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Topological Berry phase and semiclassical quantization of cyclotron orbits for two dimensional electrons in coupled band models

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Abstract. The semiclassical quantization of cyclotron orbits for two-dimensional Bloch electrons in a coupled two band model with a particle-hole symmetric spectrum is considered. As concrete examples, we study graphene (both mono and bilayer) and boron nitride. The main focus is on wave effects – such as Berry phase and Maslov index – occurring at order $\hbar$ in the semiclassical quantization and producing non-trivial shifts in the resulting Landau levels. Specifically, we show that the index shift appearing in the Landau levels is related to a *topological part of* the Berry phase – which is basically a winding number of the direction of the pseudo-spin $1/2$ associated to the coupled bands – acquired by an electron during a cyclotron orbit and not to the *complete* Berry phase, as commonly stated. As a consequence, the Landau levels of a coupled band insulator are shifted as compared to a usual band insulator. We also study in detail the Berry curvature in the whole Brillouin zone on a specific example (boron nitride) and show that its computation requires care in defining the "$\mathbf{k}$-dependent Hamiltonian" $H(\mathbf{k})$, where $\mathbf{k}$ is the Bloch wavevector.

1 Introduction

The dispersion relation of Bloch electrons in two dimensional (2D) crystals generally exhibit regions of closed orbits in reciprocal space. As a consequence, it is expected that applying a perpendicular magnetic field gives rise to quantized cyclotron orbits and the corresponding Landau levels. A semiclassical approach to obtain these Landau levels consists of first computing the area of the classical cyclotron orbits and then imposing the Bohr-Sommerfeld quantization condition in the form suggested by Onsager for Bloch electrons [1]. The semiclassical quantization condition (see Appendix A) for a cyclotron orbit C reads:

$$S(C)l_B^2 = 2\pi[n + \gamma] \qquad (1)$$

where $S(C) \equiv \iint d^2k$ is the $\mathbf{k}$-space area enclosed by the cyclotron orbit, $\mathbf{k}$ is the (gauge-invariant) Bloch wavevector, $l_B \equiv \sqrt{\hbar/eB}$ is the magnetic length, $-e$ is the electron charge and n is an integer. The quantity γ is called a phase mismatch ($0 \leq \gamma < 1$) and is not given by the semiclassical quantization rule [1]. The precise determination of γ requires the inclusion of wave effects and therefore to include terms of order $\hbar$ in the semiclassical expansion. For free electrons, and for a single (uncoupled) band of Bloch electrons, $\gamma = 1/2$ as a result of the presence of two caustics on the cyclotron orbit [2,3]. The number of caustics

on an orbit is known as the Maslov index [3,4]. From the dependence of the cyclotron surface $S(C)$ on the energy ε, one can usually rewrite the above quantization condition as:

$$S(\varepsilon)l_B^2 = 2\pi[n + \gamma_L]. \qquad (2)$$

Then by inverting $S(\varepsilon)$, one obtains the (semiclassical) Landau levels

$$\varepsilon_n = S^{-1}\left[\frac{2\pi}{l_B^2}(n + \gamma_L)\right] = \text{function}[B(n + \gamma_L)] \qquad (3)$$

where n is now interpreted as the Landau index. Usually, the shift γ_L is trivially equal to the phase mismatch γ introduced above. For example, the Landau levels for a free electron of mass m and dispersion relation $\varepsilon = \hbar^2 k^2/2m$ are given by a harmonic oscillator $\varepsilon_n = (n + 1/2)\hbar eB/m$, and $\gamma_L = \gamma = 1/2$ in that case. Indeed the area of the cyclotron orbit is $S(C) = \pi k^2$ and therefore $S(\varepsilon) = 2\pi m\varepsilon/\hbar^2$ such that $S(\varepsilon)l_B^2 = 2\pi(n + 1/2)$. One of the goals of this paper is to show that these two quantities, γ and γ_L, are not necessary equal.

A relation between the phase mismatch γ and the nature of the electronic Bloch functions was obtained by Roth [5]. She found that γ can depend on the cyclotron orbit C and that $\gamma(C)$ can be related to a quantity $\Gamma(C)$ later identified by Wilkinson [2] as a Berry phase [6–8] acquired by the Bloch electron during a cyclotron orbit C,

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see also reference [9]. The relation reads

$$\gamma(C) = \gamma_M + \gamma_B = \frac{1}{2} - \frac{\Gamma(C)}{2\pi} \tag{4}$$

where $\gamma_M = 1/2$ refers to the Maslov index contribution and $\gamma_B = -\Gamma(C)/2\pi$ to the Berry phase contribution. The Berry phase is given by

$$\Gamma(C) = i \oint_C d\boldsymbol{k} \cdot \langle u_{\boldsymbol{k}} | \boldsymbol{\nabla}_{\boldsymbol{k}} u_{\boldsymbol{k}} \rangle \tag{5}$$

in terms of the Bloch function $u_{\boldsymbol{k}}(\boldsymbol{r})$, where $\boldsymbol{k}$ is the gauge-invariant Bloch wavevector, and is computed along the cyclotron orbit C.

A case which is particularly interesting from the perspective of semiclassical quantization is that of coupled bands. In the present paper, we will restrict to two coupled bands with electron-hole symmetry, having in mind the examples of graphene (the two bands touch at two inequivalent valleys known as Dirac points) and boron nitride (the two bands are separated by a gap). In a two coupled band system, the Bloch electron is endowed with a pseudo-spin 1/2 associated with the freedom of being in the two bands and its wavefunction is therefore a bi-spinor. In the context of graphene or boron nitride, this internal degree of freedom is usual called "sublattice pseudo-spin" as it results from having two inequivalent sites A and B in the unit cell.

The Landau levels of electrons in graphene were first obtained by McClure [10], who performed a fully quantum mechanical calculation and obtained the now well-known behavior

$$\varepsilon_{n,\alpha} = \alpha v \sqrt{2neB\hbar} \tag{6}$$

where $\alpha = \pm 1$ is the band index and v is the constant Fermi velocity. From a semiclassical perspective [10], this result and the value $\gamma_L = 0$ that it implies – via equation (3) – seem to imply that the phase mismatch is now $\gamma = 0$ instead of the usual $\gamma = 1/2$. Using the Roth-Wilkinson relation (4), Mikitik and Sharlai [9] were able to show that this value of γ can be attributed to a Berry phase $\Gamma = \pi$, which exactly cancels the Maslov contribution. This Berry phase of π is actually the phase appearing in Hilbert space when rotating a bi-spinor by an angle of 2π in real space, which is familiar in the context of spin 1/2 physics, see e.g. reference [11]. The conclusion is that $\gamma_L = \gamma = 0$ in graphene and this value has indeed been observed in Shubnikov-de Haas and quantum Hall effect measurements [12,13].

In this paper, we focus on a situation where the assumption that $\gamma_L = \gamma$ gives a wrong result for the Landau levels. This is, for example, the case of boron nitride[1], whose low energy effective theory is that of

massive Dirac fermions [16], with a dispersion relation $\varepsilon(\boldsymbol{k}) = \alpha \sqrt{\Delta^2 + (v\hbar k)^2}$ where the gap $2\Delta = \varepsilon_B - \varepsilon_N$ is the energy difference between a boron and a nitrogen $2p_z$ atomic orbital. Haldane [17] computed the Landau levels of two dimensional massive Dirac fermions quantum mechanically and found[2]:

$$\varepsilon_{n,\alpha} = \alpha \sqrt{\Delta^2 + 2neB\hbar v^2}. \tag{7}$$

From a semiclassical perspective Haldane's result raises the following question. When comparing massless (graphene) and massive (boron nitride) Dirac fermions, it appears that in both cases, the Landau level shift is the same $\gamma_L = 0$. However, as we will show below, the Berry phase $\Gamma(C)$ depends on the magnitude of the gap and is therefore different in both cases. We are led to conclude that the two quantities γ and γ_L are different in this case. The main goal of this paper is to relate these two quantities. We will show that while γ entering the quantization (1) of cyclotron orbits is correctly related to the Berry phase, γ_L entering the energy quantization (2) is related to a topological part of the Berry phase, which is essentially a winding number of the pseudo-spin 1/2. The key point to understand this difference is to account for the orbital magnetization of Bloch electrons and we will see that when quantizing the cyclotron orbit one needs to consider the change in energy due to this magnetization. In the Onsager quantization condition, the contribution of the orbital magnetization exactly cancels the non-topological part of the Berry phase. As a consequence, the Landau index shift γ_L is only the topological part of the Berry phase and not the whole Berry phase.

Recently Carmier and Ullmo [18] have computed the semiclassical Green functions for similar systems (graphene, boron nitride, etc.). With a different approach, they reach essentially the same conclusion as ours: the phase appearing in the Landau levels is in general not the complete Berry phase but is what they call the semiclassical phase. In the same vein, see also reference [19]. Another related work, which appeared recently, is that of Gosselin et al. [20]. Compared to these three works, on the one hand, ours treats more general coupled band systems and do not require to take the continuum limit but also applies to discrete models on a lattice. For example, the quantization of cyclotron orbits can be performed anywhere in the Brillouin zone and not only close to specific points. On the other hand, and contrary to references [18–20], we restrict ourselves to homogeneous systems.

The structure of the paper is as follows. In Section 2, we review the semiclassical description of Bloch electrons at order $\hbar$ having in mind the quantization of cyclotron orbits and introduce various Berry quantities. Section 3

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[1] More generally, we consider the case where a gap is opened in graphene's band structure as a result of inversion symmetry breaking. Two-dimensional boron nitride is the most obvious example. However it has a very large gap of roughly $2\Delta \sim 6$ eV, that is even larger than that of silicon dioxide, and it cannot be used as a semiconductor [14]. A more interesting system

for electronic transport is graphene on a commensurate (bulk) boron nitride substrate. It is predicted [15] to have a gap $2\Delta \sim 50$ meV. In the following, we will assume that the gap is smaller than the bandwidth.

[2] This result is valid for $n > 0$. When $n = 0$, the result requires the inclusion of both valleys at the same time: $\varepsilon_{n=0} = -\xi\Delta$, where $\xi = \pm 1$ is the valley index (K or K').

is the core of the article. It contains a study of a two coupled band model for which we show that the Landau index shift γ_L is related to a winding number and not to the complete Berry phase. Then in the following sections, we consider several examples: a tight-binding model for boron nitride (Sect. 4), massive Dirac electrons (Sect. 5), massless Dirac electrons (Sect. 6), and eventually chiral electrons of bilayer graphene (Sect. 7). The conclusion is presented in Section 8.

2 Semiclassical description of a Bloch electron on a cyclotron orbit

In this section, we review known results about the semi-classical description (including terms at order $\hbar$) of Bloch electrons in a crystal under the influence of a magnetic field. When describing a Bloch electron confined to a single band, the presence of other bands shows up in the semiclassical equation of motions at order $\hbar$ (classical order being $\hbar^0$) in the form of Berry phase type corrections. Our goal is to discuss the effect of these corrections on the quantization of cyclotron orbits. It should be kept in mind in the following that the electron is described by a wavefunction which is a bi-spinor – because of the band structure – and that the true spin is neglected. For a general review see reference [21].

2.1 Semiclassical equations of motion for a Bloch electron in a magnetic field

One way [21–23] of obtaining the semiclassical equations of motion for a Bloch electron in a uniform magnetic field $\boldsymbol{B}$ is to study the motion of a (typically Gaussian) *wavepacket* of Bloch waves restricted to a *single band* (indexed by α) of average position $\boldsymbol{r}_c(t)$, average crystal momentum $\hbar\boldsymbol{q}_c(t)$ – $\boldsymbol{q}_c$ is the average Bloch wavevector – and fixed width. The width of the wavepacket should be larger than the lattice spacing and much smaller than the typical length scale on which the external fields (e.g. magnetic and electric) vary. One then uses the time-dependent variational principle to obtain an effective Lagrangian for the *independent* variables $\boldsymbol{r}_c$ and $\boldsymbol{q}_c$. Minimizing the action with respect to these variational parameters one obtains the following equations of motion:

$$\hbar\dot{\boldsymbol{k}}_c = -e\dot{\boldsymbol{r}}_c \times \boldsymbol{B} \tag{8}$$

and

$$\dot{\boldsymbol{r}}_c = \hbar^{-1}\boldsymbol{\nabla}_{\boldsymbol{k}_c}\varepsilon_\alpha - \dot{\boldsymbol{k}}_c \times \boldsymbol{\Omega}_\alpha(\boldsymbol{k}_c) \tag{9}$$

where $\hbar\boldsymbol{k}_c \equiv \hbar\boldsymbol{q}_c + e\boldsymbol{A}(\boldsymbol{r}_c)$ is the average gauge-invariant crystal momentum[3], $\boldsymbol{A}$ is the vector potential and $-e <$

0 is the electron charge. The Berry curvature $\boldsymbol{\Omega}_\alpha(\boldsymbol{k}_c)$ is defined below. The electron energy is

$$\varepsilon_\alpha(\boldsymbol{k}_c) = \varepsilon_{\alpha,0}(\boldsymbol{k}_c) - \boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}_c) \cdot \boldsymbol{B} \tag{10}$$

where $\varepsilon_{\alpha,0}(\boldsymbol{k}_c)$ is the band energy in absence of a magnetic field and $\boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}_c)$ is the orbital magnetic moment of the Bloch electron (also defined below).

Compared to the usual equations of motion of Bloch and Peierls (see e.g. Ref. [24]) obtained at order $\hbar^0$, there are two additional terms in equations (8, 9), which appear at order $\hbar$. One is the so-called anomalous velocity $-\dot{\boldsymbol{k}}_c \times \boldsymbol{\Omega}_\alpha(\boldsymbol{k}_c)$. It is a kind of Lorentz magnetic force but in $\boldsymbol{k}$-space and due to Berry curvature $\boldsymbol{\Omega}_\alpha$, rather than to a real magnetic field. It takes into account the effect on the average velocity of virtual transitions to other bands $\alpha' \neq \alpha$. The other is the magnetization correction to the band energy, which gives the energy of a Bloch electron in a magnetic field as $\varepsilon_\alpha = \varepsilon_{\alpha,0} - \boldsymbol{\mathcal{M}}_\alpha \cdot \boldsymbol{B}$. The correction to the band energy is the extra magnetic energy due to the coupling of the orbital magnetic moment $\boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}_c)$ to the external magnetic field. This orbital magnetic moment comes from the self-rotation[4] of the wavepacket and exists because of the finite wavepacket width, which cannot be made arbitrary small due to the restriction to a single band [21]. Just as the Berry curvature, the orbital magnetic moment is also an effect of virtual transitions to other bands. In the present work, we neglect the electron spin and therefore do not discuss the Zeeman effect. Note that the magnetization appears as resulting from an internal structure, which is not the electron spin but rather the pseudo-spin related to the two coupled bands.

Berry-type corrections, such as $\Omega_\alpha(\boldsymbol{k}_c)$ and $\boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}_c)$, appear at first order in the external field. Therefore, to this order, $\Omega_\alpha(\boldsymbol{k}_c) \approx \Omega_\alpha(\boldsymbol{q}_c)$ and $\boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}_c) \approx \boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{q}_c)$ and it is therefore not important to distinguish between $\boldsymbol{k}$ and $\boldsymbol{q}$ when computing these quantities.

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[3] When studying an electron in a periodic potential in the presence of a magnetic field, one should be careful in defining various momenta. Here we consider four such momenta. First, there is the canonical (or linear) momentum $\boldsymbol{p}$ which is canonically conjugated to the position $\boldsymbol{r}$. Second, there is the crystal momentum $\hbar\boldsymbol{q}$ (where $\boldsymbol{q}$ is the Bloch wavevector) defined by the Bloch theorem. Third, in the presence of a vector potential, there is the gauge invariant momentum $\boldsymbol{\Pi}$ which is obtained from the canonical momentum by minimal coupling $\boldsymbol{\Pi} = \boldsymbol{p} + e\boldsymbol{A}$ (in the absence of a periodic potential, it is directly related to the velocity $\boldsymbol{\Pi} = m\boldsymbol{v}$). Fourth, there is the gauge invariant crystal momentum $\hbar\boldsymbol{k}$, which is related to the crystal momentum by $\hbar\boldsymbol{k} = \hbar\boldsymbol{q} + e\boldsymbol{A}$ (in the absence of a magnetic field, the two are equal $\boldsymbol{k} = \boldsymbol{q}$ and we therefore usually use $\boldsymbol{k}$). The gauge invariant crystal momentum is the one appearing in the semiclassical equations of motion. It is sometimes a valid approximation to neglect the difference between linear momentum and crystal momentum (think of the Peierls substitution), in such a case $\boldsymbol{p} \simeq \hbar\boldsymbol{q} = \hbar\boldsymbol{k} - e\boldsymbol{A}$.

[4] Note that in addition to the self-rotation $\boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}_c)$ the magnetic moment of the electron also gets a more familiar contribution from its center of mass motion, which is taken care of by $\varepsilon_{\alpha,0}(\boldsymbol{k}_c = \boldsymbol{q}_c + e\boldsymbol{A}(\boldsymbol{r}_c)) \approx \varepsilon_{\alpha,0}(\boldsymbol{q}_c) + e\boldsymbol{A}(\boldsymbol{r}_c) \cdot \boldsymbol{\nabla}_{\boldsymbol{k}_c}\varepsilon_{\alpha,0} = \varepsilon_{\alpha,0}(\boldsymbol{q}_c) + \frac{e}{2\hbar}(\boldsymbol{r}_c \times \boldsymbol{\nabla}_{\boldsymbol{k}_c}\varepsilon_{\alpha,0}) \cdot \boldsymbol{B}$ in the symmetric gauge where $\boldsymbol{A}(\boldsymbol{r}_c) = \boldsymbol{B} \times \boldsymbol{r}_c/2$. The corresponding magnetic moment is $-\frac{e}{2\hbar}\boldsymbol{r}_c \times \boldsymbol{\nabla}_{\boldsymbol{k}_c}\varepsilon_{\alpha,0} \approx -\frac{e}{2}\boldsymbol{r}_c \times \dot{\boldsymbol{r}}_c$ as expected.

2.2 Berry-ology

Here we consider the effective dynamics of an electron restricted to a single band and define several quantities related to a Berry phase appearing because of the coupling between bands. In particular, we consider a 2D crystalline system described by a Hamiltonian $\hat{H}$ containing only two bands (band index $\alpha = \pm 1$). Typically, we think of a tight-binding model with two sites in the unit cell. In the Bloch basis it reads:

$$\hat{H} = \sum_{\boldsymbol{k},\alpha} \varepsilon_{\alpha,0}(\boldsymbol{k})|\boldsymbol{k},\alpha\rangle\langle\boldsymbol{k},\alpha| \tag{11}$$

where $\varepsilon_{\alpha,0}(\boldsymbol{k})$ is the band energy, $|\boldsymbol{k},\alpha\rangle = \exp(i\boldsymbol{k}\cdot\hat{\boldsymbol{r}})|u_{\boldsymbol{k},\alpha}\rangle$ is a Bloch state and $\hat{\boldsymbol{r}}$ is the complete position operator (and not just the Bravais lattice position, e.g.). Its wavefunction is $\varphi_{\boldsymbol{k},\alpha}(\boldsymbol{r}) = \langle\boldsymbol{r}|\boldsymbol{k},\alpha\rangle = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})u_{\boldsymbol{k},\alpha}(\boldsymbol{r})$, where $u_{\boldsymbol{k},\alpha}(\boldsymbol{r})$ is the Bloch function. In the case of two bands, $\varphi_{\boldsymbol{k},\alpha}(\boldsymbol{r})$ and $u_{\boldsymbol{k},\alpha}(\boldsymbol{r})$ are bi-spinors (in sublattice space). Next, we perform a unitary transform to define a $\boldsymbol{k}$-dependent Hamiltonian [21]:

$$\hat{H}(\boldsymbol{k}) = \exp(-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}})\hat{H}\exp(i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}). \tag{12}$$

The wavevector $\boldsymbol{k}$ is a parameter spanning the first Brillouin zone and on which the Hamiltonian $\hat{H}(\boldsymbol{k})$ depends. By virtue of the unitary transform $\exp(-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}})$, one has $\hat{H}(\boldsymbol{k})|u_{\boldsymbol{k},\alpha}\rangle = \varepsilon_{\alpha,0}(\boldsymbol{k})|u_{\boldsymbol{k},\alpha}\rangle$. Using the projection operators $P(\boldsymbol{k}) = \sum_\alpha |u_{\boldsymbol{k},\alpha}\rangle\langle u_{\boldsymbol{k},\alpha}|$, we also define the following 2×2 $\boldsymbol{k}$-dependent Hamiltonian:

$$H(\boldsymbol{k}) = P(\boldsymbol{k})\hat{H}(\boldsymbol{k})P(\boldsymbol{k}) = \sum_\alpha \varepsilon_{0,\alpha}(\boldsymbol{k})|u_{\boldsymbol{k},\alpha}\rangle\langle u_{\boldsymbol{k},\alpha}| \tag{13}$$

which is the restriction of $\hat{H}(\boldsymbol{k})$ to the $\boldsymbol{k}$ subspace. For more details on the three different types of Hamiltonians we are using [$\hat{H}$, $\hat{H}(\boldsymbol{k})$ and $H(\boldsymbol{k})$] see Appendix B.

Following the general result of reference [6–8], the Berry phase acquired by a Bloch electron on a cyclotron orbit [9,25] C in the band α is:

$$\Gamma_\alpha(C) = \oint_C d\boldsymbol{k} \cdot i\langle u_{\boldsymbol{k},\alpha}|\boldsymbol{\nabla}_{\boldsymbol{k}} u_{\boldsymbol{k},\alpha}\rangle. \tag{14}$$

Note that in general this quantity depends on the cyclotron orbit C. The Berry connection (equivalent to a $\boldsymbol{k}$-space vector potential) in the band α is given by:

$$\boldsymbol{\mathcal{A}}_\alpha(\boldsymbol{k}) = i\langle u_{\boldsymbol{k},\alpha}|\boldsymbol{\nabla}_{\boldsymbol{k}} u_{\boldsymbol{k},\alpha}\rangle \tag{15}$$

so that the Berry phase appears as an Aharonov-Bohm phase in $\boldsymbol{k}$-space. The corresponding Berry curvature (equivalent to a $\boldsymbol{k}$-space magnetic field) is

$$\boldsymbol{\Omega}_\alpha(\boldsymbol{k}) = \boldsymbol{\nabla}_{\boldsymbol{k}} \times \boldsymbol{\mathcal{A}}_\alpha = \Omega_\alpha \boldsymbol{e}_z \tag{16}$$

where

$$\Omega_\alpha(\boldsymbol{k}) = \partial_{k_x}\mathcal{A}_y - \partial_{k_y}\mathcal{A}_x = i[\langle\partial_{k_x}u|\partial_{k_y}u\rangle - \langle\partial_{k_y}u|\partial_{k_x}u\rangle]. \tag{17}$$

It can also be written as:

$$\boldsymbol{\Omega}_\alpha(\boldsymbol{k}) = i\langle\boldsymbol{\nabla}_{\boldsymbol{k}} u_{\boldsymbol{k},\alpha}| \times |\boldsymbol{\nabla}_{\boldsymbol{k}} u_{\boldsymbol{k},\alpha}\rangle. \tag{18}$$

Another useful formulation, especially convenient when performing numerical calculations as, contrary to equation (18), it does not require the Bloch wavefunctions to be single-valued in parameter space [21], is:

$$\boldsymbol{\Omega}_\alpha(\boldsymbol{k}) = i\sum_{\alpha'\neq\alpha} \frac{\langle u_{\boldsymbol{k},\alpha}|\partial_{k_x}H(\boldsymbol{k})|u_{\boldsymbol{k},\alpha'}\rangle\langle u_{\boldsymbol{k},\alpha'}|\partial_{k_y}H(\boldsymbol{k})|u_{\boldsymbol{k},\alpha}\rangle}{[\varepsilon_{\alpha,0}(\boldsymbol{k}) - \varepsilon_{\alpha',0}(\boldsymbol{k})]^2}$$
$$+ \text{c.c.} \tag{19}$$

It shows explicitly, that the Berry curvature is due to the restriction to a single band α and to the resulting virtual transitions to other bands $\alpha' \neq \alpha$.

The orbital magnetic moment $\boldsymbol{\mathcal{M}}_\alpha = \mathcal{M}_\alpha \boldsymbol{e}_z$ of a Bloch electron described by a wavepacket of average position $\boldsymbol{r}_c$ and average gauge-invariant crystal momentum $\hbar\boldsymbol{k}_c$ restricted to the band α is [21–23]:

$$\boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}_c) = -\frac{e}{2m}\langle(\hat{\boldsymbol{r}} - \boldsymbol{r}_c) \times \hat{\boldsymbol{p}}\rangle \tag{20}$$
$$= -i\frac{e}{2\hbar}\langle\boldsymbol{\nabla}_{\boldsymbol{k}_c}u_{\boldsymbol{k}_c,\alpha}| \times [\varepsilon_{\alpha,0} - H(\boldsymbol{k}_c)]|\boldsymbol{\nabla}_{\boldsymbol{k}_c}u_{\boldsymbol{k}_c,\alpha}\rangle$$

where the average in the first expression is taken over the wavepacket, $\hat{\boldsymbol{p}}$ is the canonical momentum operator, and m is the bare electron mass. As the Berry curvature, this quantity also has an expression revealing the virtual transitions to other bands:

$$\boldsymbol{\mathcal{M}}_\alpha(\boldsymbol{k}) = i\frac{e}{2\hbar}$$
$$\times \sum_{\alpha'\neq\alpha} \frac{\langle u_{\boldsymbol{k},\alpha}|\partial_{k_x}H(\boldsymbol{k})|u_{\boldsymbol{k},\alpha'}\rangle\langle u_{\boldsymbol{k},\alpha'}|\partial_{k_y}H(\boldsymbol{k})|u_{\boldsymbol{k},\alpha}\rangle}{\varepsilon_{\alpha,0}(\boldsymbol{k}) - \varepsilon_{\alpha',0}(\boldsymbol{k})} + \text{c.c.}$$
$$\tag{21}$$

This shows that in the case of a single isolated band, both the Berry curvature and the orbital magnetic moment vanish. Note that both quantities depend on the off-diagonal (in band index) matrix elements $\hbar^{-1}\langle u_{\boldsymbol{k},\alpha}|\boldsymbol{\nabla}_{\boldsymbol{k}}H(\boldsymbol{k})|u_{\boldsymbol{k},\alpha'}\rangle$ of the velocity operator.

In the particular case of a two-band model with electron-hole symmetry, the orbital magnetic moment is directly related to the Berry curvature:

$$\boldsymbol{\mathcal{M}}_\alpha = \frac{e}{\hbar}\varepsilon_{\alpha,0}\boldsymbol{\Omega}_\alpha. \tag{22}$$

This relation was already obtained in reference [26] and we present a proof in Appendix C.

According to general symmetry arguments [22,23], the Berry phase and the magnetization of a single band should vanish in a crystal which is inversion and time reversal invariant. Indeed, time-reversal symmetry implies $\boldsymbol{\Omega}(-\boldsymbol{k}) = -\boldsymbol{\Omega}(\boldsymbol{k})$ and inversion symmetry implies $\boldsymbol{\Omega}(-\boldsymbol{k}) = \boldsymbol{\Omega}(\boldsymbol{k})$.

All the above definitions are valid for an electron in a single Bloch band, which is well separated from other bands. We will nevertheless apply them in the case of touching bands (such as graphene at its Dirac points) remembering that the correct procedure is to calculate these quantities in presence of a finite gap Δ and to send it to zero at the end.

2.3 Cyclotron orbit, phase mismatch and Landau index shift

In the following, the aim is to quantize the cyclotron motion in order to find the Landau levels. Classically, a free electron in a uniform and constant magnetic field performs a motion at constant energy in a plane perpendicular to the magnetic field. For a Bloch electron, the classical cyclotron orbit is a cut at constant energy in the band structure, i.e. an iso-energy line $\varepsilon_\alpha(\mathbf{k}) = $ constant. The semiclassical quantization of a cyclotron orbit is explained in detail in the introduction – see equations (1), (4) and (5) – we therefore do not recall it here. Nevertheless, we would like to precise the definition of the Landau index shift γ_L, which is related, but not identical, to the phase mismatch $\gamma(C)$ appearing in the Onsager semiclassical quantization condition (1). The Landau index shift appears in the energy quantization condition (2). It can also be defined via the exact Landau levels ε_n by taking the semiclassical limit ($n \gg 1$, keeping terms of order n and n^0):

$$\varepsilon_n \approx \text{function}[B(n + \gamma_L)] \qquad (23)$$

where n corresponds to the dominant term, of order $1/\hbar$, and γ_L to the first correction, of order $n^0 \sim 1/\hbar^0$. To be more precise, imagine expanding the exact Landau levels as a decreasing series in powers of n: $\varepsilon_n = a_0 n^l + a_1 n^{l-1} + a_2 n^{l-2} + \ldots$. Keeping only the two first terms in the semiclassical limit $n \gg 1$, one obtains $\varepsilon_n \approx a_0[n^l + a_1 n^{l-1}/a_0] \approx a_0[n + a_1/(a_0 l)]^l = a_0[n + \gamma_L]^l$, which defines the Landau index shift $\gamma_L \equiv a_1/(a_0 l)$ modulo 1.

Often both quantities $\gamma(C)$ and γ_L are equal and are usually not distinguished. The insight here comes from recognizing that both quantities can be different as $\gamma(C)$ may depend on the precise cyclotron orbit, whereas γ_L is a constant.

3 Semiclassical quantization of cyclotron orbits in a coupled two-band model

In the following, we perform the semiclassical quantization of the cyclotron orbit for a Bloch electron in a two-band model and obtain the relation between $\gamma(C)$ and γ_L. We consider a coupled two-band Hamiltonian with a particle-hole symmetric spectrum $\hat{H}$. As explained in the previous section, we then perform a unitary transform $\exp(-i\mathbf{k} \cdot \hat{\mathbf{r}})$ to obtain a parameter-dependent Hamiltonian $\hat{H}(\mathbf{k})$ and then project on the $\mathbf{k}$ subspace to obtain a 2×2 Hamiltonian (in the following $\hbar \equiv 1$):

$$H(\mathbf{k}) = \begin{pmatrix} \Delta & f(\mathbf{k}) \\ f^*(\mathbf{k}) & -\Delta \end{pmatrix} \qquad (24)$$

where $\mathbf{k}$ is the Bloch wavevector in the first Brillouin zone (BZ). The function $f(\mathbf{k})$ is usually obtained as a sum over hopping amplitudes in a tight binding description. Time-reversal symmetry imposes $H(-\mathbf{k})^* = H(\mathbf{k})$ and therefore $f(-\mathbf{k})^* = f(\mathbf{k})$. Note that Bloch's theorem imposes that $|f(\mathbf{k} + \mathbf{G})| = |f(\mathbf{k})|$ for any reciprocal lattice vector $\mathbf{G}$.

However it does not require that $f(\mathbf{k} + \mathbf{G}) = f(\mathbf{k})$. An important assumption here is that the diagonal term Δ does not depend on the wavevector and can therefore be interpreted simply as an on-site energy. This term explicitly breaks the inversion symmetry. Introducing the energy spectrum $\varepsilon_0(\mathbf{k}) = \alpha\sqrt{\Delta^2 + |f(\mathbf{k})|^2}$, where $\alpha = \pm 1$ is the band index, and the azimuthal $\beta(\mathbf{k})$ and polar $\theta(\mathbf{k})$ angles on the Bloch sphere, such that $\cos\beta = \Delta/|\varepsilon_0|$, $\sin\beta = |f|/|\varepsilon_0|$ and $\theta \equiv -\text{Arg}f$, the Hamiltonian can be rewritten as

$$H(\mathbf{k}) = |\varepsilon_0| \begin{pmatrix} \cos\beta & \sin\beta e^{-i\theta} \\ \sin\beta e^{i\theta} & -\cos\beta \end{pmatrix}. \qquad (25)$$

The eigenfunction of energy $\varepsilon_0 = \alpha|\varepsilon_0|$ is $\psi(\mathbf{r}) = u_\mathbf{k}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ where the Bloch spinor is

$$|u_{\mathbf{k},\alpha}\rangle = \begin{pmatrix} \cos(\beta/2) \\ \sin(\beta/2)e^{i\theta} \end{pmatrix} \text{ if } \alpha = +1$$

$$= \begin{pmatrix} -\sin(\beta/2)e^{-i\theta} \\ \cos(\beta/2) \end{pmatrix} \text{ if } \alpha = -1. \qquad (26)$$

The Berry connection is given by

$$\boldsymbol{\mathcal{A}} = -\alpha \sin^2\frac{\beta}{2}\boldsymbol{\nabla}_\mathbf{k}\theta \qquad (27)$$

and the corresponding curvature is

$$\boldsymbol{\Omega} = \frac{\alpha}{2}\boldsymbol{\nabla}_\mathbf{k}\cos\beta \times \boldsymbol{\nabla}_\mathbf{k}\theta$$

$$= -\frac{\alpha}{2}\sin\beta(\partial_{k_x}\beta\partial_{k_y}\theta - \partial_{k_x}\theta\partial_{k_y}\beta)\boldsymbol{e}_z. \qquad (28)$$

An important simplification occurs in the calculation of the Berry phase Γ because the cyclotron orbit C is travelled at constant energy and the diagonal term Δ is independent of the wavevector. As a consequence, the azimuthal angle β is a constant along the trajectory. Indeed $\cos\beta = \Delta/|\varepsilon_0|$ and $\sin\beta = \sqrt{\varepsilon_0^2 - \Delta^2}/|\varepsilon_0|$ are both functions of ε_0 only. Therefore the calculation of the Berry phase along a cyclotron orbit is easily performed:

$$\Gamma(C) = \oint_C d\mathbf{k} \cdot \boldsymbol{\mathcal{A}}$$

$$= -\alpha \sin^2\frac{\beta}{2}\oint_C d\mathbf{k} \cdot \boldsymbol{\nabla}_\mathbf{k}\theta = \pi W_C[1 - \cos\beta] \qquad (29)$$

where $W_C \equiv -\alpha \oint_C d\theta/2\pi$ is the winding number, which is a topological invariant. Indeed the relevant mapping is from a cyclotron orbit in the Brillouin zone to a circle (because β is fixed) on the Bloch sphere: therefore, the relevant homotopy group is $\pi_1(S^1) = \mathbb{Z}$. Note that $d(|\varepsilon_0|\Gamma)/d|\varepsilon_0| = $ constant $= \pi W_C$. We call this quantity the topological Berry phase. It is a local quantity as it depends on the precise path C. The winding number W_C counts the total charge of the vortices in θ, which are encircled by the cyclotron orbit (see Fig. 2). Note that this topological Berry phase is not directly related to the

Chern number, which is the Berry curvature integrated over the entire BZ [31,32].

Starting from the Onsager-Roth relation (see Eqs. (1, 4, 5))

$$S(\varepsilon_0)l_B^2 = 2\pi[n + \frac{1}{2}] - \Gamma(C) \tag{30}$$

where ε_0 is the band energy in zero magnetic field, we search the quantization of $S(\varepsilon)$ where ε is the energy in presence of a magnetic field. Using the relation between the energy and the curvature $\varepsilon_0 = \varepsilon + \mathcal{M}B$ with $\mathcal{M} = e\varepsilon_0\Omega$, we obtain

$$S(\varepsilon_0)l_B^2 = S(\varepsilon)l_B^2 + \bar{\Omega}(\varepsilon_0)|\varepsilon_0|\frac{dS}{d|\varepsilon_0|}. \tag{31}$$

In the previous equation, we introduced the Berry curvature $\bar{\Omega}$ averaged over a constant energy orbit[5]:

$$\bar{\Omega}(\varepsilon_0) \equiv \frac{1}{(2\pi)^2\nu(\varepsilon_0)}\frac{d\Gamma}{d|\varepsilon_0|} = \frac{d\Gamma}{dS}. \tag{32}$$

Therefore, we obtain

$$S(\varepsilon_0)l_B^2 = S(\varepsilon)l_B^2 + |\varepsilon_0|\frac{d\Gamma}{d|\varepsilon_0|}. \tag{33}$$

which does not require the cyclotron orbit to be circular. The energy quantization condition can now be rewritten as

$$S(\varepsilon)l_B^2 = 2\pi\left[n + \frac{1}{2}\right] - \frac{d(|\varepsilon_0|\Gamma)}{d|\varepsilon_0|}$$
$$= 2\pi\left[n + \frac{1}{2}\right] - \pi W_C \tag{34}$$

in which we recognized the topological Berry phase. Inverting this last relation $S(\varepsilon)l_B^2 = 2\pi[n + (1 - W_C)/2]$ allows one to obtain the (semiclassical) Landau levels for the whole energy band. Finally, the Landau index shift is

$$\gamma_L = \frac{1}{2} - \frac{W_C}{2} \tag{35}$$

and the winding number only matters modulo 2. This last equation is the central result of the paper. It shows that the Landau index shift γ_L is related to the topological part of the Berry phase πW_C and not to the complete Berry phase $\Gamma(C)$. The important point in the proof is the cancellation in the phase $S(\varepsilon)l_B^2$ between the non-topological part of the Berry phase $\Gamma(C) - \pi W_C = -|\varepsilon_0|d\Gamma/d|\varepsilon_0|$ and the orbital magnetic moment contribution $\mathcal{M}Bd(Sl_B^2)/d|\varepsilon_0| = |\varepsilon_0|d\Gamma/d|\varepsilon_0|$. Physically, the topological Berry phase πW_C is just the usual π phase that a bi-spinor acquires in Hilbert space as a result of a

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2π rotation in position space. Here the spin $1/2$ is actually the sublattice pseudo-spin.

In the following, we consider several concrete examples such as boron nitride, graphene mono- and bilayer. These examples are treated either in discrete lattice models or in their continuum limit (effective low energy models).

4 Example 1: tight-binding model of boron nitride

In this section, we consider a single layer of boron nitride, which has a honeycomb lattice with two crystallographically and energetically inequivalent atoms (boron and nitride, usually called A and B) as a basis. Because of the two different on-site energies $\varepsilon_A - \varepsilon_B = 2\Delta \neq 0$, the inversion symmetry is explicitly broken leading to a gap opening. We use a tight binding model, with hopping amplitude t and nearest-neighbour distance a, given by the following 2×2 Hamiltonian in (A, B) subspace:

$$H(\mathbf{k}) = \begin{pmatrix} \Delta & f(\mathbf{k}) \\ f^*(\mathbf{k}) & -\Delta \end{pmatrix}$$
$$\text{with} \quad f(\mathbf{k}) = -t[e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_1} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_2} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_3}] \tag{36}$$
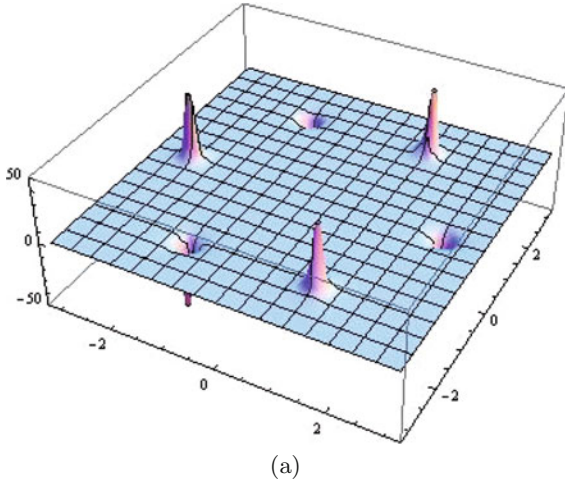
where $\mathbf{k}$ is the wavevector in the entire Brillouin zone [$\mathbf{k} = 0$ corresponds to the center of the BZ, i.e. Γ point], $\boldsymbol{\delta}_1, \boldsymbol{\delta}_2, \boldsymbol{\delta}_3$ are vectors connecting an A atom with its three nearest B neighbours and $\mathbf{a}_1, \mathbf{a}_2$ span the Bravais lattice (we follow the notations of Bena and Montambaux [27]: our $H(\mathbf{k})$ corresponds to what they call basis II[6]). Note that, contrary to $|f(\mathbf{k})|$, $f(\mathbf{k})$ does not have the periodicity of the reciprocal lattice but satisfies $f(\mathbf{k} + \mathbf{G}) = f(\mathbf{k})\exp(i\mathbf{G}\cdot\boldsymbol{\delta}_3)$ where $\boldsymbol{\delta}_3$ is the vector relating the two atoms A, B of the basis. This case exactly corresponds to that of Section 3 with a specific form for $f(\mathbf{k})$. The quantities of interest (Berry curvature, orbital magnetic moment, Berry phase, winding number) can be directly computed from the results obtained there.

The curvature is given by

$$\Omega(\mathbf{k}) = a^2\frac{\sqrt{3}\alpha t^2\Delta}{|\varepsilon_0(\mathbf{k})|^3}\sin\left(\mathbf{k}\cdot\frac{\boldsymbol{\delta}_2 - \boldsymbol{\delta}_3}{2}\right)$$
$$\times \sin\left(\mathbf{k}\cdot\frac{\boldsymbol{\delta}_3 - \boldsymbol{\delta}_1}{2}\right)\sin\left(\mathbf{k}\cdot\frac{\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2}{2}\right) \tag{37}$$

where $|\varepsilon_0(\mathbf{k})|^2 = \Delta^2 + |f(\mathbf{k})|^2$, see Figure 1. Note that the curvature has both the C_3 symmetry and the translational

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[5] When the dispersion relation $\varepsilon_0(\mathbf{k})$ is not isotropic, the cyclotron orbit in $\mathbf{k}$ space is not circular and the Berry curvature explicitly depends on the wavevector. Hence the necessity of defining an averaged Berry curvature. Another expression for this quantity is $\bar{\Omega}(\varepsilon_0) = [(2\pi)^2\nu(\varepsilon_0)]^{-1}d\Gamma/d|\varepsilon_0|$ where $\nu(\varepsilon_0) = (2\pi)^{-2}dS/d|\varepsilon_0|$ is the density of states per unit area.

[6] When computing the Berry curvature and related quantities, there is no "choice of basis" for $H(\mathbf{k})$ in the sense of reference [27]. Indeed, the basis is fixed by the unitary transform $\exp(-i\mathbf{k}\cdot\hat{\mathbf{r}})$ used to define $H(\mathbf{k})$ and this gives basis II. Writing $H(\mathbf{k})$ in basis I, instead of II, amounts to replace $f(\mathbf{k})$ by $f_I(\mathbf{k}) = -t[1 + e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2}]$. To check that this is not correct, we computed the Berry curvature by boldly replacing f by f_I in the corresponding formulas and found a different Berry curvature, which did not have the C_3 symmetry.
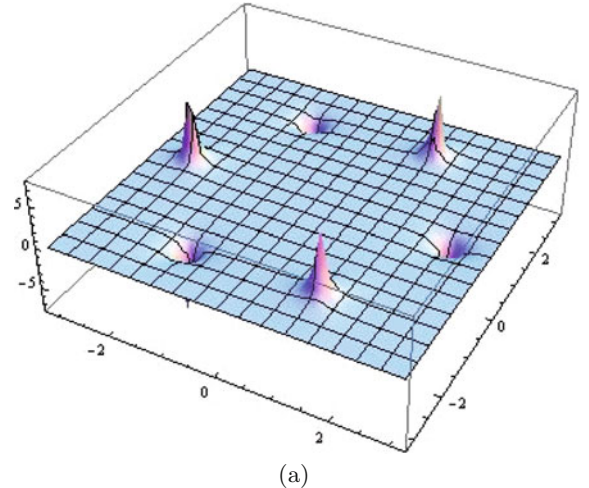
(a)
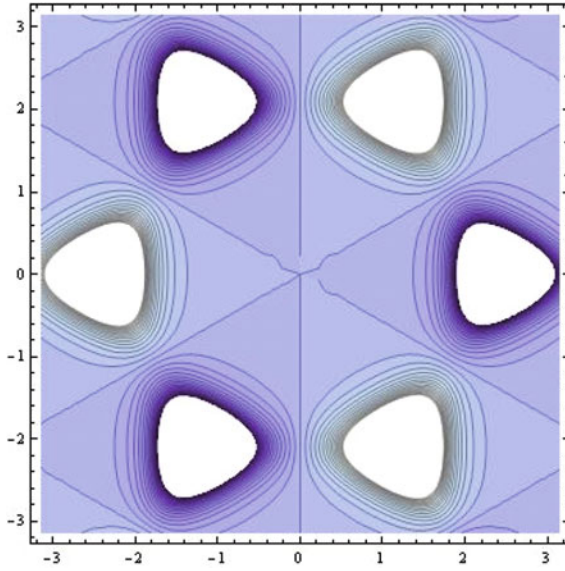
(b)

Fig. 1. Berry curvature Ω (in units of a^2) in the conduction band of boron nitride as a function of the Bloch wavevector (k_x, k_y) (in units of $1/a$) in the entire Brillouin zone for $\Delta/t = 0.1$. The lattice vectors have been taken as $\boldsymbol{a}_1 = \frac{\sqrt{3}}{2}a\boldsymbol{e}_x + \frac{3}{2}a\boldsymbol{e}_y$, $\boldsymbol{a}_2 = -\frac{\sqrt{3}}{2}a\boldsymbol{e}_x + \frac{3}{2}a\boldsymbol{e}_y$. (a) Three dimensional plot (k_x, k_y, Ω). (b) Contours of iso-curvature in the Brillouin zone.

symmetry $(\Omega(\boldsymbol{k} + \boldsymbol{G}) = \Omega(\boldsymbol{k}))$ of the triangular Bravais lattice.

The orbital magnetic moment is easily obtained from $\mathcal{M} = e\varepsilon_0\Omega$ and is shown in Figure 2.

Because of time reversal symmetry, the curvature satisfies $\Omega(-\boldsymbol{k}) = -\Omega(\boldsymbol{k})$ and its integral over the entire BZ vanishes. As inversion symmetry is absent $\Omega(-\boldsymbol{k}) \neq \Omega(\boldsymbol{k})$.

The Berry phase for a cyclotron orbit C of constant energy ε_0 is $\Gamma(C) = \pi W_C[1 - \frac{\Delta}{|\varepsilon_0|}]$ where $W_C \equiv -\alpha \oint_C d\theta/2\pi$ is the winding number, which is ± 1 when encircling a valley (because of a vortex in θ) and 0 when the orbit is around the Γ point, see Figure 3.


(a)
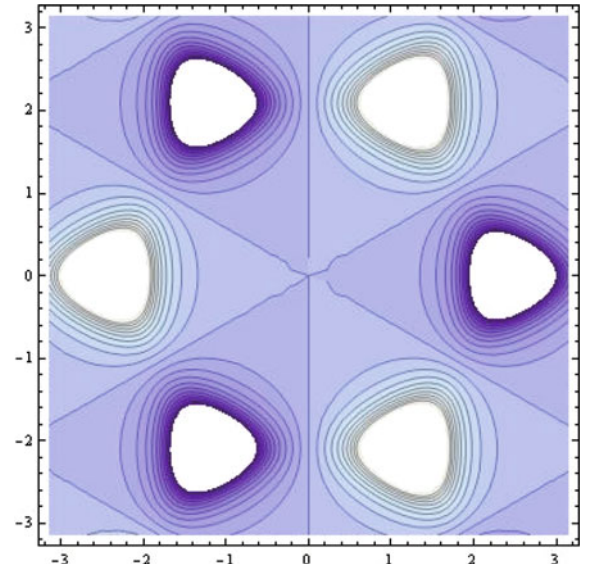
(b)

Fig. 2. Orbital magnetic moment $\mathcal{M}$ (in units of $e\,t\,a^2/\hbar$) in the conduction band of boron nitride as a function of the Bloch wavevector (k_x, k_y) (in units of $1/a$) in the entire Brillouin zone for $\Delta/t = 0.1$. (a) Three dimensional plot $(k_x, k_y, \mathcal{M})$. (b) Contours of iso-$\mathcal{M}$ in the Brillouin zone.

A saddle point in the energy dispersion at $|\varepsilon_0| = \sqrt{\Delta^2 + t^2}$ separates the cyclotron orbits which encircle the two valleys from the cyclotron orbit which encircle the Γ point in the BZ. As a consequence,

$$\Gamma(C) = -\alpha\xi\pi[1 - \Delta/|\varepsilon_0|] \text{ if } \Delta \leq |\varepsilon_0| < \sqrt{\Delta^2 + t^2}$$
$$\text{(i.e. } W_C = -\alpha\xi = \pm 1)$$
$$= 0 \text{ if } \sqrt{\Delta^2 + t^2} < |\varepsilon_0| \leq \sqrt{\Delta^2 + (3t)^2}$$
$$\text{(i.e. } W_C = 0). \tag{38}$$

We checked this simple expression for the Berry phase along a cyclotron orbit numerically by directly computing the integral of the curvature in $\boldsymbol{k}$ space over the area encircled by the cyclotron orbit.

(a)

(b)
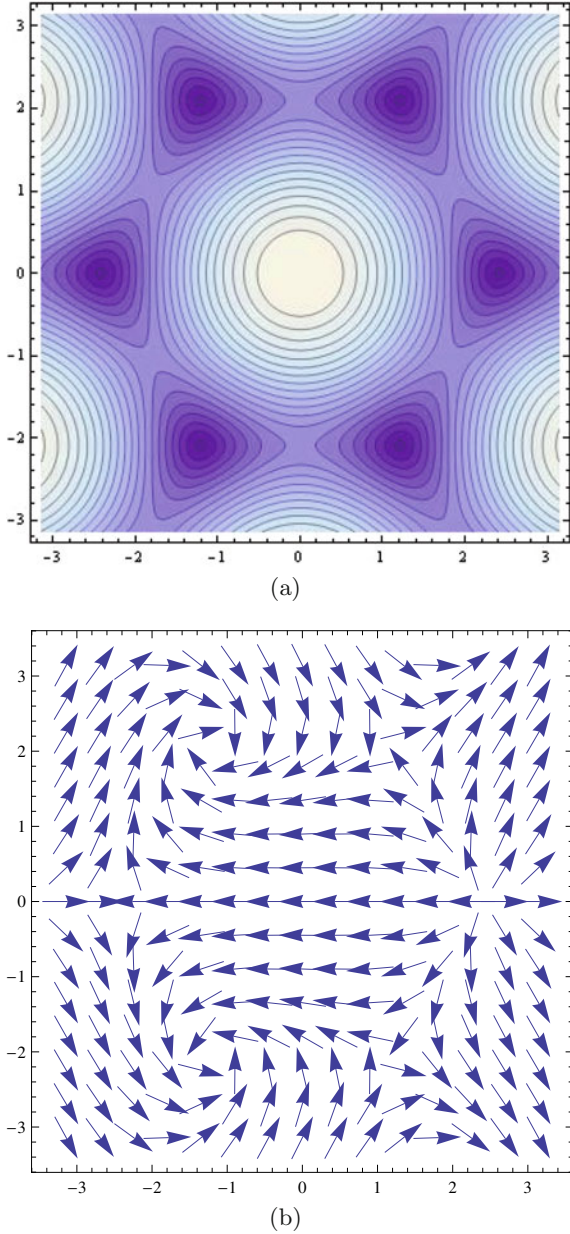
Fig. 3. (a) Isoenergy lines ($\varepsilon_0(\boldsymbol{k})$=constant) of boron nitride in the first Brillouin zone for $\Delta = 0.1$ (energies in units of t). In the semiclassical limit, cyclotron orbits in reciprocal space follow the isoenergy lines. (b) Polar angle on the Bloch sphere $\theta(\boldsymbol{k}) \equiv -\mathrm{Arg} f(\boldsymbol{k})$ in the BZ. The winding number W_C measures the topological charge of vortices in the polar angle θ.

From the energy quantization relation $S(\varepsilon)l_B^2 = 2\pi[n + 1/2] - \pi W_C$ it is now possible to obtain the (semiclassical) Landau levels for the whole energy band of boron nitride. It shows that the Landau index shift $\gamma_L = 1/2 \pm 1/2 = 0$ (modulo 1) vanishes for cyclotron orbits encircling a single valley (K or K'). Whereas for orbits around the Γ point, it is $\gamma_L = 1/2 + 0 = 1/2$.

5 Example 2: low energy model of boron nitride (massive 2D Dirac fermions)

We now take the continuum limit of a single layer of boron nitride. The low energy effective theory close to two inequivalent corners of the Brillouin zone (called valleys K and K') is now given by a massive 2D Dirac Hamiltonian [16]:

$$H_\xi(\boldsymbol{k}) = \xi \boldsymbol{k} \cdot \boldsymbol{\sigma}_\xi + \Delta \sigma_z = |\varepsilon_0| \begin{pmatrix} \cos\beta & \xi\sin\beta e^{-i\xi\theta} \\ \xi\sin\beta e^{i\xi\theta} & -\cos\beta \end{pmatrix}$$
$$\tag{39}$$

where $\cos\beta = \Delta/|\varepsilon_0|$, $\sin\beta = k/|\varepsilon_0|$ with $|\varepsilon_0| = \sqrt{\Delta^2 + k^2} \geq 0$ and $0 \leq \beta \leq \pi/2$, $\theta(\boldsymbol{k}) = \mathrm{Arg}(k_x + ik_y)$ and $f_\xi(\boldsymbol{k}) = \xi|\boldsymbol{k}|e^{-i\xi\theta(\boldsymbol{k})}$. The wavevector $\boldsymbol{k}$ is now defined from the K or K' points and not in the entire BZ. The Pauli operator vector is defined as $\boldsymbol{\sigma}_\xi \equiv (\sigma_x, \xi\sigma_y)$ where $\xi = \pm 1$ is the valley index ($\xi = 1$ corresponding to the K valley). The Fermi velocity $v = 3ta/2$ has been taken to 1. The most general single valued eigenfunction with eigenenergy $\varepsilon_0 = \alpha|\varepsilon_0|$ is $\psi(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ where the Bloch spinor is

$$|u_{\boldsymbol{k},\alpha}\rangle = \begin{pmatrix} \cos(\beta/2) \\ \xi\sin(\beta/2)e^{i\xi\theta} \end{pmatrix} \text{ if } \alpha = +1$$
$$= \begin{pmatrix} -\xi\sin(\beta/2)e^{-i\xi\theta} \\ \cos(\beta/2) \end{pmatrix} \text{ if } \alpha = -1. \tag{40}$$

The Berry connection is given by:

$$\boldsymbol{\mathcal{A}} = -\alpha\xi\sin^2(\beta/2)\nabla\theta. \tag{41}$$

Upon integration over the circular cyclotron orbit C of radius k, we obtain the Berry phase:

$$\Gamma(k) = -\alpha\xi 2\pi\sin^2(\beta/2) = -\alpha\xi\pi(1 - \cos\beta) \tag{42}$$

and the topological Berry phase:

$$\pi W_C = -\alpha\xi\pi. \tag{43}$$

The connection can be rewritten as:

$$\boldsymbol{\mathcal{A}} = \frac{\Gamma(k)}{2\pi}\boldsymbol{\nabla}_{\boldsymbol{k}}\theta = \frac{\Gamma(k)}{2\pi k}\boldsymbol{e}_\theta. \tag{44}$$

Note that

$$\sum_{\xi=\pm} \Gamma_{\alpha,\xi}(k) = 0 \tag{45}$$

which is a manifestation of time-reversal cancellation. The Berry phase depends on the magnitude of the gap, which means that it now depends on k and therefore on the magnetic field B. Two limits of interest are the "ultra-relativistic" limit ($\Delta/k \to 0$, $\beta \to \pi/2$)

$$\Gamma(k \gg \Delta) \approx -\alpha\xi\pi = \pi W_C \tag{46}$$

and the "non-relativistic" limit ($\beta \approx k/\Delta \to 0$):

$$\Gamma(k \ll \Delta) \approx 0 = \Gamma(0) \tag{47}$$

when $\Delta \neq 0$. The corresponding Berry curvature is:

$$\Omega = \frac{1}{2\pi k}\frac{d\Gamma}{dk} = -\alpha\xi\frac{\Delta}{2|\varepsilon_0|^3}. \tag{48}$$

It does not contain a singular term, except when $\Delta \to 0^+$: $\Omega = 0$ when $k \neq 0$ and $\Omega \to -\alpha\xi\infty$ when $k = 0$. Details of the calculation are given in Appendix D.

The orbital magnetic moment is [26]

$$\mathcal{M} = e\varepsilon_0\Omega = -\xi\frac{e\Delta}{2\varepsilon_0^2}. \tag{49}$$

As a side remark, we note that this orbital magnetic moment leads to a valley-Zeeman effect in presence of a magnetic field. In particular, at the bottom of the band $k \to 0$, the orbital magnetic moment is $\mathcal{M}(0) = -\xi e/2\Delta$ and the valley-Zeeman gap would be $2\Delta_{vZ} = 2\mathcal{M}(0)B$. Some effects related to this valley magnetic moment are discussed in reference [26]. Here, we would like to point out one more effect, which could be relevant for graphene in the quantum Hall regime. In graphene – which is gapless $\Delta = 0$ in the absence of a magnetic field – it is possible to imagine a self-consistent mechanism at finite B leading to a valley-dependent gap opening for the $n = 0$ Landau level. Indeed asking that the gap leading to a valley magnetic moment is itself the valley-Zeeman gap $\Delta = \Delta_{vZ}$ leads to $\Delta = \hbar v/l_B\sqrt{2} \propto \sqrt{B}$. This single electron mechanism is similar but not identical to that proposed by Lukyanchuk and Bratkovsky [28], as can be seen from the different magnetic field dependence of the gap (square root versus linear). A valley splitting of the $n = 0$ Landau level of graphene has indeed been observed in a strong magnetic field [29]. However it is not yet clear what is the relevant microscopic mechanism (for a review see Ref. [30]).

From the Onsager relation and the Berry phase just obtained, we find the energy quantization condition $S(\varepsilon)l_B^2 = 2\pi n + 1/2 - \pi W_C$ with $W_C = -\alpha\xi$.

The area $S(\varepsilon) = \pi[\varepsilon^2 - \Delta^2]$ has the same functional form as $S(C) = \pi[\varepsilon_0^2 - \Delta^2]$, but the two quantities differ by the term $-2\pi\varepsilon_0\mathcal{M}B$. It is $S(\varepsilon)$ which is directly related to the Landau levels (and not $S(C)$). By inverting $S(\varepsilon)$, the semiclassical Landau levels are:

$$\varepsilon_n = S^{-1}\left[2\pi eB\left(n + \frac{1}{2} - \frac{W_C}{2}\right)\right]$$
$$= \alpha\sqrt{\Delta^2 + 2eB\left(n + \frac{1}{2} - \frac{W_C}{2}\right)}. \tag{50}$$

The energy is therefore quantized as

$$\varepsilon_{n'} = \alpha\sqrt{\Delta^2 + eB2n'} \tag{51}$$

where $n' = n + (1 + \alpha\xi)/2$ is an integer. This result agrees with the exact expression for the Landau levels (7), including $n' = 0$. Indeed, $n' = n = 0$ implies $\alpha = -\xi$, which gives $\varepsilon = \alpha\Delta = -\xi\Delta$. It is a bit surprising that a semiclassical calculation (including terms of order $\hbar$) is able to recover exactly a fully quantum result. This is actually a peculiarity of massive Dirac fermions and does not occur in more general cases.

6 Example 3: low energy model of graphene (massless 2D Dirac fermions)

As another example, we consider the case of graphene, which is a two-dimensional honeycomb lattice of carbon atoms. It can be seen as the limit of boron nitride when the gap closes because the two carbon atoms in the unit cell have the same on-site energy. It is a zero-gap semiconductor and its low energy effective theory – close to K or K' – is given by a massless 2D Dirac Hamiltonian:

$$H_\xi(\boldsymbol{k}) = \xi v\boldsymbol{k} \cdot \boldsymbol{\sigma}_\xi = \xi vk\begin{pmatrix} 0 & e^{-i\xi\theta} \\ e^{i\xi\theta} & 0 \end{pmatrix} \tag{52}$$

where $\theta = \mathrm{Arg}(k_x + ik_y)$ depends on the direction of the Bloch wavevector $\boldsymbol{k}$ (here defined from the K or K' points) and $\xi = \pm 1$ is the valley index ($\xi = 1$ corresponding to the K valley). The 2×2 matrix is written in (A, B) space. In the following, we take the Fermi velocity $v \equiv 1$. The most general single valued eigenfunction with eigenenergy αk is $\psi(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ where the Bloch spinor is

$$|u_{\boldsymbol{k},\alpha}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \xi e^{i\xi\theta} \end{pmatrix} \text{ if } \alpha = +1$$
$$= \frac{1}{\sqrt{2}}\begin{pmatrix} -\xi e^{-i\xi\theta} \\ 1 \end{pmatrix} \text{ if } \alpha = -1 \tag{53}$$

where α is the band index: $\alpha = +1$ (resp. -1) corresponding to the conduction (resp. valence) band. The first (resp. second) component of the spinor is the amplitude on the A (resp. B) sublattice for both valleys and the area of the system was taken as unity.

The Berry connection is given by:

$$\boldsymbol{\mathcal{A}} = -\frac{\alpha\xi}{2}\boldsymbol{\nabla}_{\boldsymbol{k}}\theta = -\frac{\alpha\xi}{2k}\boldsymbol{e}_\theta \tag{54}$$

which shows that it is a pure gauge except for the singularity at the origin. Because of this vortex, it gives a topological (quantized) Berry phase:

$$\Gamma = \oint_C d\boldsymbol{k} \cdot \boldsymbol{\mathcal{A}} = -\alpha\xi\pi \tag{55}$$

which is independent of the cyclotron orbit. Here the winding number $W_C = -\alpha\xi = \pm 1$, where $\alpha\xi$ is the chirality of the massless electron. This allows one to rewrite the Berry connection as:

$$\boldsymbol{\mathcal{A}} = \frac{\Gamma}{2\pi}\boldsymbol{\nabla}_{\boldsymbol{k}}\theta. \tag{56}$$

The corresponding Berry curvature is singular

$$\Omega = \Gamma\delta^2(\boldsymbol{k}) \tag{57}$$

and the Roth-Wilkinson relation (4) between the phase mismatch γ and the Berry phase Γ gives:

$$\gamma = \frac{1}{2} - \frac{\Gamma}{2\pi} = \frac{1 + \alpha\xi}{2} \equiv 0 \bmod. 1 \tag{58}$$

which is consistent with the Landau levels found by McClure $\varepsilon_n = \alpha\sqrt{2neB}$. The Berry phase is non-zero

here because of the band degeneracy (Dirac point) and despite the inversion symmetry being present (which results in $\Omega = 0$ in the absence of band degeneracy [22,23]). A singular Berry phase in a system with inversion and time-reversal symmetry is a signature of the presence of a Dirac point.

The orbital magnetic moment is also singular:

$$\mathcal{M} = e\Gamma\delta(k)\delta(\theta) = -\alpha\xi\pi e\delta(k)\delta(\theta) \qquad (59)$$

However, it plays no role in the quantization of cyclotron orbits for massless Dirac fermions because the area of the cyclotron orbit at constant energy $S(\varepsilon) = S(C) - 2\pi\varepsilon_0\mathcal{M}B$ is equal to $S(C)$ as $\varepsilon_0\mathcal{M} \propto k\delta(k) = 0$.

7 Example 4: low energy model of a gapped graphene bilayer

The low energy effective theory close to K and K' of a gapped bilayer graphene is given by the following Hamiltonian [33]:

$$H_\xi(\boldsymbol{k}) = \begin{pmatrix} \Delta & -\frac{\boldsymbol{k}^2}{2m}e^{i\xi 2\phi} \\ -\frac{\boldsymbol{k}^2}{2m}e^{-i\xi 2\phi} & -\Delta \end{pmatrix} \qquad (60)$$

where m is an effective mass and $\phi = \text{Arg}\,(k_x + ik_y)$. The function f_ξ is therefore $f_\xi(\boldsymbol{k}) = (-\boldsymbol{k}^2/2m)\exp{(i2\xi\phi)}$, which shows that $\theta(\boldsymbol{k}) = 2\xi\phi(\boldsymbol{k}) - \pi$ and $|\varepsilon_0| = \sqrt{\Delta^2 + (\boldsymbol{k}^2/2m)^2}$.

The Berry phase is $\Gamma(C) = \pi W_C[1 - \Delta/|\varepsilon_0|]$ where the winding number is:

$$W_C = 2\alpha\xi \qquad (61)$$

because the phase θ rotates twice as fast as ϕ. From the previous analysis of the semiclassical quantization condition (34) including the effect of the orbital magnetic moment, we find the energy quantization condition $S(\varepsilon)l_B^2 = 2\pi n + 1/2 - \pi W_C$. Inverting $S(\varepsilon) = 2\pi m\sqrt{\varepsilon^2 - \Delta^2}$, we obtain the semiclassical Landau levels:

$$\varepsilon_n = \alpha\sqrt{\Delta^2 + \omega_c^2(n + \frac{1}{2} - \alpha\xi)^2} = \alpha\sqrt{\Delta^2 + \omega_c^2(n' + \frac{1}{2})^2} \qquad (62)$$

where the cyclotron pulsation $\omega_c \equiv eB/m$ and $n' = n - \alpha\xi$ is an integer. The quantum mechanical result [33] is $\varepsilon_n = \alpha\sqrt{\Delta^2 + \omega_c^2 n(n-1)}$, which agrees with the semiclassical result including the n^0 order. Here, however, the semiclassical results does not match the quantum result to all orders in $\hbar$.

8 Conclusion

We have studied wave effects in the semiclassical quantization of cyclotron orbits in coupled two-band mod-

els, focusing especially on the case of boron nitride. Two main results of the article are the following:

First, although the phase mismatch $\gamma(C)$ appearing in the Onsager quantization condition is related to the complete Berry phase $\Gamma(C)$, the Landau index shift γ_L only gets a contribution from the topological part of the Berry phase πW_C (winding number of the pseudo-spin $1/2$). The latter is a topological invariant, which allows one to distinguish between two types of band insulators. On the one hand, zero topological Berry phase indicates that if inversion symmetry is restored, the bands are well separated and no Dirac points are present. On the other hand, a non-zero topological Berry phase is a signature of the presence of Dirac points in crystals with inversion symmetry. Therefore a shift in the Landau level index is related to a non-zero topological Berry phase, which signals the presence of underlying Dirac points (which are only revealed if inversion symmetry is restored).

Second, computing the Berry curvature in the entire Brillouin zone requires care in defining the $\boldsymbol{k}$-dependent Hamiltonian. In particular this Hamiltonian should be written in what Bena and Montambaux [27] call basis II and not in basis I, which is the basis that automatically emerges when performing the unitary transformation (12). The Berry curvature is a local physical quantity that in principle could be measured. A challenge would be to design a "Berrymeter" to measure this curvature in the entire Brillouin zone. An idea would be to measure the anomalous g-factor, which is due to the orbital magnetic moment $\mathcal{M}_\alpha$ and contains the same information as the Berry curvature. This could be done as a function of doping – e.g. electric doping in graphene with a gate – giving access to local quantities.

Appendix A: Physical interpretation of the semiclassical quantization condition

Here we give a physical interpretation of the semiclassical quantization condition for the cyclotron orbit. These results are certainly not new, but we collect them because they seem not to be so well-known. Physically Onsager's quantization is the condition for the single-valuedness of the semiclassical wavefunction. It states that the total stationary phase ϕ accumulated by an electron around its cyclotron orbit is the sum of four terms and should equal zero modulo 2π:

$$\phi = \hbar k \times 2\pi r/\hbar - eB \times \pi r^2/\hbar + \Gamma(k) - \pi = 2\pi n \quad (A.1)$$

where n is an integer and $-e < 0$ is the electron charge. These four terms are: the spatial de Broglie phase $k \times 2\pi r$; the Aharonov-Bohm phase $-eB \times \pi r^2/\hbar$; the Berry phase $\Gamma(k)$; and the Maslov contribution of $-\pi$.

The two first terms are classical (they arrive at order $\hbar^0$). The de Broglie phase is just the accumulated

phase of a (quasi) plane wave on a trajectory of length $2\pi r$. For the cyclotron orbit, because classically $\hbar k = eBr$ as $\hbar\dot{\boldsymbol{k}} = -e\dot{\boldsymbol{r}} \times \boldsymbol{B}$, it can be rewritten as $eB \times 2\pi r^2/\hbar$. The Aharonov-Bohm phase comes from the fact that the electron surrounds a region of non-zero magnetic flux $\Phi = B \times \pi r^2$ and the minus sign comes from the negative electric charge of the electron. It is given by $-2\pi\Phi/\Phi_0 = -eB \times \pi r^2/\hbar$, where $\Phi_0 \equiv h/e$ is the flux quantum. The Aharanov-Bohm phase can be seen as a Berry phase due to magnetic curvature in real space. Together these two terms form the classical reduced action (divided by $\hbar$): $A_{\mathrm{cl}}/\hbar = \oint d\boldsymbol{r}\cdot\boldsymbol{p}/\hbar = \pi k^2 \times \hbar/eB = S(k)l_B^2$ where $\boldsymbol{p} \approx \hbar\boldsymbol{k} - e\boldsymbol{A}$.

The two other terms are the first quantum corrections to the classical action (they appear at order $\hbar$ and represent wave effects): the Berry phase and the Maslov contribution. The Berry phase is due to curvature in $\boldsymbol{k}$-space because of the torus-like topology of the Brillouin zone. It can be seen as an Aharonov-Bohm phase due to a "magnetic field in $\boldsymbol{k}$ space" $\boldsymbol{\Omega}$, whose flux is $\Omega \times \pi k^2$. The Maslov contribution comes from two caustics (Maslov index of 2) on the cyclotron orbit, each contributing a factor $-\pi/2$. The caustics represent singularities in the semiclassical wavefunction, where the probability density diverges and the phase picks an extra $-\pi/2$ factor. The caustics are actually not properties of a single orbit but of a family of classical orbits. For a detailed discussion of caustics and the extra $\pi/2$ phase (in the context of optics) see reference [34].

Collecting these four terms, equation (A.1) can be rewritten as:

$$\frac{A_{\mathrm{cl}}}{\hbar} = S(k)l_B^2 = 2\pi\left[n + \frac{1}{2} - \frac{\Gamma(k)}{2\pi}\right] \qquad (A.2)$$

which is precisely the semiclassical quantization of a cyclotron orbit including terms of order $\hbar$, with $\gamma = 1/2 - \Gamma(k)/2\pi$, see equation (1,4).

Appendix B: Hamiltonians

In this appendix, we discuss the relation between the three kinds of Hamiltonians used in the main text, namely $\hat{H}$, $\hat{H}(\boldsymbol{k})$ and $H(\boldsymbol{k})$. Hats are used to distinguish operators acting in the complete Hilbert space from those solely acting on band indices.

(1) The original Hamiltonian of the system is called $\hat{H}$. In its eigenbasis of Bloch states it reads:

$$\hat{H} = \sum_{\boldsymbol{k},\alpha} \varepsilon_{\alpha,0}(\boldsymbol{k})|\boldsymbol{k},\alpha\rangle\langle\boldsymbol{k},\alpha|. \qquad (B.1)$$

(2) Next, we define the unitary operator $\hat{U}(\boldsymbol{k}) = \exp(-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}})$ – where $\hat{\boldsymbol{r}}$ is the complete position operator and not, for example, merely the Bravais lattice position operator –, which transforms Bloch states $|\boldsymbol{k},\alpha\rangle$ into

their u-part: $\hat{U}(\boldsymbol{k})|\boldsymbol{k},\alpha\rangle = |u_{\boldsymbol{k},\alpha}\rangle$. This transformation is just a translation by $\boldsymbol{k}$ in reciprocal space. Performing this unitary transform on $\hat{H}$, we define the $\boldsymbol{k}$-dependent Hamiltonian:

$$\hat{H}(\boldsymbol{k}) \equiv \hat{U}(\boldsymbol{k})\hat{H}\hat{U}(\boldsymbol{k})^\dagger \qquad (B.2)$$
$$= \sum_{\boldsymbol{k}',\alpha} \varepsilon_{\alpha,0}(\boldsymbol{k}')e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}}|u_{\boldsymbol{k}',\alpha}\rangle\langle u_{\boldsymbol{k}',\alpha}|e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}}.$$

It is still an operator in the complete Hilbert space but it depends on $\boldsymbol{k}$ as a parameter. This transformation actually defines a whole family of Hamiltonians (one for each wavevector $\boldsymbol{k}$ in the Brillouin zone).

(3) The 2×2 $\boldsymbol{k}$-dependent Hamiltonian is defined as the restriction of $\hat{H}(\boldsymbol{k})$ on the fixed $\boldsymbol{k}$ subspace:

$$H(\boldsymbol{k}) \equiv P(\boldsymbol{k})\hat{H}(\boldsymbol{k})P(\boldsymbol{k}) = \sum_\alpha \varepsilon_{\alpha,0}(\boldsymbol{k})|u_{\boldsymbol{k},\alpha}\rangle\langle u_{\boldsymbol{k},\alpha}| \qquad (B.3)$$

where $P(\boldsymbol{k}) \equiv \sum_\alpha |u_{\boldsymbol{k},\alpha}\rangle\langle u_{\boldsymbol{k},\alpha}|$ are projectors on the $\boldsymbol{k}$ subspace. Note that $H(\boldsymbol{k})$ is only an operator in band index subspace. In the case of only two bands, it is therefore a 2×2 matrix. Note that $H(\boldsymbol{k})$ is not periodic in reciprocal lattice vectors but its eigenvalues are.

Appendix C: Orbital magnetic moment for an electron-hole symmetric two-band Hamiltonian

In this Appendix, we prove that there is a simple relation between the orbital magnetic moment and the Berry curvature in the case of a two-band model with particle-hole symmetry [26]. The 2×2 Hamiltonian is

$$H(\boldsymbol{k}) = \sum_\alpha \varepsilon_{0,\alpha}(\boldsymbol{k})P_\alpha(\boldsymbol{k}) \qquad (C.1)$$

where $P_\alpha(\boldsymbol{k}) \equiv |u_{\boldsymbol{k},\alpha}\rangle\langle u_{\boldsymbol{k},\alpha}|$ are projectors on each of the two bands (labeled by $\alpha = \pm1$) and $\varepsilon_{0,\alpha}(\boldsymbol{k})$ are the band energies. Particle-hole symmetry together with time-reversal symmetry implies that

$$\varepsilon_{0,-\alpha}(-\boldsymbol{k}) = -\varepsilon_{0,\alpha}(\boldsymbol{k}) = -\varepsilon_{0,\alpha}(-\boldsymbol{k}) \qquad (C.2)$$

and the Hamiltonian becomes

$$H(\boldsymbol{k}) = \varepsilon_{0,+}(\boldsymbol{k})[P_+(\boldsymbol{k}) - P_-(\boldsymbol{k})]$$
$$= \varepsilon_{0,-}[P_-(\boldsymbol{k}) - P_+(\boldsymbol{k})]. \qquad (C.3)$$

Using the unit operator in the reduced $\boldsymbol{k}$-space $I(\boldsymbol{k}) = P_+(\boldsymbol{k}) + P_-(\boldsymbol{k})$, we can write:

$$\varepsilon_{0,\alpha}(\boldsymbol{k})I(\boldsymbol{k}) - H(\boldsymbol{k}) = 2\varepsilon_{0,\alpha}(\boldsymbol{k})[I(\boldsymbol{k}) - P_\alpha(\boldsymbol{k})]. \qquad (C.4)$$

Therefore the orbital magnetic moment (in the upper band, e.g., $\alpha = +1$) is

$$\boldsymbol{\mathcal{M}}_+ = i\frac{e}{2\hbar}\langle\boldsymbol{\nabla}u_+| \times [\varepsilon_{0,+} - H(\boldsymbol{k})]|\boldsymbol{\nabla}u_+\rangle$$
$$= i\frac{e}{\hbar}\varepsilon_{0,+}\langle\boldsymbol{\nabla}u_+| \times [I - P_+]|\boldsymbol{\nabla}u_+\rangle \qquad (C.5)$$

But $\langle \boldsymbol{\nabla} u_+| \times I|\boldsymbol{\nabla} u_+\rangle = -i\boldsymbol{\Omega}_+$ by definition of the Berry curvature and $\langle \boldsymbol{\nabla} u_+| \times P_+|\boldsymbol{\nabla} u_+\rangle = \langle \boldsymbol{\nabla} u_+|u_+\rangle \times \langle u_+|\boldsymbol{\nabla} u_+\rangle = \boldsymbol{\mathcal{A}}_+ \times \boldsymbol{\mathcal{A}}_+ = 0$ by definition of the Berry connection, therefore

$$\boldsymbol{\mathcal{M}}_\alpha = \frac{e}{\hbar}\varepsilon_{0,\alpha}\boldsymbol{\Omega}_\alpha. \tag{C.6}$$

Appendix D: Berry curvature of a massive Dirac fermion

The Berry connection is given by:

$$\boldsymbol{\mathcal{A}} = \frac{\Gamma(k)}{2\pi}\boldsymbol{\nabla}_{\boldsymbol{k}}\theta. \tag{D.1}$$

Therefore:

$$\boldsymbol{\Omega} = \nabla \times \boldsymbol{\mathcal{A}} = \frac{\nabla\Gamma(k)}{2\pi} \times \nabla\theta + \frac{\Gamma(k)}{2\pi}\nabla \times \nabla\theta. \tag{D.2}$$

Using that $\nabla \times \nabla\theta = 2\pi\delta^2(\boldsymbol{k})\boldsymbol{e}_z$, we obtain:

$$\Omega = \frac{1}{2\pi k}\frac{d\Gamma(k)}{dk} + \Gamma(0)\delta^2(\boldsymbol{k}). \tag{D.3}$$

Therefore, if $\Delta \neq 0$, $\Gamma(0) = 0$ and the Berry curvature is $\Omega = (d\Gamma/dk)/(2\pi k) = -\alpha\xi\Delta/(2|\varepsilon_0|^3)$. But if $\Delta = 0$, $\Gamma(k) = \Gamma = -\alpha\xi\pi = \Gamma(0) \neq 0$, $d\Gamma/dk = 0$ and the curvature is $\Omega = \Gamma\delta^2(\boldsymbol{k})$.

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