# On exponential localization of magnetic Wannier functions



2004 J. Phys.: Condens. Matter 16 2357

(http://iopscience.iop.org/0953-8984/16/13/015)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) 2357–2369 PII: S0953-8984(04)68131-8

# On exponential localization of magnetic Wannier functions

**Gagik Avanesyan**

Institute of Problems of Chemical Physics, RAS, Chernogolovka, 142432, Russia

E-mail: avangt@icp.ac.ru

Received 26 August 2003
Published 19 March 2004
Online at stacks.iop.org/JPhysCM/16/2357 (DOI: 10.1088/0953-8984/16/13/015)

**Abstract**
A triple of quantum numbers of conventional zone theory, namely the quasi-momentum, described in terms of Bloch functions, the lattice coordinate, described in terms of Wannier functions, and the associated energy band index, are modified to describe the space of states of a charged particle in magnetic field, in a translation covariant manner. A quartet of Bloch functions that belong to an invariant subspace, and define an irreducible representation of an anticommutative subgroup of the magnetic translation group, lead to Wannier function sets at a single Landau level that satisfy the exponential localization criterion. The degrees of freedom within the invariant subspace of this physically irreducible representation match those of spin $1/2$. With a view to possible experimental studies, it is shown how a set of four regular arrays of connected wires or a similar quantum device may be used to access the pseudo-spin degree of freedom described, by observation of the effects of a controlled doubly periodical electric potential applied to a 2DEG in a strong and commensurate magnetic field.

## 1. Introduction

The problem of magnetic Wannier functions may be described by showing an analogy with the non-magnetic case, as follows. In the absence of an external magnetic field, the space of states for a single electron in a periodic field of the crystal lattice, its dynamics restricted to a single energy band, may be represented both in terms of Bloch states (definite quasi-momenta) and in terms of Wannier states (definite lattice coordinates). Both classes of states form complete sets on the subspace of states in the band, and the unitary equivalence of these two descriptions is guaranteed by the properties of Fourier transformation. When necessary, the spin degree of freedom may be easily incorporated into this non-relativistic picture. The historical role of these two pictures in understanding electronic structure and transport in crystalline solids, as well as in classifying the solids, is well known. The fact that one may describe Bloch states as superpositions of Wannier states, and vice versa, means that for an electron restricted to a single energy band one may think of 'here' and 'there' in terms of (Bravais) lattice coordinates. The respective Wannier states are mutually orthogonal and form a complete set, and thus the *position* of the electron is represented in the probabilistic manner of quantum mechanics. The localization of Wannier states in solids is exponential, and this is an important point. However, the case of a magnetic band is different.

If there existed well-localized Wannier states for a two-dimensional electron restricted to a single Landau level, then these states could represent 'here' and 'there', and a regular array of 'point' detectors spaced such that the unit cell area of this two-dimensional lattice was equal to $2\pi$, in magnetic length units, could represent a complete set of quantum observables. This is not the case, since the product of the respective uncertainties cannot be made finite, as discussed below in a more detail.

Consider a quantum electronic device, which makes use of two-dimensional spin-polarized electrons in the lowest Landau level as charge carriers. Suppose there is a well-defined plane created within a MOSFET or a heterojunction. The plane, as 'seen' by an electron, is by no means merely a Euclidean plane: despite the fact that one may attribute a distinct coherent state to any point in the plane, one cannot describe the collection of such states as 'here' and 'there', since these states are not mutually orthogonal. In other words, these states do not form a quantum probabilistic sample space for allowed positions in the plane. (Imagine position detectors in the plane to develop something like Wilson chamber tracks, as collections of dots.) What should a quantum device engineer think then of the *loci* for charge carriers in the plane, when dealing with electrons restricted to a single Landau level?

The new dimension introduced by Zak (1997) to the problem of magnetic Wannier functions is its connection to Balian–Low theorem (Balian 1981, Low 1985) which may be viewed as a global form of the position–momentum uncertainty relation—in contrast with the conventional, 'local' formulation, in the form of the Heisenberg uncertainty relation. The 'incompatibility of localization and orthogonality' described by Zak is in accord with the 'impossibility of constructing a well-localized representation of the magnetic translation group' discussed by Thouless (1984). A set of magnetic Wannier functions on a Gabor–von Neumann lattice, in the weak form of localization, is studied in detail by Rashba *et al* (1997).

The studies cited above make it explicit that no simple description of a Hilbert space of states on a single Landau level is possible, with account taken of the magnetic translation symmetry, in terms of both localized and orthogonal states, simultaneously. This contrasts with intuitive expectations, especially when compared to exponential localization in the absence of a magnetic field, known due to the seminal paper by Kohn (1959). One could say that the belief in the existence of a local description of an electron in a Landau level that guided the pursuit of magnetic Wannier functions for decades has had no grounds, and one could leave it at that. On the other hand, a variety of questions, as regards the solid-state theory basics, are raised by the statement of such impossibility. Fortunately, a description in terms of strong (exponential) localization still exists, and the aim of this paper is to present it explicitly.

To construct such a set, the usage of Jacobi theta functions is critical. An equivalent description of translational symmetry in the Landau level is possible in terms of Weierstrass sigma functions, and this possibility is exploited by Dubrovin and Novikov (1980). The substantial usage of Jacobi identities for theta functions in the present paper seems to be a novel feature. The other procedures belong to traditional approaches, and, in particular, the transparent conventional orthogonalization procedure developed by Wannier (1937) does not require any essential modification.

The paper is organized as follows. For reading convenience, some simplifying assumptions, as well as conventions used, are listed in section 2. In section 3, the context is created which allows construction of strongly localized magnetic Wannier functions, within a framework of two-dimensional representation of an anticommutative subgroup of the magnetic translation group. Mathematical proofs and detailed description of some important properties of the representation constructed are discussed in section 4. In section 5, the pseudo-spin observable that naturally enters the translation invariant representation of the space of states is described, in its coupling to external electric fields, and possible experimental studies are discussed. A summary and discussion follow in section 6.

## 2. Some definitions, simplifying assumptions and notation

Without loss of generality, the lowest Landau level is considered; mapping to higher levels is an easy task, and will not be discussed here. The Landau gauge $A_y = A_z = 0$, $A_x = -y$ is used, along with representation in magnetic length units. Magnetic translations of a single coherent state centred at the origin of the coordinate frame,

$$c(x, y) = \mathrm{e}^{-(x^2+2\mathrm{i}xy+y^2)/4}, \tag{1}$$

lead to a two-dimensional continuum of coherent states in the lowest Landau level, and this forms the largest (and, of course, an overcomplete) set of functions relevant to the problem of basis construction. Normalization of the coherent state $\|c\| = \sqrt{2\pi}$ is convenient for avoiding unnecessary constant factors. One takes wavefunctions of the coherent states centred about some lattice sites $(\mathrm{l}_x, \mathrm{l}_y) \in \mathrm{L}$ and, after performing summation, a set of (non-normalized) Bloch functions is obtained:

$$\varphi_{k_x k_y}(x, y) = \sum \mathrm{e}^{\mathrm{i}(k_x \mathrm{l}_x + k_y \mathrm{l}_y)} c_{\mathrm{l}_x \mathrm{l}_y}(x, y). \tag{2}$$

It may be said that Bloch functions are maps $\mathrm{L} \to \varphi_{k_x,k_y}$, in a special sense, of these lattices into Hilbert space. (Later it will be shown that the choice of lattice is an analogue of the choice of quantization axis for a spin 1/2.) In standard zone theory, any lattice may be used. To construct a conventional orthonormal set in the magnetic case, one has to take a lattice with the Wigner–Seitz cell area equal to $2\pi$, corresponding to a single (normal) magnetic flux quantum per unit cell. That is expected from the viewpoint of the density of states in a single Landau level. Then the actual orthogonalization is performed, and so one obtains the Wannier function set on a Gabor–von Neumann lattice.

To prepare for modification of the method, existing choices for translational periodicity of the point sets are described below in a more detail. When constructing Bloch functions in the presence of a magnetic field, a distinction is to be made between the lattices as collections of lattice sites, on one hand, and the lattices as collections of translation vectors, on the other. The latter vectors represent symmetry transformations in the Hilbert space of states, magnetic translations, which belong to a subgroup of the magnetic translation group. Such a distinction is to be made mainly because of the fact that a uniform and stationary magnetic field enters the Hamiltonian of the problem via a vector potential, and the latter is not a uniform field. In the construction of magnetic Wannier functions one has to deal with both meanings, and that is illustrated in figure 1; both lattice sites and translation vectors are shown, for some choices relevant to the problem under discussion. The magnetic flux through the smallest unit cell of area $\pi$ is equal to half a flux quantum. The four sublattices labelled as 3, 4, 1 and 2 have unit cells of area $4\pi$. Since a special choice of a subgroup of the magnetic translation group is needed, it is convenient to introduce special notation for the lattices: $\mathrm{L}_3$, $\mathrm{L}_1$, $\mathrm{L}_4$ and $\mathrm{L}_2$, respectively, for future reference. The $\mathrm{L}_3$ lattice sites $(\mathrm{l}_x, \mathrm{l}_y)$ could be taken as $\mathrm{l}_x = \sqrt{\pi}m$ and $\mathrm{l}_y = \sqrt{\pi}n$, $m$ and $n$ being even integers here and odd integers for the $\mathrm{L}_1$ lattice, and similarly for $\mathrm{L}_4$, and $\mathrm{L}_2$; for the sake of simplicity, the special case $a = b = \sqrt{\pi}$ will be considered. This fixes the lattices with respect to the vector potential gauge.

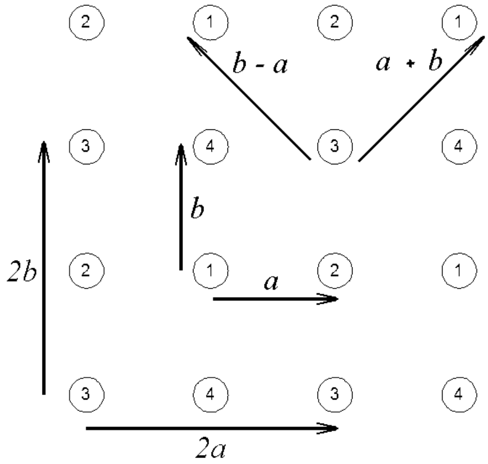


**Figure 1.** The four lattices labelled as 3, 4, 1 and 2, and described by periods $2a$ and $2b$, are shown. The union of these is a lattice characterized by unit cell area $\pi$, which corresponds to half a magnetic flux quantum per unit cell. Also shown are the periods $a+b$ and $b-a$ of a lattice which represents the conventional Gabor–von Neumann set that is in one-to-one correspondence with the density of states in the Landau level.

It will be convenient to have special notation for collections of periods, representing translational symmetry, such as lattices generated by vectors $2a$ and $2b$. The latter will be denoted as $L_{4\pi}$, showing the unit cell area in magnetic length units. When this is a real (position) space lattice, the reciprocal (quasi-momentum) space lattice is $L_{\pi}$, and vice versa. Therefore, the lattices $L_{\mu}$, $\mu = 3, 4, 1, 2$, are $L_{4\pi}$ lattices. The vectors $a+b$ and $b-a$ generate a square lattice with a unit cell of area $2\pi$, $L_{2\pi}$, which is represented in figure 1 by the union of the third and the first sublattices, $L_{31} = L_3 \cup L_1$ (equivalently, the fourth and the second could be taken instead, $L_{42} = L_4 \cup L_2$); in this case both real and quasi-momentum spaces have $L_{2\pi}$ symmetry, and this is the conventional Gabor–von Neumann lattice. Also of interest is the union of all four lattices that may be thought of as a union of the mutually dual lattices $L_{31}$ and $L_{42}$; $L_{3412} = L_{42} \cup L_{31}$ is an $L_{\pi}$ lattice.

Bloch functions constructed in a standard manner, on a Gabor–von Neumann lattice, form a basis consisting of states that belong to (and define) one-dimensional generalized subspaces of the Hilbert space of states in Landau level, and their norm with respect to these subspaces is defined by integration over the Wigner–Seitz cell area, i.e. the integration domain is defined modulo $L_{2\pi}$:

$$\|\varphi_{k_x k_y}\|^2 = \int\int |\varphi_{k_x k_y}(x, y)|^2 \, \mathrm{d}x \, \mathrm{d}y. \tag{3}$$

The corresponding resolution of the identity is written as an integral in reciprocal space modulo $L_{2\pi}$ too. (In the context of the following discussion, the integration domain in (3) would be doubled later, integrating modulo $L_{4\pi}$ in real space, which means turning to another (two-dimensional) invariant subspace.) For performing normalization of the corresponding set of Bloch functions, and, as a result, orthogonalization of Wannier functions, a convenient procedure is that developed by Wannier, which essentially involves division by the norm defined by (3) with respect to magnetic translations on an $L_{2\pi}$ lattice.

In the case of magnetic sub-bands, the overcompleteness of the set under consideration is known due to the identity proved by Perelomov (1971). Using the standard orthogonalization procedure described above, the magnetic Wannier functions set may be constructed as a set of weakly localized states for which the product $\Delta x \Delta y$ cannot be made finite, because of the restrictions due to the Balian–Low theorem; note that $2\Delta x \Delta y = (\Delta x)^2 + (\Delta y)^2$ in this geometry. A set of this type was studied by Rashba *et al*. The authors found that (despite infinite uncertainty products) about 95% of the probability density is contained in the Wigner–Seitz cell, which may be satisfactory for some problems.

Obviously, in a great number of problems exponential localization is necessary. In the next section, a modified approach is presented which allows construction of such a strongly localized Wannier set. Within the scope of this, other interesting features of translational symmetry in an external magnetic field are also revealed.

## 3. A quartet of Bloch functions and localization of Wannier functions

A subtlety in the construction of the set of magnetic Wannier functions described is in that, despite the commutativity of the magnetic translations $T_{a+b}$, and $T_{b-a}$, these do not form an Abelian group as a subgroup of the magnetic translation group, $T_{b-a}T_{a+b} = -T_{2b}$. This may be seen from the fact that the magnetic translations $T_a$ and $T_b$ are *anti*-commutative, because of the half of a magnetic flux quantum threading the unit cell of area $\pi$ of the $L_{3412}$ lattice:

$$T_b T_a + T_a T_b = 0. \tag{4}$$

That is why the conventional, as in the absence of the magnetic field, argumentation based on irreducibility of the one-dimensional representation of the translation group does not apply in the magnetic case. The dimension of the representation as an irreducibility criterion here also does not work properly, and not only from the physical viewpoint. Note that the minimal dimension for the twice-larger subgroup of the magnetic translation group is 2, which may be seen from anticommutation relation (4), e.g. by relating it to an $SU(2)$ group representation (see below). The above statements will become clear after the construction of an alternative, in a special sense, representation, which is worth treating as physically irreducible.

To be able to deal with strongly localized states and finite uncertainties only, in consonance with requirements introduced by Kohn, a more sophisticated approach is needed, such as follows from the context created by the Balian–Low theorem. There is no alternative to allowing some non-orthogonality, as follows from the discussion presented by Zak. Then, in order to preserve translational invariance, relaxing the orthogonality condition with respect to the states centred on the sites that belong to two complementary $L_{4\pi}$ lattices is a physically correct procedure. Moreover, this is what creates the context for the present study. Thus, mutual orthogonality is required for the functions centred on each of $L_3$ and $L_1$ lattices only. Non-orthogonality between the states centred at the sites of the complementary sublattices is allowed. In this context the two sets of Bloch functions are obtained, before actual normalization is performed: $\varphi_{3,k_x k_y}(x, y)$ and $\varphi_{1,k_x k_y}(x, y)$. The Brillouin zone area is $\pi$, and not $2\pi$, as for the conventional one-to-one correspondence between the numbers of flux quanta and unit cells. These two sets of Bloch functions together represent the two-dimensional subspace $H_{k_x k_y}$ of the physically irreducible representation. Note that the smaller subgroup of the magnetic translation group generated by the magnetic translations $T_{2a}$ and $T_{2b}$ is an ordinary (non-magnetic) translation group, in contrast with that generated by the magnetic translations $T_{a+b}$ and $T_{b-a}$. Although $\varphi_{3,k_x k_y}(x, y)$ and $\varphi_{1,k_x k_y}(x, y)$ are not, in general, mutually orthogonal, for the same $(k_x, k_y)$ modulo $L_\pi$, the linear envelope of these generalized vectors in Hilbert space covers two-dimensional invariant subspace. (There is an exception for a single point in quasi-momentum space, as discussed below.) The reason for the numbers '3' and '1' in the notation becomes clear from the fact that summation (2) for $(l_x, l_y) \in L_\mu$ leads to a product of Jacobi theta functions:

$$\varphi_{\mu,k_x k_y}(x, y) = c(x, y)\vartheta_{\bar{\mu}}(2k_x + \mathrm{i}x - y)\vartheta_\mu(2k_y + x + \mathrm{i}y). \tag{5}$$

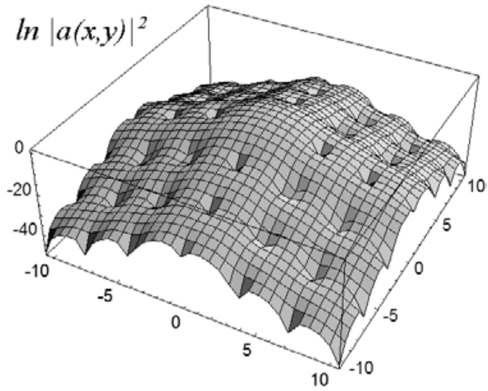


**Figure 2.** The exponentially localized magnetic Wannier function centred at the origin; distances are shown in magnetic length units. In this logarithmic plot of the probability density, the exponential fall-off is seen clearly. Also seen are the zeros of the magnetic Wannier function.

Throughout this paper, the following convention is used: $\vartheta_\mu(\sqrt{\pi}z/2, \mathrm{e}^{-\pi}) \to \vartheta_\mu(z)$. The other two functions may be constructed in the same way, but they are linearly dependent on the former two. These four sets are orthogonal for different quasi-momenta, as follows from their Bloch function-like definitions, but they are not, for the same quasi-momentum. An example of using four non-orthogonal sets of functions with non-orthogonality between them, in signal processing, is given by Grochenig (2000).

A pair of complementary sets treated as a single set then lead to a conventional set on the Gabor–von Neumann lattice, which is overcomplete by just one state, due to the Perelomov identity, and, consequently, one returns to the weakly localized magnetic Wannier functions set.

The sets of magnetic Wannier functions constructed here are strongly localized, which is seen clearly from the exponential fall-off in the logarithmic plot in figure 2. The function is oscillating, and this is seen in the plot. Orthogonalization is performed in a standard manner by dividing the function sets $\varphi_{\mu,k_xk_y}(x, y)$ by their norm and calculating the integral over the Brillouin zone, as in conventional zone theory. The norm is calculated by using transformations of the theory of theta functions, and since these are extremely important in the context of the construction of a special representation of the magnetic translation group, the mathematical description and derivations are presented in the next section.

## 4. Jacobi identities and symmetry properties of Bloch functions

The four sets of Bloch functions constructed transform under the action of the smallest relevant subgroup of the magnetic translation group, i.e. that generated by $T_{2a}$ and $T_{2b}$, in the same way:

$$\varphi_{\mu,k_xk_y}(x + 2a, y) = \mathrm{e}^{-2\mathrm{i}ak_x}\varphi_{\mu,k_xk_y}(x, y), \tag{6}$$

$$\mathrm{e}^{2\mathrm{i}bx}\varphi_{\mu,k_xk_y}(x, y + 2b) = \mathrm{e}^{-2\mathrm{i}bk_y}\varphi_{\mu,k_xk_y}(x, y). \tag{7}$$

This is because of the fact that a subgroup of the magnetic translations group corresponding to the $\mathrm{L}_{4\pi}$ lattice and the ordinary translation group are isomorphic. The relations (6) and (7) may be viewed, in addition to the standard interpretation as eigenvectors of unitary operators, as definitions of a functional subspace by imposition of boundary conditions. The next step is to prove that this generalized subspace, which represents the states of a charged particle in a Landau level, is effectively two dimensional. Then the normalization integral (3) should be redefined as over a domain modulo $\mathrm{L}_{4\pi}$.

The functions (5) obtained by direct summation over one of the four lattices $\mathrm{L}_\mu$ may be transformed, by first using the following formulae for the Jacobi imaginary transformation, Whittaker and Watson (1927), as for the case of the square lattice:

$$\vartheta_3(z) = \mathrm{e}^{-z^2/4}\vartheta_3(\mathrm{i}z), \qquad \vartheta_1(z) = -\mathrm{i}\mathrm{e}^{-z^2/4}\vartheta_1(\mathrm{i}z),$$
$$\vartheta_4(z) = \mathrm{e}^{-z^2/4}\vartheta_2(\mathrm{i}z), \qquad \vartheta_2(z) = \mathrm{e}^{-z^2/4}\vartheta_4(\mathrm{i}z).$$

The Bloch functions are transformed as follows:

$$\varphi_{\mu,k_xk_y}(x,y) \to c(x,y)\mathrm{e}^{(-\mathrm{i}k_x+(x+\mathrm{i}y)/2)^2}\vartheta_\mu(-2\mathrm{i}k_x + x + \mathrm{i}y)\vartheta_\mu(2k_y + x + \mathrm{i}y).$$

The periodicity in $k_x$ is preserved now due to an exponential factor. The form above is essential for further consideration, since the pair of Bloch function sets constructed is to be transformed further into another pair of function sets with somewhat different properties. To do so we use Jacobi identities. As a next step the theta functions are transformed to forms with different arguments with the help of the identities

$$\vartheta_3(u+v)\vartheta_3(u-v)\vartheta_3(0)^2 = \vartheta_1(v)^2\vartheta_1(u)^2 + \vartheta_3(v)^2\vartheta_3(u)^2,$$
$$\vartheta_1(u+v)\vartheta_1(u-v)\vartheta_3(0)^2 = \vartheta_3(v)^2\vartheta_1(u)^2 - \vartheta_1(v)^2\vartheta_3(u)^2.$$

It should be noted that the latter relation is specific to the case of a square lattice, since in this case

$$\vartheta_4(z)^2 = \frac{1}{\sqrt{2}}(\vartheta_3(z)^2 + \vartheta_1(z)^2), \qquad \vartheta_2(z)^2 = \frac{1}{\sqrt{2}}(\vartheta_3(z)^2 - \vartheta_1(z)^2). \tag{8}$$

For the two Bloch functions the following expressions are obtained (the factor $\vartheta_3(0)^{-2}$ in the right-hand side is omitted):

$$\varphi_{3,k_xk_y}(x,y) \propto \mathrm{e}^{-k_x^2-y^2/2+k_x(y-\mathrm{i}x)}\big(\vartheta_3(k_y+\mathrm{i}k_x)^2\vartheta_3(k_y-\mathrm{i}k_x+x+\mathrm{i}y)^2 + \vartheta_1(k_y+\mathrm{i}k_x)^2\vartheta_1(k_y-\mathrm{i}k_x+x+\mathrm{i}y)^2\big), \tag{9}$$

$$\varphi_{1,k_xk_y}(x,y) \propto \mathrm{e}^{-k_x^2-y^2/2+k_x(y-\mathrm{i}x)}\big(-\vartheta_1(k_y+\mathrm{i}k_x)^2\vartheta_3(k_y-\mathrm{i}k_x+x+\mathrm{i}y)^2 + \vartheta_3(k_y+\mathrm{i}k_x)^2\vartheta_1(k_y-\mathrm{i}k_x+x+\mathrm{i}y)^2\big). \tag{10}$$

As a result, the products of theta functions in the expressions for the Bloch functions transform to linear combinations of squares of theta functions, and this is different in many respects, as discussed below. While the functions $\varphi_{\mu,k_xk_y}(x,y)$ are periodic in $(k_x,k_y)$, the functions defined as

$$\psi_{\mu,k_xk_y}(x,y) = \mathrm{e}^{-k_x^2/2-y^2/2+k_x(y-\mathrm{i}x)}\vartheta_\mu(k_y-\mathrm{i}k_x+x+\mathrm{i}y)^2 \tag{11}$$

are not: instead, they are quasi-periodic. So are the coefficients in the linear combinations of $\psi_{\mu,k_xk_y}(x,y)$ in (9) and (10), but the quasi-periodicity multipliers for the latter cancel with those of the former to give functions periodic in $(k_x,k_y)$, $\varphi_{\mu,k_xk_y}(x,y)$. We rewrite (9) and (10) as

$$\varphi_{3,k_xk_y}(x,y) \propto \overline{\psi_{3,k_xk_y}(0,0)}\psi_{3,k_xk_y}(x,y) + \overline{\psi_{1,k_xk_y}(0,0)}\psi_{1,k_xk_y}(x,y), \tag{12}$$

$$\varphi_{1,k_xk_y}(x,y) \propto -\overline{\psi_{1,k_xk_y}(0,0)}\psi_{3,k_xk_y}(x,y) + \overline{\psi_{3,k_xk_y}(0,0)}\psi_{1,k_xk_y}(x,y). \tag{13}$$

The functions $\varphi_{\mu,k_xk_y}(x,y)$ and $\psi_{\mu,k_xk_y}(x,y)$ coincide at the centre of Brillouin zone. Now that the sets of Bloch functions are expressed in terms of squares of theta functions, as if obtained by magnetic translations of the 'central' pair, the structure of the functional subspace may be studied explicitly by use of linear identities (8) for squares of theta: any pair of them may be expressed linearly via the other pair. Moreover, the pair of functions $\psi_{3,k_xk_y}(x, y)$ and $\psi_{1,k_xk_y}(x, y)$ form a generalized orthonormal set in the $H_{k_xk_y}$ subspace. This is proved by calculating the scalar product within the subspace $H_{k_xk_y}$ defined by (6) and (7), and the norm defined by (3) where integration is performed modulo $L_{4\pi}$.

The $L_4$, $L_2$ pair is transformed similarly to give

$$\varphi_{4,k_xk_y}(x, y) \propto \overline{\psi_{4,k_xk_y}(0, 0)}\psi_{3,k_xk_y}(x, y) + \overline{\psi_{2,k_xk_y}(0, 0)}\psi_{1,k_xk_y}(x, y), \tag{14}$$

$$\varphi_{2,k_xk_y}(x, y) \propto \overline{\psi_{2,k_xk_y}(0, 0)}\psi_{3,k_xk_y}(x, y) - \overline{\psi_{4,k_xk_y}(0, 0)}\psi_{1,k_xk_y}(x, y). \tag{15}$$

Expressions (12)–(15) above may be given an interpretation that connects the lattice origin choice to the Bloch amplitudes constructed. It may be shown that there is a relativity relation between the position of the critical quasi-momentum in the reciprocal space and the real space lattice origin position, as for $L_3$. Then, the origin of the amplitudes $\overline{\psi_{\mu,k_xk_y}(0, 0)}$ in (12)–(15) is to be interpreted as a consequence of that choice. Such effects are typically described as Aharonov–Bohm effects.

Here it is worth mentioning that there exists a physically clear analogy between the 'space' and 'body' descriptions of the rotations of a solid body with fixed centre of mass, on one hand, and the two types of Bloch function, (5) and (11), on the other. A distinctive feature of $\psi_{3,k_xk_y}(x, y)$ and $\psi_{1,k_xk_y}(x, y)$, as compared to $\varphi_{3,k_xk_y}(x, y)$ and $\varphi_{1,k_xk_y}(x, y)$, is that the functions of the former pair are orthogonal, and so form an orthonormal basis in any two-dimensional invariant $(k_x, k_y)$ subspace $H_{k_xk_y}$.

The normalization $c(x, y) \to a(x, y)$ in (2), which leads to the Wannier function that is plotted in figure 2, is performed easily in this basis by using an identity that may be proved with the help of the following identity for Jacobi theta functions:

$$|\vartheta_3(\xi + \mathrm{i}\eta)|^4 + |\vartheta_1(\xi + \mathrm{i}\eta)|^4 = |\vartheta_4(\xi + \mathrm{i}\eta)|^4 + |\vartheta_2(\xi + \mathrm{i}\eta)|^4 \propto \vartheta_3(2\xi)\vartheta_3(2\eta). \tag{16}$$

Similar identities,

$$\begin{aligned} &\overline{\vartheta_3(\xi + \mathrm{i}\eta)^2}\vartheta_1(\xi + \mathrm{i}\eta)^2 - \overline{\vartheta_1(\xi + \mathrm{i}\eta)^2}\vartheta_3(\xi + \mathrm{i}\eta)^2 \propto \vartheta_1(2\xi)\vartheta_1(2\eta), \\ &\overline{\vartheta_4(\xi + \mathrm{i}\eta)^2}\vartheta_2(\xi + \mathrm{i}\eta)^2 - \overline{\vartheta_2(\xi + \mathrm{i}\eta)^2}\vartheta_4(\xi + \mathrm{i}\eta)^2 \propto \vartheta_1(2\xi)\vartheta_1(2\eta), \end{aligned} \tag{17}$$

play an important role in the description of the non-orthogonality of the Bloch functions, illustrating the Balian–Low theorem as interpreted by Zak, and responsible for non-locality effects. The scalar product of Bloch functions that describes non-orthogonality takes the form

$$\int\int \overline{\varphi_{1,k_xk_y}(x, y)}\varphi_{3,k_xk_y}(x, y)\,\mathrm{d}x\,\mathrm{d}y \propto \vartheta_1(2k_x)\vartheta_1(2k_y),$$

which follows from the expressions (9), (10) and (17), written above. At the same time, relations (17) are used to describe the intrinsic (with respect to the invariant subspace) degree of freedom of the charged particle. An approach based on the formulae presented above is a convenient framework for studying non-locality in this context. The respective operators of projection onto the states $\varphi_{3,k_xk_y}(x, y)$ and $\varphi_{1,k_xk_y}(x, y)$ are not commutative; nevertheless they present a convenient framework for further detailed discussion of any relevant physical phenomenon. In this sense, the representation constructed may be treated as physically irreducible, despite the twice-larger dimension of the representation.

The operator of projection onto the $H_{k_xk_y}$ subspace may be written in the form

$$P_{k_xk_y} = |\psi_{3k_xk_y}\rangle\langle\psi_{3k_xk_y}| + |\psi_{1k_xk_y}\rangle\langle\psi_{1k_xk_y}| = |\psi_{4k_xk_y}\rangle\langle\psi_{4k_xk_y}| + |\psi_{2k_xk_y}\rangle\langle\psi_{2k_xk_y}|.$$

So any pair may be used just as well, and their equivalence follows from the identities of the theory of theta functions. $P_{k_xk_y}$ is $L_\pi$ periodic in quasi-momentum space. A simple expression for the kernel of the projection operator may be proved to hold, with the help of relation (16), but we will not go into further detail here.

Here is a brief description of the representation for the anticommutative subgroup of the magnetic translation group. The quasi-momentum $(k_x, k_y)$ is defined modulo $\mathrm{L}_\pi$ and thus belongs to a Brillouin zone that has area $\pi$, and not $2\pi$, as in the conventional case, and any point of the Brillouin zone represents a two-dimensional subspace, $H_{k_x k_y}$, of the Hilbert space of states $H$ in a single Landau level. By representing the subspace with the help of a pair of functions, $\psi_{3,k_x k_y}(x, y)$ for 'spin'-up states and $\psi_{1,k_x k_y}(x, y)$ for 'spin'-down states, a two-dimensional representation for the subgroup that is generated by the magnetic translations $T_a$ and $T_b$ of the magnetic translation group is obtained:

$$T_a(k_x, k_y) = \frac{\mathrm{e}^{-\mathrm{i}ak_x}}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad T_b(k_x, k_y) = \frac{\mathrm{e}^{-\mathrm{i}bk_y}}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix},$$
$$(T_b T_a)(k_x, k_y) = \mathrm{i}\mathrm{e}^{-\mathrm{i}(ak_x + bk_y)} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}. \tag{18}$$

The third matrix is the Pauli matrix $\sigma_2$, and the two others are rotated Pauli matrices, $(\sigma_3 \pm \sigma_1)/\sqrt{2}$. Transformations (18) resemble those for spin 1/2 wavefunctions due to rotations in three dimensions. At the critical (with respect to the origin chosen) quasi-momentum, $k_x = \pm\sqrt{\pi}/2$, $k_y = \pm\sqrt{\pi}/2$, the rank of the pair of transformations (9) and (10) is 1, and this is an independent proof of the Perelomov identity, and the infinite uncertainties discussed above. At this point $T_a^2 = T_b^2 = (T_b T_a)^2 = -1$, and magnetic translations act as pure (with no multiplicative phase factor) three-dimensional rotations by angle $\pi$. Therefore, the internal, with respect to any subspace $H_{k_x k_y}$, degree of freedom is commutative with operators $T_{2a}$ and $T_{2b}$, and matches that of spin 1/2. This could be guessed from the anticommutativity relation (4).

The two-dimensional representation of the magnetic translation group constructed here has remarkable features, in addition to the strong, exponential localization of magnetic Wannier functions: a twice-larger set of sites on the real space lattice are involved in the representation, exactly those belonging to the sites of the half-flux-quantum unit cell lattice. In addition, a quartet of Bloch functions in each two-dimensional $(k_x, k_y)$ subspace, namely $\varphi_{\mu,k_x k_y}(x, y)$, $\mu = 1, 2, 3, 4$, is present.

## 5. The pseudo-spin observable

The solution to the magnetic Wannier functions problem that is given by the description in terms of two-dimensional invariant subspaces is not complete, since the question of the physical meaning of the intrinsic, to those subspaces, degree of freedom, which arises from the construction scheme above, remains unanswered. To have a complete set of observables, along with the quasi-momentum, there must be defined something like a quasi-coordinate observable, as is done in zone theory, in the absence of a magnetic field. In the latter case a quasi-coordinate replaces the zone number observable. Here the case is somewhat different. An obvious definition follows from (18), apart from exponential phase factors, on recalling the definition of rotations in quantum mechanics as exponential functions of the angular momentum. The physical meaning of this observable is revealed further by its behaviour in an electric field. Therefore, the next question is the effect of an electric potential applied to a two-dimensional charge in a strong magnetic field, in its coupling to the pseudo-spin degree of freedom.

First, consider an example of a potential that is antiperiodic with respect to an $\mathrm{L}_\pi$ lattice in real space, such as $V(x, y) \propto \sin(bx)\sin(ay)$. The calculation of the only non-zero matrix element on an invariant subspace, in perturbative analysis,

$$\int\int V(x,y)\frac{1}{\mathrm{i}}(\overline{\psi_{3,k_xk_y}(x,y)}\psi_{3,k_xk_y}(x,y)-\overline{\psi_{1,k_xk_y}(x,y)}\psi_{3,k_xk_y}(x,y))\,\mathrm{d}x\,\mathrm{d}y,$$

with the help of (17), reduces the matrix element value to a product of two similar terms such as

$$\frac{1}{\sqrt{\pi}}\int_0^{\sqrt{\pi}}\vartheta_1(2(k_y+x))\sin(\sqrt{\pi}x)\,\mathrm{d}x=\mathrm{e}^{-\frac{1}{4}\pi}\cos(\sqrt{\pi}k_y),$$

and we get a simple product expression for a dispersion law possessing electron–hole symmetry, on an invariant subspace:

$$V(x,y)\to V_c\cos(ak_x)\cos(bk_y)\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}.$$

In this particular case the spectrum may be described both in terms of a single conventional Brillouin zone, i.e. quasi-momentum defined modulo $\mathrm{L}_{2\pi}$ in reciprocal space, by diagonalization of the matrix above, and in terms of a twice-smaller, $\mathrm{L}_{\pi}$ Brillouin zone with an additional 'spin' degree of freedom. This is a single 'spin' component aligned along the quantization axis, taken 'parallel' to the 'diagonal' magnetic translation. In the calculation of the matrix elements of antiperiodic potentials

$$V(x+a,y)=V(x,y+b)=-V(x,y)=-V(x+a,y+b),$$

which are anticommutative with $T_a$ and $T_b$, the role played by relations (17) for theta functions allowing the definition of the pseudo-spin component with respect to an arbitrarily chosen 'quantization axis' in an invariant way is important. The two other operators present in (18) may be described similarly.

Thus, along with the projection operator defined in section 4, which is equivalent to scalar observables on an invariant subspace, and is represented by $\mathrm{L}_{\pi}$ periodic operators, three other operators may be constructed. These may be interpreted as a single vector operator.

The pseudo-spin degree of freedom may also be interpreted as a quasi-coordinate with non-commutative components, coupled to the charge, and resembling the electric dipole moment. The physical meaning of this observable is revealed by its coupling to the external doubly periodic electric potential, and it is equivalent to a scalar and a vector, on an invariant subspace.

Potential landscapes of appropriate periodicity would not affect the conservation of the quasi-momentum; i.e. any potential such that $V(x+2a,y)=V(x,y+2b)=V(x,y)$ does conserve the quasi-momentum $(k_x,k_y)$. The effect of an electric potential applied to a two-dimensional charge in a strong magnetic field, in its coupling to the pseudo-spin degree of freedom, may be described as follows. With respect to the magnetic translations $T_a$ and $T_b$, four types of translational symmetry for the potentials which conserve the quasi-momentum are allowed. For instance, imagine a four-pole gate, instead of the conventional single-poled ones in 2DEG experiments, as in figure 3. The obvious correspondence of this to the lattices in figure 1 is exploited, and the only pole, the third, is shown for viewing convenience. Similarly connected are the conductors of the three other poles, producing a periodic potential landscape that conserves quasi-momentum and makes accessible the pseudo-spin degree of freedom. The four voltages applied to the gate poles correspond to the four possible symmetries of the potentials conforming with the quasi-momentum conservation condition, and the relations between them are as follows:

$$V_0=(V_1+V_2+V_3+V_4)/4,$$
$$V_a=(-V_1-V_2+V_3+V_4)/4,$$
$$V_b=(-V_1+V_2+V_3-V_4)/4,$$
$$V_c=(V_1-V_2+V_3-V_4)/4.$$

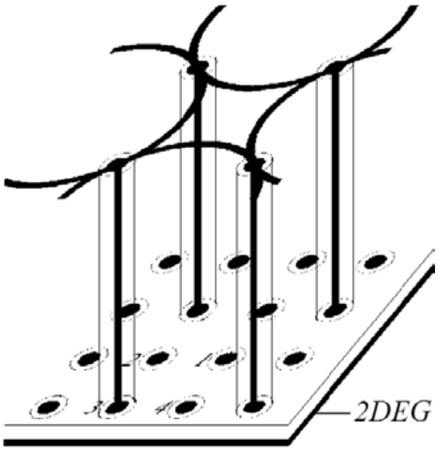


**Figure 3.** One of the four isolated arrays of connected conducting wires positioned perpendicular to the surface of a semiconductor. The array forms one of the four 'poles' of a gate that replaces the conventional gate made of a uniform metallic film. The potential landscape created by the four independently applied voltages conserves the quasi-momentum, thus allowing access to the pseudo-spin degrees of freedom exclusively.

The energy of the particle may be written in a form analogous to that for a magnetic dipole, namely, as $V(x, y) = \sigma_0 V_0(x, y) - \vec{\sigma} \cdot \vec{V}(x, y)$, using standard Pauli matrices, with the vector function $\vec{V}(x, y) : \vec{V} = (V_a, V_b, V_c)$, its components being defined with respect to anticommutative magnetic translations $T_a$ and $T_b$ that represent three-dimensional rotations in 'spin' space.

The possibility of new resonance phenomena may be predicted within this scope; this involves the detection of the precession of the pseudo-spin introduced. There are also methods other than the four-pole gate method described above which could work, e.g. creating two-dimensional superlattices with complex structures of the unit cell, with respect to the double-flux Bravais lattice. Direct observation of non-locality effects should contribute significantly to the understanding of quantum phenomena.

With the proof of the possibility of accessing the 'spin' degree of freedom, in principle, by applying periodic potentials of a special configuration, the set of physical observables becomes complete, as required in quantum mechanics.

## 6. Summary and discussion

The role played by the concept of quasi-momentum is at the heart of condensed matter physics. While the description in terms of quasi-momentum in the absence of an external magnetic field leads naturally to a scalar 'complementary' observable, namely, the energy band index (or, equivalently, to a quasi-coordinate vector), the study presented shows how this description is to be modified in the magnetic case. Because of the Balian–Low theorem, one has either to use a description in terms of non-orthogonal and 'non-commutative bands', as subspaces of the Hilbert space of states, or to tolerate weak localization, and infinite uncertainty products. The context created by relaxing the orthogonality condition, in order to preserve translation invariance and strong localization, leads to non-orthogonal subspaces, and, as a consequence, to pseudo-spin. It is the imposition of a (global) localization condition, in view of the 'discretization' of the plane 'seen' by a 2D charged particle restricted to a single Landau level, that dramatically affects the structure of the representation of the space of states induced by magnetic translation symmetry. In contrast with the case in conventional theory where the energy bands represent mutually orthogonal subspaces of states, the band index observable is replaced by non-commutative components of the pseudo-spin vector observable.

The quasi-momentum defined in the present paper is an *additive conserving* quantity. This may be seen, for a pair of particles, from the fact that corresponding operators commute with the commutative subgroup of the magnetic translation group, and it may be checked easily, with the help of the Bloch functions constructed, that any interaction that depends on inter-particle distance only does conserve the quasi-momentum. In fact, there is no need to check it literally since the quasi-momentum constructed is analogous to the ordinary quasi-momentum, due to group isomorphism. One may recall that the main purpose of the study conducted by Rashba *et al* (1997) was to give a framework convenient for solving interaction problems. The description in terms of quasi-momentum introduced in the present paper opens up new possibilities for such studies.

The sets of strongly localized Wannier functions constructed make it possible to clarify the question of 'here' and 'there' posed in the introduction. Critical is the understanding of the fact that the pseudo-spin degree of freedom appears in the spatial description of the charged particle in a magnetic field, restricted to a single Landau level, with no reference to the actual spin. The two (complementary) schemes of description, i.e. in terms of extended (Bloch) and in terms of localized (Wannier) states, are preserved due to the introduction of 'spin'. Thus one may think of electrons being 'here' and 'there' in terms of 'spin'-polarized states, with respect to the double flux quantum Bravais lattice.

The physical meaning of the 'spin' may be revealed in the Bloch representation by considering application of an electric field. Stationary states in a doubly periodic electric field and a uniform magnetic field in the case of a single flux quantum per unit cell may alternatively be described as polarized ones with definite quasi-momenta. From the physical viewpoint, the most intriguing possibility is that of observing resonance phenomena in electric fields varying in time, their spatial periodicity being commensurate with the magnetic field half-value. Recent advances in nanotechnology present new possibilities for creating quantum devices on the magnetic length scale. The simplest and a quite direct experiment in this area is the detection of precession of pseudo-spin by standard methods of magnetic resonance. There are also many other methods, including observation of echo phenomena, but further discussion of these seems to be inappropriate until any is established unambiguously. Apart from the practical goals in quantum device engineering, observation of resonant non-linear effects on the magnetic length scale could be a step towards a better understanding of the concepts of quantum mechanics.

At least four aspects of the problem of magnetic Wannier functions are of interest. Formally speaking, the mathematical aspect consists in a problem of square integrable basis sets in Hilbert space, related to a subgroup of the Weyl–Heisenberg group unitary representation action, the latter being isomorphic to the magnetic translation group. Dubrovin and Novikov (1980) do mention this isomorphism. The second aspect is signal processing. Due to the paper by Zak (1998), the bridge between the areas was established. The questions of physical analogies have to be a subject of special study. The third aspect is the phase space quantum mechanics, and there is need for a separate discussion of this too. It is the problem of the 2D Bloch electron in a strong magnetic field that is explicitly intuitive and does not raise unnecessary questions as regards interpretation. One clearly has an in-plane particle, and the magnetic translations form a symmetry group that may be treated unambiguously, with no reference to the particular mechanics (either classical, or non-relativistic quantum, or other). The 2D electrons that are moving within a heterojunction or a MOSFET present the best-known example for particles in a plane. That is why this fourth aspect had to be considered first in a line of problems related to the general problem of magnetic Wannier functions. The parallels and analogies may wait for a while.

The actual spin degrees of freedom of electrons, which are irrelevant to the spatial degrees of freedom, in the non-relativistic approximation, have so far been neglected completely; their inclusion into the consideration is trivial. An interesting question then is the possible coupling of these two spins.

## Acknowledgments

I would like to thank S P Novikov for useful discussions. The provision of the reference Grochenig (2000) by a referee is acknowledged.

## References

Balian R 1981 Un principe d'incertitude fort en théorie du signal ou en mécanique quantique *C. R. Acad. Sci., Paris* **292** 1357–62

Dubrovin B E and Novikov S P 1980 Ground states of a two-dimensional electron in a periodic magnetic field *JETP* **79** 1006–16

Grochenig K 2000 *Foundations of Time–Frequency Analysis* (Boston, MA: Brikhauser)

Kohn W 1959 Analytic properties of Bloch waves and Wannier functions *Phys. Rev.* **115** 809–21

Low F 1985 Complete sets of wave packets *A Passion for Physics—Essay in Honour of Geoffrey Chew* ed C DeTar (Singapore: World Scientific) pp 17–22

Perelomov A M 1971 Remark on the completeness of the coherent state system *Teor. Mat. Fiz.* **6** 213–24

Rashba E I, Zhukov L E and Efros A L 1997 Orthogonal localized wave functions of an electron in a magnetic field *Phys. Rev.* B **55** 5306–12

Thouless D J 1984 Wannier functions for magnetic sub-bands *J. Phys. C: Solid State Phys.* **17** L325–7

Wannier G H 1937 The structure of electronic excitation levels in insulating crystals *Phys. Rev.* **52** 191–7

Whittaker E T and Watson G N 1927 *A Course of Modern Analysis* (Cambridge: Cambridge University Press)

Zak J 1997 Balian–Low theorem for Landau levels *Phys. Rev. Lett.* **79** 533–6

Zak J 1998 Orthonormal sets of localized functions for a Landau level *J. Math. Phys.* **39** 4195–200