ by

$$\begin{aligned}
\mathcal{L}_\eta \;&:\; L^2(\mathbb{R}^2) \otimes \ell^2(\mathbb{N}) \;\to\; L^2(T_\eta^2) \otimes \mathbb{C}^M \otimes \mathbb{C}^N \otimes \ell^2(\mathbb{N}) \otimes \ell^2(\mathbb{N}), \\
&(\mathcal{L}_\eta f)(p, j, k, l, n) = N^{-\frac{1}{2}} \sum_{m=-\infty}^{\infty} \exp\left(2\pi i m \frac{p_2 + k}{N}\right) \qquad (3.7) \\
&\qquad\qquad \times \int_{\mathbb{R}^2} d^2x f(x, n) \psi_0^*(x; p_1 + \eta j + m, l)\,, \\
&(\mathcal{L}_\eta^{-1} \widetilde{f})(x, n) = N^{-\frac{1}{2}} \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} \sum_{l=0}^{\infty} \sum_{m=-\infty}^{\infty} \int_0^{1/M} dp_1 \int_0^1 dp_2 \widetilde{f}(p, j, k, l, n) \\
&\qquad\qquad \times \exp\left(-2\pi i m \frac{p_2 + k}{N}\right) \psi_0(x; p_1 + \eta j + m, l)\,,
\end{aligned}$$

where $\psi_0(x; q, l)$ with $q \in \mathbb{R}$ and $l = 0, 1, \dots,$ are generalized eigenfunction of the operator h (the 'planar' part of the Hamiltonian H_0) associated with the lattice Λ,

$$\begin{aligned}
\psi_0(x; q, l) = &\left(\frac{b_2}{\eta} \frac{\pi^{3/2}}{|B|^{3/2}} 2^{l+1}\, l!\right)^{-\frac{1}{2}} \exp\left(i\pi \frac{b_1}{a_1 \eta} q^2\right) \exp\left(2\pi i \frac{x_1}{a_1}\left(\frac{\eta}{b_2} \frac{x_2}{2} + q\right)\right) \\
&\times \exp\left(-|B|\left(x_2 + \frac{b_2}{\eta} q\right)^2\right) H_l\left(|B|^{\frac{1}{2}}\left(x_2 + \frac{b_2}{\eta} q\right)\right),
\end{aligned}$$

with H_l being the lth-order Hermite polynomial. As in the two-dimensional case, we get the following claims.

Theorem 3.1 *Assume that the flux is a rational number, $\eta = N/M$. Then the Landau-Zak transformation (3.7) decomposes the representation T of a magnetic translation $(\vec{v}, \zeta) \in W_\eta$ into a direct integral of multiples of irreducible representations $\triangle(\cdot)$, in other words*

$$\mathcal{L}_\eta T(\vec{v}, \zeta) \mathcal{L}_\eta^{-1} = \int_{T_\eta^2}^{\oplus} d^2p\, \triangle(\vec{v}, \zeta; p) \otimes I_{\mathbb{C}^N} \otimes I_{\ell^2(\mathbb{N})} \otimes I_{\ell^2(\mathbb{N})}. \qquad (3.8)$$

In particular, if the flux η is integer, then the irreducible representations are one-dimensional and their characters are given by the expression (3.5).

The second important feature of the Landau-Zak transformation is that it diagonalizes the free Hamiltonian in the space $L^2(T^2_\eta)$, as well as any other operator which exhibits the magnetic-translation symmetry:

Theorem 3.2 *Assume that a self-adjoint operator H acting on $L^2(\Sigma)$ is invariant w.r.t. the group W_η; then it can be decomposed into a direct integral*

$$\widetilde{H} = \int_{T^2_\eta}^{\oplus} d^2p\, \widetilde{H}(p)\,, \tag{3.9}$$

where $\widetilde{H} = (\mathcal{L}_\eta \otimes \mathcal{M})H(\mathcal{L}_\eta \otimes \mathcal{M})^{-1}$ and the fiber operator $\widetilde{H}(p)$ acts on the space $\mathbb{C}^M \otimes \mathbb{C}^N \otimes \ell^2(\mathbb{N}) \otimes \ell^2(\mathbb{N})$.

4 The perturbed Hamiltonian

Now let us consider perturbation of the free Hamiltonian H_0 by point potentials placed at the points of the lattice Γ. To define the perturbed operator H_A, where A are the coupling-parameter matrix introduced by the relation (4.1) below, we employ the standard technique based on theory of self-adjoint extensions of symmetric operators. First we pass to the symmetric operator S_Γ which is the restriction of H_0 to the domain $D(S_\Gamma) := \{f \in D(H_0) : f(\vec\gamma) = 0,\ \vec\gamma \in \Gamma\}$, which is well defined in view of the usual Sobolev embedding. The sought Hamiltonian H_A is then an appropriate self-adjoint extension of the operator S_Γ. There is a family of such extensions which can be parametrized in different ways, the most traditional of which is the von Neumann one using unitary maps between deficiency subspaces. For our purposes it is more suitable to employ the mentioned self-adjoint operator A which acts in $\ell^2(\Gamma)$; its properties will be specified later.

One of possible characterizations of the extensions starts from the (generalized) boundary values. In this approach one determines the domain $D(H_A)$ as the set of all functions having prescribed behavior in the vicinity of the point-potential sites $\vec\gamma \in \Gamma$, namely

$$\psi(\vec x) = L_0(\psi;\vec\gamma)\frac{1 + i\vec A(\vec\gamma).(\vec x - \vec\gamma)}{|\vec x - \vec\gamma|} + L_1(\psi;\vec\gamma) + \mathcal{O}(|\vec x - \vec\gamma|),$$

where the vectors $L_j(\psi) := \{ L_j(\psi;\vec\gamma) :\ \vec\gamma \in \Gamma \}\,, j = 0, 1\,,$ are related by

$$L_1(\psi) = -4\pi A L_0(\psi)\,. \tag{4.1}$$

This is a generalization of the usual point-interaction definition – see [AGHH] – the latter corresponds to a diagonal A and represents the physically most interesting situation, at least from the viewpoint of modeling semiconductor layers with impurities, as we pointed out in the introduction.

Spectral properties of the Hamiltonian can be found by means of its resolvent. Krein's formula gives us its kernel, i.e. the Green's function of H_A for a fixed operator A,

$$G(\vec x,\vec x\,';z) = G_0(\vec x,\vec x\,';z) - \sum_{\gamma,\gamma'\in\Gamma} [Q(z)+A]^{-1}(\vec\gamma,\vec\gamma\,')G_0(\vec x,\vec\gamma;z)G_0(\vec\gamma\,',\vec x\,';z)\,. \tag{4.2}$$

with $Q(z)$ given by the relation (4.4) below. If we use the transverse-mode representation of the Hamiltonian in the space $L^2(\mathbb{R}^2)\otimes\ell^2(\mathbb{N})$ we get

$$\begin{aligned} G(x,n;x',n';z) \;&=\; \delta_{nn'}G_0^{2D}\left(x,x';z-\left(\frac{\pi n}{d}\right)^2\right) \qquad (4.3)\\ &- \sum_{\vec\gamma,\vec\gamma\,'\in\Gamma}[Q(z)+A]^{-1}(\vec\gamma,\vec\gamma\,')G_0^{2D}\left(x,\gamma;z-\left(\frac{\pi n}{d}\right)^2\right)\\ &\times G_0^{2D}\left(\gamma',x';z-\left(\frac{\pi n'}{d}\right)^2\right)\chi_n(\gamma_3)\chi_{n'}(\gamma_3').\end{aligned}$$

Since the Krein formula (4.2) was originally meant for a finite number of point potentials and the set Γ is infinite, we have to be a bit more precise. One possible way how to define the Hamiltonian H_A is via strong resolvent limit of the family of "restricted" operators $H_A(\bar\Gamma)$ which are point-interaction Hamiltonians referring to finite subsets $\bar\Gamma\subset\Gamma$, an example for diagonal A and $B=0$ can be found in [AGHH, III.1.1]. But the limit is not necessary; the existence of the operator H_A and the generalized Krein formula have been already proven for a larger class of operators, – see, e.g., [GMC] or [Po].

The matrix Q in (4.2) is given by

$$Q(\vec\gamma,\vec\gamma\,';z) = \begin{cases} G_0(\vec\gamma,\vec\gamma\,';z) & \vec\gamma\neq\vec\gamma\,' \\ Q_0(\gamma_3;z) & \vec\gamma=\vec\gamma\,' \end{cases}\,, \tag{4.4}$$

where $Q_0(\gamma_3;z)$ is the regularized Green's function (stripped off the pole singularity) which is defined by $\lim_{|\vec{x}-\vec{\gamma}|\to 0}(G_0(\vec{x},\vec{\gamma};z)-\frac{1}{4\pi}|\vec{x}-\vec{\gamma}|^{-1})$. We know from [EN] how it looks like,

$$\begin{aligned} Q_0(\gamma_3;z) &= \frac{1}{2\pi d}\sum_{n=1}^{\infty}\left[\ln\left(\frac{(\pi n)^2}{2|B|d^2}\right)-\psi\left(\frac{|B|-z+\left(\frac{\pi n}{d}\right)^2}{2|B|}\right)\right]\sin^2\left(\frac{\pi n\gamma_3}{d}\right) \\ &\quad +\frac{1}{4\pi d}\left[C_E+\psi\left(\frac{\gamma_3}{d}\right)+\frac{\pi}{2}\cot\left(\frac{\pi\gamma_3}{d}\right)\right]. \end{aligned} \tag{4.5}$$

In case when two point potentials are arranged vertically, i.e. $\gamma=\gamma'$ and $\gamma_3\neq\gamma_3'$, the corresponding element of Q is well defined but the expression (2.4) makes no sense and has to be recast into the form

$$\begin{aligned} Q(\vec{\gamma},\vec{\gamma}';z) &= \frac{1}{2\pi d}\sum_{n=1}^{\infty}\left[\ln\left(\frac{(\pi n)^2}{2|B|d^2}\right)-\psi\left(\frac{|B|-z+\left(\frac{\pi n}{d}\right)^2}{2|B|}\right)\right] \\ &\qquad \times\sin\left(\frac{\pi n\gamma_3}{d}\right)\sin\left(\frac{\pi n\gamma_3'}{d}\right) \\ &\quad +\frac{1}{4\pi d}\left[C_E+\psi\left(\frac{\gamma_3+\gamma_3'}{2d}\right)+\frac{\pi}{2}\cot\left(\frac{\pi(\gamma_3+\gamma_3')}{2d}\right)\right] \\ &\quad -\frac{1}{4\pi d}\left[C_E+\psi\left(\frac{|\gamma_3-\gamma_3'|}{2d}\right)+\frac{\pi}{2}\cot\left(\frac{\pi|\gamma_3-\gamma_3'|}{2d}\right)\right]. \end{aligned}$$

For the sake of brevity it is useful to rewrite the Krein's formula in a compact form,

$$R_A(z)=R_0(z)-\Gamma_z[Q(z)+A]^{-1}\Gamma_z^*, \tag{4.6}$$

where Γ_z is a map from $\ell^2(\Gamma)$ to $L^2(\mathbb{R}^2)\otimes\ell^2(\mathbb{N})$ defined by

$$(\Gamma_z\phi)(x,n):=\sum_{\vec{\gamma}\in\Gamma}\phi(\vec{\gamma})G_0^{2D}\left(x,\gamma;z-\left(\frac{\pi n}{d}\right)^2\right)\chi_n(\gamma_3). \tag{4.7}$$

The operator H_0 is invariant under magnetic translations from the group W_η. One can easily check that the free resolvent kernel satisfies the relation

$$G_0(\vec{x}-\vec{\lambda},\vec{x}'-\vec{\lambda};z)=\exp(\pi i\xi\,(x-x')\wedge\lambda)G_0(\vec{x},\vec{x}';z). \tag{4.8}$$

Our aim is to study the situation when the operator H_A is also W_η-invariant, which is the case when the operator A is assumed to satisfy the same condition. Notice that this is trivially satisfied if A is a diagonal matrix. We will assume only that A is a self-adjoint operator invariant w.r.t. W_η, and furthermore, that it is bounded and there exist two positive constants c_1 and c_2 such that

$$|A(\vec{\gamma},\vec{\gamma}')| \le c_1 \exp(-c_2|\gamma-\gamma'|) \quad \text{for all } \vec{\gamma},\gamma' \in \Gamma\,. \tag{4.9}$$

The last condition means a restriction on the non-locality we have allowed mathematically: it means that the probability of particle hoping between two points of the lattice Γ decays exponentially with their distance.

A similar estimate is valid for the operator Q – for any given $z \notin \sigma(H_0)$ there exist two positive constants c_3 and c_4 such that

$$|Q(\vec{\gamma},\vec{\gamma}';z)| \le c_3 \exp(-c_4|\gamma-\gamma'|) \quad \text{for all } \vec{\gamma},\gamma' \in \Gamma \tag{4.10}$$

as it follows from the definition (4.4) of the function Q and the free resolvent kernel (2.4). The infinite sum contained in the second formula converges because the term $\Gamma(u)U(u,1;s)$ can be written for large positive u as $2K_0(2\sqrt{us})$ (see [AS, 13.3.3]) and the Macdonald function K_0 decays exponentially for large argument. Using the asymptotics of the function $U(u,1;s)$ we conclude that the sum grows with $|\gamma|$ at most as a polynomial; hence the exponential term $\exp(-\frac{1}{4}|B||\gamma|^2)$ is sufficient to yield the estimate.

If z approaches a point from the spectrum of the free Hamiltonian H_0 the elements of Q may diverge – cf. [EN] – in other words the functions $Q(\vec{\gamma},\vec{\gamma}';\cdot)$ are in general meromorphic. We summarize the above discussion in the following theorem:

Theorem 4.1 *Suppose that an operator A acting on $\ell^2(\Gamma)$ is self-adjoint and W_η-invariant. Then there is exactly one self-adjoint extension H_A of the operator S_Γ with Green's function given by*

$$G(\vec{x},\vec{x}';z) = G_0(\vec{x},\vec{x}';z) - \sum_{\gamma,\gamma'\in\Gamma} [Q(z)+A]^{-1}(\vec{\gamma},\vec{\gamma}')G_0(\vec{x},\vec{\gamma};z)G_0(\vec{\gamma}',\vec{x}';z)\,,$$

where the operator $Q(z)$ is defined by the relations (4.4) and (4.5). As an operator in $\ell^2(\Gamma)$, i.e. an infinite matrix, $Q(\vec{\gamma},\vec{\gamma}';z)$ satisfies the estimate (4.10) for some $c_3, c_4 > 0$ and it is W_η-invariant. As a function of z, Q is meromorphic and all its poles belong to the spectrum $\sigma(H_0)$. Finally, the operator H_A is also W_η-invariant.

5 The case of integral flux and a monoatomic crystal

We begin with the simplest case assuming that the flux η through the elementary cell is integral, $\eta = N \geq 1$, and that this cell contains only one potential placed at $\vec{\kappa} = (0, 0, \kappa_3)$; in other words in this section we have $\Gamma = \Lambda + \{\vec{\kappa}\}$.

We already know from Thm. 3.1 that to diagonalize the representation T acting in $L^2(\Sigma)$ we have to employ the Landau-Zak transformation. Since $M = 1$ in the present case we drop the parameter j. Diagonalization of the representation D acting in $\ell^2(\Gamma)$ is achieved by the Fourier transformation $\mathcal{F}_\eta : \ \ell^2(\Lambda) \mapsto L^2(T^2)$ which is defined by

$$(\mathcal{F}_\eta \phi)(p) = \sum_{\vec{\lambda} \in \Lambda} \phi(\vec{\lambda} + \vec{\kappa}) e_\lambda(p) \tag{5.1}$$

with the basis $e_\lambda(p) := \exp(-2\pi i(\lambda_a p_1 + \lambda_b p_2 + N\lambda_a \lambda_b/2))$. It reduces the action of the magnetic translation to multiplication by the function $e_\lambda(p)$. In view of the W_η-invariance of G_0, the transformed function $\widetilde{Q}$ equals

$$\widetilde{Q}(p; z) = (\mathcal{F}_\eta Q(z) \mathcal{F}_\eta^{-1})(p) = \sum_{\vec{\lambda} \in \Lambda} Q(\vec{\lambda}, \vec{\kappa}; z) e_\lambda(p). \tag{5.2}$$

With the exponential estimate (4.10) of the function Q in mind, we infer that the function $\widetilde{Q}$ is well defined. It is also meromorphic in z with simple poles, which lie in $\sigma(H_0)$. Both the functions $\widetilde{Q}(p; z)$ and $\widetilde{A}(p)$ are real-analytic with respect to $p_1, p_2 \in \mathbb{R}$.

Our goal now is to find the $\mathcal{L}_\eta$-transformation of the Green's function given by Krein's formula (4.6). To this aim we denote

$$\begin{aligned} \widetilde{R}_A(z) &= \mathcal{L}_\eta R_A(z) \mathcal{L}_\eta^{-1}, \\ \widetilde{R}_0(z) &= \mathcal{L}_\eta R_0(z) \mathcal{L}_\eta^{-1}, \\ \widetilde{\Gamma}_z &= \mathcal{L}_\eta \Gamma_z \mathcal{F}_\eta^{-1}. \end{aligned}$$

After a straightforward computation we arrive at the formula

$$\begin{aligned} G(p; k, l, n; k', l', n'; z) &= \delta_{kk'} \, \delta_{ll'} \, \delta_{nn'} \, \frac{1}{\varepsilon(l, n) - z} \\ &- [\widetilde{Q}(p; z) + \widetilde{A}(p)]^{-1} \frac{\widetilde{\delta}_0(p; k, l)}{\varepsilon(l, n) - z} \, \frac{\widetilde{\delta}_0^*(p; k', l')}{\varepsilon(l', n') - z} \chi_n(\kappa_3) \, \chi_{n'}(\kappa_3) \, , \end{aligned} \tag{5.3}$$

where $\widetilde{\delta}_0(p;k,l)$ is the $\mathcal{L}_\eta$-transformed delta-function in $\mathbb{R}^2$,

$$\widetilde{\delta}_\gamma(p;k,l) = N^{-1/2} \sum_{m=-\infty}^{\infty} \exp\left(2\pi i m \frac{p_2+k}{N}\right) \psi_0^*(\gamma, p_1+m, l)\,; \tag{5.4}$$

we have used here the relation

$$\widetilde{\delta}_{\lambda+\gamma}(p;k,l) = \exp(\pi i \xi\, \gamma \wedge \lambda)\, e_\lambda(p)\, \widetilde{\delta}_\gamma(p;k,l)\,, \tag{5.5}$$

which follows from the W_η-invariance of the free resolvent kernel and the fact that $\widetilde{\delta}_\gamma(p;k,l) = (|B|(2l+1)-z)(\mathcal{L}_\eta G_0^{2D}(\cdot,\gamma;z))(p;k,l)$. Recall that although the Landau-Zak transformation $\mathcal{L}_\eta$ acts on $L^2(\mathbb{R}^2)\otimes \ell^2(\mathbb{N})$, it can be viewed as two-dimensional since it does not affect the transverse modes.

To perform the spectral analysis we need to know the behavior of the function $\widetilde{Q}(p;z)$ for fixed p and real z. It is convenient to treat this problem separately in each of the (infinitely many) intervals corresponding to gaps in the free Hamiltonian spectrum. To this end, we denote the points of $\sigma(H_0)$ arranged in the ascending order by $\varepsilon_i,\ i=0,1,\dots$. The function $\widetilde{Q}(p,\cdot)$ diverges at a chosen point ε_i if and only if there exists at least one pair of integer numbers $(l,n)\in J(\varepsilon_i)$ such that $\chi_n(\kappa_3)\neq 0$ and p belongs to $U_l = \{p\in T^2:\ \widetilde{\delta}_0(p;\cdot,l)\neq 0\}$, where the expression $\widetilde{\delta}_0(p;\cdot,l)$ stands for an N-dimensional vector. By [KL] the residues in Krein's formula (4.6) are given by $dQ/dz = \Gamma_{z^*}^*\Gamma_z$; the transformed form of this relation reads

$$\frac{\partial \widetilde{Q}}{\partial z}(p;z) = \sum_{l=0}^{\infty}\sum_{n=1}^{\infty} \frac{1}{|\varepsilon(l,n)-z|^2}\, \chi_n^2(\kappa_3) \sum_{k=0}^{N-1} |\widetilde{\delta}_0(p;k,l)|^2. \tag{5.6}$$

For notational convenience, we also put $\varepsilon_{-1}=-\infty$ and $U_{-1}=T^2$. It is clear from (5.6) that the function $\widetilde{Q}(p,\cdot)$ is monotonously increasing in each of the intervals $(\varepsilon_{i-1},\varepsilon_i)$.

The asymptotic behaviour of $\widetilde{Q}(p,z)$ for large negative z is governed by the function $Q_0(\kappa_3;z)$, while the contribution of the rest of the series in expression (5.2) for $\widetilde{Q}$ is bounded, its convergence being ensured by the estimate (4.10). By [EN] the divergent term has the expansion

$$Q_0(\kappa_3;z) = -\frac{\sqrt{-z}}{4\pi} + \mathcal{O}(1) \qquad \text{as} \qquad z\to -\infty\,. \tag{5.7}$$

Now we are ready to analyze the spectrum of the fibre operator $\widetilde{H}_A(p)$. The first thing we would like to know is whether the Landau levels of the free system stay in the spectrum $\sigma(\widetilde{H}_A(p))$. By examining the residues of the Green's function (5.3) at $z = \varepsilon_i \in \sigma(H_0)$, $i = 0, 1, \ldots$, it is straightforward find the multiplicity of ε_i in $\sigma(\widetilde{H}_A(p))$ and the corresponding eigenspaces.

Lemma 5.1 *Assume that the flux η equals an integer number N and the lattice Γ is 'monoatomic'. Fix a point ε_i from $\sigma(H_0)$ and $p \in T^2$, then one of the following three situations occurs:*
(i) if there is at least one pair $(l,n) \in J(\varepsilon_i)$ satisfying $\widetilde{\delta}_0(p;\cdot,l) \neq 0$ and $\chi_n(\kappa_3) \neq 0$, the multiplicity $d(p;\varepsilon_i)$ equals $N|J(\varepsilon_i)| - 1$ and the eigenspace is the orthogonal complement of the vector $\omega(p;\varepsilon_i)$ in the space $\Omega(p;\varepsilon_i)$, where

$$\begin{aligned} \omega(p;\varepsilon_i) &= \Big(\widetilde{\delta}_0(p;k,l)\chi_n(\kappa_3) \sum_{(l_0,n_0)\in J(\varepsilon_i)} \delta_{ll_0}\delta_{nn_o}\Big)_{k,l,n}, \\ \Omega(p;\varepsilon_i) &= \mathbb{C}^N \otimes \Big(\bigoplus_{(l,n)\in J(\varepsilon_i)} (e_l \otimes \chi_n) \Big), \end{aligned} \tag{5.8}$$

(ii) if $\chi_n(\kappa_3)\widetilde{\delta}_0(p;\cdot,l)$ is a zero vector for all indices $(l,n) \in J(\varepsilon_i)$ and $\widetilde{Q}(p;\varepsilon_i) + \widetilde{A}(p) \neq 0$, then $d(p;\varepsilon_i) = N|J(\varepsilon_i)|$ and $\Omega(p;\varepsilon_i)$ is the eigenspace,
(iii) if $\chi_n(\kappa_3)\widetilde{\delta}_0(p;\cdot,l)$ is a zero vector for all indices $(l,n) \in J(\varepsilon_i)$ and $\widetilde{Q}(p;\varepsilon_i) + \widetilde{A}(p) = 0$, then $d(p;\varepsilon_i) = N|J(\varepsilon_i)| + 1$. In this case the eigenspace is the linear hull of $\Omega(p;\varepsilon_i)$ and the vector $\Big(\frac{\widetilde{\delta}_0(p;k,l)\chi_n(\kappa_3)}{\varepsilon(l,n)-\varepsilon_i}\Big)_{k,l,n}$, where we put $0/0 := 0$ for elements with $(l,n) \in J(\varepsilon_i)$.

This answers the question what happens with the free Hamiltonian spectrum under influence of the perturbation. However, the spectrum $\sigma(\widetilde{H}_A(p))$ contains not only the original modified Landau levels but also additional points due to the presence of the point potential. From the properties of $\widetilde{Q}(p,\cdot)$ it is obvious that there is exactly one solution $E_{i_k}(p)$ of the implicit equation

$$\widetilde{Q}(p;E) + \widetilde{A}(p) = 0 \tag{5.9}$$

in any interval $(\varepsilon_{i_{k-1}(p)}, \varepsilon_{i_k(p)})$, where $(\varepsilon_{i_k(p)})_{k=-1}^{\infty}$ is a subsequence of all points from $(\varepsilon_i)_{i=-1}^{\infty}$ at which the function $\widetilde{Q}(p;\cdot)$ diverges. If E does not belong to $\sigma(H_0)$, the said solution is a nondegenarate eigenvalue of $\widetilde{H}_A(p)$ with the unnormalized eigenvector $\Big(\frac{\widetilde{\delta}_0(p;k,l)}{\varepsilon(l,n)-E(p)}\,\chi_n(\kappa_3)\Big)_{k,l,n}$. This vector is non-trivial, which follows from the inequality (6.9) derived below applied to the derivative $\partial\widetilde{Q}/\partial z$ given in the monoatomic case by (5.6).

Let us summarize the effect of the periodic point potential on the spectrum $\sigma(\widetilde{H}_A(p))$ at a fixed point $p \in T^2$. The modified Landau level ε_i in the spectrum of the free Hamiltonian H_0 has the multiplicity equal to $N|J(\varepsilon_i)|$. In the perturbed spectrum $\sigma(\widetilde{H}_A(p))$ the generic situation is the case (i) of the above lemma, when the function $\widetilde{Q}(p;\cdot)$ diverges at ε_i. Then an eigenvalue splits off this level moving down with the increasing $\widetilde{A}(p)$ towards the neighbouring lower modified Landau levels. In particular, for $N|J(\varepsilon_i)| = 1$ the perturbation removes in this way the level ε_i from the spectrum $\sigma(\widetilde{H}_A(p))$ entirely. On the other hand, if $\widetilde{Q}(p;\cdot)$ does not diverge at ε_i, the multiplicity remains the same or it can be enlarged by one; the latter happens when an eigenvalue coming from a higher modified Landau level reaches ε_i for a particular $\widetilde{A}(p)$. These two situations correspond, of course, to cases (ii) and (iii) of Lemma 5.1, respectively.

After we have found the spectrum of the fibre operator for a fixed quasi-momentum, we can proceed to analysis of the spectrum of the full operator

$$H_A \simeq \widetilde{H}_A = \int_{T^2}^{\oplus} \widetilde{H}_A(p)\, dp\,. \tag{5.10}$$

Since the functions appearing in the equation (5.9) are real-analytic the same is true for its solution. Fix an interval $(\varepsilon_{i-1}, \varepsilon_i)$ such that there are two pairs of indices $(l_1, n_1) \in J(\varepsilon_{i-1})$ and $(l_2, n_2) \in J(\varepsilon_i)$ with $\chi_{n_1}(\kappa_3) \neq 0$ and $\chi_{n_2}(\kappa_3) \neq 0$, then by the above discussion there is a real-analytic function $E_i(\cdot)$ defined on a set $U_{l_1} \cap U_{l_2}$ with the range in $(\varepsilon_{i-1}, \varepsilon_i)$. Moreover, $\widetilde{A}(\cdot)$ is bounded as a continuous function on a compact set. Combining this observation with the asymptotics (5.7) for $i = 0$ we see that also the range of $E_i(\cdot)$ is a bounded interval. Since $\widetilde{\delta}_0(\cdot; k, l)$ is an analytic function and $U_l \neq \emptyset$ for all $l \in \mathbb{N} \cup \{0\}$, the domains U_l are dense open sets of full measure, so any intersection $U_{l_1} \cap U_{l_2}$ is also an open set of full measure. Hence the function $E_i(\cdot)$ extends by continuity to the entire torus T^2 and its range lies in the interval $[\varepsilon_{i-1}, \varepsilon_i]$, having a finite lower bound for $i = 0$.

A modification is needed in case of an 'orphan' modified Landau level, i.e. a point $\varepsilon_{i'}$ for which there is no pair of indices $(l, n) \in J(\varepsilon_{i'})$ satisfying $\chi_n(\kappa_3) \neq 0$. It is obvious that this cannot be a pole of $\widetilde{Q}(p;\cdot)$ for any p, and consequently, the implicit equation (5.9) may have no solution in one or both of the intervals $(\varepsilon_{i'-1}, \varepsilon_{i'})$ and $(\varepsilon_{i'}, \varepsilon_{i'+1})$. Instead we have to consider in this case the joint interval amended with the common endpoint. Then there is a unique solution $E_{i'+1}(p)$ of (5.9) on the interval $(\varepsilon_{i'-1}, \varepsilon_{i'+1})$, provided its endpoints belong to the 'regular' class considered above, and the dispersion function $E_{i'}(p)$ is excluded from further consideration; the argument easily extends to the situation with two or more neighbouring 'orphan' points. Note that the number of 'non-orphan' levels is infinite.

Eliminating the 'orphan' points $\varepsilon_{i'}$ from $(\varepsilon_i)_{i=0}^{\infty}$ we obtain a subsequence $(\varepsilon_{i_k})_{k=0}^{\infty}$; we add conventionally $\varepsilon_{-1} = -\infty$ as its first term. For each interval $(\varepsilon_{i_{k-1}}, \varepsilon_{i_k})$ we have then a unique dispersion function $E_{i_k}(p)$ defined on an open set of full measure as a solution to (5.9) and extended by continuity to the entire torus T^2.

Lemma 5.2 *The function $E_{i_k}(\cdot)$ defined above has following properties:*
(i) if $\varepsilon_{i_{k-1}} < E_{i_k}(p) < \varepsilon_{i_k}$, then $E_{i_k}(p)$ is the unique solution to the implicit equation (5.9) in $(\varepsilon_{i_{k-1}}, \varepsilon_{i_k})$,
(ii) if ε_{i_k} is a pole of the function $\widetilde{Q}(p;\cdot)$, then $E_{i_k}(p) < \varepsilon_{i_k} < E_{i_{k+1}}(p)$,
(iii) if ε_{i_k} is not a pole of the function $\widetilde{Q}(p;\cdot)$, then

$$\begin{aligned}
\widetilde{Q}(p;\varepsilon_{i_k}) + \widetilde{A}(p) < 0 \quad &\Rightarrow \quad E_{i_k}(p) = \varepsilon_{i_k} < E_{i_{k+1}}(p)\,,\\
\widetilde{Q}(p;\varepsilon_{i_k}) + \widetilde{A}(p) > 0 \quad &\Rightarrow \quad E_{i_k}(p) < \varepsilon_{i_k} = E_{i_{k+1}}(p)\,,\\
\widetilde{Q}(p;\varepsilon_{i_k}) + \widetilde{A}(p) = 0 \quad &\Rightarrow \quad E_{i_k}(p) = \varepsilon_{i_k} = E_{i_{k+1}}(p)\,.
\end{aligned}$$

Proof: The proof is similar to the one for point interactions on the plane [Ge]. By definition of the sequence $\{\varepsilon_{i_k}\}_{k=-1}^{\infty}$ there are pairs of indices $(l_1, n_1) \in J(\varepsilon_{i_{k-1}})$ and $(l_2, n_2) \in J(\varepsilon_{i_k})$ such that $\chi_{n_1}(\kappa_3) \neq 0$ and $\chi_{n_2}(\kappa_3) \neq 0$. The union $U_{l_1} \cap U_{l_2}$ has a full measure in T^2, so the extension of $E_{i_k}(\cdot)$ to the whole T^2 by continuity (using a sequence $\{p_n\}_{n=1}^{\infty} \in U_{l_1} \cap U_{l_2}$ tending to $p \in T^2$) is well defined. Assume first that $E_{i_k}(p)$ does not coincide with the endpoints $\varepsilon_{i_{k-1}}$ and ε_{i_k} of the interval. From the condition $\mu(p_n; E_{i_k}(p_n)) := \widetilde{Q}(p_n; E_{i_k}(p_n)) + \widetilde{A}(p_n) = 0$ and the joint continuity of $\mu(\cdot;\cdot)$ in the a neighbourhood of the point $(p, E_{i_k}(p))$ we infer that $\mu(p; E_{i_k}(p)) = 0$ for any $p \in T^2$; then the claim (i) follows from the monotonicity of the function $\mu(p;\cdot)$.

The point $E_{i_k}(p)$ defined as above cannot be a pole of the function $\mu(p;\cdot)$. To see this, consider the function $z \mapsto \beta(p; z) := \mu(p; z)(z - \varepsilon_{i_{k-1}})(z - \varepsilon_{i_k})$ which is analytic in an interval $(\varepsilon_{i_{k-1}} - \rho, \varepsilon_{i_k} + \rho)$ with a small enough $\rho > 0$. Using the continuity again we find that $\beta(p; E_{i_k}(p)) = 0$ for any $p \in T^2$, thus a pole at $E_{i_k}(p)$ is excluded. This proves the claim (ii).

To prove the last statement of the lemma, we need two auxiliary results:

$$\begin{aligned} E_{i_k}(p) = \varepsilon_{i_k} \quad &\Rightarrow \quad \lim_{z \to E_{i_k}(p)} \mu(p;z) \le 0\,, \\ E_{i_k}(p) = \varepsilon_{i_{k-1}} \quad &\Rightarrow \quad \lim_{z \to E_{i_k}(p)} \mu(p;z) \ge 0\,. \end{aligned} \tag{5.11}$$

Let us check the first relation. Assume that $E_{i_k}(p) = \varepsilon_{i_k}$ but the limit is strictly positive, then there are $E_0 \in (\varepsilon_{i_{k-1}}, \varepsilon_{i_k})$ with $\mu(p;E_0) > 0$ and $p_{\tilde{n}}$ such that $\mu(p_{\tilde{n}};E_0) > 0$ and $E_0 < E_{i_k}(p_{\tilde{n}})$. However, the monotonicity of $\mu(p;\cdot)$ leads then to a contradiction, $0 < \mu(p_{\tilde{n}};E_0) < \mu(p_{\tilde{n}};E_{i_k}(p_{\tilde{n}})) = 0$. Assume now that ε_{i_k} is not a pole of $\mu(p;\cdot)$ and $\mu(p;\varepsilon_{i_k}) < 0$. By (5.11) we would have $\varepsilon_{i_k} < E_{i_{k+1}}(p)$. There is an integer number n_0 such that $\mu(p_n;\varepsilon_{i_k}) < 0$ holds for all $n > n_0$, hence $\varepsilon_{i_k} < E_{i_k}(p_n)$ for all $n > n_0$, and consequently, $\varepsilon_{i_k} \le E_{i_k}(p)$. The case of the opposite inequality $\mu(p;\varepsilon_{i_k}) > 0$ is treated in a similar way.

Finally, let us consider the last case when ε_{i_k} is not a pole of $\mu(p;\cdot)$ and $\mu(p;\varepsilon_{i_k}) = 0$. We have to exclude both the strict inequalities $E_{i_k}(p) < \varepsilon_{i_k}$ and $\varepsilon_{i_k} < E_{i_{k+1}}(p)$. Assume, for instance, that the first one of them holds. From (5.11) and the proof of the claim (i) we know that $\lim_{z \to E_{i_k}(p)} \mu(p;z) \ge 0$. There exists E_1 satisfying $E_{i_k}(p) < E_1 < \varepsilon_{i_k}$ and we arrive at a contradiction, $0 \le \mu(p;E_{i_k}(p)) < \mu(p;E_1) \le \mu(p;\varepsilon_{i_k}) = 0$.

To finish the proof, we must check that the definition of $E_{i_k}(p)$ is independent of the choice of the approximating sequence $(p_n)_{n=1}^{\infty}$. Consider another sequence $(p'_n)_{n=1}^{\infty}$ converging to p and denote the limit of $E_{i_k}(p'_n)$ by $E'_{i_k}(p)$. Assume $E_{i_k}(p) < E'_{i_k}(p)$, then by the claim (i) it is necessary that at least one of these points coincides with one of the endpoints of the interval $(\varepsilon_{i_{k-1}}, \varepsilon_{i_k})$. Using (5.11) we arrive at the relations

$$\lim_{z \to E_{i_k}(p)} \mu(p;z) \ge 0\,, \qquad \lim_{z \to E'_{i_k}(p)} \mu(p;z) \le 0\,.$$

Choosing points E_1, E_2 such that $E_{i_k}(p) < E_1 < E_2 < E'_{i_k}(p)$, we get a contradiction, $0 \le \mu(p;E_{i_k}(p)) \le \mu(p;E_1) < \mu(p;E_2) \le \mu(p;E'_{i_k}(p)) \le 0$. ∎

Combining the above results with with the direct-integral decomposition (5.10) we arrive finally at the sought description of the spectrum $\sigma(H_A)$.

Theorem 5.3 *Suppose that the flux η is integer, $\eta = N$, and the elementary cell contains one point potential. Then $\sigma(H_A)$ consists of two parts:*

(i) The first one is the union of spectral bands denoted by J_k, $k = 0, 1, \ldots$, where J_k is the range of the function $E_{i_k}(\cdot)$ over the torus T^2, with $E_{i_k}(p)$ defined by the implicit equation (5.9). Each band J_k lies within one interval $[\varepsilon_{i_{k-1}}, \varepsilon_{i_k}]$ and two neighboring bands $J_{i_{k-1}}$ and J_{i_k} have a common endpoint ε_{i_k} if and only if there exist p_1 and p_2 from T^2 such that $\widetilde{Q}(p_1; z)$ and $\widetilde{Q}(p_2; z)$ do not have a pole at ε_{i_k} and

$$\begin{aligned} \widetilde{Q}(p_1; \varepsilon_{i_k}) + \widetilde{A}(p_1) &\geq 0\,, \\ \widetilde{Q}(p_2; \varepsilon_{i_k}) + \widetilde{A}(p_2) &\leq 0\,. \end{aligned}$$

There is at most one degenerate band corresponding to a constant $E_{i_k}(\cdot)$. In particular, the degeneracy is excluded if the matrix A is diagonal, i.e. $A = \alpha I_{\ell^2(\Gamma)}$ for some $\alpha \in \mathbb{R}$. The absolutely continuous spectrum of H_A is the union $\bigcup_{k=0}^{\infty} J_k$ with the exception of the possible degenerate band.
(ii) The point part of the spectrum consists, in addition to the mentioned degenerate band, of the modified Landau levels z_0 from $\sigma(H_0)$ which persist under the perturbation. This concerns the whole $\sigma(H_0)$ if $N \geq 2$ while for $N = 1$, the levels $z_0 \in \sigma(H_0)$ for which there is just one pair of indices $(l, n) \in J(z_0)$ and $\chi_n(\kappa_3) \neq 0$ have to be removed.

Proof: Most part follows from Lemma 5.1 and Lemma 5.2; it remains us to check the claims about the degenerate band in (i). Suppose that there are two different degenerate bands $\{E\}$ and $\{E'\}$ with E, $E' \in \mathbb{R}$ separated from the spectrum of H_0. Then we have $\widetilde{Q}(p; E) + \widetilde{A}(p) = 0$ for all $p \in T^2$ and the same for E' which yields

$$Q(\vec{\gamma}, \vec{\kappa}; E) = -A(\vec{\gamma}, \vec{\kappa}) = Q(\vec{\gamma}, \vec{\kappa}; E') \tag{5.12}$$

for all $\vec{\gamma}$ from the set Λ. In particular, choosing $\vec{\gamma}$ with a large modulus, we find different terms for the corresponding matrix elements of Q at different energies E and E', because

$$Q(\vec{\gamma}, \vec{\kappa}; E) = C(E)\, e^{-\frac{|B|}{4}|\gamma|^2} |\gamma|^{\frac{E-|B|-(\frac{\pi}{d})^2}{|B|}} \left(1 + \mathcal{O}(|\gamma|^{-\nu})\right), \tag{5.13}$$

where $\nu = \min\left\{2, \frac{3}{|B|}(\frac{\pi}{d})^2\right\}$ which leads to a contradiction with (5.12). The expansion (5.13) follows from the definition of Q by (4.4) in combination with the asymptotic behavior of the hypergeometric function, $U(a, 1; s) = s^{-a}(1 + \mathcal{O}(|s|^{-1}))$ – see [AS, 13.1.8]. Furthermore, consider a diagonal matrix

A and suppose that there is a degenerate band $\{E\}$. Then the condition $\widetilde{Q}(p;E)+\alpha=0$ holds for any $p\in T^2$. In view of the relation (5.2) it leads to the requirement $Q(\vec{\gamma},\vec{\kappa};E)=0$ for all $\vec{\gamma}\neq\vec{\kappa}$ which again contradicts the known asymptotic behavior. ∎

Thus we have obtained spectral bands between neighboring points of the unperturbed spectrum as in the planar case [Ge]. Needless to say, the bands are not the same because the dispersion functions are different and also the unperturbed spectrum is different: its points are sums of the 'two-dimensional' Landau levels and energies of transverse modes. In this sense the band structure in a layer is richer.

The most important difference from the planar case is the possible existence of a spectral gap containing the whole interval $(\varepsilon_{i-1},\varepsilon_i)$ for some integer i, so that the free-spectrum gap is preserved by the perturbation. Such a situation occurs, for example, if the positions of point potentials coincide with a node of each transverse mode corresponding to ε_i, i.e. $\chi_n(\kappa_3)=0$ for all $(l,n)\in J(\varepsilon_i)$, and if at the same time $\widetilde{Q}(p;\varepsilon_i)+\widetilde{A}(p)\leq 0$ holds for all $p\in T^2$. The last condition is satisfied, e.g., for a diagonal matrix $A=\alpha I$ with the parameter $\alpha\leq -\max_{p\in T^2}|\widetilde{Q}(p;\varepsilon_i)|$ as it follows from monotonicity of the function $\widetilde{Q}(p;\cdot)$. Although it is not a generic situation it is not purely hypothetical. On the other hand, such a preserved gap cannot occur for the lowest interval, $k=0$, or in the situation when both endpoints contain the contribution from the lowest transverse mode, i.e. $(l,1)\in J(\varepsilon_{i-1})$ and $(l',1)\in J(\varepsilon_i)$. In case of a thin layer, it means that there is exactly one spectral band between each two neighboring modified Landau levels below $\varepsilon(0,2)$, i.e. below the threshold of the second transverse mode; it is obvious that the thinness here has to be understood in comparison to the characteristic length given by the magnetic field.

6 The case of integral flux and polyatomic crystal

Consider next a polyatomic lattice Λ, i.e. suppose that the set K contains more than one point, $\vec{\kappa}_i\neq\vec{\kappa}_j$ for $i,j=1,\ldots,|K|,\ i\neq j$. The flux η is again an integer number N. Comparing to (5.1) the Fourier transformation must be modified; $\mathcal{F}_\eta :\ \ell^2(\Gamma) \mapsto L^2(T^2)\otimes \ell^2(K)$ acts now as

$$(\mathcal{F}_\eta\phi)(p;\vec\kappa) = \sum_{\vec\lambda\in\Lambda} \phi(\vec\lambda)\exp\left[\pi i\xi\,\kappa\wedge\lambda - 2\pi i(\lambda_a p_1+\lambda_b p_2 + N\lambda_a\lambda_b/2)\,,\right] \tag{6.1}$$

i.e. values of the transformed function $\mathcal{F}_\eta\phi$ of the variable $p\in T^2$ are no longer scalar but rather $|K|$-dimensional vectors. The Fourier transformed operator $\mathcal{F}_\eta D((\vec\lambda,1))\mathcal{F}_\eta^{-1}$ with $\vec\lambda\in\Lambda$ acts again as a multiplication by $e_\lambda(p)$. An argument similar to that of the monoatomic case leads to

$$\begin{aligned}(\widetilde{Q}(z)+\widetilde{A})(p;\vec\kappa,\vec\kappa') &= (\mathcal{F}_\eta(Q(z)+A)\mathcal{F}_\eta^{-1})(p;\vec\kappa,\vec\kappa) \qquad (6.2)\\ &= \sum_{\vec\lambda\in\Lambda}(Q(z)+A)(\vec\lambda+\vec\kappa,\vec\kappa')\ \exp\left[\pi i\xi\,\kappa\wedge\lambda - 2\pi i(\lambda_a p_1+\lambda_b p_2+N\lambda_a\lambda_b/2)\right].\end{aligned}$$

The matrix elements $\widetilde{Q}(p;\vec\kappa,\vec\kappa';z)$ are real-analytic with respect to $p\in T^2$ and meromorphic in z with simple poles which can be located only at the points of $\sigma(H_0)$. The matrix elements $\widetilde{A}(p;\vec\kappa,\vec\kappa')$ are real-analytic in p. Finally, the transformed Green's function reads

$$\begin{aligned}G(p;k,l,n;k',l',n';z) &= \delta_{kk'}\delta_{ll'}\delta_{nn'}\frac{1}{\varepsilon(l,n)-z} \qquad (6.3)\\ &- \sum_{\vec\kappa,\vec\kappa'\in K}[\widetilde{Q}(p;z)+\widetilde{A}(p)]^{-1}(\vec\kappa,\vec\kappa')\,\frac{\widetilde{\delta}_\kappa(p;k,l)}{\varepsilon(l,n)-z}\,\frac{\widetilde{\delta}^*_{\kappa'}(p;k',l')}{\varepsilon(l',n')-z}\,\chi_n(\kappa_3)\chi_{n'}(\kappa'_3)\,.\end{aligned}$$

Using the known relation $d\widetilde{Q}/dz = \widetilde{\Gamma}^*_{z^*}\widetilde{\Gamma}_z$ for the derivative, we get

$$\frac{\partial\widetilde{Q}}{\partial z}(p;\vec\kappa,\vec\kappa';z) = \sum_{l=0}^\infty\sum_{n=1}^\infty \frac{1}{|\varepsilon(l,n)-z|^2}\,\chi_n(\kappa_3)\chi_n(\kappa'_3)\,\sum_{k=0}^{N-1}\widetilde{\delta}^*_\kappa(p;k,l)\widetilde{\delta}_{\kappa'}(p;k,l). \tag{6.4}$$

The asymptotic behaviour of the diagonal elements of the matrix $\widetilde{Q}(p;z)$ as $z\to-\infty$ is similar to (5.7), while the non-diagonal elements are bounded,

$$\widetilde{Q}(p;\vec\kappa,\vec\kappa';z) = -\delta_{\vec\kappa\vec\kappa'}\,\frac{\sqrt{-z}}{4\pi}+\mathcal{O}(1)\,. \tag{6.5}$$

Let us begin the spectral analysis with the fiber operator $\widetilde{H}_A(p)$ for a fixed $p\in T^2$. For each point $\varepsilon_i\in\sigma(H_0)$ we define the matrix $G_{\varepsilon_i}(p)$ as the residue of $-\widetilde{Q}(p;z)$ at $z=\varepsilon_i$, i.e.

$$G_{\varepsilon_i}(p;\vec{\kappa},\vec{\kappa}') = \sum_{(l,n)\in J(\varepsilon_i)} \chi_n(\kappa_3)\chi_n(\kappa_3') \sum_{k=0}^{N-1} \widetilde{\delta}^*_\kappa(p;k,l)\widetilde{\delta}_{\kappa'}(p;k,l)\,, \tag{6.6}$$

and we denote its rank by $r_{\varepsilon_i}(p)$. We further define $P_{\varepsilon_i}(p)$ as the orthogonal projection onto $\ker G_{\varepsilon_i}(p) \subset \ell^2(K)$ and operator $D_{\varepsilon_i}(p)$ as

$$D_{\varepsilon_i}(p) = \lim_{z\to\varepsilon_i} P_{\varepsilon_i}(p)(\widetilde{Q}(p;z)+\widetilde{A}(p))|_{\ker G_{\varepsilon_i}(p)}\,. \tag{6.7}$$

The multiplicity of ε_i in the spectrum of the free Hamiltonian is equal to $N|J(\varepsilon_i)|$ with the eigenspace $\Omega(\varepsilon_i)$ defined by (5.8). The second term of the Green's function (6.3) modifies the residue at $z=\varepsilon_i$ in two possible ways:
(i) taking into account contribution from the indices (l,n), $(l',n')\in J(\varepsilon_i)$ to the kernel of the resolvent, we get the orthogonal projection to the subspace spanned by the vectors $(\chi_{n_i}(\kappa_3)\widetilde{\delta}_\kappa(p;k,l_i))_{k,i}$ with $k=0,\ldots,N-1$ and $(l_i,n_i)\in J(\varepsilon_i)$. In this way the multiplicity of ε_i is diminished by $r_{\varepsilon_i}(p)$.
(ii) On the other hand, for indices $(l,n)\notin J(\varepsilon_i)$ we get a nonzero residue when the operator $D_{\varepsilon_i}(p)$ is not invertible. The corresponding eigenspace is orthogonal to $\Omega(\varepsilon_i)$ with the maximal possible dimension equal to $|K|$.

Putting two terms of the Green's function (6.3) together, we arrive at the following result:

Lemma 6.1 *Assume that the flux η equals an integer number N and the elementary cell of the lattice Γ contains $|K|$ point interactions. Choose a point $\varepsilon_i\in\sigma(H_0)$ and fix $p\in T^2$. Then the multiplicity $d_{\varepsilon_i}(p)$ of ε_i in $\sigma(\widetilde{H}_A(p))$ is equal to*

$$d_{\varepsilon_i}(p) = N|J(\varepsilon_i)| - r_{\varepsilon_i}(p),$$

if $D_{\varepsilon_i}(p)$ is invertible, while in the opposite case it satisfies the inequalities

$$N|J(\varepsilon_i)| - r_{\varepsilon_i}(p) \le d_{\varepsilon_i}(p) \le N|J(\varepsilon_i)| + |K| - r_{\varepsilon_i}(p)\,.$$

Apart from the modified Landau levels of the free system, the spectrum of $\widetilde{H}_A(p)$ contains eigenvalues due to the presence of the point potentials. A necessary condition for $E\in\mathbb{R}\setminus\sigma(H_0)$ to be an eigenvalue is

$$\det[\widetilde{Q}(p;E)+\widetilde{A}(p)] = 0. \tag{6.8}$$

Notice that E might not be an eigenvalue of $\widetilde{H}_A(p)$ if the vectors

$$\psi_{\vec{\kappa}} = \Big(\frac{\widetilde{\delta}_\kappa(p;k,l)}{\varepsilon(l,n)-E}\, \chi_n(\kappa_3) \Big)_{k,l,n}, \qquad \vec{\kappa} \in K$$

were not linearly independent, in which case the second term in Green's function (6.3) could vanish. This cannot happen, however, because $\partial\widetilde{Q}/\partial z$ is the Gram matrix for this $|K|$-tuple of vectors and by [KL] one has for a fixed $z \notin \sigma(H_0)$ the inequality

$$\frac{\partial \widetilde{Q}(p;z)}{\partial z} \geq c_z I_{\ell^2(K)} \tag{6.9}$$

with some $c_z > 0$. Therefore $\psi_{\vec{\kappa}}$ are linearly independent and eigenvectors corresponding to E are given by $\sum_{\vec{\kappa}\in K} \beta_{\vec{\kappa}} \psi_{\vec{\kappa}}$, where the vectors $\{\beta_{\vec{\kappa}}\}$ belong to $\ker[\widetilde{Q}(p;E) + \widetilde{A}(p)]$.

A useful way to solve the implicit equation (6.8) is by examining the eigenvalues $\mu^{(j)}(p;z)$, $j = 1, \dots, |K|$ of the matrix $\widetilde{Q}(p;z) + \widetilde{A}(p)$ with the numbering which takes their multiplicity into account. Apparently, a solution of equation $\mu^{(j)}(p;E) = 0$ for some j solves also the original equation. Properties of the functions μ are described in following lemma:

Lemma 6.2 *Suppose that the flux η is an integer number N and the elementary cell of Γ contains $|K|$ point potentials, and fix $p \in T^2$. Then the eigenvalues $\mu^{(j)}(p;z)$ of the matrix $\widetilde{Q}(p;z) + \widetilde{A}(p)$ are monotonously increasing functions of z in each interval $(\varepsilon_{i-1}, \varepsilon_i)$, $i = 0, 1, \dots$. When z approaches a modified Landau level ε_i, exactly $r_{\varepsilon_i}(p)$ functions of the family $\mu^{(j)}(p;\cdot)$, $j = 1, \dots, |K|$ diverge, while the remaining ones have finite limits. When z tends to $-\infty$, all the $|K|$ functions $\mu^{(j)}(p;\cdot)$ diverge to $-\infty$.*

Proof: Since the matrix $\widetilde{Q}(p;z_2) - \widetilde{Q}(p;z_1)$ with $\varepsilon_{i-1} < z_1 < z_2 < \varepsilon_i$ is by (6.9) positive definite, the Lidskii's theorem [Ka, Thm. II.6.10] yields the inequality $\mu^{(j)}(p;z_1) < \mu^{(j)}(p;z_2)$ for each j, hence all the functions $\mu^{(j)}(p;\cdot)$ increase monotonously between every two neighboring points of $\sigma(H_0)$. To prove the second claim, take $|K|$ eigenvalues $\beta^{(j)}(p;z)$, $j = 1, \dots, |K|$, of matrix $(\varepsilon_i - z)[\widetilde{Q}(p;z) + \widetilde{A}(p)]$. By Rellich's theorem [Ka, Thm. II.6.8] the functions $\beta^{(j)}$ are continuously differentiable in some neighborhood of ε_i, an for $z = \varepsilon_i$ the matrix under considerations coincides with G_{ε_i}. Finally, using Gershgorin's circles – see [Ga, Thm. XIV.5.5] – in combination with the asymptotic formula (6.5) for the matrix $\widetilde{Q}(p;z)$ we get the last claim. ∎

The lemma implies that there are at most $|K|$ eigenvalues in each interval $(\varepsilon_{i-1}, \varepsilon_i)$, $i = 0, 1, \dots$ which is after all clear from general principles – cf. [We, Sec. 8.3]. To get a more specific information about the actual number of eigenvalues, we have to look closely at the number $r_{\varepsilon_i}(p)$.

Remark 6.3 Since the matrix $G_{\varepsilon_i}(p)$ is obviously the Gram matrix of the system of $N|J(\varepsilon_i)|$-dimensional vectors

$$\Big(\chi_{n_s}(\kappa_3)\widetilde{\delta}_\kappa(p; k, l_s)\Big)_{k,s} \qquad k = 0, \dots, N-1\,,\ (l_s, n_s) \in J(\varepsilon_i)\,,$$

the rank $r_{\varepsilon_i}(p)$ cannot exceed $\min(|K|, N|J(\varepsilon_i)|)$. There are three situations when the maximum value specified here cannot be achieved whatever point p is considered. First, the dimension of the vectors is in fact smaller if $\chi_{n_s}(\kappa_3) = 0$ holds for some index n_s and all $\vec{\kappa} \in K$. In general, the said dimension is equal to $N|\tilde{J}(\varepsilon_i)|$, where $\tilde{J}(\varepsilon_i)$ is the set $J(\varepsilon_i)$ from which the pairs (l_s, n_s) with the described property were deleted. Second, the number of the vectors is $|K|$, but when a lattice point $\vec{\kappa}$ is such that $\chi_{n_s}(\kappa_3) = 0$ holds for all $(l_s, n_s) \in J(\varepsilon_i)$, the corresponding vector is zero for any p. Excluding such elements from the set K we obtain a subset denoted as $\bar{K}(\varepsilon_i)$.

Finally, we must also examine carefully the situation when several points $\vec{\kappa}^j$, $j = 1, \dots, q$, from the elementary cell differ in the third coordinate only, i.e. they are arranged vertically in the layer. If the level ε_i is not degenerate, by neglecting all but one of the q vectors in question, we do not change the rank of the Gram matrix, provided the one which we keep is not a zero vector. If a degenerate level is admitted, then the number of linearly independent vectors among these q vectors is less or equal to the rank of the following matrix

$$\Big(\chi_{n_s}(\kappa_3^j)\Big)_{j,s} \qquad j = 0, \dots, q,\ (l_s, n_s) \in \tilde{J}(\varepsilon_i)\,.$$

Then we eliminate the remaining ones of the q vectors from $\bar{K}(\varepsilon_i)$ and obtain in this way another subset of K which we denote as $\tilde{K}(\varepsilon_i)$. The maximal possible rank $r_{\varepsilon_i}(p)$ of the matrix $G_{\varepsilon_i}(p)$ is in this way equal to

$$\min(|\tilde{K}(\varepsilon_i)|, N|\tilde{J}(\varepsilon_i)|)\,;$$

whether the maximum is achieved at a point p or not now depends on the functions $\widetilde{\delta}_\kappa(\cdot; k, l)$.

Such a dependence of $r_{\varepsilon_i}(p)$ on the parameters of the problem makes the general spectral analysis cumbersome. In what follows we will thus restrict our attention to the generic situation only by imposing additional restrictions on the Hamiltonian H_A. First of all, we assume that $(\pi/d)^2$ and $|B|$ are not rationally related, so that $J(\varepsilon_i) = 1$ holds for all modified Landau levels ε_i. Furthermore, we define the sets

$$\begin{aligned} U'_{\varepsilon_i} &:= \{p \in T^2 : \; r_{\varepsilon_i}(p) = r_{\max} \equiv \min(N, |\tilde{K}|)\}, \\ U''_{\varepsilon_i} &:= \{p \in T^2 : \; D_{\varepsilon_i} \text{ is invertible}\} \end{aligned}$$

and

$$U_{\varepsilon_i} := U'_{\varepsilon_i} \cap U''_{\varepsilon_i}, \tag{6.10}$$

where $|\tilde{K}|$ represents the number of points $\vec{\kappa} \in K$ after we have excluded $q-1$ points from every q-tuple in which the first two coordinates coincide. The set $\tilde{K}$ does not depend on ε_i any more.

In the rest of the paper, we consider only operators H_A such that the set $\bigcap_{i\geq 0} U_{\varepsilon_i}$ is nonempty which is a generic situation. First of all, one can check easily that by an arbitrarily small shift of the points $\vec{\kappa}$ in the elementary cell Q_Λ we can achieve that $\bigcap_{i\geq 0} U'_{\varepsilon_i} \neq \emptyset$, and in a similar way, by an arbitrarily small perturbation of the diagonal elements of the matrix A we can always satisfy the condition $\bigcap_{i\geq 0} U''_{\varepsilon_i} \neq \emptyset$. Recall that the possible positions $\vec{\kappa}$ of point potentials in the elementary cell are dense in $Q_\Lambda^{|K|}$, while all possible values of $A(\vec{\kappa}, \vec{\kappa})$ span $\mathbb{R}^{|K|}$, and consequently, the set

$$\left\{ (\vec{\kappa}_1, \ldots, \vec{\kappa}_{|K|}, A(\vec{\kappa}_1, \vec{\kappa}_1), \ldots, A(\vec{\kappa}_{|K|}, \vec{\kappa}_{|K|})) \in Q_\Lambda^{|K|} \times \mathbb{R}^{|K|} \; : \; \bigcap_{i\geq 0} U_{\varepsilon_i} \neq \emptyset \right\}$$

has a full measure in $Q_\Lambda^{|K|} \times \mathbb{R}^{|K|}$.

For $|K| = r_{\max}$ and $p \in U_{\varepsilon_{i-1}} \cap U_{\varepsilon_i}$, the number of the eigenvalues in the free Hamiltonian spectral gap equals $|K|$. Now we employ the assumption $\bigcap_{i\geq 0} U_{\varepsilon_i} \neq \emptyset$: since $\widetilde{\delta}_\kappa(p; k, l)$ and $\widetilde{Q}(p; z)$ with $z \notin \sigma(H_0)$ are analytic as functions of p, all sets the U'_{ε_i} and U''_{ε_i}, $i \geq 0$, have full measures, and the same is true for the intersection $U_{\varepsilon_{i-1}} \cap U_{\varepsilon_i}$. The functions $E_i^{(j)}(\cdot)$ are bounded, which follows for $i = 0$ from the asymptotic formula (6.5) and the boundedness of the matrix $\widetilde{A}$ while otherwise the claim is valid trivially. Thus we may extend the $|K|$ dispersion functions $E_i^{(j)}(\cdot)$ by continuity to the entire torus T^2. We arrive at the following result.

Lemma 6.4 *Assume that $|K| = r_{\max}$ and the Hamiltonian H_A satisfies $\bigcap_{i\geq 0} U_{\varepsilon_i} \neq \emptyset$. Consider the extended functions $E_i^{(j)}(p)$, $j = 1, \ldots, |K|$, defined on T^2 in the described way. Then the inequalities $\varepsilon_{i-1} < E_i^{(j)}(p) < \varepsilon_i$ for some j, $1 \leq j \leq |K|$, implies that $E_i^{(j)}(p)$ is a solution of the implicit equation (6.8).*

For $|K| > r_{\max}$ and $p \in U_{\varepsilon_{i-1}} \cap U_{\varepsilon_i}$, the number of eigenvalues in the interval $(\varepsilon_{i-1}, \varepsilon_i)$ is not necessarily equal to $|K|$. Consider first $p \in \bigcap_{i\geq 0} U_{\varepsilon_i}$. In this case, $|K| - r_{\max}$ functions $\mu^{(j)}(p; z)$ do not diverge when z approaches an endpoint of the interval, instead they 'meet' there one of functions μ from the neighboring interval. Then it is natural to unify these functions coming from neighboring intervals obtaining new functions $\nu_i^{(j)}(p;)$, $i = 0, 1, \ldots$, $j = 1, \ldots, r_{\max}$, which are defined on the enlarged intervals $(\varepsilon_{i-s}, \varepsilon_i)$, where $1 \leq s \leq |K|/r_{\max}$ if the fraction is integer, otherwise $1 \leq s \leq [|K|/r_{\max}] + 1$. We put $\varepsilon_{i-s} = -\infty$ and $U_{\varepsilon_{i-s}} = T^2$ whenever $i - s < 0$. On each subinterval, the corresponding families of functions $\nu(p; z)$ and $\mu(p; z)$ coincide. The function $\nu_i^{(j)}(p; z)$ tends to $\pm\infty$ as z approaches ε_i or ε_{i-s}, respectively. Thus there exists exactly one solution to the equation $\nu_i^{(j)}(p; E) = 0$ which we denote as $E_i^{(j)}(p)$. The same conclusion can be made under a weaker assumption, $p \in \bigcap_{l=0}^{s} U_{\varepsilon_{i-l}}$. This set has again a full measure and functions $E_i^{(j)}(\cdot)$ are bounded, so we can extend the dispersion functions by continuity to the entire torus T^2.

After having analyzed the fiber operator spectrum, let us run p run through the torus T^2 to get the spectrum of the Hamiltonian H_A.

Theorem 6.5 *Suppose that the flux η is an integer number N and the elementary cell of the lattice Γ contains $|K|$ points. In addition, let $(\pi/d)^2$ and $|B|$ be irrationally related and let the Hamiltonian H_A satisfy the condition $\bigcap_{i\geq 0} U_{\varepsilon_i} \neq \emptyset$, where the sets U_{ε_i} are defined by (6.10). Then the spectrum of H_A consists of two parts, namely*
(i) spectral bands I_i^j with $j = 1, \ldots, r_{\max}$ and $i = 0, 1, \ldots$, where $r_{\max} = \min(N, |\tilde{K}|)$ and $\tilde{K}$ is the maximal subset of K such that no pair of points from K' coincide in the first two coordinates. Each band I_i^j is given as the range of the extended function $E_i^{(j)}(p)$, $p \in T^2$, which is defined by the implicit equation (6.8); it lies within the interval $[\varepsilon_{i-s}, \varepsilon_i]$, where $1 \leq s \leq |K|/r_{\max}$ if the fraction is integer and $1 \leq s \leq [|K|/r_{\max}] + 1$ otherwise. The absolutely continuous spectrum of H_A is the union $\bigcup_{i=0}^{\infty} \bigcup_{j=1}^{r_{\max}} I_i^j$ except possible bands

degenerate to a point,
(ii) modified Landau levels from the spectrum of H_0. If $N \le r_{\max}$, some points of $\sigma(H_0)$ may be absent from the spectrum of H_A.

The theorem says nothing about possible common endpoint of two neighboring bands which could be compared to the analogous part of Theorem 5.3 in the monoatomic case. However, the term 'neighboring bands' does not have much sense here; the bands I_i^j with the same index i may overlap and for $|K| > r_{\max}$ also bands with different indices i may overlap.

Apart from the difference between the modified Landau levels here from the unperturbed spectrum in the planar case, the structure of the two spectra is similar with one difference: the number of bands I_i^j which neighbor with the same point ε_i from above equals $\min(N, |\tilde{K}|)$, while in the planar case [Ge] it is $\min(N, |K|)$ instead. The reason is clear: the magnetic field perpendicular to the layer does not 'distinguish' two points placed one on the top of the other, and such a situation can never occur in the planar case.

In the previous chapter we have found that the spectrum can contain a gap covering the whole interval $(\varepsilon_{i-1}, \varepsilon_i)$ for some i. In the polyatomic case it is obviously possible for $|K| \ge 2r_{\max}$, while the above discussion excludes such a situation otherwise. It might thus seem that for $|K| = r_{\max} = 1$ we get a contradiction. However, the discrepancy comes from the stronger restriction we have imposed upon the operator H_A; the condition $\bigcap_{i\ge 0} U_{\varepsilon_i} \ne \emptyset$ does not allow $\chi_n(\kappa_3) = 0$ to hold for all $(l, n) \in J(\varepsilon)$.

7 The case of a rational flux

The general case when the flux is a rational number, $\eta = \frac{N}{M}$, can be in some sense reduced to the previous analysis. We can pass to an integral flux $\eta' = N$ by enlarging the elementary cell. The new lattice Λ' is generated by vectors $\vec{a}$ and $M\vec{b}$ and the new set K' is given by $K + \{0, \vec{b}, \dots, (M-1)\vec{b}\}$.

However, the result obtained by this simple trick is not fully correct because it does not take the M-fold degeneracy into account. Recall that the Hamiltonian H_A commutes with all magnetic translations from W_η. Hence any of its eigenspaces can be written as a direct sum of spaces of the irreducible representations of W_η, which are M-dimensional. Therefore additional modifications are needed here. We define the Fourier transformation

$\mathcal{F}_\eta : \ \ell^2(\Gamma) \mapsto L^2(T^2_\eta) \otimes \mathbb{C}^M \otimes \mathbb{C}^M \otimes \ell^2(K)$ by the prescription

$$(\mathcal{F}_\eta\phi)(p;j,m,\vec{\kappa}) \;=\; \sum_{\lambda_a,\lambda_b\in\mathbb{Z}} \phi(\lambda_a\vec{a} + (\lambda_b M + m)\vec{b} + \vec{\kappa}) \times \exp\left[\pi i\xi\, \kappa \wedge (\lambda_a\vec{a} + \lambda_b M\vec{b})\right] \times \exp\left[-2\pi i\Big(\lambda_a p_1 + \lambda_b p_2 + \frac{N}{2}\,\lambda_a\Big(\lambda_b + \frac{m+2j}{M}\Big)\Big)\right]. \tag{7.1}$$

The transformed quantity $\mathcal{F}_\eta D(\cdot)\mathcal{F}_\eta^{-1}$ is then a direct integral of multiples of irreducible representations,

$$\mathcal{F}\eta D(\cdot)\mathcal{F}_\eta^{-1} = \int_{T^2_\eta}^{\oplus} d^2p\, \triangle'(\cdot;p) \otimes I_{\ell^2(K)}\,.$$

The representation $\triangle_d(\cdot;p)$ acting on $\mathbb{C}^M \otimes \mathbb{C}^M$ is given by

$$\begin{aligned} \triangle_d((\vec{a},1);p) &= \triangle((\vec{a},1);p) \otimes I_{\mathbb{C}^M}\,, \\ \triangle_d((\vec{b},1);p) &= S \otimes \triangle'(p), \end{aligned}$$

where S and $\triangle'(p)$ are operators on $\mathbb{C}^M$ which act at the basis vectors e_j, $j = 0,\dots,M-1$, in following way,

$$Se_j = e_{j\ominus 1}\,, \qquad \triangle'(p)e_j = \exp(-2\pi i p_2 \delta_{j,M-1})e_{j\oplus 1}\,,$$

with $\oplus$ and $\ominus$ representing the sum and difference in $\{0,\dots,M-1\}$ modulo M. This representation is equivalent to the representation $\triangle(\cdot;p) \otimes I_{\mathbb{C}^M}$.

Applying now the Fourier transformation to the operator $Q(z) + A$ we get

$$(\widetilde{Q}(z) + \widetilde{A})(p;j,m,\vec{\kappa},j',m',\vec{\kappa}') \;=\; \delta_{jj'} \sum_{\lambda_a,\lambda_b\in\mathbb{Z}} \exp\left[\pi i\xi\, \kappa \wedge (\lambda_a\vec{a} + \lambda_b M\vec{b})\right] \times \exp\left[-2\pi i \left(\lambda_a p_1 + \lambda_b p_2 + \frac{N}{2}\,\lambda_a\Big(\lambda_b + \frac{m+2j}{M}\Big)\right)\right] \times (Q(z) + A)(\lambda_a\vec{a} + (\lambda_b M + m)\vec{b} + \vec{\kappa}, m'\vec{b} + \vec{\kappa}')\,. \tag{7.2}$$

Finally, the transformed Green's function reads

$$G(p;j,k,l,n;j',k',l',n';z) \;=\; \delta_{jj'}\delta_{kk'}\delta_{ll'}\delta_{nn'}\frac{1}{\varepsilon(l,n) - z} \tag{7.3}$$

$$- \delta_{jj'} \sum_{\vec{\kappa},\vec{\kappa}' \in K} \sum_{m,m'=0}^{M-1} [\widetilde{Q}(p,j;z) + \widetilde{A}(p,j)]^{-1}(m,\vec{\kappa},m',\vec{\kappa}')$$
$$\times \frac{\widetilde{\delta}_{m,\kappa}(p;j,k,l)}{\varepsilon(l,n)-z} \, \frac{\widetilde{\delta}^*_{m',\kappa'}(p;j,k',l')}{\varepsilon(l',n')-z} \, \chi_n(\kappa_3)\chi_{n'}(\kappa'_3)\,,$$

where

$$\widetilde{\delta}_{m,\kappa}(p;j,k,l) = N^{-1/2} \sum_{r=-\infty}^{\infty} \exp\left(2\pi i r \frac{p_2+k}{N}\right) \psi_0^*(mb+\kappa; p_1+\eta j+r, l)\,. \tag{7.4}$$

We have employed a relation similar to (5.5) with $\lambda \in \Lambda'$ and an additional parameter j, and the M-dimensional representation $\triangle(\cdot,p)$ instead of the character $\chi(\cdot;p)$.

Next, we proceed to the spectral analysis in the same way as we did in the previous section. The implicit equation defining the dispersion function $E_i^{(r,j)}(p)$ has the form

$$\det[\widetilde{Q}(p;j;E) + \widetilde{A}(p;j)] = 0 \tag{7.5}$$

with the dimension of the matrix being equal to $|K|M$. Due to the equivalence of the two representations which we have mentioned above, the matrices $\widetilde{Q}(p;j;z) + \widetilde{A}(p;j)$ for different j are unitarily equivalent. This is the source of the M-fold degeneracy of the eigenvalues of $\widetilde{H}_A(p)$, and thus also of the spectral bands of H_A.

To simplify the description of the spectrum $\sigma(H_A)$, we consider in the following theorem a lattice with $|K| = 1$.

Theorem 7.1 *Assume that the flux η is a rational number N/M and the elementary cell contains one point potential. In addition, let $(\pi/d)^2$ and $|B|$ be irrationally related, and let the Hamiltonian H_A satisfy the condition $\bigcap_{i\geq 0}\bigcap_{j=0}^{M-1} U^j_{\varepsilon_i} \neq \emptyset$, where the sets $U^j_{\varepsilon_i}$ are defined in analogy with the expression (6.10). Then the spectrum $\sigma(H_A)$ consists of two parts:*
(i) The first one is the union of spectral bands I_i^r with $r = 1,\ldots,r_{\max}$ and $i = 0,1,\ldots,$ where $r_{\max} = \min(M,N)$. The band I_i^r is given as a range of the function $p \mapsto E_i^{(r,j)}(p)$ with $p \in T^2_\eta$, defined by the implicit equation (7.5) for some j. Each band I_i^r is M-times degenerated and it lies within the interval $[\varepsilon_{i-s},\varepsilon_i]$, where $1 \leq s \leq M$ if $N = 1$ and $1 \leq s \leq [M/N]+1$ otherwise. The absolutely continuous spectrum is the union of all bands I_i^r except possible

bands degenerated to a point.
(ii) The second part of the spectrum contains modified Landau levels from $\sigma(H_0)$*. In the case* $N \leq M$ *some points of* $\sigma(H_0)$ *may be absent from the spectrum* $\sigma(H_A)$*.*

Acknowledgement

The authors thank V.A. Geyler for useful comments. The research was partially supported by GAAS grant A1048101.

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