Spectrum structure for a three-dimensional periodic array of quantum dots in a uniform magnetic field

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\textbf{Abstract}

By means of the operator extension theory, we construct an explicitly solvable model of a simple-cubic three-dimensional regimented array of quantum dots in the presence of a uniform magnetic field. The spectral properties of the model are studied. It is proved that for each magnetic flux the band is the image of the spectrum of the tight-binding operator under an analytical transformation. In the case of rational magnetic flux the spectrum is described analytically. The flux-energy and angle-energy diagrams are obtained numerically.

\section{Introduction}

The problem of commensurability in periodic systems is a source of fascination in various branches of physics and is related to the appearance of the fractal spectrum for such systems. M. Ya. Azbel', D. R. Hofstadter, and G. H. Wannier \cite{1}–\cite{3} were the first scientists who studied the simplest model of the two-dimensional (2D) electron system in a uniform magnetic field and discovered a self-similar energy spectrum, called “Hofstadter’s butterfly”. This picture shows the dependence of the energy on the magnetic field for two-dimensional periodic system in the tight-binding approximation and confirms the conjecture that the Hamiltonian of this model (which is reduced to the so-called Harper operator) has the Cantor spectrum at irrational value of the magnetic flux (the famous “Ten Martini Problem”). Very recently this problem has been solved affirmatively \cite{4}, \cite{5}.

It was assumed the long time that in the three-dimensional (3D) case the gaps in the energy spectrum, in general, are closed and the fractal structure of the spectrum is impossible. Recently M. Koshino, H. Aoki and co-authors have considered the dependence of the energy spectrum of a 3D periodic quantum system on the orientation of the magnetic field and on the strength of the field \cite{6}–\cite{8}. Using semiclassical methods they have reduced the Schrödinger
equation with the 3D tight-binding Hamiltonian to the 1D Harper equation and shown that in the obtained angle-energy and flux-energy diagrams a fractal structure appears. Note the tight-binding method is based on a series of approximations of the initial Schrödinger equation that can change considerably the structure of the spectrum, e.g., the tight-binding Hamiltonian for a single-atomic lattice has only one magnetic band in the spectrum.

Another explicitly solvable model of 3D periodic quantum systems was presented in [9]–[11]. We have considered spectral properties of the 3D Landau operator perturbed by periodic point potential. It was shown numerically in [10], [11] that the angle-energy and flux-energy diagrams for different bands of the spectrum have a fractal structure even in case of cubic lattice. Note that the dispersion equation in this model has a transcendental form and the analytical study of the spectrum becomes very difficult.

In this paper we consider the quantum-mechanical model for the 3D periodic array of quantum dots obtained by means of operator extension theory [12]–[15]. It may be noted that this method was successfully applied for construction and spectral investigation of quantum periodic systems in two dimensions in our previous works [16], [17]. In particular, the model allows, in contrary to the tight-binding approximation method, to describe all bands of the spectrum. On the other hand, the dispersion equation of our model has more simple form than the corresponding one for the 3D Landau operator perturbed by periodic point potential, and in the case of rational magnetic flux the spectrum of 3D periodic array of quantum dots is described analytically.

In the framework of our model, each Fock–Darwin level of a single quantum dot broads into magnetic band which in its turn splits into subbands. This is stipulated by the spectrum structure of irreducible representations of the magnetic translation group (for the first time it was shown by J. Zak [18]). If the numbers of the flux quanta of the magnetic field through each face of elementary cell of the Bravais lattice Λ of the system are rational (in this case the magnetic field is said to be rational with respect to the lattice Λ), then there is a finite number of subbands for a fixed magnetic band. If the fluxes through adjacent faces of elementary cell of the Bravais lattice of the system are equal to an irreducible fractions $N_1/M_1$, $N_2/M_2$ and $N_3/M_3$, then the numbers of subbands are defined by the numbers $M_1$, $M_2$ and $M_3$. Therefore the magnetic band arising from the fixed Fock–Darwin level can transform to a Cantor set when one of these fluxes tends to an irrational number. For the simple-cubic array, we prove that in both cases of rational and irrational flux the band is the image of the spectrum of the corresponding tight-binding operator under an analytic function. Hence, a fractal structure of angle-energy and flux-energy diagrams for 3D regimented array of quantum dots inherits from such diagrams for the tight-binding operator. It should be noted that similar description of the spectrum was obtained in the 2D case in [15], [16] and for quantum graphs in [19] and [20].

Our model is directly relevant to the so-called 3D regimented arrays of semiconductor quantum dots which attract the increased attention lately [21]–[23]. The regimentation along all three directions results in the formation of an artificial crystal, where quantum dots play the role of atoms [24], [25]. O. L. Lazarenkova and A. A. Balandin in [24] have analyzed the band structure of such systems using envelope function approximation.
2 The description of the model

For construction of our model we start with the quantum-mechanical Hamiltonian $H_d$ of a single 3D quantum dot subjected to a uniform magnetic field $B$:

$$H_d = H_0 + V(r),$$

where $H_0$ is the Hamiltonian of a single electron in the magnetic field,

$$H_0 = \frac{1}{2m^*} \left( i\hbar \nabla + \frac{e}{c} A(r) \right)^2. $$

Here $e$ and $m^*$ are the charge and the effective mass of the electron respectively, and $A(r)$ is the vector potential of the field $B$ (i.e. $B = \text{rot} A$), $V(r)$ is the confining potential of a three-dimensional quantum dot. In our model we choose $V(r)$ as the potential of a spherical quantum well:

$$V(r) = V(x,y,z) = \frac{m^* \omega^2}{2} (x^2 + y^2 + z^2).$$

Here the characteristic sizes $d_x$, $d_y$ and $d_z$ of the quantum well are related to the frequency $\omega$ as follows:

$$d_x, d_y, d_z \sim \sqrt{\hbar/(m^* \omega)}.$$

Now let us consider a periodic three-dimensional array of such quantum dots. We suppose that centers of the quantum dots coincide with nodes of simple cubic crystallic lattice $\Lambda$ with the basis $(a_1, a_2, a_3)$ (Fig. 1).

The state space of our model is the direct sum of the state spaces $L^2(\mathbb{R}^3)$ of single quantum dots:

$$H = \sum_{\lambda \in \Lambda} \oplus H_\lambda, \quad H_\lambda = L^2(\mathbb{R}^3) \quad \text{for each} \quad \lambda \in \Lambda. $$

The following direct sum

$$H^0 = \sum_{\lambda \in \Lambda} \oplus H_\lambda, \quad H_\lambda = H_d \quad \text{for each} \quad \lambda \in \Lambda,$$

is the unperturbed Hamiltonian of the model. This operator is the Hamiltonian of a set of isolated quantum dots. To take into account the charge carrier tunnelling between dots we use the "restriction – extension" procedure of the operator extension theory \cite{12}, \cite{13}. We denote by $D$ the set of functions $f$ from the domain $D(H_d)$ each of which vanishes in a neighborhood of zero. Let $S_d$ be the restriction of the operator $H_d$ to the set $D$ and let $S$ is the following direct sum

$$S = \sum_{\lambda \in \Lambda} \oplus S_\lambda, \quad S_\lambda = S_d \quad \text{for each} \quad \lambda \in \Lambda.$$ 

We seek the "true" Hamiltonian $H$ of the quantum dots array among non-trivial self-adjoint extensions of the operator $S$ such as $D(H) \cap D(H^0) = D(S)$.

The resolvent $R$ of the operator $H$ and the resolvent $R^0$ of the operator $H^0$ are related with the Krein resolvent formula (see, e.g. \cite{15}):

$$R(\zeta) \equiv R_A(\zeta) = R^0(\zeta) - g(\zeta)[Q(\zeta) + A]^{-1}g^*(\bar{\zeta}),$$

where operator valued holomorphic functions $g(\zeta)$ and $Q(\zeta)$ are the so-called Krein $\Gamma$- and $Q$-functions of the operator $H^0$ respectively, and $A$ is a self-adjoint operator in the deficiency space $l^2(\Gamma)$ (the so-called "interaction" operator). The main part in the study of the spectrum is played by the $Q$–function $Q(\zeta)$ and operator $A$. 

3
2.1 The \( Q \)-function of the model

In the considered case the \( Q \)-function \( Q(z) \) has the diagonal matrix in the space \( l^2(\Lambda) \):

\[
Q(\lambda, \lambda'; z) = \delta_{\lambda\lambda'} q(z), \quad \lambda, \lambda' \in \Lambda,
\]

where \( q(z) \) is the \( Q \)-function of the operator \( H_d \). To obtain the function \( q(z) \) we find preliminarily a general expression for the \( Q \)-function \( Q_3(\zeta; q|\omega, B) \) of the operator \( H_d \) at an arbitrary point \( q \in \mathbb{R}^3 \).

We denote by \( H^{(3)}(\omega) \) the Hamiltonian of spherical quantum dot without magnetic field:

\[
H^{(3)}(\omega) = -\frac{\hbar^2}{2m^*} \Delta + \frac{m^* \omega^2}{2} (x_1^2 + x_2^2 + x_3^2).
\]

Let \( G_3(q, q'; \zeta|\omega, B) \) be the Green function of the operator \( H_d \equiv H^{(3)}(\omega, B) \), \( G_3(q, q'; \zeta|\omega') \) be the Green function of the operator \( H^{(3)}(\omega') \), and \( Q_3(\zeta; q|\omega') \) be the \( Q \)-function of the operator \( H^{(3)}(\omega') \). We denote by \( S_3(q, q'|\omega') \) and \( S_3(q, q'|\omega, B) \) the singularities of the functions \( G_3(q, q'; \zeta|\omega') \) and \( G_3(q, q'; \zeta|\omega, B) \) at a point \( q \) respectively. It is known that for each \( \omega \) and \( \omega' \) the singularities \( S_3(q, q'|\omega') \) and \( S_3(q, q'|\omega, B) \) coincide and have the following form (see, e.g. [26]):

\[
S_3(q, q'|\omega') = S_3(q, q'|\omega, B) = \frac{m^*}{2\pi\hbar^2 |q - q'|}.
\]

It implies for each \( \omega' \) the following form of the function \( Q_3(\zeta; q|\omega, B) \):

\[
Q_3(\zeta; q|\omega, B) = \lim_{q \to q'} [G_3(q, q'; \zeta|\omega') - S_3(q, q'|\omega')] = \lim_{q \to q'} [G_3(q, q'; \zeta|\omega) - G_3(q, q'; \zeta|\omega')] + Q_3(\zeta; q|\omega').
\]

We denote by \( H^{(2)}(\omega, B) \) the Hamiltonian of two-dimensional symmetric quantum dot subjected with magnetic field \( B \) (the field \( B \) is perpendicular to the quantum dot plane):

\[
H^{(2)}(\omega, B) = \frac{1}{2m^*} \left(-i\hbar \nabla - \frac{e}{c} A(r)\right)^2 + \frac{m^* \omega^2}{2} (x_1^2 + x_2^2).
\]

and by \( H^{(2)}(\omega) \) the Hamiltonian of the same dot without magnetic field:

\[
H^{(2)}(\omega) = -\frac{\hbar^2}{2m^*} \Delta + \frac{m^* \omega^2}{2} (x_1^2 + x_2^2).
\]

We use the standard notations \( \omega_c = |eB|/(cm^*) \) for the cyclotron frequency and \( \Omega = \sqrt{\omega_c^2 + 4\omega^2} \) for the hybrid frequency. It is easy to show that the eigenfunctions of the operators \( H^{(2)}(\omega, B) \) and \( H^{(2)}(\Omega/2) \) coincide and have the following form in the polar coordinates \( (\rho, \phi) \):

\[
\psi^{(2)}_{mn}(\rho, \phi) = \frac{1}{\sqrt{2\pi l_\Omega^{1+|m|}}} \sqrt{n! \over 2^m (n + |m|)!} \rho^{|m|} \exp\left(-\frac{\rho^2}{\pi l_\Omega^2}\right) L_n^{|m|} \left(\frac{\rho^2}{\pi l_\Omega^2}\right) \exp(im\phi),
\]

\[
m \in \mathbb{Z}, \ n = 0, 1, 2, \ldots,
\]

where \( l_\Omega = \sqrt{\hbar/(m^*\Omega)} \), \( L_n^{|m|} \) is the Laguerre-Sonin polynomial of the power \( n \). Corresponding eigenvalues \( E^{(2)}_{mn}(\omega, B) \) and \( E^{(2)}_{mn}(\Omega/2) \) of the operators \( H^{(2)}(\omega, B) \) and \( H^{(2)}(\Omega/2) \) have the following form:

\[
E^{(2)}_{mn}(\omega, B) = \frac{\hbar \omega_c}{2} m + \frac{\hbar \Omega}{2} (2n + |m| + 1),
\]

\[
E^{(2)}_{mn}(\Omega/2) = \frac{\hbar \Omega}{2} (2n + |m| + 1).
\]
\[ E^{(2)}_{mn}(\Omega/2) = E^{(2)}_{mn}(\omega, B) - \frac{\hbar \omega_c}{2} m = \frac{\hbar \Omega}{2} (2n + |m| + 1). \]  

Further we shall denote coordinates \((\rho, \phi, z)\) of a point \(q\) by \((q_\perp, q_\parallel)\), where \(q_\perp = (\rho, \phi)\), \(q_\parallel = z\). We have the following representation of the function \(Q_3(\zeta; q|\omega, B)\):

\[ Q_3(\zeta; q|\omega, B) = \sum_{m=-\infty}^{\infty} \sum_{n=0}^{\infty} |w^{(2)}_{mn}(q_\perp)|^2 [G_1(q_\parallel; q_\parallel; \zeta - E^{(2)}_{mn}(\omega, B)|\omega) - G_1(q_\parallel; q_\parallel; \zeta - E^{(2)}_{mn}(\Omega/2)|\Omega/2)] + Q_3(\zeta; q|\Omega/2, \omega), \]

where \(G_1(x, x'; \zeta|\omega)\) is the Green function of the one-dimensional harmonic oscillator \(H^{(1)}(\omega)\):

\[ H^{(1)}(\omega) = -\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} + \frac{m^* \omega^2}{2} x^2. \]

It is known that the function \(G_1(x, x'; \zeta|\omega)\) has the following form (see, e.g. [27]):

\[ G_1(x, x'; \zeta|\omega) = \frac{1}{\sqrt{\pi \hbar \omega l_\omega}} \Gamma \left( \frac{1}{2} - \frac{\zeta}{\hbar \omega} \right) U \left( -\frac{\zeta}{\hbar \omega}, \frac{\sqrt{2} \max(x, x')}{l_\omega} \right) \times\]

\[ \times U \left( -\frac{\zeta}{\hbar \omega}, \frac{\sqrt{2} \min(x, x')}{l_\omega} \right). \]

Therefore we obtain the following expression for the function \(Q_3(\zeta; q|\omega, B)\):

\[ Q_3(\zeta; q|\omega, B) = \frac{1}{2 \pi^{3/2} \hbar l_{\Omega}^2} \exp \left( -\frac{q_\parallel^2}{l_{\Omega}^2} \right) \sum_{m=-\infty}^{\infty} \frac{(q_\perp^2 / l_{\Omega}^2)^{|m|}}{(2l_{\Omega}^2)^{|m|}} \sum_{n=0}^{\infty} \frac{n!}{(n + |m|)!} \times\]

\[ \times \left[ L_n^{\left|m\right|} \left( \frac{q_\perp^2}{2l_{\Omega}^2} \right) \right]^2 \Gamma \left( \frac{1}{2} + \frac{E^{(2)}_{mn}(\omega, B) - \zeta}{\hbar \omega} \right) U \left( \frac{E^{(2)}_{mn}(\omega, B) - \zeta}{\hbar \omega}, \frac{\sqrt{2} q_\parallel}{l_\omega} \right) \times\]

\[ \times U \left( \frac{E^{(2)}_{mn}(\omega, B) - \zeta}{\hbar \omega}, -\frac{\sqrt{2} q_\parallel}{l_\omega} \right) - \sqrt{2} \Gamma \left( \frac{1}{2} + \frac{2(E^{(2)}_{mn}(\Omega/2) - \zeta)}{\hbar \Omega} \right) \]

\[ \times U \left( \frac{2(E^{(2)}_{mn}(\Omega/2) - \zeta)}{\hbar \Omega}, q_\parallel / l_{\Omega} \right) U \left( \frac{2(E^{(2)}_{mn}(\Omega/2) - \zeta)}{\hbar \Omega}, -q_\parallel / l_{\Omega} \right) + Q_3(\zeta; q|\Omega/2, \omega), \]

Now we turn to the desired \(Q\)-function \(q(z) = Q_3(\zeta; 0|\omega, B)\). It is known that for each \(\omega\) the function \(Q_3(\zeta; 0|\omega)\) has the following form (see, e.g. [26]):

\[ Q_3(\zeta; 0|\omega) \equiv q_0(\zeta) = -\frac{m^*}{\pi \hbar^2 l_{\omega}} \Gamma \left( \frac{3}{4} - \frac{\zeta}{2 \hbar \omega} \right) \frac{\Gamma \left( \frac{3}{4} + \frac{\Omega}{2 \hbar} (n + \frac{1}{2}) - \frac{z}{2 \hbar \omega} \right)}{\Gamma \left( \frac{3}{4} + \frac{n}{2 \hbar} - \frac{z}{2 \hbar \omega} \right)} - \sqrt{2} \Gamma \left( \frac{3}{4} + n - \frac{z}{2 \hbar \omega} \right) \frac{\Gamma \left( \frac{3}{4} + \frac{n}{2 \hbar} - \frac{z}{2 \hbar \omega} \right)}{\Gamma \left( \frac{3}{4} + n - \frac{z}{2 \hbar \omega} \right)} + q_0(z). \]

Then it is easy to show that the \(q(z)\) has the following form:

\[ q(z) = \frac{1}{4 \pi \hbar l_{\Omega}^2} \sum_{n=0}^{\infty} \left\{ \frac{1}{\omega l_{\omega}} \frac{\Gamma \left( \frac{3}{4} + \frac{\Omega}{2 \hbar} (n + \frac{1}{2}) - \frac{z}{2 \hbar \omega} \right)}{\Gamma \left( \frac{3}{4} + \frac{n}{2 \hbar} - \frac{z}{2 \hbar \omega} \right)} - \sqrt{2} \frac{\Gamma \left( \frac{3}{4} + n - \frac{z}{2 \hbar \omega} \right)}{\Gamma \left( \frac{3}{4} + n - \frac{z}{2 \hbar \omega} \right)} + q_0(z) \right\}. \]
2.2 The "interaction" operator of the model

The matrix \((A(\lambda, \lambda'))_{\lambda, \lambda' \in \Lambda}\) of the "interaction" operator \(A\) in our model is described by the following conditions (cf. [15]):

1) \(A\) is the bounded self-adjoint operator in \(l^2(\Lambda)\), i.e. \(A(\lambda, \lambda') = A(\lambda', \lambda)\) for each \(\lambda, \lambda' \in \Lambda\);
2) \(A\) is the nearest-neighbour-interaction operator, i.e. \(A(\lambda, \lambda') = 0\), if \(|\lambda - \lambda'| > \inf\{|\lambda - \lambda'| : \lambda, \lambda' \in \Lambda, \lambda \neq \lambda'|\};
3) \(A\) is invariant with respect to a natural unitary representation of the magnetic translation group in the space \(l^2(\Lambda)\), i.e.

\[
A(\lambda, \lambda + \mu) = \exp[\pi i \xi \cdot (\mu \times \lambda)]A(0, \mu), \quad \lambda, \mu \in \Lambda,
\]

(22)

where \(\xi = B/\Phi_0\) is the vector of magnetic flux density (here \(\Phi_0 = 2\pi hc/e\) is the magnetic field quantum).

Therefore in the case of simple cubic crystallic lattice \(\Lambda\) the matrix of the operator \(A\) is fully determined only by the elements \(A(\lambda, 0), \lambda \in \Lambda:\)

\[
A(\lambda, 0) = \begin{cases} 
\alpha_1, & \lambda = \pm a_1, \\
\alpha_2, & \lambda = \pm a_2, \\
\alpha_3, & \lambda = \pm a_3, \\
0, & \text{in the other cases.}
\end{cases}
\]

(23)

Here \(\alpha_1, \alpha_2\) and \(\alpha_3\) are some real numbers (the so-called "coupling constants").

The construction of the Hamiltonian \(H \equiv H_A\) of 3D periodic quantum dots array in a uniform magnetic field is complete.

3 The structure of the spectrum of the Hamiltonian \(H_A\)

In the framework of our model it is possible to show that the spectrum of the model Hamiltonian \(H_A\) consists of the pure point and the band parts. The description of each band of the spectrum is mathematically reduced (without any additional simplifications or approximations) to the investigation of the only energy band in the tight-binding model. Moreover in the case of so-called rational magnetic flux the structure of the bands may be described analytically.

To investigate the spectrum of the operator \(H_A\) we start with the spectrum of the Hamiltonian \(H_d\) of single quantum dot. The spectrum \(\sigma(H_d)\) is discrete and consists of the eigenvalues \(E_{mn,\rho,\nu}\) (the Fock–Darwin levels),

\[
E_{mn,\rho,\nu} = \frac{\omega_c}{2}m + \frac{\Omega}{2}(2n_\rho + |m| + 1) + \frac{\omega}{2}(2n_\nu + 1),
\]

(24)

\(m \in \mathbb{Z}, \quad n_\rho, n_\nu, \in \mathbb{N} \cup \{0\}\).

Thus, the spectrum of the Hamiltonian \(H^0\) (the Hamiltonian of a set of isolated quantum dots) is pure point one and consists of the same points \(E_{mn,\rho,\nu}\), and each point \(E_{mn,\rho,\nu}\) is infinitely degenerated in the spectrum of \(H^0\). The Krein formula implies the following proposition.

**Proposition 1.** Let a real number \(E\) be not a point of the spectrum of \(H^0\), then the following assertions are equivalent:
1) \( E \in \sigma(H_A) \);

2) the operator \( q(E)I + A \) is not continuously invertible in the space \( l^2(\Lambda) \). ■

Therefore, to describe the spectrum of the Hamiltonian \( H_A \) we can consider the spectrum of the operator \( A \) and the behavior of the function \( q(x) \) on the real axis.

We denote by \( H_{TB} \) the standard tight-binding Hamiltonian:

\[
H_{TB} = -\sum_{\lambda, \lambda'} t_{\lambda, \lambda'} \exp(i\theta_{\lambda, \lambda'})C^\dagger_\lambda C_{\lambda'},
\]

where the summation is over nearest-neighbor nodes of \( \Lambda \), \( C^\dagger_\lambda \) and \( C_\lambda \) are the standard creation and annihilation operators at the node \( \lambda \), \( \theta_{\lambda, \lambda'} = -\frac{e}{\hbar c} \int A \cdot dl \) is the Peierls phase factor arising from the magnetic flux. It is easy to show that the interaction operator \( A \) coincides with the operator \( H_{TB} \) with \( t_{\lambda, \lambda'} = -A(\lambda, \lambda') \) for each \( \lambda, \lambda' \in \Lambda \).

As for the function \( q \), it is known that for real \( x \) the function \( q(x) \) monotone increases from \(-\infty\) to \(+\infty\) on each of the intervals \((-\infty, \varepsilon_0)\), \((\varepsilon_0, \varepsilon_1)\), \((\varepsilon_1, \varepsilon_2)\), \ldots, where the numbers \( \varepsilon_0, \varepsilon_1, \ldots \) are the eigenvalues \( E_{mn,\rho} \) putting in ascending order (Fig. 2):

\[
E_{000} = \varepsilon_0 < \varepsilon_1 < \ldots < \varepsilon_n < \ldots.
\]

Hence, there exists the multivalued real-analytical inverse function \( \chi(x) \) \((x \in \mathbb{R})\) having continuos branches \( \chi_n(x) \) \((n = 0, 1, \ldots)\) with the values in the intervals \((-\infty, \varepsilon_0)\), \((\varepsilon_0, \varepsilon_1)\), \((\varepsilon_1, \varepsilon_2)\), \ldots (Fig. 3). Let us denote by \( \tau_n \) the function \( \tau_n(x) = -\chi_n(x) \).

The following theorem describes the structure of the spectrum of the Hamiltonian \( H_A \).

**Theorem 1.** The spectrum \( \sigma(H_A) \) of the Hamiltonian \( H_A \) is the union of two parts, \( \sigma(H_A) = \Sigma_1 \cup \Sigma_2 \). The part \( \Sigma_1 \) consists of infinitely degenerated eigenvalues \( E_{mn,\rho} \), where \( m \neq 0 \). The band part \( \Sigma_2 \) of the spectrum of the operator \( H_A \) has the following form: \( \Sigma_2 = \bigcup_{n=0}^{\infty} Y_n \), where the set \( Y_n \) is the image of the spectrum \( \sigma(H_{TB}) \) of the tight-binding operator \( H_{TB} \) under the real-analytical function \( \tau_n \). ■

Therefore the every band \( Y_n \) is a result of deformation of a unique energy band in the tight-binding model under the corresponding function \( \tau_n \). This fact explains, in particular, various form of the spectrum in different energy bands.

To continue the study of the spectrum of the operator \( H_A \) we consider the case of a rational field \( B \). In this case the part \( \Sigma_2 \) of the spectrum \( \sigma(H_A) \) may be described analytically.

Fix a basis \((a_1, a_2, a_3)\) in \( \Lambda \) and denote

\[
\eta_1 = \frac{B(a_2 \times a_3)}{\Phi_0}, \quad \eta_2 = \frac{B(a_3 \times a_1)}{\Phi_0}, \quad \eta_3 = \frac{B(a_1 \times a_2)}{\Phi_0};
\]

by the supposition, the numbers \( \eta_j \) are rational. Therefore, a basis \((a'_1, a'_2, a'_3)\) can be chosen in such a way that \( \eta_1 = \eta_2 = 0 \),

\[
\eta_3 \equiv \eta = \frac{B(a'_1 \times a'_2)}{\Phi_0} = \frac{N}{M} > 0,
\]

where \( N \) and \( M \) are coprime positive integers.

Then by means of harmonic analysis on the magnetic translation group we reduce the spectral problem for the operator \( H_A \) to the eigenvalue problem of linear algebra. Namely, to
where $p$ define the band part of the spectrum of $H$ × $M$ $N/M$.

Theorem 2. Let a basis $(a_1', a_2', a_3')$ of the lattice $\Lambda$ be choosen in such a way that

$$\eta = \frac{B(a_1' \times a_2')}{\Phi_0} = \frac{N}{M} > 0, \quad B(a_2' \times a_3') = B(a_3' \times a_1') = 0,$$

where $N/M$ is the irreducible rational fraction. Then the spectrum of the operator $H_A$ is essential and is divided into two parts $\Sigma_1$ and $\Sigma_2$. The first one, $\Sigma_1$, consists of infinitely degenerated Fock–Darwin levels $E_{mn,n_1}$, where $m \neq 0$. The second part $\Sigma_2$ is the band spectrum of $H_A$. This spectrum consists of bands $I_n$, $n \geq 0$, lying on the intervals $(\varepsilon_n, \varepsilon_{n+1})$ (here $\varepsilon_{-1} = -\infty$):

$$\Sigma_2 = \bigcup_{n=0}^{\infty} I_n, \quad I_n \subset (\varepsilon_n, \varepsilon_{n+1}).$$

The each band $I_n$, $n \geq 0$, splits into $M$ ”magnetic” subbands $I_{n,l}$, $l = 1, 2, \ldots, M$:

$$I_n = \bigcup_{l=1}^{M} I_{n,l},$$

where $I_{n,l} = \{E_{n,l}(p) : p \in \mathbb{T}_3\}$, and for fixed $p$ the collection $\{E_{n,1}(p), \ldots, E_{n,M}(p)\}$ is the set of all solutions of the dispersion equation

$$\det[q(E) + \widetilde{A}(p)] = 0,$$

lying on the interval $(\varepsilon_n, \varepsilon_{n+1})$.

The subbands $I_{n,l}$ of the band $I_n$ can be overlapped. Some of subbands can be degenerated to a point.

Therefore there are three kinds of points in the spectrum of the operator $H_A$. The following physical interpretation of the described structure of the energy spectrum of our model may be proposed. The points of the first kind (the levels of the single quantum dot) correspond to the classical orbits lying wholly in the single dot. The points of the second kind (the extended states) correspond to the classical propagation trajectories in the periodic system. Finally, the points of the third kind (the bound states satisfying the dispersion equation) correspond to the classical orbits lying in compact domain (cf. [14], [16]).

As a result of numerical analysis of the dispersion equation [27] we obtain angle–energy and flux–energy diagrams represented on Fig. 4 and Fig. 5 respectively (we use a system of units such that $c = \hbar = e = 1$ and $m^* = 1/2$). According to Theorem 2, the bands of the spectrum look like deformed Hofstadter butterflies (cf. [17]).
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Fig. 1. Three-dimensional quantum dots array and basic vectors of array lattice.

Fig. 2. The behaviour of the function $q(x)$.

Fig. 3. The behaviour of the functions $\tau_n(x)$.

Fig. 4. The angle-energy diagram for the simple-cubic array of spherical quantum dots.

Fig. 5. The flux-energy diagram for the simple-cubic array of spherical quantum dots.
