An Explicitly Solvable Model for Tunneling through a Quantum Dots Array in a Magnetic Field

D. A. Eremin,1 E. N. Grishanov,1 D. A. Ivanov,1
A. A. Lazutkina,2 E. S. Minkin,1 and I. Yu. Popov2

1Mordovian State University, Bolshevistskaya, 68, Saransk, 430000, Russia
2St. Petersburg National Research University of Information Technologies, Mechanics and Optics, Kronverkskiy, 49, St. Petersburg, 197101, Russia

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An explicitly solvable model for electron tunneling through a periodic quantum dots array in a magnetic field is suggested. It is based on the theory of self-adjoint extensions of symmetric operators. Two types of arrays are considered: a honeycomb lattice of point-like potentials and a square lattice of quantum dots with parabolic confinement. Ranges of the electron energies corresponding to zero transmission coefficients are observed. The dependence of the positions of these “zero transmission bands” on the magnetic field is investigated.

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I. INTRODUCTION

The interest of physicists and mathematicians in the spectral properties of 2D periodic quantum systems in a magnetic field has risen continuously starting from the well known Hofstadter paper [1]. The magnetic field leads to the appearance of specific spectral features, e.g., fractal structure of the spectrum [2, 3]. This unusual spectral property was obtained as a result of sophisticated theoretical exercises, but later the progress of nanotechnology has allowed one to observe it in experiments [4]. There are several theoretical approaches to the description of the periodic arrays of quantum dots. In the present paper we use a zero-range potential model [5, 6] based on the theory of self-adjoint extensions of symmetric operators [7–12]. The model is explicitly solvable and gives one realistic results in spite of its simplicity. In particular, it allows one to get results appropriate for practical applications [13]. The goal of the present paper is to study electron tunneling through a periodic array of quantum dots in a homogeneous magnetic field. Tunneling of such a type was actively investigated during the last decade because of its significance for nanotechnology applications [14–16]. Our starting points are as follows: the works [17, 18] where the model of the array was suggested and the papers [19, 20] describing the mathematical scheme for tunneling through a nanodevice. The first result for this tunneling problem was obtained for the simplest case [21] (square lattice, point-like potentials). It was observed that there exists a range of electron energies for which the transmission coefficient is very close to zero. This range depends on the magnetic field. A natural question appears whether it is a particular case or the effect has general features. In the present paper we investigate this problem. Namely, we consider two cases. First, we deal with tunneling through the array of quantum dots (point-like potentials) with a honeycomb lattice. Second, we return to the
square lattice, but consider another, more realistic, model of the quantum dot—a quantum well with parabolic confinement.

We deal with the ballistic regime of electron transport. In this case one can use the Landauer-Buttiker formalism to derive the conductivity $\sigma$ for the nanostructure with two leads from the transmission coefficient $T(E)\big|_{E=E_F}$, $F$ is the Fermi energy (see, e.g., [22]):

$$\sigma = \left(\frac{e^2}{h}\right) T(1-T)^{-1}.$$

In the present paper we consider tunneling in the system consisting of a 2D periodic array of quantum dots with two laterally coupled semi-infinite leads orthogonal to the plane of the array. We study the influence of the magnetic field on the transmission coefficient and observe an interesting phenomenon: for some values of the magnetic field one has zero transmission.

II. MODEL

II-1. General scheme of the model construction

Let us start from the Hamiltonian of a charged spinless particle of mass $m$ in a constant homogeneous magnetic field $\mathbf{B}$ in the space $L^2(\mathbb{R}^3)$. We choose the standard basis $\mathbf{i}, \mathbf{j}, \mathbf{k}$ in $\mathbb{R}^3$ and assume that $\mathbf{B}$ is parallel to $\mathbf{k}: \mathbf{B} = B\mathbf{k}$, $B \neq 0$. After separation of the free motion along the $z$-axis, one obtains the Hamiltonian $H_0$ in the space $L^2(\mathbb{R}^2)$, where $\mathbb{R}^2$ is a plane orthogonal to $\mathbf{B}$ and having a basis $\mathbf{i}, \mathbf{j}$:

$$H_0 = \frac{1}{2m}(\mathbf{p} - e\mathbf{c})^2.$$

Here $\mathbf{p}$, $\mathbf{p} = -i\hbar\nabla$, is the two-dimensional momentum operator, $e$ is the particle charge, $c$ is the speed of light, $\mathbf{A}(\mathbf{r})$ is a vector potential of the field ($\mathbf{B} = \text{curl} \mathbf{A}$), $\mathbf{r}$ is the radius-vector of the point. The choice of this vector potential isn’t unique. Usually, one uses the symmetric or Landau gauge. In each case the operator $H_0$ is essentially self-adjoint in $L^2(\mathbb{R}^2)$. A change of the gauge leads to the replacement of $H_0$ by a unitary equivalent operator [23]. Further, we shall use the symmetric gauge for which one has $\mathbf{A} = -\mathbf{B} \times \mathbf{r}$.

Let us introduce the following standard notations: $\omega_c = |eB|/cm$ – the cyclotron frequency; $\Phi_0 = 2\pi\hbar c/|e|$ – the quantum of magnetic flux. Let us mark as $\xi$ the following ratio: $\xi = \pm B/\Phi_0$. Here the sign ($\pm$) is chosen in such a way that $\xi > 0$. The value of $|\xi|$ equals the number of the flux quantum through a unit area in $\mathbb{R}^2$. To simplify the formulas we shall use the system of units in which $e = \hbar = c = 2m = 1$. Then the Hamiltonian $H_0$ takes the following form:

$$H_0 = -\frac{1}{2} \left[ \left( \frac{\partial}{\partial x} + \pi \xi iy \right)^2 + \left( \frac{\partial}{\partial y} - \pi \xi ix \right)^2 \right].$$

The spectrum of $H_0$ is pure point and consists of infinitely degenerate eigenvalues (Landau levels) [6]:

$$\varepsilon_l = (l + 1/2)\omega_c.$$
Below we shall use the Green function of the operator $H_0$ (i.e., the resolvent kernel of $R^0(z) = (H_0 - z)^{-1}$), which has the form \[24\]:

$$G_0(r_i, r_j; z) = \frac{1}{2\pi} \Gamma \left( \frac{1}{2} - \frac{z}{\omega} \right) \exp \left[ -\pi i r_i \wedge r_j - \frac{\pi \xi(r_i - r_j)^2}{2} \right] \Psi \left( \frac{1}{2} - \frac{z}{\omega}, 1, \pi \xi(r_i - r_j)^2 \right).$$

Here $\Gamma(x)$ is the Euler $\Gamma$-function and $\Psi(a; c; x)$ is the confluent hypergeometric function of second type \[25\].

Consider a two-dimensional periodic array of quantum dots $\Lambda$. The centers of the quantum dots coincident with the nodes of a square lattice $\Lambda$. Let us fix two basic vectors $a_1, a_2$ from $\Lambda$ such that for any $\lambda, \lambda' \in \Lambda$, we have a unique representation $\lambda = \lambda_1 a_1 + \lambda_2 a_2$, where $\lambda_1, \lambda_2$ are integers. The Hamiltonian of the array of quantum dots can be represented in the following form

$$H = H_0 + \sum \gamma V(r - \gamma).$$

We use the zero-range potential model based on the operator extension theory, i.e., we replace the potential $V$ by $\delta$-like one. The Hamiltonian $H$ of the array in this case is constructed in the following way (see \[17\]). First, we restrict the initial self-adjoint operator $H_0$ onto the set of smooth functions vanishing at nodes of the lattice and construct its closure. It is a symmetric non-self-adjoint operator with infinite deficiency indices. The model Hamiltonian is given by a self-adjoint extension $H$ of this symmetric restriction. The Green function $G$ of the operator $H$ can be obtained by Krein’s resolvent formula \[17, 26\]:

$$G(r, r'; E) = G_0(r, r'; E) - \sum \gamma, \mu [Q(E) + A_{\gamma, \mu}^{-1}] \sum \gamma, \mu \gamma, \mu G_0(r, \gamma; E) G_0(\mu, r'; E).$$

The Hermitian matrix $A$ parameterizes the self-adjoint extension of the operator $H_0$. Due to the periodicity of the system, its Hamiltonian should be invariant with respect to the magnetic translation group \[6\]. As a consequence, one gets that terms of $A$ satisfy the following property:

$$A_{\gamma - \gamma, \mu - \mu} = \exp [\pi i \xi(\gamma \times (\lambda - \mu)) e_2] A_{\lambda, \mu}.$$

We take into account the nearest neighbors interaction only, hence, the matrix inputs have the form

$$A_{\lambda, 0} = \sigma [\delta_{\lambda_1, 0}(\delta_{\lambda_2, 1} + \delta_{\lambda_2, -1}) + \delta_{\lambda_2, 0}(\delta_{\lambda_1, 1} + \delta_{\lambda_1, -1})].$$

Here $\sigma$ is a constant related to the intensity of the interaction with the nearest neighbor.

Let us consider now the tunneling problem. We deal with the plane of our quantum dots array with two connected semi-infinite leads orthogonal to the plane (see Fig. 1).
model is analogous to that in [7, 19] and is based on the operator extension theory. The Hilbert space for the array described above will be marked as $H_d$ (it corresponds to the “internal” states). The state spaces of the channels are $H_+ = L^2(\mathbb{R}_+)$, $H_- = L^2(\mathbb{R}_-)$. Thus, the whole state space for the system $\mathcal{H}$ is as follows:

$$\mathcal{H} = H_- \oplus H_d \oplus H_+.$$ 

We start from the Hamiltonian $H^0$ which corresponds to the system having no interaction between the channels and the array. It is the orthogonal sum of the corresponding operators

$$H^0 = H_- \oplus H_d \oplus H_+.$$ 

Here $H_\pm$ is the operator $-\frac{d^2}{dx^2}$ in $L^2(\mathbb{R}_\pm)$ with the Neumann condition (absence of transmission through the contact point) at the edge (point 0), $H_d$ is the Hamiltonian of the charged particle in the quantum dots array in the homogeneous magnetic field described above.

The Green functions $G_\pm$ are well known:

$$G_\pm(x, 0; E) = ik^{-1} \exp(\pm ik(x + y)), \text{ for } x > 0,$$

where $E = k^2$, $\Im k \geq 0$. We restrict the initial operator on the set of functions vanishing at the contact points $r_1, r_2$ for $\mathbb{R}^2$ and 0 for $\mathbb{R}_\pm$. A self-adjoint extension of this operator gives us the model operator. Extensions are determined by the Hermitian matrix $A^w$. We assume that all contacts are ideal, therefore the matrix $A^w$ for this extension should be chosen in the form

$$A^w = \begin{pmatrix}
0 & \alpha_- & 0 & 0 \\
\alpha_- & 0 & 0 & 0 \\
0 & 0 & 0 & \alpha_+ \\
0 & 0 & \alpha_+ & 0
\end{pmatrix},$$

where $\alpha_-, \alpha_+$ are the real parameters which characterize the contacts.

We denote by $Q, \bar{Q}$ the Krein $Q$-functions of the quantum dots array and of the full model operator correspondingly. Let us introduce the values $Q_{ij}$:

$$Q_{11} = q(E) + \sum_{\lambda, \mu} (Q + A)^{-1}_{\lambda, \mu} G_0(r_1, \lambda; E)G_0(\mu, r_1, E),$$

$$Q_{22} = q(E) + \sum_{\lambda, \mu} (Q + A)^{-1}_{\lambda, \mu} G_0(r_2, \lambda; E)G_0(\mu, r_2, E),$$

$$Q_{12} = Q_{21} = G(r_1, r_2; E),$$

$q(E)$ are the $Q$-functions for the plane:

$$q(E) = -\frac{m}{2\pi \hbar^2} \left( \psi \left( \frac{1}{2} - \frac{E}{\hbar \omega_c} \right) + \log \pi|\xi| + 2C_E \right),$$
where $\psi(x)$ is the logarithmic derivative of the Euler gamma-function (digamma function), $C_E$ is the Euler constant.

Hence, the corresponding matrix for the full model operator has the form

$$
\tilde{Q} + \tilde{A} = \begin{pmatrix}
Q_\alpha & 0 & 0 & 0 \\
0 & Q_{11} & Q_{12} & 0 \\
0 & Q_{21} & Q_{22} & \alpha_+ \\
0 & 0 & \alpha_+ & Q_+ \\
\end{pmatrix},
$$

where $Q_\alpha$, $Q_+$ are the Krein functions for the wires.

Finally, solving the scattering problem, we obtain the formula for the transmission coefficient:

$$
T(E) = \frac{|Q_{12}|^2}{E((Q_{11} - 1)(Q_{22} - 1) - |Q_{12}|^2)}.
$$

II-2. Model for honeycomb lattice

We deal with two-dimensional honeycomb lattice with two semi-infinite wires orthogonal to the lattice plane (see Fig. 1).

The honeycomb lattice can be considered in a conventional way as a union of two square lattices: $A + K, K = \{0, b\}, b = 2(a_1 + a_2)/3$ (see Fig. 2). The model construction is the same as has been described earlier. Modification is related with the type of symmetry (the magnetic translation group is changed). It leads to another matrix $A$ for the nearest neighbor interaction case. Namely, one has the following matrix entries:

$$
A_{\lambda,\lambda'} = \sigma(\delta_{\lambda-a_1,\lambda'-b} + \delta_{\lambda-a_2,\lambda'-b} + \delta_{\lambda-a_1-a_2,\lambda'-b} + \exp(2\pi i \eta(\delta_{\lambda+a_1-b,\lambda'} + \delta_{\lambda+a_2-b,\lambda'})/3) \\
(\delta_{\lambda+a_1-a_2-b,\lambda'} + \delta_{\lambda+a_2-b,\lambda'} + \delta_{\lambda+a_1+a_2-b,\lambda'}).)
$$

Here the constant $\sigma$ characterizes the intensity of interaction with the nearest neighbor, $\eta$ is the number of the flux quantum through the lattice cell.
FIG. 2: The honeycomb lattice as a union of two square lattices.

II-3. Model of quantum dots array with parabolic confinement

In this section we deal with a more realistic model of the quantum dots—we consider a parabolic confinement instead of point-like potentials. The procedure is as follows. We consider the orthogonal sum of the Hilbert spaces $H_{\text{plane}} \oplus \sum_\lambda \mathcal{H}_\lambda$, $H_{\text{plane}} = \mathcal{H}_\lambda = L_2(R^2), \lambda \in \Lambda$. The space $H_{\text{plane}}$ is related with the plane of the periodic array of quantum dots (as in the general scheme described above). Correspondingly, we consider the Landau operator (the Schrödinger operator with a magnetic field without additional potential) for $H_{\text{plane}}$. As for $\mathcal{H}_\lambda$, we deal with the Landau operator with parabolic confinement $V_\lambda(r) = \Omega^2_0 (r - \lambda)^2 / 2$. It is the operator for the quantum dot. To “switch on” the interaction between the dots and the plane, we use the conventional scheme of operator extensions (so called zero-range potentials with internal structure [27]). Namely, we restrict the operators on the set of smooth functions vanishing at the lattice nodes and at the centers of the dots, correspondingly. We get the symmetric operator with infinite deficiency indices. Its self-adjoint extension gives us the model in question. When constructing the extension, we choose non-zero entries of the matrix describing the extension in such a way that there exist tunneling between the $\lambda$ dot and the point $\lambda$ of the plane. In some sense it is similar to the model of a double layer of quantum dots [28, 29]. Correspondingly, there appears an additional line and column in the matrix for each dot. The additional diagonal terms are the Krein functions for the dots $q_d$:

$$q_d(E) = -\frac{m}{2\pi\hbar^2} \left( \frac{1}{2} - \frac{E}{\hbar \Omega} \right) + \log \frac{m\Omega}{2\pi\hbar} + 2C_E,$$

where $\Omega = \sqrt{\omega_c^2 + 4\omega_0^2}$, $\omega_0$ is the parameter of the parabolic potential. Let $\beta$ be the parameter corresponding to the tunneling from the dot to the plane. It is the additional
III. RESULTS AND DISCUSSION

Our aim is to describe the behavior of the transmission coefficient as a function of the magnetic field. Particularly, we look for the range (some bands) of the electron energy for which the transmission coefficient is very close to zero.

**Remark.** One should note that the transmission coefficient cannot be identically zero at a segment from the energy axis. Really, it is an analytic function of the energy, and if it is zero at the whole segment then it is zero at the whole analyticity domain, i.e., everywhere. But from the point of view of real experiments, we can believe that it is zero if it is less, e.g., than 0.001 of its maximum value.

Our computations show that the position, width and numbers of “zero transmission bands” depend on the lattice symmetry, types of quantum dots and positions of the wires connecting points.

Calculations for the honeycomb lattice (with unit lattice vectors) were made for two different positions of wires connecting points. If these points are inside one lattice cell we have two bands of zero transmission depending on the magnetic field (Fig. 4 (left)). If the points are in the neighboring cells, there appears a third zero transmission band (Fig. 4 (right)). Moreover, in comparison with the corresponding band for the square lattice with the same cell area (see [21]), the bands become narrower.

Calculations for the parabolic confinement type of quantum dots show that the dependence on the magnetic field is more essential (Fig. 4). This is related with the fact that...
we assume that the magnetic field exists inside the dots also.

In conclusion, we can note that the suggested model based on the operator extension theory allows one to find the transmission coefficient for different geometrical parameters and different types of quantum dots.

It is interesting to compare our formulas with the formula for the conductivity of topological insulators. Namely, the formula for the quantum correction to 2D conductivity in a magnetic field is as follows [30]:

$$\Delta \sigma = \alpha \frac{e^2}{2\pi^2 \hbar} \left( \psi \left( \frac{1}{2} + \frac{B_0}{B} \right) - \log \left( \frac{B_0}{B} \right) \right).$$

Here $B_0 = \hbar/(4eL_0^2)$ and $L_0$ is the dephasing length. In our case the analogous term appears in the expression for the transmission coefficient due to electron transition from $r_1$ to $r_2$ through the plane with quantum dots (it is a part of the expression for the Krein $q$-function). One can see that our model can be useful for topological insulator problems.

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