Pairs of Bloch electrons and magnetic translation groups

Wojciech Florek*
A. Mickiewicz University, Institute of Physics, ul. Matejki 48/49, 60-769 Poznań, Poland
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A product of irreducible representations of the magnetic translation group is considered. It leads to irreducible representations which were previously rejected as nonphysical. A very simple example indicates a possible application of these representations. In particular, they are important in descriptions of pairs of electrons in a magnetic field and a periodic potential. The periodicity of some properties with respect to the charge of a particle is briefly discussed. [S0163-1829(97)02504-6]

I. INTRODUCTION

The first attempts to describe the movement of electrons in the presence of a constant external magnetic field were done by Landau[1] and Peierls.[2] In the 1950s many authors dealt with similar problems, but a crystalline (periodic) potential was also included.[3] Pioneering works by Brown[4] and Zak[5,6] were preceded by Wannier's paper.[7] The first two authors independently introduced and investigated the so-called *magnetic translations*, i.e., unitary, mutually *noncommuting*, operators which commute with the Hamiltonian. For more than 30 years these operators have been applied in many problems concerning the movement of electrons in a crystal lattice. Recently, much attention has been paid to two-dimensional systems in an external magnetic field due their relations with high-T_c superconductors, anyons, the Hall effect, etc.[8]

From the group-theoretical point of view, magnetic translations can be considered as a projective (ray) representation of the translation group T of a crystal lattice (this is Brown's approach). However, projective representations of any group can be found as vector representations of its covering group (the so-called *magnetic translation group* MTG). This latter group can be constructed as a central extension of a given group by the group of factors, in general $U(1)\subset\mathbb{C}^*$ or its subgroup. This construction is the basis of Zak's considerations, and is very closely related to the MacLane method for a determination of all inequivalent (Abelian) extensions of the two groups.[9] In this paper irreducible representations (irreps) of MTG's are considered. In fact they were determined by Brown and Zak,[4,5] but both authors rejected most of them as "nonphysical." Here it is shown that all representations are "physical" and a very simple example of their applications is presented. Moreover, the Clebsch-Gordan coefficients are calculated in this case.

II. MAGNETIC TRANSLATIONS

The MTG appears in a natural way when one considers an electron in a periodic potential $V(\mathbf{r})$ and a uniform magnetic field $\mathbf{H}$ determined by a vector potential (a gauge) $\mathbf{A}$. This system is described by the well-known Hamiltonian

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

which does *not* commute with the usual translation operators

$$\hat{T}_0(\mathbf{R})=\exp(-\mathrm{i}\mathbf{R}\cdot\mathbf{p}/\hbar) \tag{2}$$

and

$$\hat{T}_0(\mathbf{R})\psi(\mathbf{r})=\psi(\mathbf{r}-\mathbf{R}) \tag{3}$$

(the subscript 0 corresponds to $\mathbf{H}=0$). However, the Hamiltonian (1) commutes with unitary operators

$$\hat{T}(\mathbf{R})=\exp[-\mathrm{i}(\mathbf{p}-e\mathbf{A}/c)\cdot\mathbf{R}/\hbar] \tag{4}$$

introduced by Brown.[4] It is easy to check that in this way a projective representation of the translation group is defined; the corresponding factor system is given as

$$m(\mathbf{R},\mathbf{R}')=\exp\left[-\frac{1}{2}\frac{\mathrm{i}e}{c\hbar}(\mathbf{R}\times\mathbf{R}')\cdot\mathbf{H}\right]. \tag{5}$$

It has to be stressed that these operators commute with the Hamiltonian (1) if the vector potential $\mathbf{A}$ fulfills the condition

$$\partial A_j/\partial x_k+\partial A_k/\partial x_j=0 \quad \text{for } j,k=1,2,3. \tag{6}$$

This relation holds, for example, for the (global) gauge $\mathbf{A}(\mathbf{r})=\frac{1}{2}(\mathbf{H}\times\mathbf{r})$, which was used by both authors.[4,5] It is worth noting that, introducing a *local* gauge, one can consider any vector potential $\mathbf{A}$.[10]

Projective representations of a given group are related to *vector* representations of the covering group, which can be determined as a central extension. In the considered case, one deals with representations of the translation group $T\simeq\mathbb{Z}^3$, and the magnetic translation group $\mathcal{T}$ is its covering group, i.e., $\mathcal{T}$ is included in a central extension of T by $U(1)$. Let $\mathcal{T}$ consist of pairs $(u,\mathbf{R})$, $u\in U(1)$, $\mathbf{R}\in T$, with the multiplication rule

$$(u,\mathbf{R})(u',\mathbf{R}')=(uu'm(\mathbf{R},\mathbf{R}'),\mathbf{R}+\mathbf{R}') \tag{7}$$

with $m:T\times T\to U(1)$ being a factor system, and let Ξ be an irrep of $U(1)$. An irrep of $\mathcal{T}$ is given as a product

$$\Gamma(u,\mathbf{R})=\Xi(u)\Lambda(\mathbf{R}), \tag{8}$$

where Λ is a projective representation of T with a factor system

$$\nu(\mathbf{R},\mathbf{R}')=\Xi(m(\mathbf{R},\mathbf{R}')). \tag{9}$$

Zak[5,6] introduced such a covering group by attaching to each vector $\mathbf{R}$ a path $\mathcal{P}$ drawn in the crystal lattice, i.e. consisting of vectors $\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_k\in T$, such that $\Sigma_{j=1}^{k}\mathbf{R}_j=\mathbf{R}$. The magnetic flux Φ through the polygon enclosed by a loop $\mathcal{L}=\mathcal{P}\cup\{-\mathbf{R}\}$ determines a factor $u(\mathcal{L})=\exp(-\mathrm{i}e\Phi/c\hbar)\in U(1)$. Pairs $(u(\mathcal{L}),\hat{T}_0(\mathbf{R}))$ form the magnetic translation group in Zak's approach [$\hat{T}_0$ is defined in Eq. (2)].

Zak showed that a factor system of the covering group he introduced is identical to the factor system (5). Therefore, both these approaches are equivalent if $\Xi(u)=u$. Other representations of $\mathcal{T}$ were rejected by Zak, since they were viewed as nonphysical.

MTG's were considered central extensions in some previous papers,[9,11,12] as an illustrative example of the MacLane method for determination of all inequivalent extensions of given groups (the MacLane method is discussed in a review article by Lulek[13]). This algebraic description allows deep investigations of MTG's and their representations.

III. IRREDUCIBLE REPRESENTATIONS

Let Γ^1 and Γ^2 be irreps of $\mathcal{T}$ satisfying the condition $\Xi(u)=u$. Matrix elements of their Kronecker product $\Gamma=\Gamma^1\otimes\Gamma^2$ can be found as

$$\Gamma_{jk,lm}(u,\mathbf{R})=\Gamma^1_{j,l}(u,\mathbf{R})\Gamma^2_{k,m}(u,\mathbf{R}). \tag{10}$$

Taking into account the definition of an irrep (8), one obtains

$$\Gamma_{jk,lm}(u,\mathbf{R})=u^2\Lambda^1_{j,l}(\mathbf{R})\Lambda^2_{k,m}(\mathbf{R}). \tag{11}$$

The last product in this formula determines a product $\Lambda=\Lambda^1\otimes\Lambda^2$ of two projective representations, which is a projective representation itself. To determine its factor system one has to calculate a product $\Lambda(\mathbf{R}_1)\Lambda(\mathbf{R}_2)$:

$$\begin{aligned}(\Lambda(\mathbf{R}_1)\Lambda(\mathbf{R}_2))_{jk,lm}&=\sum_{n,p}\Lambda_{jk,np}(\mathbf{R}_1)\Lambda_{np,lm}(\mathbf{R}_2)\\&=m(\mathbf{R}_1,\mathbf{R}_2)^2\Lambda_{jk,lm}(\mathbf{R}_1+\mathbf{R}_2).\end{aligned}$$

Therefore, the representation Λ has the factor system $\nu(\mathbf{R},\mathbf{R}')=m(\mathbf{R},\mathbf{R}')^2$, which means that it corresponds to the irrep $\Xi(u)=u^2$ [cf. Eq. (11)]. In the other words, a product of two physical representations gives a nonphysical one. However, there are no *a priori* rules to exclude (as nonphysical) a product of two (physical) representations. Therefore, it *has* to be assumed that also Γ is relevant for physics.

Zak rejected irreps with $\Xi(u)\neq u$ since ''representations with the correspondence $\epsilon\rightarrow\epsilon^n$ with $n\neq 1$ are nonphysical.''[14,15] However, the above-mentioned constant contains the electric charge (of an electron). If one assumes that representations with $\Xi(u)=u^2$ describe the movement of a particle (or a system of particles) with a charge $Q=-2e$, then all formulas will be consistent. The simplest interpretation says that such representations describe a *pair* of electrons. This agrees with the way in which they have been obtained: Γ describing a pair of electrons is a product of two one-electron representations Γ^1 and Γ^2. Writing Hamiltonian (1) in the form

$$\mathcal{H}=\frac{1}{2\beta m}(\mathbf{p}+\alpha e\mathbf{A}/c)^2+V(\mathbf{r}), \tag{12}$$

one can say that for $\alpha=\beta$ it describes the movement of α electrons in the magnetic field and the periodic potential. If $\beta\neq\alpha=0$, then this Hamiltonian corresponds to a particle of a mass βm without electric charge. Since $\alpha=0$, then both factor systems (for the central extension $\mathcal{T}$ and the projective representation $\hat{T}$) are trivial, and the original translation group T and its vector irreps are appropriate to describe the dynamics of the system. (The magnetic field is irrelevant if one considers classical or spinless particles, of course.)

IV. FINITE TWO-DIMENSIONAL MTG'S

One can introduce finite representations of MTG's imposing the periodic boundary conditions in the form $\hat{T}(N\mathbf{a}_j)=1$, where $\mathbf{a}_j$, $j=1,2,3$, are the unit vectors of a crystal lattice.[4] This is equivalent to considerations of a finite translation group $T=\mathbb{Z}_N^3$ (identical periods in each direction are assumed). Both approaches yield that the magnetic field should be parallel to a lattice vector. It is convenient to assume that $\mathbf{H}\|\mathbf{a}_3$ and is perpendicular to $\mathbf{a}_1$ and $\mathbf{a}_2$. This allows us to consider $T=\mathbb{Z}_N^2$ and a factor group to be C_N (the multiplicative group of the Nth roots of 1). Therefore, a finite two-dimensional magnetic translation group is a central extension of a direct product $\mathbb{Z}_N\otimes\mathbb{Z}_N$ by the cyclic group C_N.[11] This group, denoted above by $\mathcal{T}$, consists of elements $(\omega^j,[k,l])$, where $\omega=\exp(2\pi\mathrm{i}/N)$ and $j,k,l=0,1,\ldots,N-1$. The multiplication rule is given by the following formula (all additions modulo N):

$$(\omega^j,[k,l])(\omega^{j'},[k',l'])=(\omega^{j+j'+hkl'},[k+k',l+l']).$$

The parameter $h=0,1,\ldots,N-1$ labels inequivalent extensions, and corresponds to the magnetic field $\mathbf{H}$ in Eq. (5). It is evident that algebraic properties of this group depend on h or, strictly speaking, on the greatest common divisor $\gcd(h,N)$ since for $\gcd(h,N)=\gcd(h',N)$ groups labeled by h and h' are isomorphic. In the further considerations we assume $h=1$ in order to reduce a number of parameters and of different cases. It is worthwhile to mention that for $\gcd(h,N)>1$ the extension of $\mathbb{Z}_N\otimes\mathbb{Z}_N$ by $C_{N/\gcd(h,N)}$ with the multiplication rule parametrized by $h/\gcd(h,N)$ should be taken into account.

It follows from Eq. (8) that irreps of $\mathcal{T}$ are labeled by $\xi=0,1,\ldots,N-1$ corresponding to the irreps of C_N, i.e., we have $\Xi(\omega^j)=\omega^{\xi j}$. For each ξ we have to find all (inequivalent) projective representations Λ^ξ of $\mathbb{Z}_n\otimes\mathbb{Z}_N$. These representations satisfy the following conditions: (i) a factor system of Λ^ξ is given as [see Eq. (9)]

$$\nu^\xi([k,l],[k',l'])=\omega^{\xi kl'};$$

(ii) for a given factor system ν^ξ, we have

$$\sum|\Lambda^\xi|^2=N^2$$

(the sum is taken over all inequivalent projective irreps with the factor system ν^ξ).[16] It can be shown that for given ξ that there are $\gcd(\xi,N)^2$ projective representations, each of dimension $N/\gcd(\xi,N)$. These representations are labeled by numbers $\kappa,\lambda=0,1,\ldots,\gcd(\xi,N)-1$, corresponding to irreps of $\mathbb{Z}_{\gcd(\xi,N)}\otimes\mathbb{Z}_{\gcd(\xi,N)}$. [Thus for given ξ the crystal lattice is ''scaled'' $N/\gcd(\xi,N)$ times.] To make a long story short, an actual form of matrix elements will not be discussed but only some general properties will be presented. (In fact irreps so used are similar to those considered by Brown[4] and Zak.[5,6])

It follows from previous considerations that the representations (vector ones of $\mathcal{T}$ or projective ones of T) with $\xi>1$ describe the movement of a particle with a charge $-\xi e$. Note that the periodic boundary conditions imply that particles with charge q and $q+N$ behave in the same way. In particular, it also applies to products of irreps: a product of two representations labeled by ξ_1 and ξ_2, respectively, decomposes into a sum of representations labeled by $\xi_1+\xi_2$ (modulo N). Thus a system of two particles with charges $-\xi_1 e$ and $-\xi_2 e$ has total charge $-(\xi_1+\xi_2)e$. This relation follows from the form of the first factor in Eq. (8),

$$(\Xi_1\otimes\Xi_2)(\omega^j)=\omega^{(\xi_1+\xi_2)j}.$$

In particular, a square of the N-dimensional representation Γ^1 (determined by the unique projective irrep Λ) corresponds to a pair of electrons. A number of terms and the multiplicity coefficients $f(\kappa,\lambda)$ in the decomposition

$$\Gamma^{\xi_1}_{\kappa_1,\lambda_1}\otimes\Gamma^{\xi_2}_{\kappa_2,\lambda_2}=\bigoplus_{\kappa,\lambda} f(\kappa,\lambda)\Gamma^{\xi_1+\xi_2}_{\kappa,\lambda}$$

depend on the arithmetic relations between ξ_1, ξ_2, and N. In the case $\Gamma^1\otimes\Gamma^1$ one obtains different results for N odd and even. In the first case the product decomposes into N copies of the (unique) representation Γ^2, since $\gcd(2,N)=1$. On the other hand, for $N=2M$ one has $\gcd(2,2M)=2$, and the considered product decomposes into a direct sum of M-dimensional representations. There are four such inequivalent representations, and each of them appears M times.

V. EXAMPLES

If N is a prime number then $\gcd(\xi,N)=1$ or N, and it is easy to determine the decomposition of each product:

$$\Gamma^0_{\kappa,\lambda}\otimes\Gamma^0_{\kappa',\lambda'}=\Gamma^0_{\kappa+\kappa',\lambda+\lambda'},$$

$$\Gamma^0_{\kappa,\lambda}\otimes\Gamma^{\xi}=\Gamma^{\xi}\quad\text{for}\quad \xi=1,2,\ldots,N-1,$$

$$\Gamma^{\xi}\otimes\Gamma^{N-\xi}=\bigoplus_{\kappa,\lambda=0}^{N-1}\Gamma^0_{\kappa,\lambda},$$

$$\Gamma^{\xi_1}\otimes\Gamma^{\xi_2}=N\Gamma^{\xi_1+\xi_2}\quad\text{for}\quad \xi_1+\xi_2\neq N.$$

The first nontrivial case corresponds to $N=4$. However, this case does not show all the richness of possible products, since there is only one nontrivial divisor $\xi=2$. The central extension of $\mathbb{Z}_4\otimes\mathbb{Z}_4$ has 22 irreps:

(i) 16 one-dimensional ones for $\xi=0$ labeled by $\kappa,\lambda=0,1,2,3$; they are simply the ordinary vector representations of $\mathbb{Z}_4\times\mathbb{Z}_4$.

(ii) Two four-dimensional ones for $\xi=1$ and $\xi=3$.

(iii) Four two-dimensional ones for $\xi=2$ labeled by $\kappa,\lambda=0,1$.

Two-electron states form a 16-dimensional space with the basis vectors $|p_1p_2\rangle$, where $p_1,p_2=0,1,2,3$ label vectors of the representation Γ^1. This space decomposes into eight two-dimensional representations $\Gamma^2_{\kappa,\lambda}$ with $f(\kappa,\lambda)=2$ for all $\kappa,\lambda=0,1$. Hence the irreducible basis can be denoted as $|\kappa\lambda v q\rangle$, where $v=0,1$ is the repetition index, and $q=0,1$ labels vectors of $\Gamma^2_{\kappa,\lambda}$. The relatively simple form of matrix elements allows a determination of the Clebsch-Gordan coefficients. In the presented case they lead to the following formulas:

$$|0000\rangle=\frac{1}{\sqrt{2}}(|00\rangle+|22\rangle),$$

$$|0001\rangle=\frac{1}{\sqrt{2}}(|11\rangle+|33\rangle),$$

$$|0010\rangle=\frac{1}{\sqrt{2}}(|13\rangle+|31\rangle),$$

$$|0011\rangle=\frac{1}{\sqrt{2}}(|02\rangle+|20\rangle),$$

$$|0100\rangle=\frac{i}{\sqrt{2}}(|00\rangle-|22\rangle),$$

$$|0101\rangle=\frac{1}{\sqrt{2}}(|11\rangle-|33\rangle),$$

$$|0110\rangle=\frac{1}{\sqrt{2}}(|13\rangle-|31\rangle),$$

$$|0111\rangle=\frac{i}{\sqrt{2}}(|02\rangle-|20\rangle),$$

$$|1000\rangle=\frac{1}{\sqrt{2}}(|01\rangle+|23\rangle),$$

$$|1001\rangle=\frac{1}{\sqrt{2}}(|12\rangle+|30\rangle),$$

$$|1010\rangle=\frac{1}{\sqrt{2}}(|10\rangle+|32\rangle),$$

$$|1011\rangle=\frac{1}{\sqrt{2}}(|03\rangle+|21\rangle),$$

$$|1100\rangle=\frac{i}{\sqrt{2}}(|01\rangle-|23\rangle),$$

$$|1101\rangle = \frac{1}{\sqrt{2}}(|12\rangle - |30\rangle),$$

$$|1110\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |32\rangle),$$

$$|1111\rangle = \frac{\mathrm{i}}{\sqrt{2}}(|03\rangle - |21\rangle).$$

The numbers p_1 and p_2 can be interpreted as quasimomenta, since we have $\hat{T}(\mathbf{a}_2)|p_1\rangle = |p_1 - 1\rangle$ [cf. Ref. 4 in Eq. (25)]. The translation along $\mathbf{a}_2$ is distinguished due to the choice of the matrix form of the considered representations. In general, there is always one distinguished direction, and the number p labels the corresponding quasimomentum.[17] Such an interpretation of the indices p_1 and p_2 allows the introduction of a Hamiltonian which commutes with all operators $\Gamma^1 \otimes \Gamma^1(u,\mathbf{R})$ (matrix elements are given):

$$\mathcal{H}_{p_1 p_2, p_1' p_2'} = \delta_{p_1+p_2, p_1'+p_2'} a_{p_1+p_2, p_1-p_1'},$$

where

$$a_{0,0} = a_{2,0} = a_0,$$

$$a_{1,0} = a_{3,0} = a_1,$$

$$a_{p,1} = a_{p,3}.$$

All these relations follow from the symmetry requirements. The terms $a_{p,0}$ correspond to the total quasimomentum p and describe the kinetic energy ($a_{p,0} > 0$); the condition $a_{0,0} = a_{2,0}$ is connected with a rescaling of the lattice, since the representations Γ^2 are two dimensional. The terms $a_{p,q}$ for $q \neq 0$ correspond to the interchange of a quasiparticle with the quasimomentum q or, in the other words, to the interaction of electrons. In the simplest approximation one can assume that $a_{p,q}$ for $q \neq 0$ does not depend on p (so it will be hereafter denoted as b_q; recall that $b_1 = b_3$) and is negative. It is also natural to assume that $a_0 < a_1$, and that the probability of interaction with $q = 2$ is smaller than this one for $q = 1$ (to begin with, one can assume $b_2 = 0$).

In such an approximation one finds that levels corresponding to Γ^2_{01} and Γ^2_{11} are fourfold degenerated, with energies $a_0 - b_2$ and $a_1 - b_2$, respectively. The representation Γ^2_{10} leads to two twofold-degenerated levels with energies $a_1 + b_2 \pm 2b_1$. Similarly, one obtains that two representations Γ^2_{00} describe levels with energies $a_0 + b_2 \pm 2b_1$, respectively. In two later cases the following linear combinations of vectors take the form

$$\frac{1}{\sqrt{2}}(|\kappa 000\rangle \pm |\kappa 010\rangle) \quad \text{for} \quad \kappa = 0,1.$$

The ground-state energy is $E = a_0 + b_2 + 2b_1$, and the corresponding eigenvector is

$$\tfrac{1}{2}(|00\rangle + |22\rangle + |13\rangle + |31\rangle),$$

i.e., it is the sum of states $|p,-p\rangle$. Such a result resembles the BCS state, but it is not antisymmetric. However, the performed investigations are semiclassical and electrons have been considered as spinless particles.

VI. FINAL REMARKS

The algebraic analysis of the magnetic translation groups (or, equivalently, of the projective irreducible representations of the translation group) gives us a deeper insight into their structure. This relates to many physical problems: movement of charged particles in a magnetic (or an electromagnetic) field and a periodic potential, high-T_c superconductors, the Hall effects (especially the fractional quantum Hall effect), anyons, finite phase spaces, etc. The above-presented considerations indicate the importance of the product of representations. The discussed examples are very simple, and a physical interpretation is a bit naïve, but they have shown the main (mathematical) properties of the proposed picture.

Let $\varphi = hc/e$ be a fluxon and $\mathbf{H} = \mathbf{h}\varphi$. Replacing the electron charge e by a charge $Q = -\xi e$, the factor system (5) determined by Brown can be written

$$m(\mathbf{R},\mathbf{R}') = \exp[2\pi \mathrm{i}\xi \tfrac{1}{2}(\mathbf{R}\times\mathbf{R}')\cdot\mathbf{h}].$$

This formula shows that physical properties, which depend on this factor, are periodic with respect to the magnetic field, lattice vectors, and the charge. The first case was pointed out by Azbel[18] and also noted by Zak.[6] The second is, in a sense, the basis of introduction of magnetic cells[4,5,14,19] ($\mathbf{R}$ and $\mathbf{R}'$ are linear combinations with integer coefficients of basis vectors $\mathbf{a}_j$). This work has shown that the periodicity with respect to the charge of a particle should also be taken into account.

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*Electronic mail: florek@phys.amu.edu.pl

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