Hofstadter's butterfly in a two-dimensional lattice consisting of two sublattices

This article has been downloaded from IOPscience. Please scroll down to see the full text article.
2004 J. Phys. A: Math. Gen. 375763
(http://iopscience.iop.org/0305-4470/37/22/004)
View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.90
The article was downloaded on 02/06/2010 at 18:04

Please note that terms and conditions apply.

# Hofstadter's butterfly in a two-dimensional lattice consisting of two sublattices 

G A Vugalter and A S Pastukhov

Department of Physics, Nizhny Novgorod State University, 23 Gagarin Avenue, Nizhny Novgorod 603950, Russia

E-mail: vugalter@phys.unn.ru
Received 16 February 2004, in final form 13 April 2004
Published 18 May 2004
Online at stacks.iop.org/JPhysA/37/5763
DOI: 10.1088/0305-4470/37/22/004


#### Abstract

Harper's equations for simple and complex two-dimensional lattices subject to a magnetic field have been derived in the tight-binding approximation. In our derivation we do not neglect the influence of the magnetic field on the electron eigenfunctions and eigenvalues in isolated atoms. Using a variational procedure for finding eigenfunctions and eigenvalues, we have self-consistently obtained Hofstadter's butterflies. Even for a simple square lattice Hofstadter's butterfly differs from the butterfly obtained in the case in which the influence of the magnetic field on the electron eigenvalues and eigenfunctions in isolated atoms is not taken into account.


PACS numbers: 71.70.-d, 75.10.-b

## 1. Introduction

The problem of an electron on a two-dimensional periodic lattice subject to a magnetic field has been of interest in solid state physics for several decades. After Hofstadter had numerically studied the electron spectrum of the Harper model [1] and discovered the fractal structure of the spectrum as a function of the magnetic flux per lattice cell [2], the interest in the problem especially grew (see, for example, theoretical [3-10] and experimental [11-13] works and references therein). The problem of two interacting particles in a two-dimensional potential and a magnetic field was studied in [14].

So far the Harper model and Hofstadter's butterfly have been considered for a simple two-dimensional lattice. Moreover, in the papers in which the tight-binding approximation is used in order to derive Harper's equation, it is assumed that the influence of the magnetic field on the electron eigenfunctions and eigenvalues in isolated atoms is negligible. The latter assumption is justified for real atoms. However, at present, the most appropriate objects for experimental investigation of electrons in a high magnetic field are artificial two-dimensional
lattices of quantum dots or anti-dots. In such structures the number of magnetic flux quanta per lattice cell can exceed unity for the magnetic field values (of order 10 MGs ) achievable in experiments. The coupling energy of an electron in a quantum dot is much lower than in a real atom, therefore the influence of the high magnetic field on the electron eigenfunctions and eigenvalues in a quantum dot is more significant than in an atom. It should be noted that the influence of the magnetic field on the atomic energy level and on the hopping integrals was discussed by Alexandrov and Capellmann [15] in connection with the orbital diamagnetism of two-dimensional electrons. The importance of the magnetic shift of the atomic level in the theory of electronic diamagnetism of two-dimensional electrons was mentioned in [16]. However, in both [15, 16] Harper's equation and Hofstadter's butterfly were not considered.

The purpose of our paper is to derive Harper's equations for a simple two-dimensional square lattice and for a complex two-dimensional lattice consisting of two simple square sublattices. In both cases the lattices are subject to a magnetic field perpendicular to the lattice plane. Our derivation is based on the tight-binding approximation and takes into account the influence of the magnetic field on the electron eigenfunctions and eigenvalues in isolated atoms (despite our results being applicable rather to a lattice of quantum dots than to a lattice of real atoms, we will use the term 'atom' instead of the term 'quantum dot'). We do not take into account the electron spin.

The paper is organized as follows. In section 2, we derive Harper's equation for a simple square lattice. In section 3, we consider a complex two-dimensional lattice. In section 4, we discuss numerical results. Some mathematical proofs are given in the appendix.

## 2. Harper's equation for a simple square lattice

Let us consider an electron on a two-dimensional square lattice subject to a dc magnetic field $\mathbf{B}$ perpendicular to the lattice plane. The lattice consists of atoms whose positions are characterized by two-dimensional radius vectors $\mathbf{a}_{n m}=$ ( $a n, a m$ ) where $a$ is the minimal period of the lattice, $n, m=0, \pm 1, \pm 2, \ldots$ We denote the potential energy of interaction of the electron at a point $\mathbf{r}=(x, y)$ with the atom at the point $\mathbf{a}_{n m}$ as $U\left(\mathbf{r}-\mathbf{a}_{n m}\right)$. This function is assumed to be cylindrically symmetric, i.e. $U\left(\mathbf{r}-\mathbf{a}_{n m}\right)$ depends only on $\left|\mathbf{r}-\mathbf{a}_{n m}\right|$. We choose the vector potential of the magnetic field in the Landau gauge $\mathbf{A}=(0, B x)$.

To find the electron energy spectrum, we should solve a stationary Schrödinger equation for the electron wavefunction $\psi(\mathbf{r})$

$$
\begin{equation*}
\left[\frac{1}{2 \mu}\left(\hat{\mathbf{p}}-\frac{e}{c} \mathbf{A}\right)^{2}+V_{1}(\mathbf{r})\right] \psi(\mathbf{r})=E \psi(\mathbf{r}) . \tag{1}
\end{equation*}
$$

Here $\mu, e$ are the electron mass and charge; $c$ is the velocity of light;

$$
\begin{equation*}
V_{1}(\mathbf{r})=\sum_{n, m} U\left(\mathbf{r}-\mathbf{a}_{n m}\right) \tag{2}
\end{equation*}
$$

is the periodic potential of the lattice.
In what follows we suppose that the magnetic field obeys the condition

$$
\begin{equation*}
B a^{2} / \Phi_{0}=\Phi / \Phi_{0}=p / q \tag{3}
\end{equation*}
$$

where $\Phi$ is the magnetic flux per lattice cell, $\Phi_{0}=2 \pi \hbar c /|e|$ is a magnetic flux quantum; $\hbar$ is the Planck constant; $p$ and $q$ are integers, $p / q$ is an irreducible fraction. Then the wavefunction $\psi_{\mathbf{k}}(\mathbf{r})$ being a solution of equation (1) and corresponding to a wavevector $\mathbf{k}=\left(k_{x}, k_{y}\right)$ should satisfy the Bloch-Peierls conditions

$$
\begin{equation*}
\psi_{\mathbf{k}}(x+q a, y)=\exp \left(\mathrm{i} k_{x} q a-\mathrm{i} 2 \pi p y / a\right) \psi_{\mathbf{k}}(x, y) \tag{4a}
\end{equation*}
$$

$$
\begin{equation*}
\psi_{\mathbf{k}}(x, y+a)=\exp \left(\mathrm{i} k_{y} a\right) \psi_{\mathbf{k}}(x, y) \tag{4b}
\end{equation*}
$$

If we fulfil the operation of complex conjugation and reverse the direction of the magnetic field in equation (1), we will come to the latter again. Therefore, if the function $\psi_{\mathbf{k}}(\mathbf{r}, \mathbf{B})$ is an eigenfunction of equation (1), then the function $\psi_{\mathbf{k}}^{*}(\mathbf{r},-\mathbf{B})$ is an eigenfunction of this equation too (the asterisk means the operation of complex conjugation). On the other hand, according to equations $(4 a)$ and $(4 b)$, the function $\psi_{\mathbf{k}}^{*}(\mathbf{r},-\mathbf{B})$ transforms as $\psi_{-\mathbf{k}}(\mathbf{r}, \mathbf{B})$, i.e.

$$
\begin{align*}
& \psi_{\mathbf{k}}^{*}(x+q a, y ;-\mathbf{B})=\exp \left(-\mathrm{i} k_{x} q a-\mathrm{i} 2 \pi p y / a\right) \psi_{\mathbf{k}}^{*}(x, y ;-\mathbf{B})  \tag{5a}\\
& \psi_{\mathbf{k}}^{*}(x, y+a ;-\mathbf{B})=\exp \left(-\mathrm{i} k_{y} a\right) \psi_{\mathbf{k}}^{*}(x, y ;-\mathbf{B}) \tag{5b}
\end{align*}
$$

(we assume that $q$ is positive, the integer $p$ can be either positive or negative; the reverse of the direction of the magnetic field means the change of the sign of the number $p$ ). Thus, we conclude that

$$
\begin{equation*}
E(\mathbf{k},-\mathbf{B})=E(-\mathbf{k}, \mathbf{B}) \tag{6}
\end{equation*}
$$

We emphasize that the wavefunction $\psi_{\mathbf{k}}(\mathbf{r})$ found approximately should satisfy not only the Bloch-Peierls conditions ( $4 a$ ) and (4b), but also conditions ( $5 a$ ) and ( $5 b$ ).

In the tight-binding approximation we seek the wavefunction $\psi_{\mathbf{k}}(\mathbf{r})$ in the form

$$
\begin{equation*}
\psi_{\mathbf{k}}(\mathbf{r})=\sum_{n, m} g_{n}(\mathbf{k}) \exp \left(\mathrm{i} \mathbf{k} \mathbf{a}_{n m}-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a} n\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right) \tag{7}
\end{equation*}
$$

Here $g_{n}(\mathbf{k})(n=0, \pm 1, \pm 2, \ldots)$ are unknown coefficients; $\psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)$ is the normalized wavefunction of an electron interacting only with the atom at the site $\mathbf{a}_{n m}$. The wavefunction $\psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)$ obeys a Schrödinger equation
$\left[\frac{1}{2 \mu}\left(\hat{\mathbf{p}}+\frac{|e| B}{c}(x-n a) \mathbf{y}_{0}\right)^{2}+U\left(\mathbf{r}-\mathbf{a}_{n m}\right)\right] \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)=E_{0} \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)$
where $\mathbf{y}_{0}$ is the unit vector of the $y$ axis; $E_{0}$ is the energy of the electron in the state $\psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)$. It should be noted that the wavefunction in the form (7) was used in [17] in which electron states in a three-dimensional cubic lattice subject to a high magnetic field were studied; however, the authors of [17] neglected the influence of the magnetic field on the atomic wavefunction $\psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)$.

The wavefunction (7) is a linear combination of the atomic wavefunctions of the form

$$
\exp \left(-\mathrm{i} 2 \pi \frac{p}{q} \frac{y}{a} n\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)=\exp (\mathrm{i} e B y n /(\hbar c)) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)
$$

This expression is similar to, but does not coincide with the atomic wavefunction at the site $\mathbf{a}_{n m}$, used in [15] (see equation (17) therein). The distinction is connected with different gauges of the vector potential in [15] and in our work.

Below we shall suppose that, if we make a gauge transformation of the wavefunction $\psi_{0}(\mathbf{r})$ in order to go over from the Landau gauge $\mathbf{A}=(0, B x)$ to the symmetric gauge $\mathbf{A}^{\prime}=[\mathbf{B} \times \mathbf{r}] / 2$, we shall get a wavefunction $\Psi_{0}(r)$ with the angular momentum equal to zero. The latter wavefunction is real, does not depend on the direction of the vector $\mathbf{r}$ and obeys the equation

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 \mu r} \frac{\mathrm{~d}}{\mathrm{~d} r}\left(r \frac{\mathrm{~d} \Psi_{0}}{\mathrm{~d} r}\right)+\left(\frac{e^{2} B^{2}}{8 \mu c^{2}} r^{2}+U(r)\right) \Psi_{0}=E_{0} \Psi_{0} \tag{9}
\end{equation*}
$$

Since $\mathbf{A}=\mathbf{A}^{\prime}+\nabla f$ with $f=B x y / 2$, we obtain

$$
\begin{equation*}
\psi_{0}(\mathbf{r})=\Psi_{0}(r) \exp (\mathrm{i} e f /(\hbar c))=\Psi_{0}(r) \exp \left(-\mathrm{i} x y /\left(2 l_{H}^{2}\right)\right) \tag{10}
\end{equation*}
$$

where $l_{H}=\sqrt{c \hbar /(|e| B)}$ is the magnetic length. Obviously, $\psi_{0}(-\mathbf{r})=\psi_{0}(\mathbf{r})$. The authors of [15] replaced the atomic potential by a harmonic-oscillator potential and obtained an explicit expression for the function $\Psi_{0}(r)$. However, such a choice of the atomic potential is not suitable for calculating the coefficients of Harper's equations. These coefficients contain not only the atomic potential, but also the lattice potential (see, for example, equations (14a)$(14 c)$ ). If the atomic potential is chosen in the harmonic-oscillator form, the series for the lattice potential does not converge. When deriving Harper's equations for simple and complex lattices, we do not choose any concrete form of the atomic potential $U(r)$.

One can verify that, under the condition of periodicity $g_{n+q}=g_{n}$, function (7) satisfies the Bloch-Peierls conditions $(4 a)$ and $(4 b)$. We assume that the condition of periodicity holds. Moreover, in this case function (7) satisfies conditions (5a) and (5b) as well.

Substituting the wavefunction (7) into the Schrödinger equation (1) and taking into account that

$$
\begin{align*}
& \left(\hat{p}_{y}+\frac{|e| B}{c} x\right)^{2} \exp \left(-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a} n\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right) \\
& \quad=\exp \left(-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a} n\right)\left(\hat{p}_{y}+\frac{|e| B}{c}(x-n a)\right)^{2} \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right) \tag{11}
\end{align*}
$$

we obtain

$$
\begin{equation*}
\sum_{n, m} g_{n}(\mathbf{k}) \exp \left(\mathrm{i} \mathbf{k} \mathbf{a}_{n m}-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a} n\right)\left(E_{0}-E+V_{1}(\mathbf{r})-U\left(\mathbf{r}-\mathbf{a}_{n m}\right)\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}\right)=0 \tag{12}
\end{equation*}
$$

We multiply the latter equation by

$$
\exp \left(-\mathrm{i} \mathbf{k} \mathbf{a}_{n^{\prime} m^{\prime}}+\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m^{\prime} a}{a} n^{\prime}\right) \psi_{0}^{*}\left(\mathbf{r}-\mathbf{a}_{n^{\prime} m^{\prime}}\right)
$$

and carry out integration over $x, y$. In the tight-binding approximation the overlapping of the wavefunctions localized at different sites of the lattice is negligible, and it is enough to take into account the electron transitions between the nearest neighbouring sites of the lattice. Then on the left-hand side of equation (12) we can retain the term with $n=n^{\prime}, m=m^{\prime}$, two terms with $n=n^{\prime} \pm 1, m=m^{\prime}$ and two terms with $n=n^{\prime}, m=m^{\prime} \pm 1$. As a result, we have (below we write $n, m$ instead of $n^{\prime}, m^{\prime}$ )

$$
\begin{align*}
\left(E-E_{0}-A\right) & g_{n}-B_{1}^{+} g_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}-B_{1}^{-} g_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a} \\
& -\left(B_{2}^{+} \mathrm{e}^{\mathrm{i}\left(k_{y} a+2 \pi(p / q) n\right)}+B_{2}^{-} \mathrm{e}^{-\mathrm{i}\left(k_{y} a+2 \pi(p / q) n\right)}\right) g_{n}=0 \tag{13}
\end{align*}
$$

where
$A=\int\left(V_{1}(\mathbf{r})-U(\mathbf{r})\right)\left|\psi_{0}(\mathbf{r})\right|^{2} \mathrm{~d}^{2} \mathbf{r}$
$B_{1}^{ \pm}=\int \psi_{0}^{*}(\mathbf{r})\left(E_{0}-E+V_{1}(\mathbf{r})-U\left(\mathbf{r} \mp a \mathbf{x}_{0}\right)\right) \psi_{0}\left(\mathbf{r} \mp a \mathbf{x}_{0}\right) \mathrm{e}^{\mp \mathrm{i} 2 \pi p y /(q a)} \mathrm{d}^{2} \mathbf{r}$
$B_{2}^{ \pm}=\int \psi_{0}^{*}(\mathbf{r})\left(E_{0}-E+V_{1}(\mathbf{r})-U\left(\mathbf{r} \mp a \mathbf{y}_{0}\right)\right) \psi_{0}\left(\mathbf{r} \mp a \mathbf{y}_{0}\right) \mathrm{d}^{2} \mathbf{r}$.
The vector $\mathbf{x}_{0}$ is the unit vector of the $x$ axis.
In the tight-binding approximation the radius of localization of the wavefunction $\psi_{0}(\mathbf{r})$ is small as compared to the lattice period. If the function $V_{1}(\mathbf{r})-U(\mathbf{r})$ slowly changes in the domain of localization of $\psi_{0}(\mathbf{r})$, we can assume that

$$
\begin{equation*}
A \simeq \lim _{r \rightarrow 0}\left[V_{1}(\mathbf{r})-U(\mathbf{r})\right] . \tag{15}
\end{equation*}
$$

If we completely neglect the overlapping of the wavefunctions localized at different sites of the lattice, equation (13) reduces to $\left(E-E_{0}-A\right) g_{n}=0$. Therefore, $E=E_{0}+A$, and in the small overlap integrals $B_{1,2}^{ \pm}$we can replace $E_{0}-E$ by $-A$.

Since $U(\mathbf{r})=U(r), V_{1}(-\mathbf{r})=V_{1}(\mathbf{r})$ and $\psi_{0}(-\mathbf{r})=\psi_{0}(\mathbf{r})$, one can verify that $B_{1}^{+}=B_{1}^{-}$ and $B_{2}^{+}=B_{2}^{-}$. The lattice has a symmetry axis of the fourth order $\left(V_{1}(x, y)=V_{1}(y,-x)\right)$, therefore, by replacing the integration variables $x=y^{\prime}, y=-x^{\prime}$ in equation (14b) and using equation (10), one can prove that $B_{1}^{+}=B_{2}^{+}$. Lastly, the lattice has a symmetry plane $\left(V_{1}(x, y)=V_{1}(-x, y)\right)$, and the overlap integral $B_{2}^{+}$can be represented in the form
$B_{2}^{+}=\int\left(-A+V_{1}(\mathbf{r})-U\left(\mathbf{r}-a \mathbf{y}_{0}\right)\right) \Psi_{0}(r) \Psi_{0}\left(\left|\mathbf{r}-a \mathbf{y}_{0}\right|\right) \cos \left(\frac{x a}{2 l_{H}^{2}}\right) \mathrm{d}^{2} \mathbf{r}$
i.e. this integral is real. Thus, all the overlap integrals $B_{1,2}^{ \pm}$are equal and real. We emphasize that these integrals contain both the atomic and lattice potentials (see equation (16)) and do not reduce to the hopping integral of [15], containing only the atomic potential.

Now we can rewrite equation (13) as
$\left(E-E_{0}-A\right) g_{n}-B_{2}^{+}\left(g_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}+g_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}\right)-2 B_{2}^{+} g_{n} \cos \left(k_{y} a+2 \pi(p / q) n\right)=0$.
This is Harper's equation. However, in contrast to the traditional Harper's equation, the energy $E_{0}$ and the overlap integral $B_{2}^{+}$depend on the magnetic field. Since the unknown coefficients $g_{n}(\mathbf{k})$ are periodic in $n$ with a period $q$, equation (17) reduces to a system of $q$ linear equations. Therefore, for a fixed $q$, the energy spectrum contains $q$ subbands defined in the magnetic Brillouin zone

$$
\begin{equation*}
-\pi /(q a)<k_{x} \leqslant \pi /(q a) \quad-\pi / a<k_{y} \leqslant \pi / a . \tag{18}
\end{equation*}
$$

However, the energy is a periodic function of $k_{y}$ with a period $2 \pi /(q a)$ [4, 5]. (A straightforward proof of this statement is as follows. Replacing $k_{y}$ in equation (17) by $k_{y}+2 \pi /(q a)$, we have

$$
\cos \left(k_{y} a+2 \pi / q+2 \pi(p / q) n\right)=\cos \left(k_{y} a+2 \pi(p / q) n^{\prime}+2 \pi s\right)
$$

where $n^{\prime}, s$ are integer solutions of a Diophantine equation $p n^{\prime}+q s=p n+1$. Introducing $\tilde{g}_{n^{\prime}}=g_{n}$, we restore equation (17). Therefore, $E\left(k_{x}, k_{y}+2 \pi /(q a)\right)=E\left(k_{x}, k_{y}\right)$.) Thus, it is enough to consider the energy spectrum in a part of the magnetic Brillouin zone,

$$
\begin{equation*}
-\pi /(q a)<k_{x, y} \leqslant \pi /(q a) \tag{19}
\end{equation*}
$$

## 3. Harper's equations for a complex lattice

In the present section, we derive Harper's equations for a complex plane lattice consisting of two identical square sublattices one of which is displaced with respect to the other sublattice by a vector $\mathbf{d}=\left(d_{x}, d_{y}\right)$ (see figure 1 ). We restrict ourselves to the case in which $d_{x}=d_{y}$, i.e. the vector of displacement is directed along a diagonal of a cell of the lattice. Obviously, it is enough to consider the domain $0<d<a / \sqrt{2}$ of the parameter $d$. The wavefunction of an electron obeys the Schrödinger equation (1) in which the potential $V_{1}(\mathbf{r})$ should be replaced by

$$
\begin{equation*}
V_{2}(\mathbf{r})=\sum_{n, m}\left[U\left(\mathbf{r}-\mathbf{a}_{n m}^{-}\right)+U\left(\mathbf{r}-\mathbf{a}_{n m}^{+}\right)\right] \tag{20}
\end{equation*}
$$

where $\mathbf{a}_{n m}^{ \pm}=\mathbf{a}_{n m} \pm \mathbf{d} / 2 ; \mathbf{a}_{n m}=(a n, a m)$ and $n, m=0, \pm 1, \pm 2, \ldots$ The atomic potential $U(\mathbf{r})$ is the same as in the preceding section. The magnetic field satisfies condition (3). In the


Figure 1. Plane lattice consisting of two identical square sublattices. One sublattice (white circles) is displaced with respect to the other sublattice (black circles) by a vector $\mathbf{d}$. The origin of coordinates is in the midpoint between two nearest atoms belonging to the different sublattices.
tight-binding approximation we seek the wavefunction $\psi_{\mathbf{k}}(\mathbf{r})$ in the form

$$
\begin{align*}
& \psi_{\mathbf{k}}(\mathbf{r})=\sum_{n, m} g_{n}(\mathbf{k}) \exp \left(\mathrm{i} \mathbf{k} \mathbf{a}_{n m}-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a}\left(n-\frac{d_{x}}{2 a}\right)\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}^{-}\right) \\
&+\sum_{n, m} f_{n}(\mathbf{k}) \exp \left(\mathrm{i} \mathbf{k} \mathbf{a}_{n m}-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a}\left(n+\frac{d_{x}}{2 a}\right)\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}^{+}\right) . \tag{21}
\end{align*}
$$

Here $g_{n}(\mathbf{k}), f_{n}(\mathbf{k})$ are unknown coefficients; the wavefunctions $\psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}^{\mp}\right)$ obey the Schrödinger equation (8) in which $x-n a, \mathbf{r}-\mathbf{a}_{n m}$ should be replaced by $x-n a \pm d_{x} / 2$, $\mathbf{r}-\mathbf{a}_{n m}^{\mp}$, respectively. The function $\psi_{0}(\mathbf{r})$ has the form (10). We suppose that the conditions of periodicity $g_{n+q}=g_{n}, f_{n+q}=f_{n}$ hold. In this case the wavefunction (21) satisfies the Bloch-Peierls conditions ( $4 a$ ), ( $4 b$ ) and conditions ( $5 a$ ), ( $5 b$ ). We substitute the wavefunction (21) into the Schrödinger equation, take into account that

$$
\begin{align*}
& \left(\hat{p}_{y}+\frac{|e| B}{c} x\right)^{2} \exp \left(-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a}\left(n \mp \frac{d_{x}}{2 a}\right)\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}^{\mp}\right) \\
& \quad=\exp \left(-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a}\left(n \mp \frac{d_{x}}{2 a}\right)\right)\left(\hat{p}_{y}+\frac{|e| B}{c}\left(x-n a \pm \frac{d_{x}}{2}\right)\right)^{2} \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}^{\mp}\right) \tag{22}
\end{align*}
$$

and obtain

$$
\begin{align*}
\sum_{n, m} g_{n}(\mathbf{k}) \exp & \left(\mathrm{i} \mathbf{k} \mathbf{a}_{n m}-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a}\left(n-\frac{d_{x}}{2 a}\right)\right)\left(E_{0}-E+V_{2}(\mathbf{r})-U\left(\mathbf{r}-\mathbf{a}_{n m}^{-}\right)\right) \\
& \times \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}^{-}\right)+\sum_{n, m} f_{n}(\mathbf{k}) \exp \left(\mathrm{i} \mathbf{k} \mathbf{a}_{n m}-\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m a}{a}\left(n+\frac{d_{x}}{2 a}\right)\right) \\
& \times\left(E_{0}-E+V_{2}(\mathbf{r})-U\left(\mathbf{r}-\mathbf{a}_{n m}^{+}\right)\right) \psi_{0}\left(\mathbf{r}-\mathbf{a}_{n m}^{+}\right)=0 \tag{23}
\end{align*}
$$

We multiply the latter equation by

$$
\exp \left(-\mathrm{i} \mathbf{k} \mathbf{a}_{n^{\prime} m^{\prime}}+\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m^{\prime} a}{a}\left(n^{\prime}-\frac{d_{x}}{2 a}\right)\right) \psi_{0}^{*}\left(\mathbf{r}-\mathbf{a}_{n^{\prime} m^{\prime}}^{-}\right)
$$

and integrate the result over $x, y$. In the tight-binding approximation we take into account the electron transitions between the nearest neighbouring sites. The sites nearest to the site $\mathbf{a}_{n^{\prime} m^{\prime}}^{-}$are $\mathbf{a}_{n^{\prime} m^{\prime}}^{+}, \mathbf{a}_{n^{\prime}, m^{\prime}-1}^{+}$and $\mathbf{a}_{n^{\prime}-1, m^{\prime}}^{+}$, except for the case in which the displacement $d$ is close to $a / \sqrt{2}$ (if $d=a / \sqrt{2}$, the distances between the site $\mathbf{a}_{n^{\prime} m^{\prime}}^{-}$and the sites $\mathbf{a}_{n^{\prime} m^{\prime}}^{+}, \mathbf{a}_{n^{\prime}, m^{\prime}-1}^{+}, \mathbf{a}_{n^{\prime}-1, m^{\prime}}^{+}$ and $\mathbf{a}_{n^{\prime}-1, m^{\prime}-1}^{+}$are equal; however, in this case the lattice consisting of two identical square
sublattices can be considered as a simple square lattice with a period $a / \sqrt{2}$ ). Thus, on the left-hand side of equation (23) we can retain the term with $n=n^{\prime}, m=m^{\prime}$ in the first sum and three terms (with $n=n^{\prime}, m=m^{\prime} ; n=n^{\prime}, m=m^{\prime}-1$ and $n=n^{\prime}-1, m=m^{\prime}$ ) in the second sum. The latter three terms describe the electron transitions between the site $\mathbf{a}_{n^{\prime} m^{\prime}}^{-}$of one sublattice and three sites of the other sublattice. Using notation $n, m$ instead of $n^{\prime}, m^{\prime}$, we find
$\left(E-E_{0}-D\right) g_{n}-B_{1} f_{n}-B_{2} f_{n} \mathrm{e}^{-\mathrm{i} k_{y} a-\mathrm{i} 2 \pi(p / q)\left(n+d_{x} /(2 a)\right)}-B_{3} f_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}=0$
where
$D=\int\left(V_{2}(\mathbf{r})-U(\mathbf{r}+\mathbf{d} / 2)\right)\left|\psi_{0}(\mathbf{r}+\mathbf{d} / 2)\right|^{2} \mathrm{~d}^{2} \mathbf{r}$
$B_{1}=\int \psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2)\left(E_{0}-E+V_{2}(\mathbf{r})-U(\mathbf{r}-\mathbf{d} / 2)\right) \psi_{0}(\mathbf{r}-\mathbf{d} / 2) \mathrm{e}^{-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}$
$B_{2}=\int \psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2)\left(E_{0}-E+V_{2}(\mathbf{r})-U\left(\mathbf{r}+a \mathbf{y}_{0}-\mathbf{d} / 2\right)\right)$

$$
\begin{equation*}
\times \psi_{0}\left(\mathbf{r}+a \mathbf{y}_{0}-\mathbf{d} / 2\right) \mathrm{e}^{-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r} \tag{25c}
\end{equation*}
$$

$B_{3}=\int \psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2)\left(E_{0}-E+V_{2}(\mathbf{r})-U\left(\mathbf{r}+a \mathbf{x}_{0}-\mathbf{d} / 2\right)\right)$

$$
\begin{equation*}
\times \psi_{0}\left(\mathbf{r}+a \mathbf{x}_{0}-\mathbf{d} / 2\right) \mathrm{e}^{\mathrm{i} 2 \pi p y\left(a-d_{x}\right) /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r} \tag{25d}
\end{equation*}
$$

Similarly, multiplying equation (23) by

$$
\exp \left(-\mathrm{i} \mathbf{k} \mathbf{a}_{n^{\prime} m^{\prime}}+\mathrm{i} 2 \pi \frac{p}{q} \frac{y-m^{\prime} a}{a}\left(n^{\prime}+\frac{d_{x}}{2 a}\right)\right) \psi_{0}^{*}\left(\mathbf{r}-\mathbf{a}_{n^{\prime} m^{\prime}}^{+}\right)
$$

and carrying out integration over $x, y$, we obtain
$\left(E-E_{0}-\tilde{D}\right) f_{n}-\tilde{B}_{1} g_{n}-\tilde{B}_{2} g_{n} \mathrm{e}^{\mathrm{i} k_{y} a+\mathrm{i} 2 \pi(p / q)\left(n-d_{x} /(2 a)\right)}-\tilde{B}_{3} g_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}=0$
where
$\tilde{D}=\int\left(V_{2}(\mathbf{r})-U(\mathbf{r}-\mathbf{d} / 2)\right)\left|\psi_{0}(\mathbf{r}-\mathbf{d} / 2)\right|^{2} \mathrm{~d}^{2} \mathbf{r}$
$\tilde{B}_{1}=\int \psi_{0}^{*}(\mathbf{r}-\mathbf{d} / 2)\left(E_{0}-E+V_{2}(\mathbf{r})-U(\mathbf{r}+\mathbf{d} / 2)\right) \psi_{0}(\mathbf{r}+\mathbf{d} / 2) \mathrm{e}^{\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}$
$\tilde{B}_{2}=\int \psi_{0}^{*}(\mathbf{r}-\mathbf{d} / 2)\left(E_{0}-E+V_{2}(\mathbf{r})-U\left(\mathbf{r}-a \mathbf{y}_{0}+\mathbf{d} / 2\right)\right)$
$\times \psi_{0}\left(\mathbf{r}-a \mathbf{y}_{0}+\mathbf{d} / 2\right) \mathrm{e}^{\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}$
$\tilde{B}_{3}=\int \psi_{0}^{*}(\mathbf{r}-\mathbf{d} / 2)\left(E_{0}-E+V_{2}(\mathbf{r})-U\left(\mathbf{r}-a \mathbf{x}_{0}+\mathbf{d} / 2\right)\right)$
$\times \psi_{0}\left(\mathbf{r}-a \mathbf{x}_{0}+\mathbf{d} / 2\right) \mathrm{e}^{-\mathrm{i} 2 \pi p y\left(a-d_{x}\right) /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}$.
When deriving equations (24) and (26), we have neglected the amplitudes of electron transitions from a site of one sublattice to the nearest sites of the same sublattice as compared to the amplitudes of electron transitions to the nearest sites of the other sublattice. This is justified under the reasonable assumption that the displacement of one sublattice with respect to the other sublattice is not very small, namely the parameter $d$ is larger than the radius of localization of the wavefunction $\psi_{0}(\mathbf{r})$.

Using the symmetry properties $U(\mathbf{r})=U(r), V_{2}(-\mathbf{r})=V_{2}(\mathbf{r})$ and $\psi_{0}(-\mathbf{r})=\psi_{0}(\mathbf{r})$, one can prove that $\tilde{D}=D, \tilde{B}_{1}=B_{1}, \tilde{B}_{2}=B_{2}$ and $\tilde{B}_{3}=B_{3}$. If the function $V_{2}(\mathbf{r})-U(\mathbf{r}+\mathbf{d} / 2)$ slowly changes in the domain of localization of $\psi_{0}(\mathbf{r}+\mathbf{d} / 2)$, equation (25a) reduces to

$$
\begin{equation*}
D \simeq \lim _{\mathbf{r} \rightarrow-\mathbf{d} / 2}\left[V_{2}(\mathbf{r})-U(\mathbf{r}+\mathbf{d} / 2)\right] . \tag{28}
\end{equation*}
$$

It follows from equations (25b) and (27b) that
$B_{1}-\tilde{B}_{1}^{*}=\int(U(\mathbf{r}+\mathbf{d} / 2)-U(\mathbf{r}-\mathbf{d} / 2)) \psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2) \psi_{0}(\mathbf{r}-\mathbf{d} / 2) \mathrm{e}^{-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}$.
The latter integral is equal to zero (see the appendix), therefore $B_{1}=\tilde{B}_{1}^{*}=B_{1}^{*}$, and we conclude that the overlap integral $B_{1}$ is real.

Introducing $\mathbf{r}^{\prime}=\mathbf{r}-a \mathbf{x}_{0}$ in equation (27d) and using the periodicity property $V_{2}\left(\mathbf{r}^{\prime}+\right.$ $\left.a \mathbf{x}_{0}\right)=V_{2}\left(\mathbf{r}^{\prime}\right)$, we come to the expression

$$
\begin{aligned}
\tilde{B}_{3}=\int \psi_{0}^{*}\left(\mathbf{r}^{\prime}\right. & \left.+a \mathbf{x}_{0}-\mathbf{d} / 2\right)\left(E_{0}-E+V_{2}\left(\mathbf{r}^{\prime}\right)-U\left(\mathbf{r}^{\prime}+\mathbf{d} / 2\right)\right) \\
& \times \psi_{0}\left(\mathbf{r}^{\prime}+\mathbf{d} / 2\right) \mathrm{e}^{-\mathrm{i} 2 \pi p y^{\prime}\left(a-d_{x}\right) /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}^{\prime}
\end{aligned}
$$

From this expression and equation ( $25 d$ ) it follows that

$$
\begin{align*}
B_{3}-\tilde{B}_{3}^{*}=\int & \left(U(\mathbf{r}+\mathbf{d} / 2)-U\left(\mathbf{r}+a \mathbf{x}_{0}-\mathbf{d} / 2\right)\right) \\
& \times \psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2) \psi_{0}\left(\mathbf{r}+a \mathbf{x}_{0}-\mathbf{d} / 2\right) \mathrm{e}^{\mathrm{i} 2 \pi p y\left(a-d_{x}\right) /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r} \tag{30}
\end{align*}
$$

The latter integral is equal to zero (see the appendix), therefore $B_{3}=\tilde{B}_{3}^{*}=B_{3}^{*}$. Thus, the overlap integral $B_{3}$ is real.

Similarly one can obtain that

$$
B_{2}=\tilde{B}_{2}^{*} \exp \left(\mathrm{i} 2 \pi p d_{x} /(q a)\right)=B_{2}^{*} \exp \left(\mathrm{i} 2 \pi p d_{x} /(q a)\right)
$$

therefore $B_{2} \exp \left(-\mathrm{i} \pi p d_{x} /(q a)\right)$ is real.
The plane perpendicular to the lattice plane and containing the vector $\mathbf{d}$ is a symmetry plane of the lattice, therefore $V_{2}(x, y)=V_{2}(y, x)$. By replacing the integration variables $x=y^{\prime}, y=x^{\prime}$ in equation (25c) and using equation (10), we find

$$
\begin{aligned}
B_{2} \mathrm{e}^{-\mathrm{i} \pi p d_{x} /(q a)} & =\int\left(E_{0}-E+V_{2}(\mathbf{r})-U\left(\mathbf{r}+a \mathbf{x}_{0}-\mathbf{d} / 2\right)\right) \Psi_{0}(|\mathbf{r}+\mathbf{d} / 2|) \\
& \times \Psi_{0}\left(\left|\mathbf{r}+a \mathbf{x}_{0}-\mathbf{d} / 2\right|\right) \exp \left[\mathrm{i}\left((y-x) d_{x}-a y-a d_{x} / 2\right) /\left(2 l_{H}^{2}\right)\right] \mathrm{d}^{2} \mathbf{r}
\end{aligned}
$$

The right-hand side of this expression coincides with the expression complex conjugate to the right-hand side of equation (25d), therefore $B_{2} \exp \left(-\mathrm{i} \pi p d_{x} /(q a)\right)=B_{3}^{*}=B_{3}$.

Thus, we can rewrite equations (24) and (26) in the form

$$
\begin{align*}
& \left(E-E_{0}-D\right) g_{n}=B_{1} f_{n}+B_{3} f_{n} \mathrm{e}^{-\mathrm{i}\left(k_{y} a+2 \pi(p / q) n\right)}+B_{3} f_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}  \tag{31}\\
& \left(E-E_{0}-D\right) f_{n}=B_{1} g_{n}+B_{3} g_{n} \mathrm{e}^{\mathrm{i}\left(k_{y} a+2 \pi(p / q) n\right)}+B_{3} g_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a} \tag{32}
\end{align*}
$$

where the overlap integrals $B_{1}$ and $B_{3}$ are real. We introduce new unknown coefficients

$$
\begin{equation*}
G_{n}=\left(g_{n}+f_{n}\right) / \sqrt{2} \quad F_{n}=\left(g_{n}-f_{n}\right) / \sqrt{2} \tag{33}
\end{equation*}
$$

The new coefficients are periodic in $n$, namely $G_{n+q}=G_{n}, F_{n+q}=F_{n}$. From equations (31) and (32) it follows that

$$
\begin{align*}
\left(E-E_{0}-D\right. & \left.-B_{1}\right) G_{n}=B_{3}\left[G_{n} \cos \left(k_{y} a+2 \pi(p / q) n\right)+\frac{1}{2}\left(G_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}+G_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}\right)\right] \\
& +B_{3}\left[\mathrm{i} F_{n} \sin \left(k_{y} a+2 \pi(p / q) n\right)+\frac{1}{2}\left(F_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}-F_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}\right)\right] \tag{34}
\end{align*}
$$

$$
\begin{gather*}
\left(E-E_{0}-D+B_{1}\right) F_{n}=-B_{3}\left[F_{n} \cos \left(k_{y} a+2 \pi(p / q) n\right)+\frac{1}{2}\left(F_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}+F_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}\right)\right] \\
-B_{3}\left[\mathrm{i} G_{n} \sin \left(k_{y} a+2 \pi(p / q) n\right)+\frac{1}{2}\left(G_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}-G_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}\right)\right] . \tag{35}
\end{gather*}
$$

If the displacement $d$ is not very close to $a / \sqrt{2}$ (i.e. an atom of one sublattice is not very close to the midpoint of a cell of the other sublattice), the distance between the sites $\mathbf{a}_{n m}^{-}$and $\mathbf{a}_{n m}^{+}$is markedly smaller than the distance between the sites $\mathbf{a}_{n m}^{-}$and $\mathbf{a}_{n-1, m}^{+}$. As a consequence, the overlap integrals satisfy the inequality

$$
\begin{equation*}
\left|B_{3} / B_{1}\right| \ll 1 \tag{36}
\end{equation*}
$$

In the zero approximation in the ratio $B_{3} / B_{1}$ we find from equations (34) and (35)

$$
\begin{align*}
& E_{1}=E_{0}+D+B_{1}\left(E_{1}\right)  \tag{37}\\
& E_{2}=E_{0}+D-B_{1}\left(E_{2}\right) \tag{38}
\end{align*}
$$

(we remind that the overlap integrals $B_{1}$ and $B_{3}$ depend on $E$ ). The levels $E_{1}$ and $E_{2}$ form a doublet into which the one-atomic level $E_{0}$ would split due to the electron interaction with two nearest neighbouring atoms (for example, $\mathbf{a}_{n m}^{-}$and $\mathbf{a}_{n m}^{+}$) if electron transitions to other atoms were impossible. To express the quantities $E_{1}$ and $E_{2}$ in the explicit form, we rewrite $B_{1}$ as

$$
\begin{equation*}
B_{1}(E)=\left(E_{0}-E\right) J_{1}+I_{1} \tag{39a}
\end{equation*}
$$

where
$J_{1}=\int \psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2) \psi_{0}(\mathbf{r}-\mathbf{d} / 2) \mathrm{e}^{-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}$
$I_{1}=\int \psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2)\left(V_{2}(\mathbf{r})-U(\mathbf{r}-\mathbf{d} / 2)\right) \psi_{0}(\mathbf{r}-\mathbf{d} / 2) \mathrm{e}^{-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \mathrm{d}^{2} \mathbf{r}$.
Then we obtain

$$
\begin{align*}
& E_{1}=E_{0}+\left(D+I_{1}\right) /\left(1+J_{1}\right)  \tag{40}\\
& E_{2}=E_{0}+\left(D-I_{1}\right) /\left(1-J_{1}\right) \tag{41}
\end{align*}
$$

For the energy values close to $E_{1}$, equation (35) shows that $F_{n} \sim\left(B_{3} / B_{1}\right) G_{n} \ll G_{n}$. Therefore, we can neglect the terms with $F_{n}, F_{n \pm 1}$ on the right-hand side of equation (34). As a result, we have
$\left(E-E_{1}\right) G_{n}=\frac{B_{3}\left(E_{1}\right)}{2\left(1+J_{1}\right)}\left(2 G_{n} \cos \left(k_{y} a+2 \pi(p / q) n\right)+G_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}+G_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}\right)$.
Similarly, for the energy values close to $E_{2}$, we neglect the terms with $G_{n}, G_{n \pm 1}$ on the right-hand side of equation (35) and come to the equation
$\left(E-E_{2}\right) F_{n}=-\frac{B_{3}\left(E_{2}\right)}{2\left(1-J_{1}\right)}\left(2 F_{n} \cos \left(k_{y} a+2 \pi(p / q) n\right)+F_{n+1} \mathrm{e}^{\mathrm{i} k_{x} a}+F_{n-1} \mathrm{e}^{-\mathrm{i} k_{x} a}\right)$.
We emphasize that, calculating the overlap integral $B_{3}$ for equation (42), one has to substitute $E=E_{1}$ into the right-hand side of equation (25d), while, calculating $B_{3}$ for equation (43), one has to substitute $E=E_{2}$ into the right-hand side of equation (25d).

Equations (42) and (43) have the form of Harper's equation (see equation (17)) with the energies $E_{1,2}$ and overlap integrals depending on the magnetic field. Thus, we have shown that a complex lattice consisting of two identical square sublattices one of which is displaced along a diagonal of a cell of the other sublattice is described by two Harper's equations.

The unknown coefficients $G_{n}(\mathbf{k})$ and $F_{n}(\mathbf{k})$ are periodic in $n$ with a period $q$, therefore each of equations (42) and (43) reduces to a system of $q$ linear equations. As a consequence, for any fixed $q$, the energy spectrum contains $q$ subbands in the vicinity of the energy value $E=E_{1}$ and $q$ subbands in the vicinity of the energy value $E=E_{2}$. As explained at the end of section 2, it is enough to consider the energy spectrum in the part (19) of the magnetic Brillouin zone.

## 4. Numerical results

To numerically solve Harper's equations derived in sections 2 and 3, we need to know the coefficients of these equations (for example, $E_{0}, A$ and $B_{2}^{+}$in equation (17)). We find the coefficients self-consistently, namely we choose the atomic potential, find the eigenvalue $E_{0}$ and the corresponding eigenfunction $\Psi_{0}(r)$ by using a variational procedure, and then calculate the integrals defining the coefficients of Harper's equations (for example, integrals (14a) and (16)).

We choose the atomic potential in the form

$$
\begin{equation*}
U(r)=-\left(\hbar^{2} /(2 \mu b r)\right) \exp \left(-r / a_{0}\right) \tag{44}
\end{equation*}
$$

where $b$ and $a_{0}$ are parameters with the dimension of length. Our choice of the atomic potential provides that the series for the lattice potential converges sufficiently quickly. We use a trial function

$$
\begin{equation*}
\Psi_{0}(r ; \alpha, \beta)=C(\alpha, \beta) \exp \left(-\alpha r / b-\beta r^{2} /\left(4 l_{H}^{2}\right)\right) \tag{45}
\end{equation*}
$$

where $\alpha>0, \beta \geqslant 0$ are dimensionless parameters, $C(\alpha, \beta)$ is the normalizing factor. In practice, it is more convenient to represent the trial wavefunction as

$$
\begin{equation*}
\Psi_{0}(r ; \alpha, \beta)=C(\alpha, \beta) \exp \left(-\alpha r / b-\beta \pi p r^{2} /\left(2 q a^{2}\right)\right) \tag{46}
\end{equation*}
$$

We choose such values of the parameters $\alpha, \beta$, for which the functional

$$
\begin{equation*}
E_{0}(\alpha, \beta)=2 \pi \int_{0}^{\infty} \Psi_{0}(r ; \alpha, \beta) \hat{H}_{0} \Psi_{0}(r ; \alpha, \beta) r \mathrm{~d} r \tag{47}
\end{equation*}
$$

reaches its minimum ( $\hat{H}_{0}$ in the integrand means the Hamiltonian on the left-hand side of equation (9)). We suppose the energy $E_{0}$ in equation (9) to be approximately equal to $\min _{\alpha, \beta} E_{0}(\alpha, \beta)$.

One can observe that if we measure all lengths in units of $a$ and the magnetic flux per lattice cell in units of $\Phi_{0}$, then all quantities with the dimension of energy are measured in units of $\hbar^{2} /\left(\mu a^{2}\right)$, and we do not need to give either $a$ or $\mu$.

### 4.1. Simple square lattice

The dependences of the electron energy $E_{0}$ in an isolated atom and the overlap integral $B_{2}^{+}$ in Harper's equation (17) on the magnetic field for the chosen parameters $b / a=0.1$ and $a_{0} / a=0.5$ are depicted in figure 2 (we express the magnetic field through the magnetic flux $\Phi$ per cell of the lattice). The energy shift $A$, in practice, does not depend on the magnetic field (see equation (15)) and equals $A \simeq-4.11 \hbar^{2} /\left(\mu a^{2}\right)$. One can see that the larger the magnetic field, the higher the electron energy in an isolated atom and the smaller the absolute value of the overlap integral $B_{2}^{+}$. As we have mentioned, the diamagnetic shift of the atomic level for the atomic potential in the harmonic-oscillator form was found in [15], but such a choice of the atomic potential leads to a divergent series for the lattice potential and, therefore, is unsuitable for calculating the overlap integral $B_{2}^{+}$.

Using the dependences of $E_{0}$ and $B_{2}^{+}$on the magnetic field, we have numerically found allowed values of energy for different values of the magnetic flux per lattice cell (Hofstadter's butterfly, see figure 3). If we neglected the influence of the magnetic field on the atomic eigenfunction and eigenvalue, Hofstadter's butterfly would be periodic in the magnetic flux with a period $\Phi_{0}$. Figure 3 demonstrates that, if we take into account the influence of the magnetic field more accurately, Hofstadter's butterfly is no longer periodic in the magnetic flux. In particular, the interval of allowed energy values at $\Phi=\Phi_{0}$ is narrower than at $\Phi=0$.


Figure 2. The dependences of the electron energy in an isolated atom (a) and the overlap integral in Harper's equation for a simple lattice (b) on the magnetic field. The parameters of the atomic potential are $b / a=0.1$ and $a_{0} / a=0.5$.


Figure 3. Hofstadter's butterfly for a simple square lattice. The parameters of the atomic potential are the same as in figure 2.

### 4.2. Complex lattice

First of all, we calculate the integrals $I_{1}$ and $J_{1}$ and then find the energies $E_{1}, E_{2}$ (see equations (40) and (41)) as functions of the magnetic field. All these functions are depicted in figure 4. As in the preceding subsection, we have chosen the parameters $b / a=0.1$ and $a_{0} / a=$ 0.5. The modulus of the displacement vector is supposed to be $d=\sqrt{2} a / 4$. The energy shift $D$, in practice, is independent of the magnetic field (see equation (28)) and is approximately equal to $-16.33 \hbar^{2} /\left(\mu a^{2}\right)$. Then we calculate the overlap integrals $B_{3}\left(E_{1}\right)$ and $B_{3}\left(E_{2}\right)$ in Harper's equations (42) and (43) (figure 5). One can see that the absolute value of the overlap integral corresponding to the energy level $E_{1}$ is markedly smaller than the absolute value of the overlap integral corresponding to the level $E_{2}$. Our derivation of equations (42) and (43) is based on condition (36). One can verify that the overlap integrals $B_{3}\left(E_{1}\right)$ and $B_{3}\left(E_{2}\right)$ depicted in figure 5 satisfy this condition.

Hofstadter's butterfly for the complex lattice is shown in figure 6 . The butterfly is an aggregate of two simple butterflies. The left-hand simple butterfly is markedly narrower than the right-hand one. This is a consequence of the difference in the magnitudes of the overlap integrals $B_{3}\left(E_{1}\right)$ and $B_{3}\left(E_{2}\right)$. However, it seems natural that the broadening of the lower level $E_{1}$ is smaller than the broadening of the higher level $E_{2}$. As in the case of a simple lattice, the butterfly is not periodic in the magnetic flux due to the dependence of the atomic eigenfunction and eigenvalue on the magnetic field.


Figure 4. The dependences of the integrals $I_{1}$ (a), $J_{1}$ (b) and energies $E_{1}$ (c), $E_{2}$ (d) on the magnetic field. The parameters of the atomic potential are $b / a=0.1$ and $a_{0} / a=0.5$. The distance between two nearest atoms belonging to different sublattices is $d=\sqrt{2} a / 4$.


Figure 5. The dependences of the overlap integrals $B_{3}\left(E_{1}\right)$ (a) and $B_{3}\left(E_{2}\right)$ (b) in Harper's equations (42) and (43) on the magnetic field. The atomic potential parameters and the displacement of one sublattice with respect to the other sublattice are the same as in figure 4 .


Figure 6. Double Hofstadter's butterfly for a complex lattice consisting of two identical sublattices. The parameters of the atomic potential and the displacement of one sublattice with respect to the other sublattice are the same as in figures 4 and 5 .

## 5. Conclusion

Taking into account the influence of the magnetic field on the atomic eigenfunction and eigenvalue, we have derived Harper's equations for a simple two-dimensional square lattice and for a complex two-dimensional square lattice. The latter consists of two simple square sublattices one of which is displaced along a diagonal of a cell of the other sublattice. We have shown that the complex lattice is described by two Harper's equations. Hofstadter's butterfly for the simple lattice is not periodic in the magnetic flux per lattice cell. The periodicity would
occur if one neglected the influence of the magnetic field on the atomic eigenfunction and eigenvalue. Hofstadter's butterfly for the complex lattice is an aggregate of two nonoverlapping butterflies and is not periodic in the magnetic flux per lattice cell.

## Acknowledgments

This work was supported by ISTC (grant no 2293) and the Ministry of Education (grant no E02-3.1.-336).

## Appendix

The function $\psi_{0}(\mathbf{r}+\mathbf{d} / 2)$ in the integrand (29) satisfies the Schrödinger equation

$$
\begin{equation*}
\left[\frac{1}{2 \mu}\left(\hat{\mathbf{p}}+\frac{|e| B}{c}\left(x+\frac{d_{x}}{2}\right) \mathbf{y}_{0}\right)^{2}+U\left(\mathbf{r}+\frac{\mathbf{d}}{2}\right)\right] \psi_{0}\left(\mathbf{r}+\frac{\mathbf{d}}{2}\right)=E_{0} \psi_{0}\left(\mathbf{r}+\frac{\mathbf{d}}{2}\right) \tag{A1}
\end{equation*}
$$

while the function $\psi_{0}(\mathbf{r}-\mathbf{d} / 2) \exp \left(-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)\right)$ satisfies the equation

$$
\begin{gather*}
{\left[\frac{1}{2 \mu}\left(\hat{\mathbf{p}}+\frac{|e| B}{c}\left(x+\frac{d_{x}}{2}\right) \mathbf{y}_{0}\right)^{2}+U\left(\mathbf{r}-\frac{\mathbf{d}}{2}\right)\right] \mathrm{e}^{-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \psi_{0}\left(\mathbf{r}-\frac{\mathbf{d}}{2}\right)} \\
=E_{0} \mathrm{e}^{-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)} \psi_{0}\left(\mathbf{r}-\frac{\mathbf{d}}{2}\right) . \tag{A2}
\end{gather*}
$$

We fulfil the operation of complex conjugation in equation (A1), multiply the result by $\psi_{0}(\mathbf{r}-\mathbf{d} / 2) \exp \left(-\mathrm{i} 2 \pi p y d_{x} /\left(q a^{2}\right)\right)$ and subtract equation (A2) preliminarily multiplied by $\psi_{0}^{*}(\mathbf{r}+\mathbf{d} / 2)$. Then we carry out integration over $x, y$ and take into account that the operator $\hat{\mathbf{p}}+(|e| B / c)\left(x+d_{x} / 2\right) \mathbf{y}_{0}$ is selfadjoint. As a result, we obtain that the integral on the righthand side of equation (29) is equal to zero.

Similarly, using equation (A1) and the equation

$$
\begin{gather*}
{\left[\frac{1}{2 \mu}\left(\hat{\mathbf{p}}+\frac{|e| B}{c}\left(x+\frac{d_{x}}{2}\right) \mathbf{y}_{0}\right)^{2}+U\left(\mathbf{r}+a \mathbf{x}_{0}-\frac{\mathbf{d}}{2}\right)\right] \mathrm{e}^{\mathrm{i} 2 \pi p y\left(a-d_{x}\right) /\left(q a^{2}\right)} \psi_{0}\left(\mathbf{r}+a \mathbf{x}_{0}-\frac{\mathbf{d}}{2}\right)} \\
=E_{0} \mathrm{e}^{\mathrm{i} 2 \pi p y\left(a-d_{x}\right) /\left(q a^{2}\right)} \psi_{0}\left(\mathbf{r}+a \mathbf{x}_{0}-\frac{\mathbf{d}}{2}\right) \tag{A3}
\end{gather*}
$$

and repeating the reasoning given above, one can prove that the integral on the right-hand side of equation (30) is equal to zero.

## References

[1] Harper P G 1955 Proc. Phys. Soc. London A 68874
[2] Hofstadter D R 1976 Phys. Rev. B 142239
[3] Claro F H and Wannier J H 1979 Phys. Rev. B 196068
[4] Kohmoto M 1989 Phys. Rev. B 3911943
[5] Kohmoto M and Hatsugai Y 1990 Phys. Rev. B 419527
[6] Hiramoto H and Kohmoto M 1992 Int. J. Mod. Phys. 6281
[7] Barelli A and Fleckinger R 1992 Phys. Rev. B 4611559
[8] Silberbauer H 1992 J. Phys.: Condens Matter 47355
[9] Sandhu P S, Kim J H and Brooks J S 1997 Phys. Rev. B 5611566
[10] Han S Y, Brooks J S and Kim J H 2000 Phys. Rev. Lett. 851500
[11] Weiss D, Roukes M L, Menschig A, Grambow P, von Klitzing K and Weimann G 1991 Phys. Rev. Lett. 662790
[12] Schlösser T, Ensslin K, Kotthaus J P and Holland M 1996 Semicond. Sci. Technol. 111582
[13] Albrecht C, Smet J H, von Klitzing K, Weiss D, Umansky V and Schweizer H 2001 Phys. Rev. Lett. 86147
[14] Barelli A, Bellissard J, Jacquod P and Shepelyansky D L 1997 Phys. Rev. B 559524
[15] Alexandrov A S and Capellmann H 1991 Phys. Rev. Lett. 66365
[16] Nicopoulos N and Trugman S A 1990 Phys. Rev. Lett. 64237
[17] Demikhovskii V Ya, Perov A A and Khomitsky D V 2000 Phys. Lett. A 267408

