The magnetic translation group for a finite system and the Born-Karman boundary condition

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Abstract. The symmetry of the electron on the square planar lattice and in the magnetic field perpendicular to it is described by the magnetic translation group. The boundary condition applied to the system provides, as a consequence of the boundary equivalence, the additional equations for the possible value of magnetic fluxes penetrating the elementary cell of the lattice. These restrictions depend on the chosen gauge.

1. Introduction
The translational symmetry of moving electron in the periodic potential of a planar lattice is broken by introducing a perpendicular magnetic field $B$ described by the vector potential $A$. The symmetry group of a system in this case is the magnetic translation group (MTG) which was introduced by Zak [1] and Brown [2]. An element of this group consists of the translation $t$ and the phase $\phi$ which is connected with the path of the electron in the planar lattice and with a magnetic flux penetrating the crystal cells. The physical interpretation of the phase is given in the frame of the Bohm-Aharanow effect [3].

We restrict ourselves to the finite systems which are intensively studied nowadays due to the expected practical applications in a context of nanoelectronic. In order to describe the symmetry of such a system we should introduce boundary conditions. It can be realized in two ways: by application of the Haldane sphere [4, 5] or by the Born-Karman condition [1]. Here we use the latter condition which provides the quasimomentum as a good quantum number.

This approach requires relations between the quantized magnetic field and the Born-Karman boundary condition. This results in restriction of the possible values of magnetic field penetrating the planar lattice. The problem is discussed in detail in this paper in relation to the Landau and symmetric gauges. The Hamiltonian being considered is treated within the frame of tight binding approximation reduced to the one-band model.

2. Magnetic translation group for finite lattices
The Hamiltonian describing the system is given by the formula:

$$\mathcal{H} = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}A(r))^2 + V$$

(1)

where $A$ is the vector potential of magnetic field, $V$ is periodic potential and $p$ is the momentum of the particle. Elements $g = (t, \lambda)$ of the MTG commute with the Hamiltonian (1) and the
multiplication rule for this group is following [6]:

$$g_1 g_2 = (t_1, \lambda_1)(t_2, \lambda_2) = \omega(t_1, t_2)(t_1 + t_2, \lambda_1 + \lambda_2) = \omega(t_1, t_2)g_3$$  \hspace{1cm} (2)

where the factor $\omega(t_1, t_2)$ states the nonabelity of the group, and the element $\lambda$ is connected with the phase (we use the convention to write only the index $\lambda$ instead of the full phase $\exp(2\pi i \lambda)$). The complete form of the equation (2) depends on the gauge which can be chosen for the vector potential, and on the type of the planar lattice [6, 7].

Let us consider the square lattice with elementary vectors $a$ and $b$. Each translation within it can be written as $t = na + mb$, with $n, m$ being integers. For the model being discussed basis vectors of the Hilbert space can be labelled by these numbers $(n, m)$.

2.1. The symmetric gauge for the square planar lattice

For the symmetric gauge the vector potential is expressed by relations

$$A^S = \frac{1}{2} B \times r, \enspace A^S = -\frac{1}{2} B y \hat{x} + \frac{1}{2} B x \hat{y},$$  \hspace{1cm} (3)

where $\hat{x}, \hat{y}$ are the unit vectors of the planar square lattice. For this gauge the factors system (2)

$$\omega(t_1, t_2) = \exp \left( \frac{2\pi i}{hc/e} B(t_1 \times t_2) \right) = \exp \left( 2\pi i \frac{B_n(a \times b)}{h c / e} \right) = \exp (2\pi i \eta n).$$  \hspace{1cm} (4)

have a simple physical interpretation. The parameter $n$ is an integer expressing the area of polygon spanned by vector $t_1$ and $t_2$ in the unit of elementary cell area $a \times b$. Since the quantum of elementary flux is given by $hc/e$, the ratio $\eta = \frac{B_n(a \times b)}{hc/e}$ is the number of quanta of magnetic fluxes passing through the elementary cell. Then the multiplication rule can be written as

$$(t_1, \lambda_1)(t_2, \lambda_2) = (t_1 + t_2, \lambda_1 + \lambda_2 + \frac{1}{2} \eta n)$$  \hspace{1cm} (5)

2.2. The Landau gauge

The vector potential in the Landau gauge is given by the equation $A^L(r) = Bx \hat{y}$. The factor system for this gauge takes the form [6]

$$\omega_{A^L}(t_1, t_2) = \exp \left( -2\pi i \frac{B y t_1 y}{hc/e} \right) = \exp (-2\pi in \eta),$$  \hspace{1cm} (6)

where $t_1 y$ and $t_2 y$ are the $y$ component of $t_1$ and $x$ component of $t_2$ respectively, $n$ and $\eta$ have the same meaning as in the symmetric case, but this time the rectangle is spanned by vectors $t_1 y$ and $t_2 y$. Then the multiplication rule is given by

$$(t_1, \lambda_1)(t_2, \lambda_2) = (t_1 + t_2, \lambda_1 + \lambda_2 + \eta n)$$  \hspace{1cm} (7)

3. The Born-Karman boundary condition

For the finite planar lattice it is convenient to use periodic, e.g Born - Karman boundary condition. In this approach we identify those elements $g \in MTG$ for which translations $t$ differ by the distance $Na$ (or $Nb$)

$$(t, \lambda) = (t + Na, \lambda) = (t + Nb, \lambda) = (t + Na + Nb, \lambda).$$  \hspace{1cm} (8)

The conditions used for the multiplication rule provide the restrictions (if any exist) to the possible value of $\eta$. It is a consequence of the fact that multiplication of elements $g_1$ and $g_2$ should give the same element as multiplication of $g_1'$ and $g_2'$ which differ from $g_1$, $g_2$ by translation of the Born-Karman period. Let us consider these relations for selected gauges.
3.1. The symmetric gauge

For the symmetric gauge the multiplication rule, given by the equation (5), for any two arbitrary equivalent elements presented by the equation (8) provides 16 equations which should be fulfilled regarding the boundary conditions. They are collected in the Table 1.

Table 1. The equations being the results of Born-Karman boundary conditions applied to all pairs of elements \( g_1, g_2 \) from the equation (8). The column ‘Equation’ is obtained as the result of subtraction \( (t_1 + \alpha_1 Na + \beta_1 Nb, \lambda_1)(t_2 + \alpha_2 Na + \beta_2 Nb, \lambda_2) - (t_1, \lambda_1)(t_2, \lambda_2) \), where elements \( \alpha_1, \alpha_2, \beta_1, \beta_2 \in \{0, 1\} \), and only the indices \( \lambda \) are written in the third column.

| No. | \( g_1 \) | \( g_2 \) | Equation |
|-----|----------|----------|----------|
| 1   | \( t_1 + Na + Nb, \lambda_1 \) | \( t_2 + Na, \lambda_2 \) | \( \frac{1}{2} \eta(N(t_2^y - t_1^y) - Nt_2^z - NN) \) |
| 2   | \( t_1 + Na + Nb, \lambda_1 \) | \( t_2 + Na + Nb, \lambda_2 \) | \( \frac{1}{2} \eta N((t_1^y - t_2^y + t_2^y - t_1^y) \) |
| 3   | \( t_1 + Na + Nb, \lambda_1 \) | \( t_2, \lambda_2 \) | \( \frac{1}{2} \eta N(t_2^y - t_2^y) \) |
| 4   | \( t_1 + Na + Nb, \lambda_1 \) | \( t_2 + Nb, \lambda_2 \) | \( \frac{1}{2} \eta N(t_2^y - t_1^y + N - t_2^y) \) |
| 5   | \( t_1 + Na, \lambda_1 \) | \( t_2 + Na, \lambda_2 \) | \( \frac{1}{2} \eta N(t_2^y - t_2^y) \) |
| 6   | \( t_1 + Na, \lambda_1 \) | \( t_2 + Na + Nb, \lambda_2 \) | \( \frac{1}{2} \eta N(t_1^y + t_2^y - t_1^y + N) \) |
| 7   | \( t_1 + Na, \lambda_1 \) | \( t_2 + Nb, \lambda_2 \) | \( \frac{1}{2} \eta N(t_1^y + t_2^y + N) \) |
| 8   | \( t_1 + Na, \lambda_1 \) | \( t_2, \lambda_2 \) | \( \frac{1}{2} \eta Nt_2^y \) |
| 9   | \( t_1 + Nb, \lambda_1 \) | \( t_2 + Na, \lambda_2 \) | \( \frac{1}{2} \eta N(t_1^y - t_1^y - t_2^y - N) \) |
| 10  | \( t_1 + Nb, \lambda_1 \) | \( t_2 + Na + Nb, \lambda_2 \) | \( \frac{1}{2} \eta N(t_1^y - t_1^y - t_1^y) \) |
| 11  | \( t_1 + Nb, \lambda_1 \) | \( t_2, \lambda_2 \) | \( \frac{1}{2} \eta Nt_2^y \) |
| 12  | \( t_1 + Nb, \lambda_1 \) | \( t_2 + Nb, \lambda_2 \) | \( \frac{1}{2} \eta N(t_1^y - t_2^y) \) |
| 13  | \( t_1, \lambda_1 \) | \( t_2 + Na, \lambda_2 \) | \( \frac{1}{2} \eta Nt_2^y \) |
| 14  | \( t_1, \lambda_1 \) | \( t_2 + Na + Nb, \lambda_2 \) | \( \frac{1}{2} \eta N(t_1^y - t_1^y) \) |
| 15  | \( t_1, \lambda_1 \) | \( t_2, \lambda_2 \) | \( 0 \) |
| 16  | \( t_1, \lambda_1 \) | \( t_2 + Nb, \lambda_2 \) | \( \frac{1}{2} \eta Nt_2^y \) |

Let us consider as an example the equation labelled by the number 2 in the Table 1. It should be valid for all vectors \( t_1 \) and \( t_2 \). This means that we have two equations: \( \frac{1}{2} \eta N(t_2^y - t_1^y) = n_1 \) and \( \frac{1}{2} \eta N(t_2^y - t_1^y) = n_2, n_1, n_2 \in Z \). If the equations are valid for \( t_2^y - t_1^y = 1 \) and \( t_2^y - t_1^y = 1 \) they will be valid for all other values of \( t_2^y - t_1^y \) and \( t_2^y - t_1^y \) as well. Then we obtain

\[
\eta = \frac{2n}{N}, \tag{9}
\]

where \( n \in Z \) and \( N \) denotes the Born-Karman period. Using the same technique we can solve all other equations which are listed in the Table 1. The common solutions of this system of equations is given in the form (9).

3.2. The Landau gauge

To find the equations for \( \eta \) being the consequence of the boundary conditions we should consider, as in the symmetric case, the product of any two elements of MTG described be the equation (8). The resulted equations obtained in this way are listed in the third column of the Table 2.

Let us consider as an example the equation 3 from the Table 2. This equation should have the solution for each arbitrary values of \( t_1 \) and \( t_2 \) which yield three equations: \( \eta t_1^y N = n_1, \eta t_2^y N = n_2, \eta NNN = n_3, n_1, n_2, n_3 \in Z \). If we find solutions for \( t_1^y = t_2^y = 1 \) then we will be able to find solutions for all other values of \( t_1^y, t_2^y \) as well. Finally the solution for \( \eta \) can be written in
The equations being the results of Born-Karman boundary conditions applied to each pair of elements \( g_1, g_2 \) from equation (8) for Landau gauge. The notation is the same as in the Table 1.

| No. | \( g_1 \) | \( g_2 \) | Equation         |
|-----|----------|----------|-----------------|
| 1   | \( (t_1, \lambda_1) \) | \( (t_2, \lambda_2) \) | 0               |
| 2   | \( (t_1 + Nb, \lambda_1) \) | \( (t_2, \lambda_2) \) | \( \eta N t_2^z \) |
| 3   | \( (t_1 + Nb, \lambda_1) \) | \( (t_2 + Na, \lambda_2) \) | \( \eta N (t_{1y} + t_{2y} + N) \) |
| 4   | \( (t_1, \lambda_1) \) | \( (t_2 + Na, \lambda_2) \) | \( \eta N t_1^y \) |

the form:

\[
\eta = \frac{n}{N}. \tag{10}
\]

The common solution of equations presented in the Table 2 is equal to (10).

4. Conclusions
The Born-Karman boundary conditions applied to the electron in the finite square planar lattice with perpendicular magnetic field provide the restrictions to the possible value of parameter \( \eta \) describing this field. It is a consequence of the boundary equivalence among the elements of the symmetry group of the system, i.e. the magnetic translation group. The equations for \( \eta \) are sensitive to the choice of a gauge for the vector potential. For the symmetric gauge this parameter should be the ratio of \( 2n/N \), where \( n \) is an integer and \( N \) is the Born-Karman period, while the Landau gauge gives the condition \( \eta = n/N \). It appears that the Landau gauge is well adapted to the boundary conditions for square planar lattice, because it allows to consider, in the frame of MTG approach, more possible values of \( \eta \) then the symmetric gauge.

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