Generalized Bloch theorem and topological characterization

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The Bloch theorem enables reduction of the eigenvalue problem of the single-particle Hamiltonian that commutes with translational group. Based on a group theory analysis we present generalization of the Bloch theorem that incorporates all additional symmetries of a crystal. The generalized Bloch theorem constrains the form of the Hamiltonian which becomes manifestly invariant under additional symmetries. In the case of isotropic interactions the generalized Bloch theorem gives a unique Hamiltonian. This Hamiltonian coincides with the Hamiltonian in the periodic gauge. In the case of anisotropic interactions the generalized Bloch theorem allows a family of Hamiltonians. Due to the continuity argument we expect that even in this case the Hamiltonian in the periodic gauge defines observables, such as Berry curvature, in the inverse space. For both cases we present examples and demonstrate that the average of the Berry curvatures of all possible Hamiltonians in the Bloch gauge is the Berry curvature in the periodic gauge.

I. INTRODUCTION

The Bloch theorem [1] is very useful in description of a quasi-particle (electron, phonon, etc.) in crystals. The solution of the Bloch problem can be stated in a representation-independent form. Namely, the Bloch vector \[ |\psi(k)\rangle \] can be written as a linear superposition of the localized, in the unit cell \( \mathbf{R} \) at position \( \mathbf{a}_j \), orbitals \( |\mathbf{R}, \mathbf{a}_j\rangle \) of a crystal with coefficients, \( c_j(k) \), that depend on Bloch momentum \( k \) and type of orbital \( j \) in the unit cell:

\[
|\psi(k)\rangle = \sum_{\mathbf{R}, j} c_j(k) e^{i\mathbf{k} \cdot \mathbf{R}} |\mathbf{R}, \mathbf{a}_j\rangle. \tag{1}
\]

It is obvious that this form satisfies the Bloch theorem \( T_{\mathbf{R}} |\psi(k)\rangle = \exp(-i\mathbf{k} \cdot \mathbf{R}) |\psi(k)\rangle \), where \( T_{\mathbf{R}} \) is the translation operator for the vector \( \mathbf{R}' \).

In this work we present a generalization of the Bloch theorem that incorporates all additional (beside translational) symmetries of a crystal. The generalized Bloch theorem constrains the form of the Hamiltonian which becomes manifestly invariant under additional symmetries. In the following we will concentrate on a single aspect, among many others, of band physics for which the generalized Bloch theorem is important.

The coefficients \( c_j(k) \) in Eq. (1) naturally represent the Bloch vector in the space of Bloch momentum, and therefore can be used in the definition of Berry connection. Berry connection provides a way to describe how the phase of the Bloch vector varies as we change Bloch momentum. The choice of the coefficients in the expansion of \( |\psi(k)\rangle \) is by no means unique. There is a freedom of choosing their phase, but two choices stand out. The choice in Eq. (1) implies Berry connection

\[
\mathbf{A}^B = i \sum_j c_j^*(k) \nabla_k c_j(k),
\]

where \( B \) stands for “Bloch gauge”. A different choice,

\[
|\psi(k)\rangle = \sum_{\mathbf{R}, j} u_j(k) e^{i\mathbf{k} \cdot (\mathbf{R} + \mathbf{a}_j)} |\mathbf{R}, \mathbf{a}_j\rangle,
\]

on the other hand, implies

\[
\mathbf{A}' = i \sum_j u_j^*(k) \nabla_k u_j(k),
\]

where \( P \) stands for “periodic gauge”. These are the most natural choices; they coincide with two possibilities to define the Fourier transform in the space of the Bloch vectors: \( |\mathbf{k}, j\rangle_B = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} |\mathbf{R}, \mathbf{a}_j\rangle \) and \( |\mathbf{k}, j\rangle_P = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot (\mathbf{R} + \mathbf{a}_j)} |\mathbf{R}, \mathbf{a}_j\rangle \) [2]. Although physics should be invariant under these choices, and we speak of two gauges, we will show in examples that they define two different Berry curvatures. So the word gauge in this sense is a misnomer and we must look for a “physical gauge”. In this gauge we would be certain that we are defining a physical Berry curvature, a suitable candidate for the intrinsic magnetic field in the inverse space. This would define a local magnetic length that is important to know for example in the case of fractional physics in the bands with non-zero Chern number. There are proposals [3, 4] how to measure Berry curvature in experiments, and thus it is important to know in which gauge it is defined.

From the Karpus-Luttinger argument [5, 6] that the coordinate operator in the inverse space can be represented as

\[
\mathbf{r} \rightarrow -i \nabla_{\mathbf{p}} + \mathbf{A}'
\]

we expect that the periodic gauge is the right choice. This choice in the literature is commonly used without a complete understanding why it is physical. On the other hand, there are references that use the Bloch gauge (and reach wrong expectations). By establishing the generalized Bloch theorem we provide strong arguments that the periodic gauge is the natural choice given that it, i.e. the Hamiltonian that this gauge defines, respects the symmetries of the underlying lattice.
Thus the symmetry is a determining factor that provides the right choice. In the past researchers were finding in certain examples that the Berry curvature calculated in the periodic gauge is the most symmetric \[7\|9\]. Here we explore the symmetry aspect by using the techniques of the group theory, and finding the form of the Hamiltonian in which any symmetry action can be made explicit. In most cases, after simple rewritings, the manifestly invariant Hamiltonian is equal to the Hamiltonian in the periodic gauge.

We demonstrate that in the case of the isotropic interactions (which will be precisely defined below) the Hamiltonian that respects the symmetries of the lattice is uniquely defined by the generalized Bloch theorem and coincides with the Hamiltonian in the periodic gauge. In the case of anisotropic interactions we find, due to a phase freedom in the construction, a family of generalized Bloch Hamiltonians that respect the symmetries of the lattice. One of the Hamiltonians corresponds to the periodic gauge choice. This choice seems a natural choice even in this case of anisotropic interactions because it can be viewed as an extension of the isotropic case. In addition we find that the average Berry curvature of the eigenstates of all possible Bloch Hamiltonians is equal to the Berry curvature in the periodic gauge.

The paper is organized as follows: In Sec. II we review the Bloch theorem and its Hamiltonian construction. In Sec. III, to begin the generalization, we assume an existence of a basis in which the action of crystal symmetries is made explicit, i.e. a symmetry adapted basis. In the same section we seek for a realization - a basis defined by a special class of projectors that represent an invariance of the action of symmetries, and reach the form of the Hamiltonian in that basis. In Sec. IV, we find explicit expressions for the vectors of the basis and therefore Hamiltonian. In the same section we discuss when the Hamiltonian that respects all additional symmetries beside translation is unique or represents a family of Hamiltonians. In Sec. V, to illustrate the formal procedure described in the previous sections (III and IV), we discuss concrete examples of lattices and constructions of the generalized Bloch Hamiltonians. Sec. VI is a short summary.

II. BLOCH THEOREM

A crystal is the system of periodically arranged atoms along \(d\) linearly independent directions. A part of a crystal, called unit cell (UC), contains minimal set of atoms sufficient to build the whole crystal by the action of discrete translations for the Bravais lattice vectors \(\mathbf{R} = \sum_{i=1}^{d} n_i \mathbf{b}_i\), where \(n_i\) are integers and \(\mathbf{b}_i\) are called primitive vectors of direct lattice. Quasi-particle basis \(|\mathbf{k}, j\rangle\) (\(j\) enumerates basis vectors-orbitals) is described by the quasi-momentum quantum numbers \(\mathbf{k} = \sum_{i=1}^{d} k_i \mathbf{g}_i\), where \(k_i \in \{-1/2, 1/2\}\) and \(\mathbf{g}_i\) are called primitive vectors of reciprocal lattice \((\mathbf{b}_i \cdot \mathbf{g}_j = 2\pi \delta_{ij}, \delta_{ij}\) is Kronecker delta). The Bloch theorem states that the basis vector \(|\mathbf{k}, j\rangle\) translated for the Bravais vector \(\mathbf{R}\) changes as

\[
T_{\mathbf{R}}|\mathbf{k}, j\rangle = e^{-ik \cdot \mathbf{R}}|\mathbf{k}, j\rangle
\]

(2)

where \(T\) is the translation operator. In other words, if the \(j\)th basis vector in the zeroth unit cell \((\mathbf{R} = 0, \mathbf{a}_j)\), then in the unit cell \(\mathbf{R}\) it is \(e^{ik \cdot \mathbf{R}}|\mathbf{a}_j\rangle\) and consequently \(|\mathbf{k}, j\rangle = \sum_{\mathbf{R}} e^{ik \cdot \mathbf{R}}|\mathbf{a}_j\rangle\). Vectors \(|0, a_j\rangle\) and \(|\mathbf{R}, a_j\rangle\) are identical, but belong to different blocks, 0 and \(\mathbf{R}\), of the vector \(|\mathbf{k}, j\rangle\), respectively.

Reduction of operators describing quasi-particle in a crystal such as the Hamiltonian, dynamical matrix, overlap matrix, etc. invariant under discrete translations, is straightforward with the help of Eq. (2). Any Hamiltonian eigenvector \(|\psi(\mathbf{k})\rangle\) can be expressed as a linear combination with coefficients \([\mathbf{c}_j(\mathbf{k})]\) \(\sum_{j} c_j(\mathbf{k})|\mathbf{k}, j\rangle = \sum_{\mathbf{R}, j} c_j(\mathbf{k})e^{-ik \cdot \mathbf{R}}|\mathbf{R}, a_j\rangle\).

(3)

Now, the eigenvalue problem of the Hamiltonian can be replaced by the set of homogeneous equations in coefficients \(c_j(\mathbf{k})\),

\[
\sum_{j'} \left[ \sum_{\mathbf{R}} e^{ik \cdot \mathbf{R}'} H_{\mathbf{R}'}^{0, j} - E(\mathbf{k}) \delta_{j, j'} \right] c_{j'}(\mathbf{k}) = 0,
\]

(4)

for all \(j\), where \(H_{\mathbf{R}}^{0, j}\) are Hamiltonian matrix elements in the basis \(|\mathbf{R}, a_j\rangle\),

\[
H_{\mathbf{R}'}^{0, j} = \langle 0, a_j | H | \mathbf{R}', a_{j'} \rangle.
\]

(5)

This set of equations can be written in the form of the eigenvalue problem of the Bloch Hamiltonian \(H(\mathbf{k})\)

\[
H(\mathbf{k}) c(\mathbf{k}) = E(\mathbf{k}) c(\mathbf{k}), \quad H(\mathbf{k}) = \sum_{\mathbf{R}} e^{ik \cdot \mathbf{R}} H_{\mathbf{R}}^{0, \mathbf{R}},
\]

(6)

where \(c(\mathbf{k})\) is a column with components \(c_j(\mathbf{k})\) and \(H_{\mathbf{R}}^{0, \mathbf{R}}\) is matrix having matrix elements \(H_{\mathbf{R}'}^{0, j}(\mathbf{k})\). In some approximations, e.g. tight-binding (not using Löwdin [10] nor Wannier [11, 12] functions), the Kronecker delta in Eq. (4) is replaced by the overlap integrals, \(\delta_{\mathbf{R}'}^{0, j} = \langle 0, a_j | H | \mathbf{R}', a_{j'} \rangle\), and the Bloch reduced overlap matrix \(S(k) = \sum_{\mathbf{R}} e^{ik \cdot \mathbf{R}} \delta_{\mathbf{R}}^{0, \mathbf{R}}\) appears on the right hand side of Eq. (6).

There are many single-particle approximations [13-16] which can be solved by using the Bloch theorem. In the nearly free electron approximation the basis consists of functions \(|\mathbf{r}, \mathbf{G}\rangle = \psi^{\mathbf{k}}(\mathbf{r}) = e^{i(k-G)\cdot\mathbf{r}} (\mathbf{G} = \sum_{i=1}^{d} m_i \mathbf{g}_i\) are vectors of reciprocal lattice and \(m_i\) are integers), and the finite set of reciprocal lattice vectors \(\mathbf{G}\) depends on the physical situation. The tight binding approximation deals with basis functions \(|\mathbf{k}, \alpha lm\rangle\), which are electron orbitals with quantum numbers \(\alpha lm\) on atom \(\alpha\). In this approximation, previously used symbol \(j\) in enumerating basis functions is replaced by the four numbers \((\alpha lm)\). In the harmonic approximation basis \(|\mathbf{k}, \alpha\rangle\) are orthogonal unit vectors \(\mathbf{e}_i (i = x, y, z)\) on atom \(\alpha\).
III. GENERALIZATION

To begin with generalization, let $\mathcal{G}$ be the symmetry group of a crystal, and let $\Gamma$ (corresponding to the quasi-momentum quantum number $\mathbf{K}$ in the Bloch theorem) label unitary irreducible representation (IR) $D^{(\Gamma)}(A)$. The basis for IR $\Gamma$ is given by the vectors $|\Gamma, j, a\rangle$ which fulfill

$$D(A)|\Gamma, j, a\rangle = \sum_{b=1}^{d_f} D^{(\Gamma)}_{ba}(A)|\Gamma, j, b\rangle. \quad (7)$$

Here, $D^{(\Gamma)}_{ba}(A)$ is matrix element $(b, a)$ of the $d_f$-dimensional irreducible representation $D^{(\Gamma)}(A)$ and $D(A)$ is unitary representation of the group element $A$. The basis [7] is called symmetry adapted basis (SAB). If the group $\mathcal{G}$ consists of translations only, IRs are one dimensional, $D^{(1)}(R) = e^{-i\mathbf{k}\cdot \mathbf{R}}$. This is the Bloch theorem, Eq. (2). Vectors differing only in $a$ are called partners. It is also said that vectors $|\Gamma, j, a\rangle$ for fixed $\Gamma$ and $j$ belong to one multiplet.

Besides permutational representations in $D$, there are also representations $D_j$ transforming the part $|\mathbf{R}, a_j, a\rangle$ of the vector $|\Gamma, j, a\rangle$. Vector $\mathbf{R}$ in the ket is just a label and, in general, a group element changes zero unit cell, i.e. $|A0, a_j, a\rangle \neq |0, a_j, a\rangle$ holds, while vector $a_j$ is the position of the $j$th orbital. Representation $D_j$ may be the representation $D^{(l, -1/2)}$ for the atomic orbital of electron with angular momentum $l$, the vector representation for phonons, etc.

Now, from the definition of SAB for IR $\Gamma$ [Eq. (7)], we see that the part of the basis vector $|\Gamma, j, a\rangle$ on atom $a_j$ in the unit cell $\mathbf{R}$, i.e. $|\mathbf{R}, a_j, a\rangle$, satisfies the following equality

$$D_j(A)|\mathbf{R}, a_j, a\rangle = \sum_{b=1}^{d_f} D^{(\Gamma)}_{ba}(A)|\mathbf{R}, a_j, b\rangle. \quad (8a)$$

Here the group element $A$ transfers the atom $a_j$ from the unit cell $\mathbf{R}$, i.e. $|\mathbf{R}, a_j\rangle$, to the atom $(A\mathbf{R}, a_j)$. Depending on the group element $A$, it could happen that $A\mathbf{R}$ and $\mathbf{R}$ are the same unit cells and/or $Aa_j$ and $a_j$ are the same orbitals. The previous transformation rule can be rewritten (remembering that all the representations are unitary) as the generalization of the Bloch theorem

$$|A\mathbf{R}, a_j, a\rangle = \sum_{b=1}^{d_f} D^{(\Gamma)}_{ab}(A)|\mathbf{R}, a_j, b\rangle, \quad (8a)$$

where the asterisk stands for the complex conjugation. Notice that for crystals with only the translational symmetry group, the representation $D_j(\mathbf{R})$ is always the identity operator and $Aa_j = a_j$. This gives the Bloch theorem, Eq. (2), i.e. $|\mathbf{R} + \mathbf{R}', a_j\rangle = e^{ik\cdot \mathbf{R}'}|\mathbf{R}, a_j\rangle$.

In the Bloch theorem, it is sufficient to define quasi-particle orbitals and construct the Bloch Hamiltonian. In our generalization of the Bloch theorem only certain, restricted by symmetry, linear combinations of orbitals are allowed. To construct these linear combinations, it is sufficient to extract group elements $A$ that do not transform the orbital $(\mathbf{R}, a_j)$, i.e. $(A\mathbf{R}, Aa_j) = (\mathbf{R}, a_j)$. These elements form the subgroup $\mathcal{S}_{\mathbf{R}, j}$ of the group $\mathcal{G}$ called stabilizer or little group of the orbital $(\mathbf{R}, a_j)$. In other words, atom $a_j$ in the unit cell $\mathbf{R}$ is the fixed point of the action of its stabilizer, $\mathcal{S}_{\mathbf{R}, j}$. The dimension (the number of the group elements of $\mathcal{S}_{\mathbf{R}, j}$) we label by $s_j$.

After introducing stabilizers, we are able to find the allowed linear combinations of orbitals. Let us build the column $|\mathbf{R}, a_j\rangle$ of the vectors $|\mathbf{R}, a_j, a\rangle$. Then, Eq. (8a) can be written in the form $|\mathbf{AR}, Aa_j\rangle = D^{(\Gamma)}(A) \otimes D_j(A)|\mathbf{R}, a_j\rangle$, where “$\otimes$” stands for tensor product operator. Summing over the stabilizer elements $A \in \mathcal{S}_{\mathbf{R}, j}$ of the previous equality we obtain projectors

$$P^{(\Gamma)}_{\mathbf{R}, j} = |\mathbf{R}, a_j\rangle \langle \mathbf{R}, a_j| \quad (8b)$$

These projectors are the identity operators in the Bloch theorem, since the stabilizer there consists of only the identity group element. Therefore the projectors $P^{(\Gamma)}_{\mathbf{R}, j}$ are unnecessary therein. In our generalization, the projectors (8b) restrict the linear combinations of the basis $|\mathbf{R}, a_j, a\rangle a = 1, \ldots, d_f$ to their range. This basis is chosen to have orthogonal columns with the non-zero components $\sqrt{s_j}|\mathbf{R}, a_j, a\rangle$ and unit length of ket. If the projector’s range is multidimensional ($\text{Tr} P^{(\Gamma)}_{\mathbf{R}, j} > 1$), it can be written, re-enumerating components if necessary, as a direct sum of one-dimensional projectors. Then the vectors are taken from the range of these one-dimensional projectors complemented by zeroes in the rest of the space, ensuring in this way vectors’ orthogonality.

From the Eq. (8a) we see that the group element $A \notin \mathcal{S}_{\mathbf{R}, j}$, transfers the vectors $|\mathbf{R}, a_j\rangle$ to the other vector $|A\mathbf{R}, Aa_j\rangle \neq |\mathbf{R}, a_j\rangle$ making it unnecessary to look for other reduced projectors. A sufficient set of reduced projectors is for the atoms not connected by the group action, i.e. for $(\mathbf{R}, a_j)$ and $(\mathbf{R}', a_j)$ if $(\mathbf{R}, a_j) \neq (A\mathbf{R}', Aa_j)$ for all $A \in \mathcal{G}$. Such atoms are called the orbit representatives of the crystal for the symmetry group $\mathcal{G}$ and are not uniquely defined. However, this has no influence on the results. Although this generalization holds for any choice of orbit representatives, even within different unit cells, we will take them from the same unit cell, $\mathbf{R}' = \mathbf{R} = \mathbf{0}$. Hereafter, index 0 in $P^{(\Gamma)}_{0, j}$ and $\mathcal{S}_{0, j}$ will be omitted.

We now follow the same steps as in the Bloch reduction of Hamiltonian. The Hamiltonian eigenvectors are expressed as linear combinations

$$|\psi_\alpha(\Gamma)\rangle = \sum_{j} \sum_{A \in \mathcal{G}_j} c_j(\Gamma) \sqrt{s_j}|A0, a_j, a\rangle, \quad (9)$$
where subset \(G_{a,j} = G_j \subseteq G\) contains elements giving each atom \((A0, Aa_j)\) ones. Then, the Hamiltonian eigenvalue problem can be written as the set of homogenous equations in constants \(c_j(\Gamma)\) with no summation over the repeated index \(a\):

\[
\sum_{j'} \left[ \sum_{A \in U_j, b} D_{ab}^{(\Gamma)*} (A) H_{A,b,j,j'}^{c,a} (\Gamma) - E(\Gamma) \delta_{j,j'} \right] c_{j'} (\Gamma) = 0.
\]

(10)

In these equations \(e\) is the unit group element and corresponds to \(R = 0\) in the Bloch theorem. This set of equations can be expressed as the eigenvalue problem

\[
H(\Gamma)c(\Gamma) = E(\Gamma)c(\Gamma)
\]

(11)
of the reduced Hamiltonian \(H(\Gamma)\) and the matrix elements of \(H_{A,b,j,j'}^{c,a}(\Gamma)\) are

\[
H_{A,b,j,j'}^{c,a} (\Gamma) = \sqrt{\frac{2\pi}{s_j}} \langle 0, a_j, a \mid H(D_{j'}(0) | 0, a_j, b) \rangle,
\]

(12)

where \(D_{j'}(0) | 0, a_j, b\) is the orbital on the atom \((A0, Aa_j)\). The index \(a\) on the left-hand side in Eq. (11) is omitted as the reduced Hamiltonian does not depend on the choice for the nonzero vector \(|0, a_j, a\rangle\).

In this section we represented the Hamiltonian in a symmetry adapted basis. Therefore the possible action of symmetries on the Hamiltonian can be made explicit and we can ask whether the Hamiltonian is invariant under an arbitrary action of the symmetries. To claim the invariance of the constructed Hamiltonian(s) we have to find and examine the structure of \(|0, a_j\rangle\) vectors, defined by \(P_j^{(\Gamma)} | 0, a_j \rangle = |0, a_j\rangle\), and their transformation properties. We will do this in the following section.

\section*{IV. THE SYMMETRY CONSTRAINT ON GAUGE}

Let the symmetry group of a crystal have, beside translations \((R)\), one or more orthogonal transformations, \(A\). An orthogonal transformation leaves the origin \((R = 0)\) intact. We will consider only the orthogonal transformations that do not commute with translations as only such transformations affect \(k\) and vectors \(|0, a_j\rangle\). Namely, it can happen that an orbit representative is not on the axis of rotation, and/or in the reflection plane, etc., and an additional translation is needed to bring the atom to its original position after some orthogonal transformation. In such situations, \(k\)-dependent phases appear in vectors \(|0, a_j, a\rangle\). To extract this dependence, we need further analysis.

If the reduced projectors \(P_j^{(\Gamma)}\) are multidimensional (\(\text{Tr} P_j^{(\Gamma)} > 1\)), the results of the analysis coincide \[29\] with the case of equal numbers of orbit representatives and atoms in the unit cell, when the reduced projectors are one-dimensional. Therefore, the symmetry group will be reduced by the factor of maximal \(\text{Tr} P_j^{(\Gamma)}\), and all projectors will be one-dimensional. Notice that, in this case, the number of orthogonal transformations is equal to \(d_k = s_j\) and all \(s_j\) are same.

In the analysis of the \(k\)-dependence of phases we will work only when \(\Gamma\) is the general irreducible representation (label \(\Gamma\) is redundant). Phases for the irreducible representations at special points and along special lines can be deduced as limits of the phases for a general IR. To find \(k\)-dependence of phases we will explicitly construct IR using the method of induction. Induction of a (general) IR is performed, usually, from (Abelian) translational group with the one-dimensional IR \(D^{(k)}(b_i) = \exp(-ik \cdot b_i)\). In this case, the IR of the orthogonal group transformations, \(D(A)\), does not depend on the quasi-momentum and the matrix element \((1,1)\) of the general \(d_k\)-dimensional IR for translation is \(D_{j1}(b_i) = \exp(-ik \cdot b_i)\). The irreducible representation of translations is diagonal and other diagonal matrix elements satisfy

\[
\sum_{a=1}^{d_k} D_{1a}(A) D_{aa}(b_i) D_{a1}(A^{-1}) = e^{-ik \cdot ab_i}.
\]

(13)

In the above equality, the sum is redundant as the index \(a\) is uniquely defined by the orthogonal group element \(A\) and vice versa, with \(A(a = 1) = e\). In other words, the equivalent translation for \(b_i\) in the reference frame of the partner \(a\) is given by \(D_{aa}(b_i) = \exp[-ikA(a)\cdot b_i]\), where \(A(a)\) is the orthogonal transformation which brings the \(a_j\) orbital to the position of partner \(a\), i.e. \(A(a)\cdot a_j\) as we will denote in the following.

The physical content of orbitals is irrelevant in the analysis, and we will take representations \(D_{j}\) to be one-dimensional identity operator. If two orbitals \(|0, a_j\rangle\) and \((A0, Aa_j)\) are connected by the orthogonal group element \(A\), then the vector \((A0, Aa_j)\) is a linear combination of vector’s \(|0, a_j\rangle\) components, see Eqs. \[8\]. On the other hand, there is a translation \(R\) that maps the initial atom \(|0, a_j\rangle\) to \((A0, Aa_j)\) and each component \(|0, a_j, a\rangle\) gains the phase factor, see Eq. \[13\]. \(D_{aa}(R) = \exp[ikA(a)\cdot R]\).

The equivalence of these two symmetry operations implies a consistency condition that has to be imposed on the vectors \(|0, a_j\rangle\). This (formally) coincides with the usual scalar condition in the quantum field theory: \(\Psi(k) = D(A)\Psi(k) = \Psi(A^{-1}k)\), where \(\Psi(k)\) fields in our case are vectors \(|0, a_j\rangle\). The solution is given in the following general form:

\[
|0, a_j, a\rangle(k) = \exp[ikA(a)\cdot a_j - ika^0_j] |0, a_j, a\rangle(k = 0).
\]

(14)

There is also an overall phase freedom given by the phase, \(\exp(-i k \cdot a^0_j)\), where \(a^0_j\) is invariant under orthogonal transformations. This invariance of \(a^0_j\) under orthogonal transformations ensures consistent definition (the same gauge) for the orbitals connected by the group action.
Let us first discuss the case of isotropic interactions. Isotropic interactions are defined by the condition that the strength between a fixed orbital $j$ and all $j'$ at the same distance from $j$ is the same. Then the only $\mathbf{a}_j^0$ invariant under all orthogonal transformations is the zero vector, i.e. $\mathbf{a}_j^0 \equiv 0$. Any orthogonal transformation will act only as an orthogonal matrix. Under an arbitrary orthogonal transformation $B$ on the $\{\mathbf{0}, \mathbf{a}_j\}$ vectors in the generalized Bloch Hamiltonian, Eq. (12), the summation over $A$ becomes the one over $B^{-1}AB = A'$, which covers again $G_j$, and makes the Hamiltonian invariant.

The unique Hamiltonian defined by $\mathbf{a}_j^0 \equiv 0$ in this generalization of the Bloch theorem coincides with the Hamiltonian in the periodic gauge. The periodic gauge is defined as the gauge in which the Bloch vector, $|\psi(k)\rangle$, is invariant under the translation by $G = \sum_{i=1}^{d} m_i \mathbf{g}_i$ in the inverse space. Then the coefficients in Eq. (9) $c_j(k)$ transform as:

$$c_j(k + G) = c_j(k) \exp\{-iG\mathbf{a}_j\}. \quad (15)$$

In the case when $\mathbf{a}_j^0 \equiv 0$ for each $j$ the Hamiltonian matrix elements transform as

$$H_{k,j}^{\alpha,j}(k + G) = H_{k,j}^{\alpha,j}(k) \exp\{iG(a_j - a_{j'})\}. \quad (16)$$

This follows from the solution [14] for the vectors that define the generalized Bloch Hamiltonian and the fact that, in each component of the vector, $A(a) \mathbf{a}_j$ in the exponent can be rewritten as $A(a) \mathbf{a}_j = \mathbf{R} + \mathbf{a}_j$, i.e. as a translation by $\mathbf{R}$, a Bravais lattice vector. The invariance of the eigenvalue problem under the translation by $\mathbf{G}$ implies [15]. Thus, in the case of isotropic interactions, the generalized Bloch Hamiltonian is the unique Hamiltonian that is invariant under orthogonal transformations and coincides with the Hamiltonian in the periodic gauge.

We showed that the requirement that the Bloch eigenvector is invariant under the translation by any $\mathbf{G}$ in the inverse space, $|\psi(k + G)\rangle = |\psi(k)\rangle$, i.e. the requirement on its coefficients in (15), or the requirement that the Hamiltonian is invariant under orthogonal transformations lead to the same Hamiltonian.

Let us now consider anisotropic interactions. In this case the invariance under orthogonal transformations does not constrain all $\mathbf{a}_j^0$ to zero, i.e. there will be non-zero $\mathbf{a}_j^0$ which are invariant under orthogonal transformations. Thus instead of a unique Hamiltonian we can have a family of Hamiltonians invariant under orthogonal transformations. The Hamiltonian that represents the periodic choice, i.e. $\mathbf{a}_j^0 \equiv 0$ for each $j$, belongs to this family. The anisotropic case may be considered as an extension of the isotropic case when we start to continuously change the interaction strength along some directions. If we demand a continuous change of Berry curvature, or any physical quantity in the inverse space, along this process, then the periodic gauge choice is a natural choice even in the case of anisotropic interactions.

We see that in the case of the anisotropic interactions the generalized Bloch theorem, which ensures the invariance under orthogonal transformations does allow various gauges with some of $\mathbf{a}_j^0$’s being non-zero. If furthermore the choice of $\mathbf{a}_j^0$’s leads to periodicity of the coefficients, $c_j(k)$, $c_j(k + G) = c_j(k)$, and of the Hamiltonian, we deal with the Bloch Hamiltonians. The periodicity in the inverse space is the usual, defining requirement for the Bloch Hamiltonians. This choice for the Hamiltonian, so-called Bloch gauge choice is often used in the literature on the fractional Chern insulators, like in Refs. [20–22], irrespective whether the Bloch Hamiltonian is invariant under orthogonal transformations. As long as we ask for physical (“gauge invariant”) quantities, like energy spectrum, degeneracy of the ground state on the torus, Chern number, this is justified. But if we seek description in the inverse space and look for quantities that may be considered as observables, like density in the inverse space, internal field, i.e. Berry curvature or the quantities that depend on local values of Berry curvature like anomalous Hall conductance, we can find them only in the periodic gauge.

As we already emphasized there is the need for the periodic gauge even in the case of anisotropic interactions where the Bloch Hamiltonian may be invariant under orthogonal transformations. In general the off-diagonal elements of the Bloch Hamiltonians under orthogonal transformations acquire phase factors that depend on the quasi-momentum $k$ - see Table I. But though the periodic gauge is unique and physical, as we demonstrated by developing the generalized Bloch theorem, there is an interesting connection between the Berry curvatures of all possible Bloch Hamiltonians and the Berry curvature in the periodic gauge. Namely, as we will demonstrate in examples, the average of the Berry curvatures of Bloch Hamiltonians, defined by a choice of the unit cell and its partner cells connected by orthogonal transformations, is equal to the Berry curvature in the periodic gauge.

| Gauge  | Bloch | Periodic | Adding $G$ |
|--------|-------|----------|------------|
| Phase $\varphi(k)$ | $0$  | $\text{const.}$ |

TABLE I: Phases $\varphi(k)$ of the phase factor $\exp[i\varphi(k)]$ that could be acquired by the certain transformations of quasi-momentum $k$ in the off-diagonal Hamiltonian matrix elements in two gauges. Diagonal elements do not change.

V. BERRY CURVATURE CHARACTERIZATION

In the following two-dimensional examples, quasi-momentum is parameterized as $k = (k_1, k_2) = (\mathbf{k} \cdot \mathbf{b}_1, \mathbf{k} \cdot \mathbf{b}_2)$. As we are interested in the Berry curvature, IRs are general and $D_j = 1$. Berry curvature is defined as

$$B = i(\langle \partial_{k_x} u_n(k) \partial_{k_y} u_n(k) \rangle - \langle \partial_{k_y} u_n(k) \partial_{k_x} u_n(k) \rangle),$$

(17)
where \( |u_n(k)\rangle \) is the Hamiltonian eigenvector, \( n \) is the band index, and derivatives are along \( k_x \) and \( k_y \) direction in reciprocal space. Besides \( U(1) \) symmetry that leaves Berry curvature unchanged, permutation of vector’s \( |u_n(k)\rangle \) components also leaves invariant Berry curvature. These permutations are, in fact, freedom in the choice of the order of the basis functions \( |0, a_i\rangle \).

All three models, analyzed here, are relevant in the description of (fractional) quantum anomalous Hall effect, i.e. (fractional) Chern insulators. The Berry curvature, usually viewed as an intrinsic magnetic field in reciprocal space, is responsible for various effects. The dispersion of its local values gives a criterion for the stability of fractional Chern insulator states \[21, 23, 25\]. Naturally, its symmetry has to be the same as the symmetry of a crystal. In the examples in this section it is shown that Hamiltonian constructed by the generalized Bloch theorem, i.e. by using full symmetry of a crystal, have its symmetry has to be the same as the symmetry of space, is responsible for various effects. The dispersion of (fractional) quantum anomalous Hall effect, in particular, leaves Berry curvature unchanged, permutation of vector’s components also leaves invariant Berry curvature. In addition, this curvature is compared with the curvatures of the Bloch Hamiltonians.

The first and most relevant example is Haldane model \[26\] for honeycomb lattice (see Fig. 1). The General IR, \( D \), for the group’s \( C_3T_2 \) generators is:

\[
D(C_3) = \begin{pmatrix}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 0
\end{pmatrix},
\]

\[
D(b_1) = \text{diag}(e^{-i\kappa_1}, e^{i(k_1+k_2)}, e^{-i\kappa_2}),
\]

\[
D(b_2) = \text{diag}(e^{-i\kappa_2}, e^{-i\kappa_1}, e^{i(k_1+k_2)}).
\]

Stabilizers of orbit representatives, for example, atoms \( A(a\sqrt{3}/2, -a/2) \) and \( B(a\sqrt{3}/2, a/2) \) (see Fig. 1) are

\[
S_A = \{ e, (C_3|b_2\rangle, (C_3^2|b_1\rangle)\},
\]

\[
S_B = \{ e, (C_3|b_1\rangle, (C_3^2|b_1 + b_2\rangle)\},
\]

where \( e \equiv (e|0\rangle \) is the identity group element and \( (A|R) \) is the group element in Koster-Seitz notation (orthogonal transformation \( A \) followed by translation for vector \( R \)). Projectors, for these stabilizers, are one-dimensional with vectors

\[
|A\rangle = (e^{\frac{i\kappa_1-k_2}{3}}, e^{-i\frac{2k_1+k_2}{3}}, e^{\frac{i\kappa_1+2k_2}{3}})^T,
\]

\[
|B\rangle = (e^{\frac{2k_1+k_2}{3}}, e^{-i\frac{2k_1+3k_2}{3}}, e^{-i\frac{2k_1-k_2}{3}})^T,
\]

in their ranges and in the necessary gauge, where \( T \) stands for transposition. Notice that previously introduced arbitrary vector \( a_0 \) is zero vector, as the only vector in the \( xy \)-plane invariant under the rotations. Nevertheless, in three dimensions this vector can be along \( z \)-axis, but by adding horizontal plane reflection it becomes zero. Moreover, vectors \( a_{A/B} \) in the phases of both \( |A, 1\rangle \) and \( |B, 1\rangle \) are positions of the orbit representatives, while the vectors in the second and third components are position of atoms \( C_3^{-1}a_{A/B} \) and \( C_3^{-2}a_{A/B} \), respectively.

Off-diagonal element \( H_{AB}^{B} \) describes interaction of the orbit \( A \) representative with its three nearest neighboring \( B \) atoms. These three atoms are images of the group elements’ \( e, C_3^{-2}, -b_2 \) action on the orbit \( B \) representative. Since the first component \( |A, 1\rangle = \exp[i(k_1-k_2)/3] \) is non-vanishing, we can take \( a = 1 \) in Eqs. (11) and (12). Now, we need matrix elements of IR \( D_{1b}(A) \), conjugate them, multiply with corresponding \( (B, b) \), and sum over \( b \). Only non-zero matrix elements of IR for previous group elements are \( D_{11}(e) = 1 \), \( D_{12}(C_3^2) = 1 \), and \( D_{11}(-b_2) = \exp(ik_2) \), and the Hamiltonian (NN interactions is \( t_1 \)) off-diagonal matrix element is

\[
(A, 1|t_1 \left[ (D_{11}^A(e) + D_{11}^A(-b_2)) |B, 1\rangle + D_{12}^A(C_3^2) |B, 2\rangle \right] = H_{AB}^B = t_1 \left( e^{\frac{i\kappa_1+2k_2}{3}} + e^{\frac{i\kappa_1-k_2}{3}} + e^{-i\frac{2k_1+k_2}{3}} \right).
\]

Element \( H_{AB}^{B} \) is equal to \( H_{AB}^{A} \). The diagonal [six interactions to sum, orbit representatives hoping amplitude with three atoms is \( t_2 \exp(i\varphi) \) and with the other three \( t_2 \exp(i\varphi) \)] Hamiltonian matrix elements \( (H_{AB}^{A} \) and \( H_{AB}^{B} \)) are

\[
\pm M + 2t_2[\cos(k_1 + \varphi) + \cos(k_2 \pm \varphi) + \cos(k_1 + k_2 \mp \varphi)],
\]
where upper signs are for $H_A^2$ and the lower ones for $H_B^2$. Although, for atoms in the dark grey area (see Fig. 1), stabilizers are different, vectors $|A/B\rangle$ are just permutations of the previous vectors, but Hamiltonian matrix elements are the same. The resulting Hamiltonian stays the same for any choice of orbit representatives, not necessarily in unit cell. Adding general reciprocal lattice vector $G = m_1 \mathbf{g}_1 + m_2 \mathbf{g}_2$ to $\mathbf{k}$, the diagonal Hamiltonian elements stay as they are, while off-diagonal element $H_B^2$ gains constant (as $m_1$ are integers) phase $2\pi(2m_1 + m_2)/3$, and this does not affect the curvature. The rotation of $\mathbf{k}$ vector for integer multiple of $2\pi/3$ does not change the Hamiltonian at all.

The Berry curvature of the lowest energy band for the Haldane model is given in Fig. 2, parameters are $M = 1$, $t_1 = t_2 = 1$, and $\varphi = 0.125\pi$. It can be seen that the

\[
\begin{align*}
\text{FIG. 2: (Color online) Berry curvatures, in the Brillouin zone, of the lowest energy band for the Haldane model, with parameters } M = 1, \ t_1 = t_2 = 1, \text{ and } \varphi = 0.125\pi. \text{ Down is for the generalized Bloch Hamiltonian constructed here (Hamiltonian in the periodic gauge). Up-left is for the Bloch Hamiltonian for the light-grey (see Fig. 1) and up-right for the dark-grey unit cell.}
\end{align*}
\]

generalized Bloch Hamiltonian has the most symmetric Berry curvature. The curvatures of the Bloch Hamiltonians for the light and dark grey unit cells (see Fig. 1) have only translational symmetry, in the reciprocal space. By rotating light and dark grey unit cells for $2\pi/3$ and $4\pi/3$ and constructing the Bloch Hamiltonians for such unit cells, Berry curvature is also rotated for the same angle. Average of all three Berry curvatures, separately for light and dark grey unit cells, is equal to the Berry curvature of the generalized Bloch Hamiltonian. Equivalent conclusion will hold in other examples. Notice that rotation of the light-grey unit cell is equivalent to fixing one atom and making the Bloch Hamiltonians for that atom and its nearest neighbors.

The second example is kagome [27, 28] lattice model (see Fig. 3). The atoms are indistinguishable, and the symmetry of the crystal is a product of axial group $C_6$ and 2D translations along $\mathbf{b}_1 = 2a(1, 0)$ and $\mathbf{b}_2 = 2a(-1/2, \sqrt{3}/2)$, where $a$ is the nearest neighbor distance. The whole crystal can be obtained by this group action on a single atom. Nevertheless, the resulting Hamiltonian is equal to the Hamiltonian constructed with symmetry group $C_2 T_2$ having three orbit representatives. For the sake of simplicity and to have the representation by vectors with lower dimension (2 instead of 6), we will take as symmetry group $C_2 T_2$ with three orbit representatives. The general irreducible representation of the generators is:

\[
\begin{align*}
D(C_2) &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\
D(\mathbf{b}_1) &= \text{diag}(e^{-ik_1}, e^{ik_1}) = e^{-i\varphi}, \\
D(\mathbf{b}_2) &= \text{diag}(e^{-ik_2}, e^{ik_2}).
\end{align*}
\]

As the resulting Hamiltonian does not depend on the choice of orbit representatives, we will take, for example, atoms from the dark-grey unit cell $R(-a/2, a\sqrt{3}/2)$, $G(-a/2, -a\sqrt{3}/2)$, and $B(-a, 0)$ (see Fig. 3). Stabilizers for these atoms are $S_R = \{e_i(C_2|\mathbf{b}_2)\}$, $S_G = \{e_i(C_2|\mathbf{b}_1 - \mathbf{b}_2)\}$, and $S_B = \{e_i(C_2|\mathbf{b}_2)\}$. Again, the projectors for these stabilizers are one-dimensional with vectors

\[
|R\rangle = \begin{pmatrix} e^{i\varphi} \\ e^{-i\varphi} \end{pmatrix}, \\
|G\rangle = \begin{pmatrix} e^{-i\varphi} \\ e^{i\varphi} \end{pmatrix}, \\
|B\rangle = \begin{pmatrix} e^{-i\varphi} \\ e^{i\varphi} \end{pmatrix},
\]

in their ranges and in the necessary gauge. Here, as in the previous example, arbitrary vectors $a_j$ are zero. Also, the first components have $a_j$ vectors equal to the positions of orbit representatives, while, in the second components, vectors are the positions of atoms rotated for $\pi$.

Now, as in the Haldane example, with the help of Eqs. (11) and (12), the generalized Bloch Hamiltonian

\[
\begin{align*}
\text{FIG. 3: (Color online) Kagome lattice model with three sublattices } R \text{ [grey (red) disks], } G \text{ [light-gray (green) disks], and } B \text{ [dark-grey (blue) disks]. Complex nearest neighbors hoping amplitude is } t_1 - i\lambda_1 = t_1 e^{-i\varphi} \text{ in the arrow direction. Vectors } \mathbf{b}_1 \text{ and } \mathbf{b}_2 \text{ are direct lattice vectors. Light and dark grey areas are two differently shaped unit cells.}
\end{align*}
\]
is

\[ H = 2t_1 \begin{pmatrix} 0 & e^{-i\phi} \cos \frac{k_1}{2} & e^{i\phi} \cos \frac{k_1+k_2}{2} \\ e^{-i\phi} \cos \frac{k_1+k_2}{2} & 0 & e^{-i\phi} \cos \frac{k_2}{2} \\ e^{i\phi} \cos \frac{k_2}{2} & e^{-i\phi} \cos \frac{k_2}{2} & 0 \end{pmatrix}. \]

It is obvious that this Hamiltonian is invariant under the rotation for \( \pi \). A rotation for \( 2\pi/6 \) and reordering basis vectors \([(RGB) \rightarrow (GRB)]\) leaves the Hamiltonian unchanged. This means that the Berry curvature is invariant under rotation for \( 2\pi/6 \). By adding an arbitrary vector of reciprocal lattice to \( \mathbf{k} \), off-diagonal elements might change their sign which is of no influence on the Berry curvature.

![FIG. 4: (Color online) Berry curvatures of the lowest energy band for the kagome model (parameters are \( t_1 = 1 \) and \( \phi = \pi/4 \)) in the Brillouin zone. Up-left is of the Bloch Hamiltonian for the light-grey (see Fig. 3) and up-right for the dark-grey unit cell. Down is for the generalized Bloch Hamiltonian constructed here.](image)

The Berry curvature of the lowest energy state of the generalized Bloch Hamiltonian is given in Fig. 4 (down). Notice that it has the full symmetry of the crystal. Above are the Berry curvatures, also for the lowest energy state, of the Bloch Hamiltonians for light (left) and dark-grey (right) unit cells (see Fig. 3). Again, the average of any of these two Berry curvatures and ones rotated for \( \pi \) (i.e. of the Bloch Hamiltonians for unit cells rotated for \( \pi \), which is the symmetry of the model), is the Berry curvature of the generalized Bloch Hamiltonian. Notice that the Berry curvature for the light-grey unit cell is symmetric under rotation for \( 2\pi/3 \), like that unit cell, while for the dark-grey unit cell has only the translational symmetry.

Finally, the third example is the brick-wall model [7]. In order to illustrate the case with anisotropic interactions with non-zero vectors \( \mathbf{a}_1^0 \), we took model without next nearest neighbors hoping amplitude \( t_2 = 0 \) (see Fig. 5). This model is invariant under the 2D translations along \( \mathbf{b}_1 = d\sqrt{2}(1,0) \) and \( \mathbf{b}_2 = d\sqrt{2}(0,1) \), where \( d \) is the NN distance, and the rotation for \( \pi \) about horizontal \( U \) axis (centerline of \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \)). The general irreducible representation for these generators is

\[ D(U) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \]

\[ D(\mathbf{b}_1) = \text{diag}(e^{-ik_1}, e^{-ik_2}), \]

\[ D(\mathbf{b}_2) = \text{diag}(e^{-ik_2}, e^{-ik_1}). \]

FIG. 5: The brick-wall lattice model \( (t_2 = 0) \) with two sublattices \( A \) (circles) and \( B \) (disks), with on-site energies \( M \) and \( -M \), respectively. The nearest neighbors hoping amplitude is \( t_1 \), only between connected atoms. The distance of NNs is \( d \). Dashed line is the group element \( U \), horizontal axis of rotation for \( \pi \). Vectors \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) are direct lattice vectors. Grey area is one choice for unit cell. Other choices are \( A \) atom from that unit cell with one of the nearest neighbors, \( B \) atom 2, 3, or 4.

The stabilizers for the atoms \( A \) and \( B \) in the grey UC are equal \( S_A = S_B = \{ e, U \} \). Vectors from the range of the projector for this stabilizer are

\[ |A\rangle = e^{-ik} a^0_A \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |B\rangle = e^{-ik} a^0_B \begin{pmatrix} e^{i(k_1+k_2)/2} \\ e^{i(k_1+k_2)/2} \end{pmatrix}, \]

with an arbitrary \( a^0_{A/B} \) along \( \mathbf{b}_1 + \mathbf{b}_2 \), \( a_A = 0 \), and \( a_B = (\mathbf{b}_1 + \mathbf{b}_2)/2 \). Since one of the vectors \( a^0_{A/B} \) is redundant, we can take \( a^0_A = 0 \) and let \( a^0_B = c(\mathbf{b}_1 + \mathbf{b}_2) \) with an arbitrary constant \( c \). With the vectors \( |A\rangle/|B\rangle \), the generalized Bloch Hamiltonian matrix elements are

\[ H^A = M = -H^B \]

and

\[ H^A = e^{-ik} a^0_B t_1 (2 \cos \frac{k_1 - k_2}{2} + e^{i(k_1+k_2)/2} \). \]

Notice that the Hamiltonian matrix elements are invariant under the rotation for \( \pi \) about \( U \), while adding general reciprocal lattice vector \( \mathbf{G} = m_1 \mathbf{g}_1 + m_2 \mathbf{g}_2 \) to \( \mathbf{k} \), brings a constant phase \( \pi + c(m_1 + m_2)2\pi \) into off-diagonal elements.

Different vectors \( a^0_B \) provide different gauges. If \( a^0_B \) is equal to zero we have for the generalized Bloch Hamiltonian the Hamiltonian in periodic gauge. If we chose \( a^0_B \) to be equal to the position of the \( B \) atoms 1 or 3.
$[a B] = \pm (b_1 + b_2)/2$, with plus for the atom 1 and minus for 3, then the generalized Bloch Hamiltonian is the Bloch Hamiltonian for the unit cells with central atom $A$ and $B$ atoms 1 or 3, respectively. Notice that the symmetry does not allow a construction of the Bloch Hamiltonian for the unit cells containing atom $A$ in the origin (see Fig. 5). Again, all the possible (by varying $a B$) Berry curvatures for the generalized Bloch Hamiltonian have the symmetry of the model. The Berry curvature of the lowest energy state of the Hamiltonian in periodic gauge ($a B = 0$) is given down in Fig. 6. Others are the curvatures for the lowest energy state of the Bloch Hamiltonians constructed with different unit cells, atom $A$ being one in the origin and the $B$ atoms 1 or 3. Unit cells with atoms 1 and 3 have $U$ symmetry and therefore their Berry curvatures, up-left and up-right in Fig. 6 have the following transformation property $U B(k_1, k_2) = -B(k_2, k_1)$. Although the symmetry of the curvatures is the same, the average of these two curvatures is the curvature of the generalized Bloch Hamiltonian for $a B = 0$, i.e. the Hamiltonian in periodic gauge. As a consequence, here, like in the Haldane model, the Berry curvature of any eigenstate of the Hamiltonian in the periodic gauge is average of the curvatures of the Bloch Hamiltonians constructed for the unit cells made of one fixed atom and its nearest neighbors.

VI. SUMMARY

The Bloch theorem is generalized to the case when a crystal is invariant under more symmetry operations than just translations. The method applied can be used even in the case of the systems without translational symmetry like molecules. In this generalization the method provides the most symmetric, in the reciprocal space, Hamiltonian. The method applied can be used even in the case of the systems without translational symmetry like molecules. In this generalization the method provides the most symmetric, in the reciprocal space, Hamiltonian and Berry curvature. The resulting Hamiltonian coincides with the Hamiltonian defined by the periodic gauge. In addition it is shown, for any energy band, the curvature of the Hamiltonian in the periodic gauge is equal to the average of the curvatures of the Bloch Hamiltonians for all possible unit cells.

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