BERRY PHASE, BERRY CURVATURE, AND THE ANOMALOUS VELOCITY OF BLOCH ELECTRONS*

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1 Introduction

Along the last decades topology has acquired an ever increasing relevance in physics, as also witnessed by the recent Nobel prize in 2016 assigned to David Thouless, Duncan Haldane e Michael Kosterlitz for topological phase transitions and topological phases of matter [1]. Their work has explicitly shown that topological concepts are crucial to understand some states of matter. In particular this emphasizes the great deal of attention that in last decades was devoted to topology in condensed matter physics, where these topological states can be realized in practice: not only Quantum Hall Effect, Berezinskii-Kosterlitz-Thouless transition, but also, more recently, the topological insulators and the Majorana Fermions (these latters having also been claimed recently to be of practical relevance for quantum computation [2]).

One of the major examples of a topological concept in fundamental quantum physics was introduced by Berry, who, contrary to a widespread belief, first showed that the phase of wavefunctions can sometimes be a gauge-invariant physical observable[4]. The Aharonov-Bohm effect (see, e.g., Ref. [3] p. 331) provides an example in this sense. This entailed other related concepts like Berry connection and Berry curvature. This latter, a gauge-invariant characteristic of some quantum states, has been shown to be crucial to explain some solid state phenomena [9], like, e.g., the Anomalous Hall Effect. Some of these effects are tightly related to the fact that the Berry curvature in the band structure of some solids induces additional terms in the velocity of the Bloch states. This is the main topic at issue in the present notes. While Sect. 2 is freely inspired by the treatment of Ref.[3], Sect. 3 and 4 are based on the approach described in Ref. [9].

*Notes for the Condensed Matter Theory course

2 General introduction to the Berry Phase

2.1 The geometric phase

Let us consider a quantum system, described by a Hamiltonian H, which is initially in an eigenstate with eigenvalue E. Let us consider the possibility that this Hamiltonian is so slowly varied in time (so slowly that the adiabatic theorem of quantum mechanics hold: if the system is in a quantum eigenstate it will remain in the same eigenstate during the time evolution). This time variation can be realized with a slow variation of its parameters, like, e.g., in the Born-Oppenheimer treatment of electron-ion systems: in this case the electron Hamiltonian and states vary through the parametric dependence on the slow ionic coordinates.

During the time evolution the system will stay in the same eigenstate $|n,t\rangle$ and the eigenvalue $E_n(t)$ so that

$$H(t)|n,t\rangle = E_n(t)\,|n,t\rangle. \tag{1}$$

Any generic state at time t can be expanded as

$$|\alpha,t\rangle = \sum_n c_n(t)\, e^{\mathrm{i}\,\theta_n(t)}\,|n,t\rangle, \tag{2}$$

with

$$\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'. \tag{3}$$

To determine the coefficients $c_n(t)$ one can consider the Schrödinger equation

$$i\hbar\,\frac{\partial}{\partial t}|\alpha,t\rangle = H(t)|\alpha,t\rangle \tag{4}$$

and insert on both sides the expansion (2). On the left hand sides one obtains

$$\begin{aligned} i\hbar\,\frac{\partial}{\partial t}|\alpha,t\rangle &= i\hbar\sum_n\left[\dot{c}_n e^{i\theta_n(t)}|n,t\rangle + c_n(t)e^{i\theta_n(t)}\frac{\partial}{\partial t}|n,t\rangle + i\frac{\partial\theta(t)}{\partial t}c_n(t)e^{i\theta_n(t)}\right] \\ &= i\hbar\sum_n e^{i\theta_n(t)}\left[\dot{c}_n(t)|n,t\rangle + c_n(t)\frac{\partial}{\partial t}\,|n,t\rangle + i\frac{\partial\theta(t)}{\partial t}c_n(t)|n,t\rangle\right] \\ &= i\hbar\sum_n e^{i\theta_n(t)}\left[\dot{c}_n(t)|n,t\rangle + c_n(t)\frac{\partial}{\partial t}\,|n,t\rangle + \frac{i}{\hbar}E_n(t)c_n(t)|n,t\rangle\right] \end{aligned} \tag{5}$$

having used Eq.(3) in the last step. On the other hand, the rhs of Eq.(4) is

$$H(t)|\alpha,t\rangle = \sum_n e^{i\theta_n(t)}E_n(t)c_n(t)|n,t\rangle. \tag{6}$$

and cancels the corresponding term on the lhs of (5), so that the Schrödinger equation can be recast as

$$\sum_n e^{i\theta_n(t)}\left[\dot{c}_n(t)|n,t\rangle + c_n(t)\frac{\partial}{\partial t}|n,t\rangle\right] = 0. \tag{7}$$

Projecting on the $\langle m,t|$ eigenstate one finds

$$\dot{c}_m(t) = -\sum_n c_n(t)\, e^{i(\theta_n(t)-\theta_m(t))}\langle m,t|\frac{\partial}{\partial t}|n,t\rangle. \tag{8}$$

Splitting the summation in $n=m$ and $n\neq m$ terms one gets

$$\dot{c}_m(t) = -c_m(t)\langle m,t|\frac{\partial}{\partial t}|m,t\rangle - \sum_{n\neq m} c_n(t)e^{i(\theta_n(t)-\theta_m(t))}\langle m,t|\frac{\partial}{\partial t}|n,t\rangle. \tag{9}$$

We assume now (and it can be shown, see Ref. [3]) that the time evolution can be chosen slow enough to make the second term on the rhs negligible thereby leading to

$$\dot{c}_n(t) = -c_n(t)\langle n,t|\frac{\partial}{\partial t}|n,t\rangle. \tag{10}$$

This equation can be solved to obtain

$$c_n(t) = c_n(0)\exp\left[-\int_0^t \langle n,t'|\frac{\partial}{\partial t}|n,t'\rangle dt'\right] \equiv c_n(0)e^{i\gamma_n(t)} \tag{11}$$

The *geometric* phase

$$\gamma_n(t) = i\int_0^t \langle n,t'|\frac{\partial}{\partial t}|n,t'\rangle dt' \tag{12}$$

can be shown to be real by imposing that the norm of the eigenstate is conserved in time

$$\begin{aligned} 0 &= \frac{\partial}{\partial t}\langle n,t|n,t\rangle = \left[\frac{\partial}{\partial t}\langle n,t|\right]|n,t\rangle + \langle n,t|\left[\frac{\partial}{\partial t}|n,t\rangle\right] \\ &= \left(\langle n,t|\left[\frac{\partial}{\partial t}|n,t\rangle\right]\right)^* + \langle n,t|\left[\frac{\partial}{\partial t}|n,t\rangle\right]. \end{aligned} \tag{13}$$

To summarize, one finds that, when the Hamiltonian is adiabatically evolved in time, $\psi_n(t)$, the $n-$th component of the wavefunction $|\alpha,t\rangle$, not only acquires the usual *dynamical* phase $\theta_n(t)$ related to the $n-$th energy eigenvalue E_n (see Eq.(3), but also acquires a *geometrical* phase factor $\gamma_n(t)$

$$|\psi_n(t)\rangle = e^{i\gamma_n(t)}\exp\left[-\frac{i}{\hbar}\int_0^t E_n(t')dt'\right]|n,t\rangle \tag{14}$$

2.2 The Berry phase

Let us now make it explicit the fact that the Hamiltonian depends on time through a set of N parameters $\xi_i(t)$ (with $i=1,...,N$). We define a vector $\boldsymbol{\xi}(t)$ having $\xi_i(t)$ as components so that $H=H(\boldsymbol{\xi})$, $\boldsymbol{\xi}=\boldsymbol{\xi}(t)$. Then also the eigenvalues and eigenvectors depend on t via $\boldsymbol{\xi}(t)$: $|n,t\rangle = |n(\boldsymbol{\xi})\rangle$ and $E_n(t) = E_n(\boldsymbol{\xi})$ so that

$$H(\boldsymbol{\xi})|n(\boldsymbol{\xi})\rangle = E_n(\boldsymbol{\xi})|n(\boldsymbol{\xi})\rangle \tag{15}$$

$$\frac{d}{dt}|n,t\rangle = \frac{\partial}{\partial\boldsymbol{\xi}}|n(\boldsymbol{\xi})\rangle\cdot\frac{d\boldsymbol{\xi}}{dt} \tag{16}$$

Eq.(12) can then be rewritten as

$$\gamma_n(C) = \int_C i\langle n(\boldsymbol{\xi})|\frac{\partial}{\partial \boldsymbol{\xi}}|n(\boldsymbol{\xi})\rangle d\boldsymbol{\xi} \equiv \int_C \mathbf{A}_n(\boldsymbol{\xi}) d\boldsymbol{\xi} \tag{17}$$

where C is a path $\xi(t')$ (cf. Eq.(12) in the parameter space starting in $\xi(t=0)$ and ending in $\xi(t=T)$. $\mathbf{A}_n(\boldsymbol{\xi})$ is a vector valued function in the same space. This vector is called the **Berry connection** or the **Berry vector potential**. Obviously, $\mathbf{A}_n(\boldsymbol{\xi})$ is gauge dependent: If we make a gauge transformation

$$|n(\boldsymbol{\xi})\rangle \to e^{i\zeta(\boldsymbol{\xi})}|n(\boldsymbol{\xi}\rangle \tag{18}$$

with $\zeta(\boldsymbol{\xi})$ an arbitrary smooth function, then A_n transforms as vector potentials usually do

$$\mathbf{A}_n(\boldsymbol{\xi}) \to \mathbf{A}_n(\boldsymbol{\xi}) - \frac{\partial}{\partial \boldsymbol{\xi}}\zeta(\boldsymbol{\xi}). \tag{19}$$

Consequently, the phase γ_n given by Eq. (17) will be changed by $\zeta(\boldsymbol{\xi}(T)) - \zeta(\boldsymbol{\xi}(0))$, after the transformation, where $\boldsymbol{\xi}(0))$ and $\boldsymbol{\xi}(T))$ are the initial and final points of the path C. This observation had led to conclude that one can always choose a suitable $\zeta(\boldsymbol{\xi})$ such that γ_n accumulated along the path C is canceled out, leaving Eq. (14) with only the dynamical phase. Because of this, the phase γ_n has long been deemed unimportant and it was usually neglected in the theoretical treatment of time-dependent problems. This conclusion remained unchallenged until Berry [4] reconsidered the cyclic evolution of the system along a **closed** path C with $\boldsymbol{\xi}(0)) = \boldsymbol{\xi}(T))$. The phase choice made earlier on the basis function $|n(\boldsymbol{\xi})\rangle$ requires $e^{i\zeta(\boldsymbol{\xi})}$ in the gauge transformation Eq. (18) to be single valued,

$$e^{i\zeta(\boldsymbol{\xi}(0))}|n(\boldsymbol{\xi}(0))\rangle = e^{i\zeta(\boldsymbol{\xi}(T))}|n(\boldsymbol{\xi}(T))\rangle$$

which implies $\zeta(\boldsymbol{\xi}(T)) - \zeta(\boldsymbol{\xi}(0)) = 2\pi\times$integer. This shows that γ_n can be only changed by an integer multiple of 2π under the gauge transformation Eq. (18) and it cannot be removed. Therefore *for a closed path*, γ_n becomes a gauge-invariant physical quantity, now known as the **Berry phase**

$$\gamma_n(C) = \oint_C d\boldsymbol{\xi} \cdot \mathbf{A}_n(\boldsymbol{\xi}). \tag{20}$$

From the above definition, we can see that the Berry phase only depends on the geometric aspect of the closed path and is independent of how $\boldsymbol{\xi}(t)$ varies in time. The explicit time dependence is thus not essential in the description of the Berry phase and will be dropped in the following discussion.

The definition of the Berry phase as a path integral over a closed curve in Eq. (20), naturally suggests the use of Stokes' theorem to define γ_n in terms of a surface integral

$$\gamma_n(C) = \int_S d\mathbf{s} \cdot \boldsymbol{\Omega}_n(\boldsymbol{\xi}). \tag{21}$$

where S is an arbitrary surface encircled by the path C and in the case of a three dimensional parameter space ($N = 3$)

$$\boldsymbol{\Omega}_n(\boldsymbol{\xi}) \equiv \boldsymbol{\nabla}_{\boldsymbol{\xi}} \times \mathbf{A}_n(\boldsymbol{\xi}). \tag{22}$$

Eq. (22) only holds for $N = 3$, while a more general form can be given in terms of gauge-field tensor in all other cases [6, 9]

$$\begin{aligned}\Omega^n_{\mu\nu}(\boldsymbol{\xi}) &= \frac{\partial}{\partial\xi^\mu}A^n_\nu(\boldsymbol{\xi}) - \frac{\partial}{\partial\xi^\nu}A^n_\mu(\boldsymbol{\xi}) \\ &= i\left[\langle\frac{\partial n(\boldsymbol{\xi})}{\partial\xi^\mu}|\frac{\partial n(\boldsymbol{\xi})}{\partial\xi^\nu}\rangle - (\nu \rightleftharpoons \mu)\right] \end{aligned} \tag{23}$$

$\boldsymbol{\Omega}_n(\boldsymbol{\xi})$ is termed **Berry curvature** and for $N = 3$ can be interpreted as a 'magnetic field' in the 3D parameter space. It is also worth noticing that compared to the Berry phase which is always associated with a closed path, **the Berry curvature is truly a local quantity** in the $\boldsymbol{\xi}$ parameter space. It provides a local description of the geometric properties of this parameter space, which, we will see, may have important consequences in electron transport properties.

In Appendix A we also derive an expression for calculating the Berry curvature, which highlights the relevance of degeneracy points in the electronic spectrum such that $E_n(\boldsymbol{\xi}) = E_m(\boldsymbol{\xi})$, (see Eq.(49)). In this case the Berry curvature $\boldsymbol{\Omega}_n(\boldsymbol{\xi})$, and therefore the Berry phase $\gamma_n(C)$, will be dominated by these points, regardless of whether or not the path C followed by the parameter vector $\boldsymbol{\xi}$ includes these points. These degenerate points are 'singularities' that contribute significantly to the integral of the curve containing them, even if the curve (as well as the surface enclosed by it) does not include such points. This means, ultimately, that the phase of the system will undergo a measurable effect resulting from possible states of energy degeneration, even if the system itself never finds itself in such degenerate states.

A very important fact is finally worth being stressed again: The Berry phase (i.e. the geometric phase on a closed path) is a **gauge-invariant quantity**, while the geometric phase on open paths of Eq. (12,14) is a gauge-dependent quantity. Thus, while the Berry phase is an intrinsic and measurable quantity, the generic geometric phase is not and can, for instance, always be eliminated by a suitable choice of the gauge vector potential $\mathbf{A}(t)$ (this particular choice is usually called the 'parallel transport gauge' and correspond to the choice $\langle n, t|\frac{\partial}{\partial t}|n, t\rangle = 0$ at any t). At first sight this choice seems at odds with a non-vanishing Berry phase because the geometric phase in Eq. (12) or (17) vanishes. However it is not so (see also Sect. 3.1 in Ref.[6] and Appendix in Ref.[9]): For a closed path in the parameter space, i.e., $\boldsymbol{\xi}(T) = \boldsymbol{\xi}(0)$, there is no guarantee that the phase at the final time $t_f = T$ is the same as the phase at the beginning $t_0 = 0$. In other words, under the parallel transport condition, even though $|n(\boldsymbol{\xi}(t))\rangle$ is uniquely determined as a function of t, it can still be a multi-valued function of $\boldsymbol{\xi}(t)$ so that $|n(\boldsymbol{\xi}(T))\rangle \neq |n(\boldsymbol{\xi}(0))\rangle$. In particular the phase difference γ_n in $|n(\boldsymbol{\xi}(T))\rangle = e^{-i\gamma_n}|n(\boldsymbol{\xi}(0))\rangle$ is precisely the Berry phase of the closed path. In fact, this can be considered as another definition of the Berry phase.

3 Berry phase in Bloch bands

Above we introduced the basic concepts of the Berry phase for a generic system described by a parameter-dependent Hamiltonian. We now consider its realization in crystalline solids. As we shall see, the band structure of crystals provides a natural platform to investigate the occurrence of the Berry phase effect. Within the independent electron approximation, the band structure of a crystal is determined by the following Hamiltonian for a single electron:

$$H = \frac{\hat{p}^2}{2m} + V(\mathbf{r}) \tag{24}$$

where $V(\mathbf{r} + \mathbf{R}_B) = V(\mathbf{r})$ is the periodic potential with $\mathbf{R}_B$ any Bravais lattice vector. According to Bloch's theorem, the eigenstates of a periodic Hamiltonian satisfy the following condition

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}_B) = e^{i\mathbf{k}\cdot\mathbf{R}_B}\psi_{n\mathbf{k}}(\mathbf{r}) \tag{25}$$

where n is the band index and $\mathbf{k}$ is the crystal momentum, which resides in the Brillouin zone. Thus the system is described by a k-independent Hamiltonian with a k-dependent (boundary) condition Eq. (25). To be coherent with the general formalism of the Berry phase, we move to the momentum dependent Hamiltonian [cf. Eq. (8.48) in Ref. [7]]

$$H(\mathbf{k}) = \frac{(\hat{\mathbf{p}} + \hbar\mathbf{k})^2}{2m} + V(\mathbf{r}) \tag{26}$$

having $u_{n\mathbf{k}}(r)$ as eigenvectors, $H(\mathbf{k})u_{n\mathbf{k}}(r) = E_{\mathbf{k}}u_{n\mathbf{k}}(r)$, and momentum independent boundary condition $u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}_B)$. We can thus identify the Brillouin zone as the parameter space of the transformed Hamiltonian $H(\mathbf{k})$ and $u_{n\mathbf{k}}(\mathbf{r})$ as the basis function (i.e. we here identify $\mathbf{k}$ with ξ). Now, if $\mathbf{k}$ is forced to vary along a path in the momentum space, then the Bloch state at time t will pick up a phase (cf. Eq.(17))[1]

$$\gamma_n = i\int_{\mathbf{k}_i}^{\mathbf{k}_f} d\mathbf{k}\cdot\langle u_n(\mathbf{k})|\nabla_{\mathbf{k}}|u_n(\mathbf{k})\rangle. \tag{27}$$

Remember that γ_n is in general gauge-dependent unless the path C is closed to make γ_n a gauge-invariant quantity with physical significance (the Berry phase)

$$\gamma_n = i\oint_C d\mathbf{k}\cdot\langle u_n(\mathbf{k})|\nabla_{\mathbf{k}}|u_n(\mathbf{k})\rangle. \tag{28}$$

According to our previous discussion, for each energy band n we can also define in any point $\mathbf{k}$ of the crystal momentum space a Berry curvature

$$\mathbf{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \langle u_n(\mathbf{k})|i\nabla_{\mathbf{k}}|u_n(\mathbf{k})\rangle \tag{29}$$

[1] To be coherent with the general treatment reported in Sect. 2, here we keep using the Dirac notation for basis $|u_n(\mathbf{k})\rangle$ so that $u_{n\mathbf{k}}(r) = \langle\mathbf{r}|u_n(\mathbf{k})\rangle$.

This Berry curvature is an intrinsic property of the band structure because it only depends on the wave function $|u_n(\mathbf{k})\rangle$. It is nonzero in a wide range of materials, in particular, crystals with broken time-reversal or inversion symmetry (see below). In fact, once we have introduced the concept of the Berry curvature, a closed loop is not necessary because the Berry curvature itself is a local gauge-invariant quantity. It is now well recognized that information on the Berry curvature is essential in a proper description of the dynamics of Bloch electrons, which has various effects on transport and thermodynamic properties of crystals.

4 Bloch electron dynamics in an electric field

The dynamics of Bloch electrons under the perturbation of an electric field is one of the oldest problems in solid-state physics. It is usually understood that while the electric field can drive electron motion in momentum space, it does not appear in the electron velocity; the latter is simply given by (see, for example, Chap. 8 and Appendix E of Ref. [7])

$$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial \mathbf{k}} \tag{30}$$

Through recent progress on the semiclassical dynamics of Bloch electrons it has been made increasingly clear that this description is incomplete. In the presence of an electric field, an electron can acquire an anomalous velocity proportional to the Berry curvature of the band [8]. This anomalous velocity is responsible for a number of peculiar transport phenomena, like, e.g. the anomalous Hall effect. To study the corrections induced on the Bloch electron velocity by the Berry curvature there are various approaches. In the following we use the approach of Xiao et al. [see Sect. II.A and Appendix in Ref. [9]][2]. An alternative approach is reported in Ref. [10].

4.1 Adiabatic evolution of Bloch states and anomalous velocity of Bloch electrons

In order to identify additional contributions to the velocity of Bloch electrons in Eq. (30), we need to identify how Bloch states are modified by an adiabatic modification of the Hamiltonian. In particular one can see that under an adiabatic time evolution of the Hamiltonian $H(\mathbf{k}, t)$, the m-th eigenvalue $|u_m(\mathbf{k}, t)\rangle$, up to first order in the rate of change of $H(\mathbf{k}, t)$, becomes

$$|u_m(\mathbf{k}, t)\rangle = |u_m(\mathbf{k})\rangle - i\hbar \sum_{n\neq m} \frac{|u_n(\mathbf{k})\rangle\langle u_n(\mathbf{k})|\frac{\partial}{\partial t}|u_m(\mathbf{k}, t)\rangle}{E_m(t) - E_n(t)}. \tag{31}$$

[2] We point out that in order to be coherent with the notation of the previous sections and the notation in the book by Ashcroft and Mermin [7] the crystal momentum $\mathbf{q}$ in the paper by Xiao et al. [9] is called $\mathbf{k}$ here

where $|u_m(\mathbf{k})\rangle \equiv |u_m(\mathbf{k},0)\rangle$. This expression is explicitly derived in the Appendix of Ref. [9]. This expression as it is is derived in a specific gauge, the so-called parallel transport gauge. A clear discussion on this choice and its relation with other possible gauge choices, is in the Sec. 3.1 of Ref. [6]. Since, however, we will only use this expression for the calculation of gauge-invariant quantities, this choice is immaterial here and we skip further details on this interesting issue.

The adiabatic time evolution of the eigenstates $|u_m(\mathbf{k},t)\rangle$ of $H(\mathbf{k},t)$ induces important modifications on the expression of velocity. The velocity **operator** in the $\mathbf{k}$ representation is given by [see, e.g., Appendix E of Ref. [7]]

$$\hat{\mathbf{v}}_n(\mathbf{k}) = \frac{\partial H(\mathbf{k},t)}{\hbar \partial \mathbf{k}} = \frac{\hbar}{m}(-i\nabla + \mathbf{k}). \tag{32}$$

When averaged over the eigenstates $|u_m(\mathbf{k},t)\rangle$ given by Eq.(31) the velocity acquires additional terms

$$\mathbf{v}_m(\mathbf{k}) = \frac{\partial E_m(\mathbf{k})}{\partial \hbar \mathbf{k}} - i \sum_{n \neq m} \left[\frac{\langle u_m(\mathbf{k}| \frac{\partial H}{\partial \mathbf{k}} |u_n(\mathbf{k})\rangle \langle u_n(\mathbf{k})| \frac{\partial}{\partial t} |u_m(\mathbf{k},t)\rangle}{E_m(t) - E_n(t)} - c.c. \right]. \tag{33}$$

Then one can use the identity $\sum_{n\neq m} |u_n(\mathbf{k})\rangle\langle u_n(\mathbf{k}| = 1 - |u_m(\mathbf{k})\rangle\langle u_m(\mathbf{k}|$ and the fact that

$$\langle u_m(\mathbf{k}| \frac{\partial H(\mathbf{k},t)}{\partial \mathbf{k}} |u_n(\mathbf{k})\rangle = (E_m - E_n) \langle \frac{\partial u_m(\mathbf{k})}{\partial \mathbf{k}} |u_n(\mathbf{k})\rangle \tag{34}$$

(we demonstrate this relation below).[3] Thus Eq. (33) becomes

$$\begin{aligned} \mathbf{v}_m(\mathbf{k}) &= \frac{\partial E_m(\mathbf{k})}{\partial \hbar \mathbf{k}} - i \left[\langle \frac{\partial u_m(\mathbf{k})}{\partial \mathbf{k}} | \frac{\partial u_m(\mathbf{k},t)}{\partial t} \rangle \right. \\ &- \left. \langle \frac{\partial u_m(\mathbf{k})}{\partial \mathbf{k}} |u_m(\mathbf{k})\rangle\langle u_m(\mathbf{k})| \frac{\partial u_m(\mathbf{k},t)}{\partial t} \rangle - c.c. \right]. \end{aligned} \tag{35}$$

The second term in the square bracket in the rhs is real because it is the product of two purely imaginary terms (this can be shown by by the same procedure

[3] We here briefly derive Eq. (34). We restart from the Schrödinger equation in $\mathbf{k}$-representation

$$H(\mathbf{k})|u_{n\mathbf{k}}\rangle = E_{n\mathbf{k}}|u_{n\mathbf{k}}\rangle$$

and differentiate both sides with respect to $\mathbf{k}$

$$\frac{\partial H(\mathbf{k})}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle + H(\mathbf{k})\frac{\partial}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle = \frac{\partial E_{n\mathbf{k}}}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle + E_{n\mathbf{k}}\frac{\partial}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle.$$

Projecting on the $\langle u_{m\mathbf{k}}|$ $(m \neq n)$ state one obtains

$$\langle u_{m\mathbf{k}}|\frac{\partial H(\mathbf{k})}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle + \langle u_{m\mathbf{k}}|H(\mathbf{k})\frac{\partial}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle = E_{n\mathbf{k}}\langle u_{m\mathbf{k}}|\frac{\partial}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle.$$

from which Eq. (34) is easily obtained.

leading to Eq. (13). See also the discussion in the Appendix after Eq. (46)). Therefore by subtracting the complex conjugate it is canceled

$$\mathbf{v}_m(\mathbf{k}) = \frac{\partial E_m(\mathbf{k})}{\partial \hbar \mathbf{k}} - i\left[\langle \frac{\partial u_m(\mathbf{k})}{\partial \mathbf{k}} | \frac{\partial u_m(\mathbf{k},t)}{\partial t}\rangle - \langle \frac{\partial u_m(\mathbf{k},t)}{\partial t} | \frac{\partial u_m(\mathbf{k})}{\partial \mathbf{k}}\rangle\right]. \quad (36)$$

The second term in the rhs can be compared with Eq.(23) to recognize that it is the Berry curvature for a parameter space of the Hamiltonian given by $\boldsymbol{\xi}(t) \equiv (\mathbf{k}, t)$

$$\mathbf{v}_m(\mathbf{k}) = \frac{\partial E_m(\mathbf{k})}{\partial \hbar \mathbf{k}} - \Omega^m_{\mathbf{k}t}. \quad (37)$$

This is a major result because it shows that the longstanding textbook relation Eq. (30) is incomplete and the second term in the rhs of Eq.(37) has also to be considered under rather general conditions that will be discussed at the end of the next subsection.

4.2 The anomalous Hall effect

The above modification of the velocity induces a modification to the electrical current when an external uniform electric field is present. Consider a crystal under the perturbation of a weak electric field $\mathbf{E}$, which enters the Hamiltonian by coupling to the electrostatic potential $\phi(\mathbf{r})$. A uniform $\mathbf{E}$ means that $\phi(\mathbf{r})$ varies linearly in space and breaks the translational symmetry of the crystal so that Bloch's theorem can no longer be applied. To avoid this difficulty, one can let the electric field enter through a uniform vector potential, $\mathbf{E}(t) = -\frac{\partial}{\partial t}\mathbf{A}(t)$, that changes over time. In this way the external vector potential is a spacially uniform vector and the periodicity of the Bravais lattice is preserved. Using the Peierls (minimal) substitution, the Hamiltonian is written as

$$H(t) = \frac{(\hat{\mathbf{p}} + e\mathbf{A}(t))^2}{2m} + V(\mathbf{r}) \quad (38)$$

Transforming to the $\mathbf{k}$ representation, one has

$$H(\mathbf{k}, t) \equiv H(\mathbf{k} + \frac{e}{\hbar}\mathbf{A}(t))$$

Let us introduce the gauge-invariant crystal momentum

$$\tilde{\mathbf{k}} = \mathbf{k} + \frac{e}{\hbar}\mathbf{A}(t). \quad (39)$$

The parameter-dependent Hamiltonian can be simply written as $H(\tilde{\mathbf{k}}(\mathbf{k}, t))$. Hence, the eigenstates of the time-dependent Hamiltonian can be labeled by a single parameter $\tilde{\mathbf{k}}$. Moreover, since $\mathbf{A}(\mathbf{t})$ preserves the translational symmetry, the Bloch momentum $\mathbf{k}$ is still a good quantum number and it is a constant of motion $\dot{\mathbf{k}} = 0$. Differentiating in time Eq.(39) it then follows that $\tilde{\mathbf{k}}$ satisfies the following equation of motion:

$$\dot{\tilde{\mathbf{k}}} = \frac{e}{\hbar}\dot{\mathbf{A}}(t) = -\frac{e}{\hbar}\mathbf{E} \quad (40)$$

This is the usual expression for the time derivative of the crystal momentum $\mathbf{k}$. On the other hand, since $\partial/\partial k_\alpha = \partial/\partial \tilde{k}_\alpha$ and $d/dt = \sum_\alpha \dot{\tilde{k}}_\alpha \partial/\partial \tilde{k}_\alpha = -(e/\hbar)\sum_\alpha E_\alpha \partial/\partial k_\alpha$, then, taking into account Eqs.(36,37), one finds

$$\mathbf{v}_m(\mathbf{k}) = \frac{\partial E_m(\mathbf{k})}{\partial \hbar \mathbf{k}} - \frac{e}{\hbar}\mathbf{E} \times \mathbf{\Omega}_m(\mathbf{k}) \tag{41}$$

where $\mathbf{\Omega}_m(\mathbf{k})$ is the Berry curvature of the m-th band. To be more explicit, let us consider the case of a two-dimensional electron system so that the parameter space of the Hamiltonian is spanned by a three-dimensional vector $[\tilde{\mathbf{k}} = (\mathbf{k}, t) = (k_x, k_y, t)]$. Then $\mathbf{\Omega}_m(\mathbf{k}) = i\langle \nabla_{\mathbf{k}} u_m(\mathbf{k})| \times |\nabla_{\mathbf{k}} u_m(\mathbf{k})\rangle$ (see Eq. (45) in the Appendix) is given by a vector perpendicular to the $k_x - k_y$ plane:

$$H_z \equiv i\left[\langle \frac{\partial u_m(\mathbf{k})}{\partial k_x}| \frac{\partial u_m(\mathbf{k})}{\partial k_y}\rangle - \langle \frac{\partial u_m(\mathbf{k})}{\partial k_y}| \frac{\partial u_m(\mathbf{k})}{\partial k_x}\rangle\right]$$

. Then the semiclassical equation for the velocity along y becomes

$$v_y(\mathbf{k}) = \frac{\partial E_m(\mathbf{k})}{\partial \hbar k_y} + \frac{e}{\hbar} E_x H_z. \tag{42}$$

We can see that, in addition to the usual band dispersion contribution, an extra term, previously known as anomalous velocity, appears 'as if a magnetic field perpendicular to the $k_x - k_y$ plane were present' (cf. Eqs. (12.45) and (12.46) in ref. [7]). This additional term is always transverse to the electric field driving the current along x, and will give rise to a Hall current (Anomalous Hall Effect). According to Ref. [9], Sect. III.D, the anomalous velocity contribution is the most important (and intrinsic) mechanism leading to the Anomalous Hall Effect, an Hall effect taking place in ferromagnetic materials under the application of an electric field only (that is without an external magnetic field). Historically the anomalous velocity was obtained by Karplus and Luttinger [11] and Kohn and Luttinger [12], while its relation to the Berry phase was realized much later.

The velocity formula Eq. (41) [as well as Eqs. (36) and (37)] reveals that, in addition to the band energy, the Berry curvature of the Bloch bands is also required for a complete description of the electron dynamics. However, the conventional formula, Eq. (32) has been successful in describing many electronic properties in the past. It is thus important to know under what conditions the Berry curvature term can be neglected and when should instead it be considered. The general form of the Berry curvature $\mathbf{\Omega}_m(\mathbf{k})$ can be obtained via symmetry analysis. The velocity formula (41) should be invariant under time-reversal and spatial inversion operations if the unperturbed system has these symmetries. Under time reversal, $\mathbf{v}_n$ and $\mathbf{k}$ change sign while $\mathbf{E}$ is fixed. Under spatial inversion, $\mathbf{v}_n$, $\mathbf{k}$, and $\mathbf{E}$ change sign. If the system has time-reversal symmetry, the symmetry condition on Eq. (41)requires that

$$\mathbf{\Omega}_n(-\mathbf{k}) = -\mathbf{\Omega}_n(\mathbf{k}). \tag{43}$$

If the system has spatial inversion symmetry, then

$$\mathbf{\Omega}_n(-\mathbf{k}) = \mathbf{\Omega}_n(\mathbf{k}). \tag{44}$$

Therefore, for crystals with simultaneous time-reversal and spatial inversion symmetry the Berry curvature vanishes identically throughout the Brillouin zone. In this case Eq. (41) reduces to the simple expression (32). However, in systems with broken either time-reversal or inversion symmetries, their proper description requires the use of the full velocity formula (41).

A The explicit expression of the Berry curvature

To complete this general presentation of the Berry phase, the Berry connection, and the Berry curvature, we now recast the Berry curvature in a more convenient form for explicit calculations.

$$\begin{aligned}
\boldsymbol{\Omega}_n(\boldsymbol{\xi}) &\equiv \frac{\partial}{\partial \boldsymbol{\xi}} \times \mathbf{A}_n(\boldsymbol{\xi}) = i \left(\frac{\partial}{\partial \boldsymbol{\xi}} \times \langle n(\boldsymbol{\xi})| \left[\frac{\partial}{\partial \boldsymbol{\xi}} |n(\boldsymbol{\xi})\rangle \right] \right) \\
&= i \left[\frac{\partial}{\partial \boldsymbol{\xi}} \langle n(\boldsymbol{\xi})| \right] \times \left[\frac{\partial}{\partial \boldsymbol{\xi}} |n(\boldsymbol{\xi})\rangle \right] + \langle n(\boldsymbol{\xi})| \left[\frac{\partial}{\partial \boldsymbol{\xi}} \times \frac{\partial}{\partial \boldsymbol{\xi}} |n(\boldsymbol{\xi})\rangle \right] \\
&= i \left[\frac{\partial}{\partial \boldsymbol{\xi}} \langle n(\boldsymbol{\xi})| \right] \times \left[\frac{\partial}{\partial \boldsymbol{\xi}} |n(\boldsymbol{\xi})\rangle \right] \qquad (45)
\end{aligned}$$

where use has been done of the fact that the rotor of a gradient vanishes. Inserting a complete basis set one obtains

$$\boldsymbol{\Omega}_n(\boldsymbol{\xi}) = i \sum_{m \neq n} \left[\frac{\partial}{\partial \boldsymbol{\xi}} \langle n(\boldsymbol{\xi})| \right] |m(\boldsymbol{\xi})\rangle \times \langle m(\boldsymbol{\xi})| \left[\frac{\partial}{\partial \boldsymbol{\xi}} |n(\boldsymbol{\xi})\rangle \right] \qquad (46)$$

The $m = n$ vanishes because, taking the gradient of the normalization condition, similarly to Eq. (13), one can show that $\left[\frac{\partial}{\partial \boldsymbol{\xi}} \langle n(\boldsymbol{\xi})| \right] |n(\boldsymbol{\xi})\rangle = -\langle n(\boldsymbol{\xi})| \left[\frac{\partial}{\partial \boldsymbol{\xi}} |n(\boldsymbol{\xi})\rangle \right]$. Then for this term the vector product acts between two parallel vectors and vanishes. The terms of the Eq. (46) can be obtained by differentiating Eq.(1) and scalarly multiplying by the $\langle m(\boldsymbol{\xi})|$ bra

$$\frac{\partial}{\partial \boldsymbol{\xi}} \left(H(\boldsymbol{\xi}) |n\boldsymbol{\xi}\rangle \right) = \frac{\partial}{\partial \boldsymbol{\xi}} \left(E_n(\boldsymbol{\xi}) |n(\boldsymbol{\xi})\rangle \right) \qquad (47)$$

$$\begin{aligned}
&\langle m(\boldsymbol{\xi})| \left(\frac{\partial}{\partial \boldsymbol{\xi}} H(\boldsymbol{\xi}) \right) |n\boldsymbol{\xi}\rangle + \langle m(\boldsymbol{\xi})| H(\boldsymbol{\xi}) \left(\frac{\partial}{\partial \boldsymbol{\xi}} |n\boldsymbol{\xi}\rangle \right) \\
= \quad &\left(\frac{\partial}{\partial \boldsymbol{\xi}} E_n(\boldsymbol{\xi}) \right) \langle m(\boldsymbol{\xi}) | n(\boldsymbol{\xi})\rangle + E_n(\boldsymbol{\xi}) \langle m(\boldsymbol{\xi}) \left(\frac{\partial}{\partial \boldsymbol{\xi}} |n(\boldsymbol{\xi})\rangle \right)
\end{aligned}$$

Then one gets

$$\langle m(\boldsymbol{\xi})| \left(\frac{\partial}{\partial \boldsymbol{\xi}} |n\boldsymbol{\xi}\rangle \right) = \frac{\langle m(\boldsymbol{\xi})| \left(\frac{\partial}{\partial \boldsymbol{\xi}} H(\boldsymbol{\xi}) \right) |n\boldsymbol{\xi}\rangle}{E_n(\boldsymbol{\xi}) - E_m(\boldsymbol{\xi})} \tag{48}$$

Inserting Eq.(48) and its conjugated in Eq.(46) one finally obtains

$$\boldsymbol{\Omega}_n(\boldsymbol{\xi}) = i \sum_{m \neq n} \frac{\langle m(\boldsymbol{\xi})| \left(\frac{\partial}{\partial \boldsymbol{\xi}} H(\boldsymbol{\xi}) \right) |n(\boldsymbol{\xi})\rangle \times \langle n(\boldsymbol{\xi})| \left(\frac{\partial}{\partial \boldsymbol{\xi}} H(\boldsymbol{\xi}) \right) |m(\boldsymbol{\xi})\rangle}{\left(E_n(\boldsymbol{\xi}) - E_m(\boldsymbol{\xi}) \right)^2}. \tag{49}$$

This summation formula has the advantage that no differentiation on the wave function is involved and therefore it can be evaluated under any gauge choice. This property is particularly useful for numerical calculations, in which the condition of a smooth phase choice of the eigenstates is not guaranteed in standard diagonalization algorithms. It has been used to evaluate the Berry curvature in crystals with the eigenfunctions supplied from first-principles band structure calculations.

Furthermore, Eq.(49) reveals a characteristic of the Berry phase that is anything but trivial: if there are points of degeneration of the eigenvalue $E_n(\boldsymbol{\xi})$ in the parameter space, i.e., there are states such that $E_n(\boldsymbol{\xi}) = E_m(\boldsymbol{\xi})$, then the Berry curvature $\boldsymbol{\Omega}_n(\boldsymbol{\xi})$, and therefore the Berry phase $\gamma_n(C)$, will be dominated by these points, regardless of whether or not the path C followed by the parameter vector $\boldsymbol{\xi}$ includes these points.

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