

Energy bands for finite two-dimensional systems in a quantised magnetic field: the symmetry of the model

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Abstract Analysis of properties of an electron (electrons) in a periodic two-dimensional potential and quantised magnetic field is presented. The key role in this description is played by the symmetry of the model determined by the magnetic translation group, together with the symmetric and unitary group according to the duality of Weyl. The magnetic translation group is described in detail along with its irreducible representations which form the Brillouin zone in magnetic field. Together with the other two mentioned groups, it allows to characterize the system providing some good quantum numbers. These groups facilitate determination of the band structure through the diagonalisation of the eigenvalue problem in the base adapted to the considered symmetry. The difference between the Brillouin zone with and without magnetic field is pointed out. Discussion is concentrated on the finite two-dimensional systems, closed by use of Born–von Karman boundary conditions.

Keywords Tight-binding model · Magnetic translation group · Itinerant electrons · Magnetic Brillouin zone

1 Introduction

The problem of a charged particle (or particles) in a magnetic field is an old one but still interesting and intensively studied. The interest in such systems has been increased after the discovery of quantum Hall effect (integer and fractional). The system exhibits a rich energy band structure which is very sensitive to the change of both magnetic field and size of the system (Hofstadter butterfly). From theoretical point of view it

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is an interesting subject of study, intimately related to composite fermions (in the context of fractional quantum Hall effect) [1–4], quantum groups, integrable systems and application of Bethe Ansatz for two-dimensional objects [5–11].

Recently developed experimental techniques allow to measure the detailed physical properties of two-dimensional electron systems, in both periodic potential and magnetic field. First of all, it is worth to mention here the implementation of optical lattices used for simulation of charged particle in a magnetic field. By this method one can achieve an 'artificial magnetic field' of the strength compatible with the details of the spectrum (the lattice length can be tuned freely up to hundred angstroms) [12–14]. The observation of the recursive structure of energy spectrum (Hofstadter's butterfly) was reported quite recently by Dean et al. [15] for moiré superlattice arising in bilayer graphene coupled to hexagonal boron nitride.

The advent of two-dimensional surface electron systems in semiconductors [16–18], as well as in topological insulators [19,20] enable high resolution measurements of the electronic probability density with the use of scanning tunneling spectroscopy [21].

We will focus in the paper on description of finite systems from the point of view of their symmetry. This restriction is motivated by the progress in technology which nowadays allows one to build such a system very precisely. From the other hand we can test the theory on such systems, since the modern computers are able to provide well approximated numerical solutions. Moreover, the modern chemistry is also interested in finite systems, because it admits a deeper understanding of objects of the size comparable to molecules [22–25]. The interplay between the physical, chemical and mathematical tools is very fruitful nowadays at the level of quantum objects.

Let us start this introduction with the main notions used in the description of charged particles in a periodic potential and magnetic field. First consider the free electron motion. The Hamiltonian \mathcal{H} for a free electron in a magnetic field consists of the kinetic energy operator

$$\mathcal{H} = \frac{1}{2m} (\mathbf{p} + e\mathbf{A})^2, \quad (1)$$

where \mathbf{p} is the canonical momentum and \mathbf{A} is a vector potential of a magnetic field, while e means the magnitude of elementary charge. There are many ways of choosing the gauge for vector potential, but the most popular are the Landau and symmetric ones. The detailed description of these two gauges is presented in the Sect. 2. The solution of an eigenvalue problem of a free electron in a magnetic field was given by Landau in the form of eigenfunctions of a one-dimensional quantum harmonic oscillator [26]. Within the Landau gauge $\mathbf{A} = [0, Bx, 0]$ and using the substitution $\Psi(x, y) = e^{ik_y y} \varphi(x)$ the equilibrium point of this oscillator is shifted $x' = x + k_y l^2$ by the distance dependent on the magnetic field through the magnetic length $l = \sqrt{\hbar/eB}$. The quasimomentum k_y is related to quantization of the motion along y axis. The choice of this direction and the associated gauge is arbitrary, i.e. is not determined by the symmetry, so that an equivalent solution is obtained by the substitution $\Psi(x, y) = e^{ik_x x} \varphi(y)$. The

magnetic field is parallel to z axis, and the motion along it is free and can be considered independently. In further discussion the perpendicular motion is omitted.

For φ being a function of x the solution of Schrödinger equation of the Hamiltonian (1) is the product of the eigenfunction of the oscillator (Hermite polynomials) and the plane wave along y axis. For movement on an infinite plane the degeneracy of these solutions is infinite. If the area admissible for an electron is restricted to a rectangle with dimensions $L_x \times L_y$, the degeneracy of energy levels becomes finite. To quantize the quasimomentum k_y we assume the periodic boundary conditions, which provide the values $k_y = \frac{2\pi}{L_y}m$, $m \in \mathbb{Z}$. The eigenfunctions of the Hamiltonian, however, do not exhibit the translational symmetry along x axis, since it is broken by the magnetic field. The quantisation in this direction is replaced by the condition for the equilibrium point (the centre of the cyclotronic orbit). It should be placed within the range $[0, L_x]$ what results in equation $0 \leq k_y l^2 \leq L_x$. This way each Landau level with energy

$$E = \left(n + \frac{1}{2}\right) \hbar\omega_c, \quad n = 0, 1, 2, \dots, \tag{2}$$

is degenerated with the value given by

$$D = \frac{L_x L_y e B}{2\pi \hbar} = \frac{\Phi}{\Phi_0}, \tag{3}$$

where n labels energy levels, $\omega_c = |e|B/m$ is the cyclotronic frequency, $\Phi = BL_x L_y$ is the magnetic flux passing through the sample, and $\Phi_0 = h/e$ is the quantum of the flux. The magnetic field B is therefore quantised in such a way that D is an integer. The density of states for a two-dimensional electron is a series of δ functions placed around the quantised energy values $\frac{1}{2}\hbar\omega_c, \frac{3}{2}\hbar\omega_c, \frac{5}{2}\hbar\omega_c, \dots$. In real crystal, however, the scattering processes lead to broadening of Landau levels.

The degeneracy can be determined also without using such quasi-classical method. One can consider also the twisted periodic boundary condition, i.e. the function is periodic along one direction, say y , whereas periodicity along the second one is connected with a phase. The elegant and convenient way of presentation of this scheme is based on the fibre bundle formalism [27,28] (definition and properties of fibre bundle can be found, e.g., in the book [29]). The base for this bundle is formed by the two-dimensional torus while one-dimensional linear space \mathbb{C} represents the standard fibre. Twisted boundary condition in this approach is related to the way of gluing of fibres on the rectangle (defined by a boundary conditions) edge, and the degeneracy level corresponds to Euler characteristic of the bundle.

Introduction of periodic potential $U(\mathbf{r})$ (a two-dimensional lattice) together with a magnetic field changes the Hamiltonian (1) to the form

$$\mathcal{H} = \frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2 + U(\mathbf{r}) \tag{4}$$

There are two different approaches which allow to analyse the motion of an electron in this case. The magnitude of the interaction between the electron and these two fields determines the choice one of them. If the periodic potential can be treated as a perturbation one can assume that the electron is placed on the Landau level and two-dimensional potential causes a splitting of the level. The magnitude of the splitting and degeneracy of sublevels are determined by the magnetic flux going through the elementary cell of the lattice. If the value of this flux is rational $\eta = p/q$, in the unit of quanta $\phi_0 = h/e$, each Landau level splits into p sublevels. However, when the magnetic field is a perturbation for the band structure of Bloch electron, the corresponding levels are splitting into q sublevels [30]. In further discussion we will consider only the last case.

There are several approximations which allow to solve quantum problem of Bloch electrons in a magnetic field. They differ essentially by choice of the base functions used in the perturbation theory. We can list the following basic functions: Bloch states [31], edge states in the $\mathbf{k} \cdot \mathbf{p}$ theory [32] and Wannier states [33,34]. For the first type, i.e. Bloch states $\Psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$, with their dispersion relation $E_n(\mathbf{k})$, one can find eigenstates of an electron in a magnetic field by use of the Peiers-Onsager substitution, i.e. substitution of the quasimomentum \mathbf{k} by the operator $\frac{\hbar}{i}\nabla + e\mathbf{A}(r)$. Dispersion relation $E(\mathbf{k})$ which is used in the Hamiltonian in a magnetic field, can be found with the help of the tight binding method. This approach is useful when the overlapping of wave functions of neighbour atoms is so substantial, that one needs to introduce some alterations to atomic functions, but simultaneously so small that we can use these functions as a base. The method is effectively used contemporary for determination of the electronic structures of semiconductor nanocrystals [35–38]

Tight binding theory together with the Peierls-Onsager substitution provides the effective Hamiltonian, whose correctness was justified by Kohn [39] and Blount [40] in the 1960s last century. In the paper of Schellnhuber and Obermair [41], on the other hand, one can find the first principle calculations which confirm the results obtained by effective Hamiltonian approach.

The equivalent method giving the band structure of electrons in a magnetic field is based on hopping Hamiltonian (it is known also as lattice tight-binding Hamiltonian)

$$\mathcal{H}_t = \sum_{i,j} t_{ij} e^{i\theta_{ij}} c_j^\dagger c_i, \quad (5)$$

where t_{ij} is a hopping integral between the lattice points i and j , operators c_j^\dagger and c_i are creation and annihilation operator on appropriate nodes, respectively, while θ_{ij} is a phase defined for the edge ij . The last quantity depends on the chosen gauge through the equation $\theta_{ij} = \frac{2\pi}{h/e} \int_i^j \mathbf{A} \cdot d\mathbf{l}$, where $d\mathbf{l}$ means the vector that is tangent to the edge along with the integral is taken. The summation of the phase along the boundary ∂S of the surface S leads to the formula

$$\frac{1}{2\pi} \sum_{\text{along } \partial S} \theta_{ij} = \frac{e}{h} \oint_{\partial S} \mathbf{A} \cdot d\mathbf{l} = \frac{1}{\phi_0} \int_S \mathbf{B} \cdot d\mathbf{S},$$

which describes the magnetic flux (in the unit of quanta ϕ_0) passing through the surface S . Both methods, i.e. effective Hamiltonian and lattice one, give the same band structure and eigenstates if the Peierls-Onsager substitution is treated carefully [42].

The structure of the bands in the magnetic field has been investigated for a long time (see papers by Harper [43,44], Hofstadter [45], Azbel [46], Wannier with coauthors [47,48], and bibliography included there). The early works concern the square lattices with isotropic hopping integral and interaction limited to nearest-neighbours (NN) [45,49]. The other values of hopping integral were also considered [42,50], as well as the different shapes of the unit cell of the lattice [51]. The interaction of distant nodes were also taken into account in calculations. It causes removing of the degeneracy in the centre of the band, which exists for NN interaction only [52]. The band structure was also designed for honeycomb lattice in the frame of tight-binding approximation [53,54], and for hexagonal lattice [55].

Thank to relations between the symmetry of the considered system and quantum group $U_q(sl_2)$ the previous one was analysed with the help of Bethe Ansatz [5]. This approach allows to express the energy, in some region of Brillouin zone, by the roots of algebraic Bethe equation. This region consists of selected quasimomenta from magnetic Brillouin zone, so called midbands points for which the Hamiltonian can be written as a linear combination of generators of quantum group $U_q(sl_2)$. The method is especially useful in the case of large value of q , because solutions of the Bethe equations draw together into structures called strings, i.e. the cluster of Bethe pseudoparticles with the same real part of the spectral parameter and imaginary values given by the simple equation [56]. This effect helps to simplify the calculations. Analytical and numerical solutions for these special points of the magnetic Brillouin can be found in the references [7,9]. Thank to the use of Bethe equations solutions of eigenvalue problems for non-rational value of magnetic field (so called incommensurate golden-mean flux) were obtained [7].

The problem of determination of the bands for model being considered is still relevant. It was pointed out quite recently that some additional effects caused by a magnetic field should be taken into account. One can mention here the field dependence of the hopping integral and influence of a magnetic field on the atomic energy level [57,58]. There is a methods which allows to go beyond the tight binding approximations for wide range of applied magnetic field [58]. It is based on a diffusion method of solving related Schrödinger equations [59,60].

The main aim of the paper is description, with the help of the symmetry given by the magnetic translation group, of the band structure of electrons on a finite planar lattice and in a quantised magnetic field. Attention is focused on the rational magnetic field, i.e. rational value of η , and this way the incommensurate case is not discussed here [45,61,62]. The eigenvalue problem is presented in the symmetry adapted basis, and operators which enable the transitions between different symmetry bases are introduced. The magnetic Brillouin zone, i.e. the Brillouin zone in magnetic field is discussed in detail. It has been shown also that use of all irreducible representations of magnetic translation group allows to consider multi-electron states in a magnetic field.

2 The symmetry of the Bloch electron in a magnetic field

2.1 Magnetic translation group

We restrict our considerations to the model of itinerant electrons on a planar, finite, square lattice with the lattice constant a . The natural basis of the Hamiltonian for single band model is the coordinate one

$$b_o = \{ \mathbf{j} = |j_x, j_y\rangle, \quad j_x, j_y = 1, 2, \dots, L \} \quad (6)$$

where L defines the size of the lattice. Within this notation the coordinates of nodes are given by formulas $x = j_x a$, $y = j_y a$. In the basis (6) the action of the Hamiltonian (5) on the element $|j_x, j_y\rangle$ reads

$$\begin{aligned} \mathcal{H}_i |j_x, j_y\rangle = t \left(|j_x + 1, j_y\rangle e^{i\theta_1} + |j_x - 1, j_y\rangle e^{i\theta_3} + |j_x, j_y + 1\rangle e^{i\theta_2} \right. \\ \left. + |j_x, j_y - 1\rangle e^{i\theta_4} \right). \end{aligned} \quad (7)$$

This action is presented on the Fig. 1. It should be noticed, however, that the sum in the above equation is restricted to four nearest neighbours of the element $|j_x, j_y\rangle$.

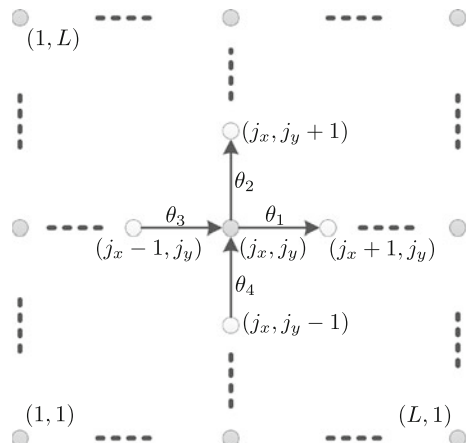
The symmetry of the Hamiltonian (7) in the absence of a magnetic field (all phases θ_i are equal to 0) is given by the translation group

$$T = \{ (t_x, t_y), \quad t_x, t_y = 1, 2, \dots, L \} \quad (8)$$

The eigenfunctions for this case are characterised by the irreducible representations of T by the formula

$$\Gamma^{k_x k_y} (t_x, t_y) = \frac{1}{L} \exp \left(-\frac{2\pi i k_x t_x}{L} - \frac{2\pi i k_y t_y}{L} \right), \quad (9)$$

Fig. 1 The action of the Hamiltonian \mathcal{H}_i on the vector $|j_x, j_y\rangle$ of position basis b_o . The white circles denote the neighbours of the node (j_x, j_y) which are included in the Hamiltonian. The phase θ_i is assigned to the edge of the cell, and arrows indicate that the value of the phase depends on the direction along with the integration of vector potential is taken. The value L means the dimension of the lattice in both directions. The magnetic field is perpendicular to the plane of the figure



where k_x and k_y form two-dimensional Brillouin zone BZ

$$\text{BZ} = \left\{ (k_x, k_y), \quad k_x, k_y \in \left\{ 0, \pm 1, \pm 2, \dots, \begin{matrix} \pm \frac{L-1}{2} \text{ for } L \text{ odd} \\ \pm \frac{L}{2} - 1, \frac{L}{2} \text{ for } L \text{ even} \end{matrix} \right\} \right\}. \quad (10)$$

The presence of the magnetic field essentially changes the symmetry of the model. The action of the translation is now accompanied by the phase, whose value depends on the gauge of the vector potential of magnetic field. This property suggests that an operator being the product of a translation and phase factor should commute with the Hamiltonian. Such operators form a group—the magnetic translation group.

This group, as a symmetry of an electron in magnetic field, was introduced by Brown [63] and Zak [64, 65]. The classification of such groups, for different vector potentials was given by Opechowski and Tam [66]. Authors showed that a change of a gauge yields an isomorphic symmetry group. The irreducible representations were also determined with their dimensions resulted from the value of the parameter η . The rational value of it is related to a finite dimension of IRRs whereas for the irrational one such a kind of representation does not exist. The detailed discussion concerning this case can be found in the paper by Boon [67]. The author demonstrated that for irrational value of η and for magnetic field along one of the crystal direction, the symmetry groups are of infinite order. These groups have infinite class of irreducible representations and all of them are of infinite order.

The analysis of symmetry of the system being considered was done also by Geyler and Popov [30]. The starting point for the discussion was the “physical representation” defined in the coordinate basis (6). The decomposition of this representation into the irreducible ones provided the quantum numbers for classification of the energy bands and their degenerations. The abelian subgroup of MTG allowed to define the Brillouin zone in a magnetic field.

The structure of magnetic translation group was also considered within the frame of extensions of translation group by the gauge group. The technique of construction of such extensions is based on the MacLane method [68]. Some of such extensions were identified as MTG [69–73].

In this paper the element of MTG can be denoted as

$$g = (t_x, t_y, \lambda), \quad (11)$$

where λ is a phase associated with the translation $\mathbf{t} = [t_x, t_y]$ (it is related to phase factor $\exp(2\pi i\lambda)$). In this notation the group multiplication rule for the symmetric gauge reads

$$(\mathbf{t}, \lambda)(\mathbf{t}', \lambda') = \left(\mathbf{t} + \mathbf{t}', \lambda + \lambda' + \frac{1}{2}\eta l \right), \quad (12)$$

where $l \in \mathbb{Z}$ and is related to the area of the parallelogram spanned by the vectors \mathbf{t} and \mathbf{t}' . Hence the last term in the Eq. (12) can be written as

$$\frac{1}{2}\eta l = \frac{1}{2} \frac{\mathbf{B}(\mathbf{t} \times \mathbf{t}')}{h/e}. \quad (13)$$

This equation can be easily interpreted. It denotes the magnetic flux $\mathbf{B}(\mathbf{t} \times \mathbf{t}')$, in the unit h/e of quanta of flux, penetrating the half area of the parallelogram spanned by vectors \mathbf{t} and \mathbf{t}' .

The multiplication rule for Landau gauge is of the similar form

$$(\mathbf{t}, \lambda)(\mathbf{t}', \lambda') = (\mathbf{t} + \mathbf{t}', \lambda + \lambda' + \eta l), \quad (14)$$

where $l \in \mathbb{Z}$ and corresponds to the area of parallelogram spanned by vectors t_y and t'_x .

2.2 The choice of a gauge and a boundary condition

The selection of a boundary condition for a finite crystal depends on the symmetry of the model and on the tentative constants of motion. One of approaches proposed by Quinn and Wojs [74] is based on the notions of a Haldane sphere [75]. Within this approach electrons are placed on the sphere with radius R and in the centre there is a magnetic monopole $B = \hbar S/eR^2$, where $2S$ denotes the magnetic flux passing through the surface. The model allows to consider multi-electrons states. This approach admits the total angular momentum as exact quantum numbers, which is a result of an artificial introduction of spherical symmetry (due to the geometry of the Haldane sphere) to the model. A drawback of the approach consists in vanishing of an ordinary linear momentum (and thus also the Brillouin zone) in description of electronic spectra.

The Born–von Karman boundary condition is the second possible approach used for description of electron properties in the magnetic field, however it should be used carefully. The standard form of these conditions for wave function $\Psi(\mathbf{r} + \mathbf{L}) = \Psi(\mathbf{r})$, where $\mathbf{L} = [L_x, L_y]$, can not be applied because an additional phase appears due to the magnetic field. However there is a set of translations for which the phase factors is equal to 1. For magnetic field whose flux ϕ is a rational multiple of the quantum $\phi_0 = h/e$, these translations for a particular choice of gauge form the magnetic cell (see the next section for detail). For a finite system the boundary conditions provide relations between the size of the system and the value of η , the so called commensurate conditions. For incommensurate values of η the states can never be repeated by the translation by lattice constant [76].

The interesting discussion concerning the boundary conditions in a magnetic field and the effective Hamiltonian theory can be found in the paper by Zak [77]. The author concludes that the effective Hamiltonian theory can only be applied for localised states in a magnetic field, not for extended ones. For the latter it leads to an “unusual” quantisation in one of the spatial coordinate (the choice of the coordinate depends on a gauge).

In this section we focus our attention on the relation between the Born–von Karman boundary condition and the magnetic translation group. In order to fulfil the

commensurate conditions, i.e. the relation between the quantisation of the magnetic field and the size of the system, the length of the crystal should be a product of the integer q entering the definition of η , and the lattice constant a . For such a system we should introduce the equivalence relation between the elements of the magnetic translation group whose translations are differing by the length of the sample

$$(\mathbf{t}, \lambda) = (\mathbf{t} + L\mathbf{a}, \lambda) = (\mathbf{t} + L\mathbf{b}, \lambda) = (\mathbf{t} + L\mathbf{a} + L\mathbf{b}, \lambda). \tag{15}$$

These conditions mean that each group element listed in the equation acts in the same way on the wave function and, according to the multiplication rule, product of any two elements provides an equivalent operator of MTG. As a result we obtain sixteen equations of the form [78]

$$(\mathbf{t}_1 + \alpha_1 L\mathbf{a} + \beta_1 L\mathbf{b}, \lambda_1)(\mathbf{t}_2 + \alpha_2 L\mathbf{a} + \beta_2 L\mathbf{b}, \lambda_2) = (\mathbf{t}_1, \lambda_1)(\mathbf{t}_2, \lambda_2), \tag{16}$$

where $\alpha_1, \beta_1, \alpha_2, \beta_2$ are integers from the set $\{0, 1\}$. The detailed form of the product depends on the chosen gauge of a vector potential of magnetic field. Let us consider this equations for the symmetric and Landau gauge.

For a symmetric gauge the Eq. (16) provides 16 conditions for possible values of phases λ , which guarantee the equivalence (15). The detailed form of these conditions can be found in our paper [78]. Let us consider here, as an example, the product $(\mathbf{t}_1 + L\mathbf{a} + L\mathbf{b}, \lambda_1)(\mathbf{t}_2 + L\mathbf{a} + L\mathbf{b}, \lambda_2)$. The result of multiplication should be equal to $(\mathbf{t}_1, \lambda_1)(\mathbf{t}_2, \lambda_2)$. The translation parts are always equal, however the phase part should fulfil some requirements. For considered example this condition means that the value of $\frac{1}{2}\eta L(t_1^x - t_2^x + t_2^y - t_1^y)$ should be an integer. This is satisfied for all values t_1 and t_2 if it holds for $t_1^x - t_2^x = 1$ and $t_2^y - t_1^y = 1$. As a result we obtain two equations for admissible value of η , both with the same form

$$\eta = \frac{2n}{L}, \quad n \in \mathbb{Z}. \tag{17}$$

The similar calculations done for others 15 equations lead to the same solutions. This means that the symmetric gauge together with the boundary conditions introduce the restriction for quantisation of a magnetic field, i.e. the numerator of η should be an even number.

For Landau gauge, according to the multiplication rule the Eq. (16) comes down to a system of four conditions. The analysis of them results in equation

$$\eta = \frac{n}{L}, \quad n \in \mathbb{Z}. \tag{18}$$

The equation provides the dependence between the quantised magnetic field and dimension of the system. It follows, that the Landau gauge is better adopted to the square lattice closed with the boundary conditions. The restriction for possible value of η is weaker than for the symmetric gauge.

2.3 The structure of MTG

The notion of magnetic translation group was introduced by Zak [64]. He presented description of the structure of MTG, distinguished its abelian subgroup, and pointed out that the order of the group depends on the parity of the period L —the dimension of the system. For even and odd value of L the number of group elements is equal to $2L^3q$ and L^3q , respectively.

Description of symmetry for different orientations of a magnetic field and different gauges was done also by Opechowski and Tam [66]. They pointed out that the set of admissible values of phase λ depends on the parity of p

$$\begin{aligned} \lambda &= 0, \frac{1}{2q}, \frac{2}{2q}, \dots, \frac{2q-1}{2q}, & \text{for } p \text{ odd,} \\ \lambda &= 0, \frac{1}{q}, \frac{2}{q}, \dots, \frac{q-1}{q}, & \text{for } p \text{ even.} \end{aligned} \quad (19)$$

They also have shown the role of the maximal abelian subgroup consisting of elements of the form $(t_x n_x, t_y n_y, \lambda)$, $n_x n_y = q$ and $n_x, n_y \in \mathbb{Z}$. This subgroup was the key for determination of the irreducible representations of MTG.

Let us focus in the following sections on the analysis of structure of MTG. Description is based on our paper [79]. It will be shown, that the order of MTG does not depend on the parity of p , however the detailed structural properties are related to it.

2.3.1 Generators of the magnetic translation group

Let us consider the rectangular lattice with its vectors \mathbf{a} and \mathbf{b} . Each point of the lattice can be reached by the translation being the linear combination of the lattice vectors. The number of sequences leading to a given node is infinite one, even for a finite system, since we can form a closed loop and repeat them as much as we want. Together with the translation guiding to a chosen point, the phase is increased according to a value of η . The path along which the translation is taken is related to the product of elements of MTG. At the end we obtain the element of the lattice (connected with the translation \mathbf{t}) and the phase, which was gathered on the way.

Let us denote the generators of MTG by $\mathbf{a} = (1, 0, 0)$ and $\mathbf{b} = (0, 1, 0)$, where the first element corresponds to a translation by a vector $\mathbf{a} = (1, 0)$ and the second to a translation by $\mathbf{b} = (0, 1)$. There is given a set of integers (α_i, β_i) denoting the translation $\alpha_i \mathbf{a} + \beta_i \mathbf{b}$ at the step i . It should be noted, however, that for the elementary transition at a given step only one of these integers is different from 0. After the N steps of such translation we reach the lattice point with the coordinates (j_x, j_y) given by

$$\sum_{i=1}^N \alpha_i = j_x, \quad \sum_{i=1}^N \beta_i = j_y. \quad (20)$$

The phase corresponding to the path can be found by a suitable product of the generators $a_i b_j$, and the coordinates (j_x, j_y) are related to a translation $\mathbf{t} = [t_x = j_x, t_y = j_y]$ which leads into that point.

The details of the discussion depend on the choice of the gauge of vector potential. Let us consider two the most popular gauges, i.e. the symmetric and Landau ones. For the symmetric gauge after the N translation (N products of group generators) we obtain [79]:

$$\begin{aligned}
 &(\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \dots + \alpha_N, \beta_1 + \beta_2 + \beta_3 + \beta_4 + \dots + \beta_N, \\
 &\frac{1}{2}\eta(\alpha_1\beta_2 - \beta_1\alpha_2) + \frac{1}{2}\eta[(\alpha_1 + \alpha_2)\beta_3 - (\beta_1 + \beta_2)\alpha_3] \\
 &+ \frac{1}{2}\eta[(\alpha_1 + \alpha_2 + \alpha_3)\beta_4 - (\beta_1 + \beta_2 + \beta_3)\alpha_4] \\
 &+ \dots \frac{1}{2}\eta[(\alpha_1 + \alpha_2 + \alpha_3 + \dots + \alpha_{N-1})\beta_N - (\beta_1 + \beta_2 + \beta_3 + \dots + \beta_{N-1})\alpha_N].
 \end{aligned}
 \tag{21}$$

Taking into account, that $\alpha_i \beta_i = 0$ the obtained phase reads

$$\begin{aligned}
 &\frac{1}{2}\eta[\alpha_1(\beta_1 + \beta_2 + \beta_3 + \beta_4 + \dots + \beta_N) \\
 &+ \alpha_2(-\beta_1 + \beta_2 + \beta_3 + \beta_4 + \dots + \beta_N) \\
 &+ \alpha_3(-\beta_1 - \beta_2 + \beta_3 + \beta_4 + \dots + \beta_N) \\
 &+ \alpha_4(-\beta_1 - \beta_2 - \beta_3 + \beta_4 + \beta_5 + \dots + \beta_N) \\
 &+ \dots \alpha_N(-\beta_1 - \beta_2 - \beta_3 + \dots - \beta_{N-1} + \beta_N)].
 \end{aligned}$$

Using the relation (20) and after some arrangements of elements we obtain the following equation for the phase λ which can be assigned to a translation $\mathbf{t} = [t_x, t_y]$

$$\frac{1}{2}\eta(t_x t_y + \eta n),
 \tag{22}$$

where $n = -\beta_1\alpha_2 - (\beta_1 + \beta_2)\alpha_3 - \dots - (\beta_1 + \beta_2 + \dots + \beta_{N-1})\alpha_N$ is an integer. The first term in (22) denotes the phase which is constant for a given translation, whereas the second one is changing according to n . The phase factor is an exponential function of phase what means that its different values correspond to n being the elements of the set $\{0, 1, 2, \dots, q - 1\}$.

The order of the magnetic translation group for the symmetric gauge is therefore independent on the parity of p and reads

$$|\text{MTG}| = |T|q.
 \tag{23}$$

All values of n mentioned above are achievable by appropriate translations. The circle around the border of the lattice cell does not change the part of the phase related to coordinates $(\frac{1}{2}\eta t_x t_y)$, whereas the whole phase is increased or decreased by

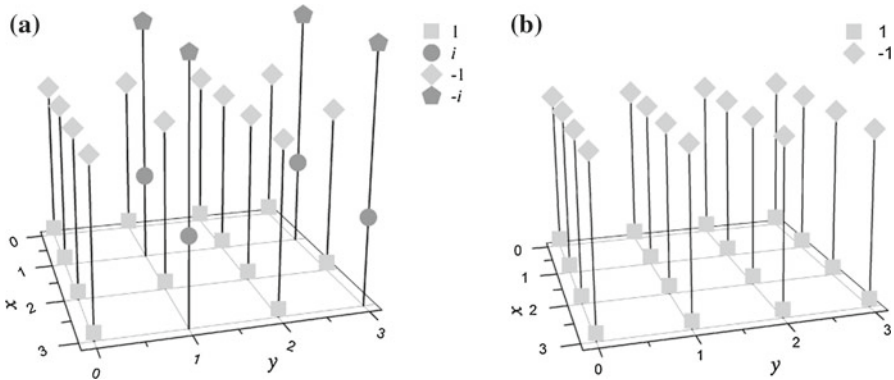


Fig. 2 The structure of the magnetic translation group. The parameters of the models are $\eta = 1/2$, $L = 4$. The part **a** corresponds to symmetric gauge whereas part **b** to Landau one. The translations are related to the lattice points, and the phases are marked by the *geometric symbol* (the values of them are explained on the legend) on the *line* associated to each point (translation)

η depending on the direction of circulation. This means that the value of n is changing by 1, so all values from the set $\{0, q - 1\}$ are possible.

Despite the fact, that the order of the group does not depend on the parity of p , what was suggested by the Eqs. (19) obtained by Opechowski and Tam, some features of the group structure are related to it. The structure of MTG can be demonstrated graphically (see Fig. 2). To each translation, denoted as lattice points, we can assign a vertical line with phases marked on it. The line we refer as a fibre. The type of fibres depends on the parity of the parameter p . For even value of it all the fibres are the same, whereas for odd value this is not the case. This time there are two types of fibres which differ by the values of phases, despite having the same number of them. The type is determined by the parity of the product $t_x t_y$ in the equation for the phase (22). In the Fig. 2 an example of the magnetic group structure for two discussed gauges and for the finite lattice of the dimension 4×4 with the magnetic field given by parameter $\eta = 1/2$ is presented.

Using the Eq. (22) each group element can be expressed by the product of generators \mathbf{a} and \mathbf{b} . It is easy to check that $\mathbf{a}^{t_x} \mathbf{b}^{t_y}$ results in element corresponding to translation $[t_x, t_y]$

$$\mathbf{a}^{t_x} \mathbf{b}^{t_y} = \left(t_x, t_y, \exp \left(2\pi i \frac{1}{2} \eta t_x t_y \right) \right).$$

The additional phase related to integer n (22) can be achieved by the product of generators corresponding to path which encircles the elementary lattice cell, located at (t_x, t_y) . This can be written as $\mathbf{a} \mathbf{b} \mathbf{a}^{-1} \mathbf{b}^{-1}$. Eventually, the element $g \in \text{MTG}$ reads

$$g = \mathbf{a}^{t_x} \mathbf{b}^{t_y} (\mathbf{a} \mathbf{b} \mathbf{a}^{-1} \mathbf{b}^{-1})^n, \quad n \in \{0, 1, 2, \dots, q - 1\}. \tag{24}$$

The similar calculation can be done for the Landau gauge. With the help of the multiplication rule (14), and using the sequence of translation described by the numbers

α_i and β_i we can find the relation for a phase factor, which can be assigned to a given lattice point (a translation vector) with coordinates (t_x, t_y) , in the form

$$\exp(-2\pi i t_x t_y \eta) \exp(2\pi i \eta n), \quad n \in \mathbb{Z}. \tag{25}$$

The analysis of this equation reveals, that each translation $\mathbf{t} = [t_x, t_y]$ is associated with exactly q distinct phases, for each parity of p . Each group element can written then, by the use of product of generators as follow

$$\begin{aligned} g &= (t_x, t_y, \exp(-2\pi i t_x t_y \eta) \exp(2\pi i \eta n)) \\ &= \mathbf{b}^{t_y} \mathbf{a}^{t_x} (\mathbf{a} \mathbf{b} \mathbf{a}^{-1} \mathbf{b}^{-1})^n, \quad n \in \{0, 1, \dots, q - 1\}. \end{aligned} \tag{26}$$

2.3.2 The maximal abelian subgroup

The determination of irreducible representations of MTG is based on the induction procedure from the maximal abelian subgroup H [30, 65, 66] of MTG. The lattice cell builds by the translations from H is called the magnetic cell and magnetic flux passing through it consists of p quanta h/e . The circulation around the magnetic cell changes the phase by a multiple of 2π . One of possible choices of such a subgroup H consists in increasing q times the elementary translation along y axis. In this case, an element of H reads

$$h = (t_x, qm, \lambda), \quad m \in \{0, 1, 2, \dots, \mu\}, \quad \mu = L/q. \tag{27}$$

There are also other ways of choosing of maximal abelian subgroup [66]. Another one is based on increasing of elementary cell q times, but along x axis. Both discussed choices lead to isomorphic group. The change of gauge of vector potential also does not alter the properties of this group.

2.4 The irreducible representations of magnetic translation group

The irreducible representation of MTG are very important in the description of dynamics of Bloch electron in a magnetic field. These representations for finite and infinite crystals were introduced by Zak together with the notion of MTG [64, 65]. The similar results were obtained by Brown, who considered the ray representation of translation group [63]. In the paper by Zak [65] a class of irreducible representations called “physical” was characterised. It is determined by the conventional choice of the one-dimensional representation Δ of the element $h = (0, 0, \lambda)$ ($h \in H$), and all irreducible representations induced from it are physical. Such a selection of IRR is justified by the argumentation that the action of an element $(0, 0, \lambda)$ should not induce different change of phase of wave function and therefore only one irreducible representation is important, whereas the others are non physical.

The representations obtained by Zak are of finite dimensions if the number of flux quanta per elementary cell is rational. For an integer value of this quantity the magnetic

translation group is isomorphic with the ordinary translation group and its irreducible representations are one-dimensional.

The classification of MTG's and their IRRs for different values and orientation of a magnetic field was given by Opechowski and Tam [66]. All the considered representations were physical. Authors discussed also cases related to non-rational value of η . This value provided the infinite dimension of IRRs.

The analysis of irreducible representation of infinite dimensions was presented also by Boon [67]. He showed that the group has the infinite number of class of irreducible representations and all of them are of infinite dimension. The more important role from mathematical and physical point of view is played then by primary representations, i.e. the representations which can not be decomposed into a direct sum of two disjoint representations.

Geyler and Popov [30] considered the symmetry group of the lattice Hamiltonian (5). They presented irreducible representations of the group generators for rational magnetic field and parametrized them by the points of the torus $T_\eta = [0, q^{-1}) \times [0, 1)$.

The relation between the magnetic translation group and Weyl-Heisenberg (WHG) group was given by Zak [80]. The latter characterizes the symmetry of an electron in a magnetic field whereas the former is related to the symmetry reduction caused by the periodic potential (MTG is a subgroup of Weyl-Heisenberg group). The irreducible representations of WHG decompose, by this reduction, into IRRs of MTG and the multipliers are constant. The properties of both groups were analysed in the phase space and the periodic boundary conditions are used.

In the next part of the section we focus our attention on the irreducible representations of symmetry group of the lattice Hamiltonian. We extend however the scope of research and consider also "nonphysical" representations ($s > 1$). Let us start the description with a basic information about the induction method used for obtaining the IRRs.

The induction procedure uses the irreducible representation of the maximal abelian subgroup, or, strictly saying, of the little group of the representation Δ [30,65,66,81,82]. The latter coincides with maximal abelian subgroup for physical representations and, as will be shown in the next part of this section, also for other representations whose parameter s is in relation with magnetic field parameter η . The further considerations are restricted to such cases therefore we present at this point only the representation of group H.

Elements of this group in the symmetric gauge are given by the formula

$$(t_x, qm, \lambda) = (t_x, 0, 0)(0, qm, 0) \left(0, 0, \lambda - \frac{1}{2} p m t_x \right), \quad (28)$$

where $m \in (0, 1, \dots, \mu - 1)$, and $\mu = L/q$. The irreducible representation of H are product of IRRs of three cyclic group and are characterised by three indices $\{\kappa_x, \kappa_y, s\}$ [66]

$$\Delta^{\kappa_x, \kappa_y, s}(t_x, qm, \lambda) = e^{2\pi i \kappa_x t_x} e^{2\pi i \kappa_y qm} e^{2\pi i s (\lambda - \frac{1}{2} m p t_x)}. \quad (29)$$

The indices κ_x and κ_y correspond to translations along axis x and y , respectively, and are determined by the boundary conditions

$$\kappa_x = l_1/L, \quad l_1 = 0, 1, \dots, L - 1, \tag{30}$$

$$\kappa_y = l_2/L, \quad l_2 = 0, 1, \dots, L/q - 1. \tag{31}$$

They are readily recognised as admissible quasimomenta in the presence of magnetic field.

It should be remarked that the choice of a maximal abelian subgroup can be done in several ways. The above equations match the condition for which the magnetic cell is broadened in y direction.

The parameter s labels the representations of the subgroup related to phase λ and its range is given by formula

$$s = 0, 1, \dots, q - 1.$$

The value $s = 1$ corresponds to the physical representation [65]. The other values we interpret as the number of electrons which occupy a state corresponding to the IRR with indices (κ_x, κ_y, s) (see Sect. 4).

The next step in the induction is determination of orbits Ω of the action of MTG on the set of representation Δ . Two representations Δ and Δ' belong to the same orbit if there is an element $g \in$ MTG for which the following equation is fulfilled

$$\Delta'(h) = \Delta(g^{-1}hg) \tag{32}$$

for all $h \in H$. It is sufficient to consider in the role of g just representatives of H -cosets in MTG. They can be chosen as $\sigma_j = (0, j, 0)$, $j \in \{0, 1, \dots, L - 1\}$. The equation is then in the form

$$\Delta^{\kappa_x \kappa_y s}(\sigma_j^{-1}h\sigma_j) = \Delta^{\kappa'_x \kappa_y s}(h), \tag{33}$$

where

$$\kappa'_x = \left(\kappa_x + \frac{p}{q}sj \right) \text{ mod } 1. \tag{34}$$

For a given $\eta = \frac{p}{q}$ and s the representation $\Delta^{\kappa'_x \kappa_y s}$ and $\Delta^{\kappa_x \kappa_y s}$ belong to the same orbit Ω for all indices κ'_x which can be obtained from the Eq. (34) substituting j by the value from the set $0, 1, \dots, q - 1$.

There are three types of orbits parametrised by the value of s

- $s = 0$: each representation Δ constitutes an orbit,
- $s = 1$: there are μ orbits consisting of q elements,
- $s > 1$:
 - if q is divisible by s ($q/s = r$) - there are μs orbits consisting of r elements,
 - if $\text{gcd}(s, q) = 1$ - there are μ orbits consisting of q elements.

The key of the method of induction is the following procedure [81]: (i) one takes a single IRR $\Delta_i \in \Omega_i$ from each orbit Ω_i , (ii) one determines the little group G_{Δ_i} of Δ_i ($H \leq G_{\Delta_i} \leq \text{MTG}$), (iii) one finds all admissible IRRs Θ of G_{Δ_i} , (iv) the set of all induced representations of the form $\Theta \uparrow \text{MTG}$ constitutes the complete set of IRRs of MTG.

The little group G_{Δ_i} consists of such elements $g' \in \text{MTG}$, which satisfy

$$\Delta(h) = \Delta(g'^{-1}hg'). \tag{35}$$

It can be shown that this group depends on the value of the parameter s :

- $s = 0$: $G_{\Delta} = \text{MTG}$
- $s = 1$: $G_{\Delta} = \text{H}$
- $s > 1$:
 q is divisible by s , $q/s = r$: $\text{H} < G_{\Delta} < \text{MTG}$,
 $\text{gcd}(s, q) = 1$: $G_{\Delta} = \text{H}$.

In the following we restrict our consideration to the case $G_{\Delta} = \text{H}$, i.e. to the condition

$$\text{gcd}(s, q) = 1. \tag{36}$$

All representations of this little group are allowed [81]. Under this conditions the IRRs of MTG are induced from the IRRs of H

$$\Gamma^{K_x K_y S} = \Delta^{K_x K_y S} \uparrow \text{MTG}.$$

The matrix of the representation Γ in the basis labelled by the coset representatives σ_j is given by the formula [81]

$$\Gamma_{(j,i)}^{K_x K_y S}(g) = \begin{cases} \Delta^{K_x K_y S}(\sigma_j^{-1}g\sigma_i) & \text{if } \sigma_j^{-1}g\sigma_i \in \text{H}, \\ 0 & \text{if } \sigma_j^{-1}g\sigma_i \notin \text{H}, \end{cases} \tag{37}$$

where indices $(j, i) \in \{0, 1, 2, \dots, q-1\}$ label the rows and the columns. The product in the Eq. (37)

$$\sigma_j^{-1}g\sigma_i = \sigma_j^{-1}(t_x, mq + j', \lambda)\sigma_i = \left(t_x, mq + j' - j + i, \lambda + \frac{1}{2}\eta t_x(j + i) \right)$$

belongs to the subgroup H if

$$j' - j + i = 0 \text{ mod } q, \tag{38}$$

what determines the coordinates of the matrix element whose value are given by the formula $\Delta^{K_x K_y S}(t_x, mq, \lambda + \frac{1}{2}\eta t_x(j + i))$. The remaining elements of the matrix are equal to 0.

3 Magnetic bands

3.1 The eigenvalue problem in the symmetry adapted basis

The lattice Hamiltonian (7) for Landau gauge is given by the formula

$$\mathcal{H}_t |j_x, j_y\rangle = t \left(|j_x + 1, j_y\rangle + |j_x - 1, j_y\rangle + e^{2\pi i \eta j_x} |j_x, j_y + 1\rangle + e^{-2\pi i \eta j_x} |j_x, j_y - 1\rangle \right). \tag{39}$$

The solution of an eigenvalue problem in the coordinate basis is nothing but the diagonalisation of the Hamiltonian matrix of the dimension $L^2 \times L^2$. As a result eigenfunctions are given in the coordinate basis and in order to obtain the band structure we should change this basis to quasimomentum one.

In the absence of a magnetic field the construction of matrix which allows the transformation from one basis to the other is done with the help of two-dimensional Fourier transform whose elements are given by the formula

$$F_{(j_x, j_y)(k_x, k_y)} = \frac{1}{L} e^{-i(j_x k_x + j_y k_y)}, \tag{40}$$

where the vectors $|j_x, j_y\rangle$ of the coordinate basis label the rows whereas quasimomenta $|k_x, k_y\rangle$ label the column of the matrix F . Hamiltonian $\mathcal{H}_t^{B=0}$ (without the magnetic field all the phases θ in the Eq. (5) are equal 0) in the quasimomentum basis

$$\mathcal{H}_t^{B=0} = F^\dagger \mathcal{H}_t^{B=0} F \tag{41}$$

is of the diagonal form.

In the presence of a magnetic field the problem of diagonalisation of the Hamiltonian is more complicated and requires the symmetry given by the magnetic translation group. It is used to determine the matrix F^B which transform the coordinate basis to symmetry adapted one [83]. The construction of such a matrix is done with the help of a projection operator

$$P_{ll}^f = \frac{n_f}{|\text{MTG}|} \sum_{g \in \text{MTG}} \Gamma_{ll}^f(g^{-1}) \delta(g). \tag{42}$$

The action of this operator on the vectors of coordinate basis gives the non-zero vectors only when they belong to the subspace V_f spanned by the basis of irreducible representation Γ^f . The index f labels the the IRRs of MTG, i.e. it is related to three numbers (κ_x, κ_y, s) . n_f means the dimension of those representations, whereas the bottom indices ll determine the row and column of their matrices. The symbol $\delta(g)$ denotes the representations of MTG in the coordinate basis and is defined by the action of the group generators on the elements of the basis $|j\rangle$

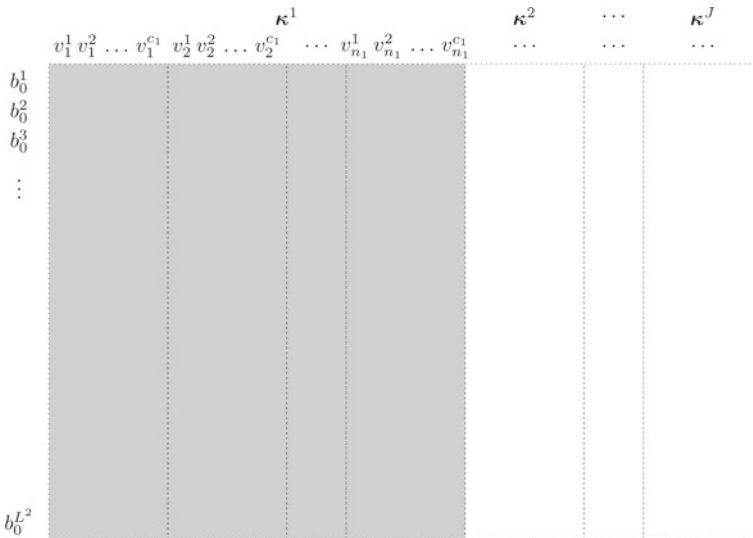
$$\delta(1, 0, 0) |j_x, j_y\rangle = |j_x + 1, j_y\rangle, \tag{43}$$

$$\delta(0, 1, 0)|j_x, j_y\rangle = e^{-2\pi i \eta j_x} |j_x, j_y + 1\rangle. \tag{44}$$

The representation δ decomposes into irreducible ones

$$\delta = \sum_f c_f \Gamma^f. \tag{45}$$

The matrix F^B is constructed with the help of projection operators (42) introduced above. Briefly speaking the procedure starts with determination of the matrix P_{11}^f , then we should choose from it c_f linear independent columns ($v_1^1, v_1^2, \dots, v_1^{c_f}$). The rest of the vectors which build the basis of subspace V^f is obtained from the equation $v_l^i = P_{ll}^f v_1^i$, for $l = 2, 3, \dots, n_f, i = 1, 2, \dots, c_f$. If this scheme is repeated for all representation Γ^f and the columns are properly arranged we finish, eventually, with the matrix of the form



The rows are label by the vectors of coordinate basis $\{b_0^1, b_0^2, \dots, b_0^{L^2}\} \in b_0$, whereas the columns are indexed by the irreducible representations with J denoting the number of them. The shadowed rectangle corresponds to the representation Γ^1 and creates the operator F_B^1 which reduces the eigenvalue problem of the Hamiltonian \mathcal{H} to selected quasimomentum $\mathbf{k}^1 = 2\pi \kappa^1 = (2\pi \kappa_x^1, 2\pi \kappa_y^1)$

$$\mathcal{H}_{\kappa^1} = (F_B^1)^\dagger \mathcal{H} F_B^1. \tag{46}$$

Similarly each of the rest operators F_B^f reduce the eigenvalue problem to given quasi-momentum $\mathbf{k}^f = (2\pi \kappa_x^f, 2\pi \kappa_y^f)$, whereas operator F^B transforms the Hamiltonian to quasi-diagonal form $\mathcal{H}' = (F^B)^\dagger \mathcal{H} F^B$ with the shape as below

$$\begin{matrix}
 & \kappa^1 & \kappa^2 & \dots & \kappa^J \\
 \kappa^1 & \boxed{} & & & \\
 \kappa^2 & & \boxed{} & & \\
 \vdots & & & \ddots & \\
 \kappa^J & & & & \boxed{}
 \end{matrix}$$

Each block on the diagonal is indexed by quasimomenta and consists of n_f identical submatrices labelled by index γ . Each of them has rows and columns labelled by index γ' according to the schema as below

$$\begin{matrix}
 & \gamma_1 & \gamma_2 & \dots & \gamma_{n_f} \\
 & \gamma'_1, \dots, \gamma'_{c_f} & \gamma'_1, \dots, \gamma'_{c_f} & \dots & \gamma'_1, \dots, \gamma'_{c_f} \\
 \gamma'_1 & \boxed{} & & & \\
 \vdots & & & & \\
 \gamma'_{c_f} & & \boxed{} & & \\
 \gamma'_1 & & & \ddots & \\
 \vdots & & & & \\
 \gamma'_{c_f} & & & & \boxed{}
 \end{matrix}$$

The dimension n_f of irreducible representations for which the Eq. (36) is fulfilled is equal to q .

From the above consideration we see that the quantum state is characterised by four quantum numbers $|\kappa_x, \kappa_y, \gamma, \gamma'\rangle$. The numbers γ and γ' correspond to degenerations of energy level and the numbers of magnetic subbands, respectively. The quantum states can be also described by the density matrices

$$\rho^{\kappa_x, \kappa_y, \gamma, \gamma'} = |\kappa_x, \kappa_y, \gamma, \gamma'\rangle \langle \kappa_x, \kappa_y, \gamma, \gamma'|. \tag{47}$$

The index s , which characterises also the IRRs of MTG is omitted in the above notations, since for one-electron states it is constant and equals 1.

One can find also another solution of eigenvalue problem presented in this section (see e.g. [42,84,85]). The Eq. (39) through the appropriate substitution can be converted to Harper equation which depends only on one variable. It can be written as a q dimensional matrix whose parameters are k_x and k_y . In the magnetic field the allowed

value of quasimomentum \mathbf{k} are different from those related to Brillouine zone without magnetic field and their values are defined by the irreducible representation of MTG. Therefore in the magnetic field we should consider the reduced Brillouine zone (see e.g. [42]). The detailed description of this Brillouine zone is presented in the next section.

The Harper matrix corresponds to Hamiltonian \mathcal{H}_{k_x, k_y} (46), i.e. Hamiltonian obtained with the help of the projection operator. This method allows to determine, in addition, the degeneracy of the energy levels denoted by index γ (\mathcal{H}_{k_x, k_y} consists of q submatrices which are identical). The method requires, however, as nearly every group theory method, laborious calculation. Fortunately, nowadays with the help of computers these computations are not so onerous as before. As the result we obtain the full set of quantum numbers which describe the states of an electron. The method provides also the set of nonequivalent quasimomenta which form the Brillouine zone in a magnetic field.

3.2 Magnetic band Brillouin zone

The band structure in solid state physics is defined over Wigner–Seitz cell of the reciprocal lattice, i.e. over the first Brillouin zone. For the discussed two-dimensional lattice and turned off magnetic field the Brillouine zone consists of the set of these quasimomenta which are the indices of IRRs of the translation group T. Their values are determined by the Born–von Karman periodic conditions.

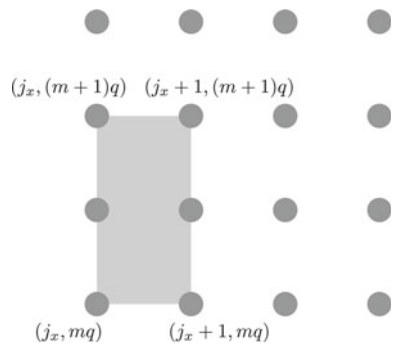
The problem is more complicated at the presence of a magnetic field. In this case the boundary condition task can be solved by applying the Haldane sphere, for which the space boundary disappears [75]. The magnetic field is generated by Dirac monopole placed in the centre of the sphere with electrons distributed on the surface. The good quantum number is a angular momentum and the technique used in description of many-electrons atoms [86] can be transferred to system of electrons on that surface (see e.g. review paper [87]).

In this paper we will use however quasimomentum \mathbf{k} as a quantum number and describe the energy band structures with help of them, i.e. consider the bands over the Brillouin zone. The choice of boundary conditions, in spite of their imperfection in application for finite crystals [88], is motivated by the benefit provided by them. As a result we obtain description of electron dynamics as a function of quasimomentum and can use the energy band scheme, widely applied in the solid state physics. The detailed description of the Brillouin zone in a magnetic field together with the discussion concerning finite crystals can be found in our paper [89].

The first step in construction of the Brillouin zone in a magnetic field is determination of abelian subgroup $H \in \text{MTG}$, which defines the magnetic cell of the lattice (see Fig. 3). Its size depends on the magnetic field through the parameter q , however the shape of it is not definitely established. We can choose it as rectangle with one of its edges q times longer than the other, but the direction of the longer edge can be selected along x , as well as along y axis. Both directions are equally good.

The magnetic cell defines the new lattice, for which one can determine the reciprocal lattice and find the corresponding Brillouine zone in magnetic field—magnetic

Fig. 3 The magnetic cell of two-dimensional square lattice, $m \in \{0, 1, \dots, \mu\}$



Brillouin zone (MBZ). The comparison between the reciprocal lattice with and without magnetic field shows that the number of allowed quasimomenta is fewer in the former [28]. We say that the Brillouin zone is rarefied in one direction. The values of quasimomenta, connected with the indices of the group H (see Eqs. 29, 30, 31) through the formulas $k_x = 2\pi\kappa_x, k_y = 2\pi\kappa_y$, are given by

$$k_x = \left\{ 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \dots, \frac{(L-1)2\pi}{L} \right\}, \tag{48}$$

$$k_y = \left\{ 0, \frac{2\pi}{L}, \dots, \frac{(L/q-1)2\pi}{L} \right\}. \tag{49}$$

All nonequivalent representations Γ of MTG are determined if the procedure of induction is carried out for selected representations Δ , being representatives of a class of nonequivalent representations of H (see Eqs. 33, 34). This means that the index κ_x and this way also the quasimomentum k_x does not take all values from Eq. (48). The energy bands are defined over the nonequivalent set of quasimomenta from Brillouin zone. According to the discussion in Sect. 2.4 the number of orbits (equivalence classes) of representations of H, under the condition $\text{gcd}(s, q) = 1$, is equal to μ , and each orbit consists of q elements. This way the original set k_x (48) is q -tuply reduced.

The set of nonequivalent quasimomenta (k_x, k_y) over which the band structure is defined will be eventually q^2 -tuply rarefied. This rarefication appears along both perpendicular directions. In one direction it is connected with the translational symmetry given by magnetic cell. The relations between the quasimomenta, as a result of equivalence between the irreducible representations of MTG, cause the rarefication in the second direction. The Brillouin zone determined in this way is referred in the literature as “small magnetic Brillouin zone” [80], however we prefer to use the name “magnetic band Brillouin zone” (MBBZ in short) since the band structure in a magnetic field is defined with help of it.

3.3 The rarefied Brillouin zone and degeneration of states

The Brillouin zone in a magnetic field is q^2 times rarefied. The number of quantum states should be constant what means that the degeneracy of energy levels is increased

in spite of creation of magnetic subbands. In the approach considered in this paper the energy band in a magnetic field splits into q subbands. These bands, however, are defined over rarefied BZ what results in q -tuply degeneration of each level. This can be easily checked

$$\text{no. of } k_x \times \text{no. of } k_y \times \text{no. of subbands} \times \text{degeneration of bands} = \frac{L}{q} \frac{L}{q} q q = L^2.$$

The complete set of quantum numbers is defined in the Sect. 3.1. Using the corresponding density matrix $\rho^{\kappa_x, \kappa_y, \gamma, \gamma'}$ (Eq. 47) we can define the operator $P^{\kappa_x, \kappa_y, \gamma'}$ which projects onto the subspace of states related to eigenvalue $E_{\kappa_x, \kappa_y, \gamma'}$

$$P^{\kappa_x, \kappa_y, \gamma'} = \sum_{\gamma=1}^q \rho^{\kappa_x, \kappa_y, \gamma, \gamma'}. \quad (50)$$

We can use it for testing concurrence between the vectors $\mathbf{k} \in \text{BZ}$ and the eigenstates of the energy $E_{\kappa_x, \kappa_y, \gamma'}$ by introducing the operator

$$c_{\mathbf{k}}^{\kappa_x, \kappa_y, \gamma'} = \frac{1}{q} \langle \mathbf{k} | P^{\kappa_x, \kappa_y, \gamma'} | \mathbf{k} \rangle. \quad (51)$$

With the help of it we obtain information how the vector \mathbf{k} matches the subspace defined by the indices γ' and $\kappa = (\kappa_x, \kappa_y)$. In this way we can determine the relations between the quasimomenta in the presence of magnetic field and those without it. The degeneration can be described then by introducing the notion of state condensations. This effect is in some way similar to the rearrangement of states in \mathbf{k} space when the magnetic field is turned on, what results in de Haas-van Alphen phenomena. Using the greatest values of the operator (51) we can select the set of \mathbf{k} , for which the concurrence between them and the state $\kappa \in \text{MBBZ}$ is the greatest. In other words in a magnetic field some of the quasimomenta disappear from BZ, but in such a way, that their residues can be observed in these quasimomenta from MBBZ, for which the value of the operator $c_{\mathbf{k}}^{\kappa_x, \kappa_y, \gamma'}$ is greater than 0. Thereby the operator can measure the concurrence of the states from BZ and MBBZ. The example of such calculations for finite system can be found in our paper [89].

4 Multi-electron states in a magnetic field

The possibility of construction of many particle Hamiltonian was mentioned already by Brown [90]. He noticed that properties of multi-electron magnetic translation operators are similar to those of the single electron ones, except that the phases are multiplied by the number of electrons in the systems. This number is related to the parameters s of appropriate irreducible representations of MTG, which we use to describe the multi-electron states.

The one-electron states in the magnetic field and periodic potential are characterised by the irreducible representations $\Gamma^{\kappa_x, \kappa_y, s}$ with parameter $s = 1$, i.e. by the “physical”

representations. It will be shown in this section that IRRs with parameter $s > 1$ are also important from physical point of view. W. Florek was the first who pointed out that such kind of representations can be used for description of system of two electrons [91]. He considered the tensor products of two representations and demonstrated that they describe the system of two charged particles in a magnetic field. Multi-electron states analysed by the use of product of IRRs can be found in others papers of this author [92,93]. The method was used also for classification of states of trion X^\pm (the system consisting of two holes and one electron or two electrons and one hole) [94]. The argument for using all IRRs of MTG, even those described by Zak as “non-physical” [65], one can find in the paper [95]. The justification was based on the algebraic relations between the charge of the particle, magnetic field and the size of finite system. The discussion was conducted for wide class of vector potentials which are the linear function of coordinates $A_\alpha = \sum_\beta a_{\alpha\beta} \beta$, $\alpha, \beta = x, y, z$.

This section concern the way of description of multi-electron states in the magnetic field proposed by us in paper [96]. The key role in it is played by the representations of magnetic translation group. Starting from the representations of MTG defined in coordinate space we build their tensor products, and finally decompose them into irreducible representations. Clearly this decomposition consists of representations Γ with parameter $s > 1$ and equal to the number of particles in the system. This method is somehow similar to that proposed by Florek, however he has used the product of IRRs. Our further consideration will be restricted to the system of identical particles—electrons. For making a presentation more clear we focus our attention on the system of three electrons (identical particles contrary to different ones considered by Florek), keeping in mind that the change of number of electrons is straightforward. It should be noticed, however, that increase in number of particles results in rise of computational complexity, especially in the case of permutation and unitary groups.

4.1 The space of three electrons

We consider as in previous sections the square lattice of the dimension $L \times L$. Electrons can jump from one node of the lattice to its nearest neighbours and their positions fully describe the orbital (spatial) state of an electron. The space available for particles is limited in a finite system and is enclosed by Born–von Karman boundary conditions. The additional restriction is provided by the Pauli principle since one has to take into account the spin of the electrons. This means that only two electrons can have the same position, having simultaneously the opposite spin projections.

We label now the base for one-electron states introduced in Sect. 2 using integers

$$b_O = \left\{ |u\rangle, u \in \left\{ 1, 2, \dots, L^2 \right\} \right\}, \quad (52)$$

where u denotes the coordinates of node $|j_x, j_y\rangle$. The space of single-electron states, referred to as orbital space, can be considered as a linear closure over the vectors of the basis b_O

$$h_O = l_{\mathbb{C}} b_O. \quad (53)$$

The spin space reads

$$h_s = lc_C \tilde{2}, \quad (54)$$

where $\tilde{2} = \{+, -\}$ is a set of projections of spin $s = 1/2$. The total single-electron space is the tensor products of both spaces $h = h_O \otimes h_s$.

The tensor product of h , in turn, allow us to consider the multi-electron states, e.g. three-electron $h^{\otimes 3} = h \otimes h \otimes h$. The electrons are fermions, so from the whole space of states

$$h^{\otimes 3} = h^{\{3\}} + h^{\{2,1\}} + h^{\{1^3\}}, \quad (55)$$

one should select only the last term. Its presentation as a tensor product of orbital and spin space reads

$$h^{\{1^3\}} = h_O^{\{3\}} \otimes h_s^{\{1^3\}} + h_O^{\{2,1\}} \otimes h_s^{\{2,1\}} + h_O^{\{1^3\}} \otimes h_s^{\{3\}}. \quad (56)$$

For electrons (spin $s = 1/2$) only the last two subspaces are available. The upper indices in formulas (55) and (56) denote the partitions λ of 3.

4.2 The Hamiltonian

The lattice Hamiltonian for a single particle is of the form

$$\mathcal{H}_1 = -t \sum_{D,C,\sigma} |C\sigma\rangle \langle D\sigma| \exp(2\pi i \vartheta_{DC}), \quad (57)$$

where D and C denote the nearest neighbours of a given node, σ is the spin projection along z axis, and ϑ_{DC} is a phase associated to the edge connecting nodes. The parameter t is a hopping integral defined as constant on each edge.

The Hamiltonian for three electrons is written as a suitable sum of tensor products of single-electron Hamiltonian and identity operator I as

$$\mathcal{H}_1^3 = \mathcal{H}_1 \otimes I \otimes I + I \otimes \mathcal{H}_1 \otimes I + I \otimes I \otimes \mathcal{H}_1. \quad (58)$$

Within the model we are able to consider Coulomb repulsion between pairs of particles with the same coordinates (but different spin projection). We can write this part of Hamiltonian as

$$\mathcal{H}_u = \mathcal{H}_{12} + \mathcal{H}_{13} + \mathcal{H}_{23}, \quad (59)$$

where the term \mathcal{H}_{ij} represents the repulsion between particle i and j and can be written as follows

$$\begin{aligned}
 \mathcal{H}_{12} &= U \sum_{C, D \neq C, \sigma} (|C \uparrow\rangle \otimes |C \downarrow\rangle \otimes |D\sigma\rangle) (\langle C \uparrow| \otimes \langle C \downarrow| \otimes \langle D\sigma|), \\
 \mathcal{H}_{13} &= U \sum_{C, D \neq C, \sigma} (|C \uparrow\rangle \otimes |D\sigma\rangle \otimes |C \downarrow\rangle) (\langle C \uparrow| \otimes \langle D\sigma| \otimes \langle C \downarrow|), \\
 \mathcal{H}_{23} &= U \sum_{C, D \neq C, \sigma} (|D\sigma\rangle \otimes |C \uparrow\rangle \otimes |C \downarrow\rangle) (\langle D\sigma| \otimes \langle C \uparrow| \otimes \langle C \downarrow|).
 \end{aligned}
 \tag{60}$$

The parameter U is a measure of repulsive force between pairs of electrons, and is given as a multiple of parameter t . The Hamiltonian \mathcal{H}_U is known as a Hubbard's Hamiltonian introduced first time in quantum chemistry by Pople [97] and Pariser and Parr [98, 99]. In solid state physics it was formulated independently by Hubbard [100], Gutzwiller [101] and Kanamori [102].

The full Hamiltonian will be taken as the sum of defined terms

$$\mathcal{H} = \mathcal{H}^3 + \mathcal{H}_U.
 \tag{61}$$

4.3 Irreducible bases for the system of three electrons

Thanks to separation of orbital and spin parts (Eq. 56), three-electron system can be studied only in orbital space since the permutational symmetry of the spin space is already fixed by the principle of Pauli. Our further description will be restricted to the symmetry in the orbital space.

In this space three groups act: the permutation group Σ_3 , the unitary group $U(L^2)$ permuting the states, and the magnetic translation group. The irreducible representations of mentioned groups introduce the symmetry adapted basis for which the Hamiltonian (61) reaches a quasideagonal form. The basis determined by the IRRs of symmetric and unitary group introduce the total spin as an exact quantum number, whereas the IRRs of MTG allow to diagonalize eigenvalue problem in the basis of quasimomenta belonging to the magnetic band Brillouin zone. The operators transforming the eigenvalue problem between discussed bases provide the whole description of the system of three electrons, i.e. a complete set of quantum numbers: total spin S , quasimomentum $\mathbf{k} \in \text{MBBZ}$ and index of magnetic subbands γ' .

Let us consider first the eigenvalue problem in the basis adapted to the symmetry given by symmetric group. The basis of IRRs of Σ_3 can be written as [103]

$$b_O^{irr} = \{|\lambda t y\rangle, \lambda \vdash 3, t \in \text{WT}(\lambda), y \in \text{SYT}(\lambda)\},
 \tag{62}$$

where $\text{WT}(\lambda)$ is the set of Weyl tableaux of the shape λ , filled in semistandardly by letters of the alphabet $\tilde{2}$, and $\text{SYT}(\lambda)$ denotes the set of all standard Young tableaux of the same shape λ in the alphabet of indices of particles ($\text{WT}(\lambda)$ and $\text{SYT}(\lambda)$ is standardly used as the basis for the irrep D^λ of $U(L^2)$ and Δ^λ of Σ^3 , respectively). Description of symmetric group and its representation can be found in the book by Sagan [104], whereas its application in quantum chemistry is described in paper by Karwowski [105]. The basis of the spin part of the space of three electron states is given by

$$b_s^{irr} = \left\{ |\tilde{\lambda}, M \rangle \right\}, \tag{63}$$

where $\tilde{\lambda}$ is a transposition of partition λ , and $M \in \text{SSYT}(\tilde{\lambda})$ is a semistandard Young tableaux, i.e. the indices are placed in the tableaux in non-decreased order in rows and strictly increased order in columns. M has the meaning of projection of the total spin of the electrons.

Basis (62) can be constructed by use of the projection operator which allows to find such states, which demonstrate requested permutational symmetry [106]

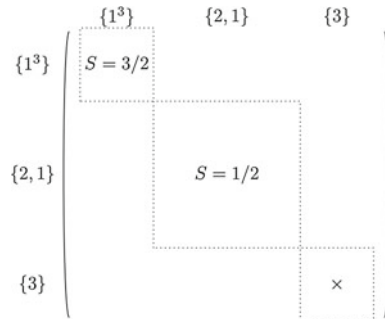
$$P^{(\lambda,t,y)} = \text{const} \sum_{\sigma} \langle y(t) | \sigma | y \rangle \sigma. \tag{64}$$

$\sigma \in \Sigma_3$ denotes a permutation of three-particle states $|j_1, j_2, j_3\rangle$, where j_i means the coordinates of the i -th particle. The term $\langle y(t) | \sigma | y \rangle$ is an element of the matrix of IRRs of the symmetric group. The symbol $y(t)$ denotes the Young tableaux obtained from Weyl tableaux through the appropriate exchange of state numbers by particle numbers (detail can be found in our paper [96]).

With the use of projection operator we can build the matrix K which transform the eigenvalue problem from coordinate basis to the symmetry adapted one. This matrix is also know in the literature as “Kostka matrix written on the level of basis” [107]. The element of this operator reads

$$K_{|j_1, j_2, j_3\rangle}^{|\lambda, t, y\rangle} = \langle j_1, j_2, j_3 | \sum_{\sigma} \langle y(t) | \sigma | y \rangle \sigma | j'_1, j'_2, j'_3 \rangle, \tag{65}$$

where the rows are labelled by $|j_1, j_2, j_3\rangle$ and columns by $|\lambda, t, y\rangle$. The Hamiltonian in this new basis is of the form



The rows and the columns in blocks (labelled by λ) on the diagonal are numbered by pairs (t, y) of Young tableaux y and Weyl tableaux t . Thanks to the relation between partitions λ and $\tilde{\lambda}$ we can assign the total spin to each submatrix. The cross in the right bottom corner of the matrix denotes the non-physical states, i.e. states impossible for three electrons due to the Pauli principle.

Diagonalization of the Hamiltonian in the basis of quasimomenta was already discussed in Sect. 3.1, where the transformation matrix F^B was also introduced. It should be adapted to the case of multi-electron system by taking the appropriate reducible and

irreducible representations with parameters $s > 1$. The single-electron representation δ is used for construction of $\delta^{\otimes 3}$ which is related to the system of three electrons. Its decomposition into irreducible representations of MTG

$$\delta^{\otimes 3} = \sum_{\kappa_x, \kappa_y, s} m(\kappa_x, \kappa_y, s) \Gamma^{\kappa_x, \kappa_y, s} \tag{66}$$

contains only such of them, whose parameter $s = 3$. The factor $m(\kappa_x, \kappa_y, s)$ determines the multiplicity of representation Γ in this decomposition. Eventually, the projection operator reads

$$P_{ll}^{\kappa_x, \kappa_y, s} = \frac{q}{|\text{MTG}|} \sum_{g \in \text{MTG}} \Gamma_{ll}^{\kappa_x, \kappa_y, s}(g^{-1}) \delta^{\otimes 3}(g). \tag{67}$$

q denotes the dimension of the Γ , and parameter s is equal to 3. With the use of this operator one can construct the matrix F^B which allows to diagonalize the Hamiltonian for three electrons. This time the blocks on the diagonal are labelled by the total quasimomenta of the system. The method results in energy band structure for three electrons defined over the magnetic band Brillouin zone.

The method presented above allows to describe the states of three electrons in a magnetic field and periodic potential. We obtain the whole set of quantum numbers: total spin of the system, the set of admissible quasimomenta which form the magnetic band Brillouin zone and, in this way, the energy band structure. It should be noticed, however, that from all obtained states one has to exclude non-physical ones, i.e. such states which are impossible for particles with the spin 1/2. For elimination of these states in the basis of quasimomenta we can use the operator $K^\dagger F_B$ which describes the transformation between the discussed bases

$$\langle \lambda, t, y | K^\dagger F_B = \langle \kappa_x, \kappa_y, s |. \tag{68}$$

In our paper [96] one can find an example of such approach concerning the finite system of the size 3×3 with a magnetic field given by parameter $\eta = 1/3$. Despite the small size of the system, it allows to present all basic properties of the model.

5 Discussion and conclusions

We have considered here the problem of structure of energy bands of a rectangular plaquette with periodic boundary conditions in a quantized magnetic field. To this aim, we have exploited the symmetry of the system, given by the magnetic translation group. It has to be stressed that the system consists of a plaquette, taken together with a definite amount of quanta of magnetic flux, so that each admissible value of total flux coresponds to a distinct MTG, characterised by the ratio $\eta = p/q$. We have presented the structure of magnetic subbands, with both indices, the label of a subband and the degeneracy index emerging as basis sets of IRR's of MTG.

The key role in description of magnetic energy bands in a finite plaquette is played by magnetic translation group, by means of its irreducible representations. The structure of this group is discussed in relation to gauges of the vector potential \mathbf{A} . It is pointed out that the detailed structural properties of MTG slightly depend on the chosen gauges (the symmetric and Landau gauges are described). This dependence is observed in the structure of group elements ($g = (t_x, t_y, \lambda)$), i.e. in the set of phases admissible for a given translation \mathbf{t} . Each translation is accompanied by the same set of phases, but their all values are identical for Landau gauge, whereas for symmetric one they form two different sets. The order of group does not depend on the value of p and is the same for both considered gauges. These properties are characteristic for both finite and infinite planar lattices.

The induction procedure, which provides irreducible representations of magnetic translation group, is extended to the case $s > 1$. This extension is straightforward under the condition $\text{gcd}(s, q) = 1$, for which the induction is carried out from the maximal abelian subgroup H . The procedure allows us to determine irreducible representations for a one-electron system, as well as for a multi-electron one. For both cases the energy bands in a magnetic field are defined over the admissible values of quasimomenta \mathbf{k} , constituting the magnetic band Brillouin zone. The IRR provides also additional quantum numbers characterising the band structure, i.e. the degeneracy number and the index of subbands.

With the help of IRRs of MTG one can construct a transformation matrix, which changes the coordinate basis to symmetry adapted one. The eigenvalue problem in the latter is of the quasi-diagonal form, and can be easily solved (even analytically) for the size related to nanosystem.

We focus our attention on description of Brillouin zone in a magnetic field. The field causes the rarefaction in the set of quasimomenta which constitute the Brillouin zone without magnetic field. The first step in rarefaction is connected with the magnetic cell, the cell related to the translational symmetry in a magnetic field. Translations by the distance being the multiplicity of size of this cell are not accompanied by the phase (strictly saying the phase is a multiplicity of 2π). Quasimomenta related to these translations constitute a new, magnetic Brillouin zone. The equivalence relation between IRRs of MTG causes additional diluteness of MBZ, and results in magnetic band Brillouin zone. Magnetic field splits an ordinary band into q -subbands, but since the order of final rarefaction becomes eventually q^2 , one can observe q -tuply degeneration of each subbands.

It should be stressed that irreducible representations of MTG with the index $s > 1$ are also important from physical point of view. They can be used to describe the system of s electrons (modulo q) in a magnetic field. The approach is similar to that used for the analysis of multi-electron atomic spectra. The essence of this approach is the separation of orbital and spin part of the space of states along with the permutational symmetry. Additional assumptions are Pauli principle and consideration of mutual Coulomb repulsion between pairs of electrons (Hubbard model). One can obtain, in this way, the energy band structure of multi-electrons states.

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