A brief note in the form of a decalogue about Berry phase, Chern number, curvature, topological Hamiltonians and much more ... an outline for beginners

Josep Planelles
Departament de Química Física i Analítica, Universitat Jaume I, E-12080, Castelló, Spain
email:josep.planelles@uji.es

July 12, 2018

A brief outline on Berry phase, Chern number, curvature, topological Hamiltonians, etc. is given, as an attempt to give some very basic hints to those students who start reading papers on the field.

1 Decalogue

1. The wave functions Ψ and $\Psi' = e^{i\gamma}\,\Psi$, with γ a constant, represent the same estate. We say that the Schrödinger equation is invariant under a *global* change of phase in the real space ($U(1)$ symmetry).

   As any other symmetry, this one is related to an invariant (Noether's theorem). In this case, the symmetry is related to the norm or particle number conservation (appendix 1).

2. The Schrödinger equation of a charged particle in a magnetic field, $\hat{H} = \frac{1}{2m}(\hat{p} - eA)^2$, where A is the vector potential, is invariant under a *local* change of phase in the real space. Actually, if we proceed with the replacement $A \rightarrow A' = A + \nabla\gamma$, with $\gamma(\mathbf{r})$, then $\Psi' = \Psi\, e^{i\gamma(\mathbf{r})}$ is eigenfunction of the Schrödinger equation and corresponds to the same eigenvalue as Ψ, i.e., represent the same state.

   It is worth saying that the physically observable magnetic field, $B = \nabla \times A$, is invariant under the change $A \rightarrow A + \nabla\gamma$ since $\nabla \times \nabla\gamma = 0$. Then, neither the state of the system changes.

3. The wave function of particle in a crystalline lattice with translational symmetry, has the form of a Bloch wave $\Psi_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r})\, e^{i\mathbf{kr}}$, the Bloch waves being invariant under a *local* change of the phase in the reciprocal or momentum space (see appendix 2).

   Can we define in this case the analog of vector potential? Yes, we can.

4. Let's consider a Hamiltonian operator $\hat{H}$ depending on a set of parameters, as e.g. the molecular electronic Hamiltonian which is a function of the nuclear coordinates. If the system undergo an adiabatic change from some time $t = 0$ up to $t = T$, following a path in the parameter space which returns to the starting point, also the system returns to the initial state. However, this initial state, reached after completing the route, is described by a function Ψ_T that may differ from Ψ_0 by a phase factor $\gamma(C)$, this phase factor being dependent on the followed path C. The phase factor $\gamma(C)$ can be determined from the Schrödinger equation $i\hbar\dot{\Psi} = \hat{H}\Psi$. Namely, should we call $|u_{nR}(\mathbf{r})\rangle$ to the n-th eigenvalue of the Hamiltonian $\hat{H}_R(\mathbf{r})$, this phase, called Berry's phase, turns out to be (appendix 3):

$$\gamma(C) = \oint_C i\,\langle u_{nR}(\mathbf{r})|\nabla_R u_{nR}(\mathbf{r})\rangle \cdot d\mathbf{R} = \oint_C \mathbf{A}_n \cdot d\mathbf{R}, \tag{1}$$

   $\mathbf{A}_n$ being referred to as Berry's connexion and represents the vector potential analog.

5. The Stokes theorem allows to transforms the above line-integral into a surface-integral:

$$\gamma(C) = \iint_S \nabla \times \mathbf{A}_n \cdot d\mathbf{S} \tag{2}$$

and, then, to define the analog of the magnetic field, $\mathbf{F}_n = \nabla \times \mathbf{A}_n$, called Berry's curvature, which, like the magnetic field, has full physical meaning.

6. The **non**-existence of magnetic monopoles entails a null divergence of the magnetic field, $\nabla B = 0$, which implies, in turn, that the net magnetic flux through a closed surface (surface without edges, like a sphere or a torus) is zero. A magnetic monopole would generate a magnetic field $B = q_m \frac{\mathbf{r}}{r^3}$. This field can be related to the vector potential $A = q_m \frac{(y,-x,0)}{r(r-z)}$ (it can be straightforwardly checked by replacement of the above A in $\nabla A = B$). This magnetic field has a non-zero net flux through a closed surface (provided the monopole being located *inside* the closed surface).

   The above vector potential A has a singularity at $z = r$. The same field B can be also derived from the potential vector $A' = q_m \frac{(-y,x,0)}{r(r+z)}$, which presents no singularity at $z = r$. But it is singular at $z = -r$. Both potential vectors are related by a *gauge* transformation: $A - A' = 2q_m \nabla \varphi$, $\varphi = \arctan \frac{y}{x}$. The presence of this *gauge*-symmetry leads to the quantization of the magnetic charge (appendix 4).

   It is worth to emphasize that no matter the gauge we may use, the vector potential of a monopole magnetic field will have at least a singularity (the absence of singularities will yield zero flux, see appendix 5).

7. In a similar way, the integral on a closed surface of the Berry's connexion $\mathbf{A}_n$ is zero, unless it has a singularity.

   Let us realize that due to the way the Berry connection has been defined, $\mathbf{A}_n = i \langle u_{nR}(\mathbf{r}) | \nabla_R u_{nR}(\mathbf{r}) \rangle$, it results ill-defined in the presence of energy degeneration (since it has been defined for **a** given state n, and in case of degeneration of the states n and m, any linear combination of them is valid to describe the dynamic state of the system, then, the connexion becomes undetermined as soon as degeneration is reached). The presence of degeneration in the parameter space $\mathbf{R}$ yields a singular connexion (as an example we may mention the Jahn-Teller conic intersection).

   In solid state, the Bloch waves phase factor $\gamma(\mathbf{k})$ arises in the reciprocal or momentum space. In this case, the effective Hamiltonian acting on the Bloch functions is $\hat{H}(\mathbf{k}) = e^{i\mathbf{kr}} \hat{H} e^{-i\mathbf{kr}}$, where $\hat{H}$ is the Hamiltonian acting on the complete wave function (envelope × Bloch). The Berry's connexion and phase can then be derived as:

$$\mathbf{A}_n = i \langle u_{nk}(\mathbf{r}) | \nabla_k u_{nk}(\mathbf{r}) \rangle \qquad ; \qquad \gamma(\mathbf{k}) = \oint_C \mathbf{A}_n \cdot d\mathbf{k} \tag{3}$$

8. As an extension of the above item, let's consider the simple case of two bands that may have a degeneration associated to a given $\mathbf{k}$ value in a two-dimensional Brillouin zone (corresponding to a 2D lattice, e.g. graphene) and an associated 2×2 Hamiltonian depending on three parameters X,Y,Z (we may consider them as the components of some 3D vector $\mathbf{R}$)[1]:

$$\hat{H}(\mathbf{R}) = \begin{bmatrix} Z & X - iY \\ X + iY & -Z \end{bmatrix} = \mathbf{R} \cdot \hat{\sigma} \tag{4}$$

   where $\hat{\sigma}(\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. The eigenvalues of this Hamiltonian can easily be calculated to be $E_\pm = \pm|\mathbf{R}|$. Please, note that degeneracy arises for $\mathbf{R} = 0$. The Berry's curvature $\mathbf{F}_n = \nabla_R \times \mathbf{A}_n$ can be written (appendix 6):

$$\mathbf{F}_n = \mathrm{Im} \sum_{\mathrm{n} \neq \mathrm{m}} \frac{\langle \mathrm{u_{nk}}(\mathbf{r}) | \nabla_{\mathrm{R}}(\hat{\mathrm{H}}) | \mathrm{u_{mk}}(\mathbf{r}) \rangle \times \langle \mathrm{u_{mk}}(\mathbf{r}) | \nabla_{\mathrm{R}}(\hat{\mathrm{H}}) | \mathrm{u_{nk}}(\mathbf{r}) \rangle}{(\mathrm{E_m} - \mathrm{E_n})^2} \tag{5}$$

   In this case, $\nabla_R(\hat{H}(\mathbf{R})) = \hat{\sigma}$.

   We may select the axes system so that z points in the $\mathbf{R}$ direction and then calculate the integrals (integrals are invariant under axes rotation). Then, $\hat{H}$ is diagonal and the eigenvalues turn into $|+\rangle = (1,0)$, $|-\rangle = (0,1)$, so that acting the Pauli matrices on these eigenvectors we find: $\sigma_z|\pm\rangle = \pm|\pm\rangle$, $\sigma_x|\pm\rangle = |\mp\rangle$, $\sigma_y|\pm\rangle = \pm i\,|\mp\rangle$. Then, after a short algebra (appendix 7) we find out: $(\mathbf{F}_n)_x = (\mathbf{F}_n)_y = 0$, and:

$$(\mathbf{F}_n)_z = \frac{\mathrm{Im}\langle + | \sigma_\mathrm{x} | - \rangle \langle - | \sigma_\mathrm{y} | + \rangle}{4R^2} = \frac{1}{2} \frac{1}{R^2} \tag{6}$$

   Let's now recover the original axes orientation: $(\mathbf{F}_n)_z = \frac{1}{2} \frac{\mathbf{R}}{R^3}$. Therefore,

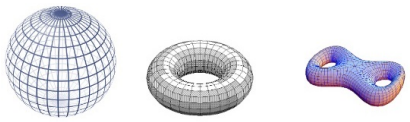
$$\gamma_n = \iint \mathbf{F}_n \cdot d\mathbf{S} = \int_0^{\pi} \int_0^{2\pi} \frac{R}{2R^3} R^2 \sin\theta \, d\theta \, d\phi = 2\pi \tag{7}$$

that represents the flux of a 1/2 magnetic charge through a R-radius sphere. Therefore, Berry's connexion has a singularity (at the degeneracy). Note that the integration of the flux of the Berry's curvature $\mathbf{F}_n$ on a close surface is zero in case the associated connexion $\mathbf{A}_n$ is free of singularities.

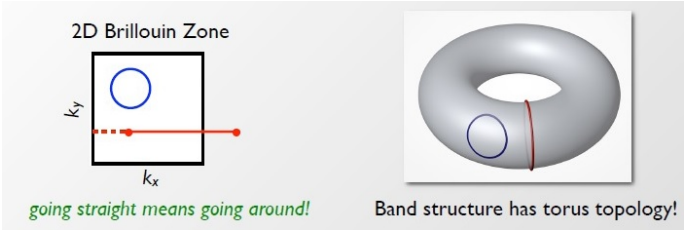
9. The curvature K at a given point on a surface is the product of the two main curvatures κ_1, κ_2 (the smallest and largest) at this point. For a R-radius sphere $\kappa_1 = \kappa_2 = \frac{1}{R}$ in every point. Then, $K = \kappa_1\kappa_2 = \frac{1}{R^2}$, and the integration over all surface results:

$$\oiint \mathbf{K} \cdot d\mathbf{S} = \int_0^{\pi} \int_0^{2\pi} \frac{1}{R^2} R \, d\theta R \sin\theta \, d\phi = 4\pi = 2\pi\chi_m \tag{8}$$

where $\chi_m = 2$. We should add here that χ_m is invariant under any deformation of the sphere (this is a general topological property. We scape its proof that can be found in any book on mathematical topology). χ_m is related to the *genus* g of the surface: $\chi_m = 2(1-g)$. The genus representing the number of holes the close surface has (zero for a sphere, one for a torus, two for a double-torus, etc).



Incidentally, the 2D first Brillouin zone has the topology of a torus, since periodicity allows to identify opposite edges of the unit lattice.



10. The *Chern number* C is the analog of χ_m. It is obtained by integration of Berry's curvature on the whole Brillouin zone. We recall here that the effective Hamiltonian acting on the Bloch functions is $\hat{H}(\mathbf{k}) = e^{i\mathbf{kr}}\hat{H}e^{-i\mathbf{kr}}$, where $\hat{H}$ is the Hamiltonian acting on the complete wave function (envolpe × Bloch). As $\hat{H}(\mathbf{k})$ depends parametrically on $\mathbf{k}$, we can define $\mathbf{A}_n(\mathbf{k}) = i\langle u_{nk}(\mathbf{r})|\nabla_k u_{nk}(\mathbf{r})\rangle$ and $\mathbf{F}_n = \nabla_k \times \mathbf{A}_n(\mathbf{k})$. The integration of $\mathbf{F}_n$ over the complete first Brillouin zone can be non-zero only when $\mathbf{A}_n$ has some singularity (like the conical intersection of graphene at the band degeneration). In such a case,

$$\oiint \mathbf{F}_n(\mathbf{k}) \cdot d\mathbf{k} = 2\pi C \tag{9}$$

where the Chern number $C \in Z$.

For the case of Haldane model[2] (a Hamiltonian for graphene with masses $\pm M$ including an imaginary *tunneling* $i\,t_2$ between second neighbors), the Hamiltonian yields a band structure where degeneracies at the K and K' points hold for different values of $t_2 = \pm\frac{M}{3\sqrt{3}}$. When we carry out integration fixing $t_2 = \frac{M}{3\sqrt{3}}$, we find out $\oiint \mathbf{F}_n(\mathbf{k}) \cdot d\mathbf{k} = 2\pi$, i.e., $C = 1$. In the graphene case ($M = t_2 = 0$) there are degeneracies at K and K' simultaneously. However, these points have same absolute value of curvatures but opposite signs, thus yielding $C = 0$ (appendix 8). This is the origin of the so-called graphene *marginal* topology[3].

2 Appendixes

2.1 Appendix 1. Norm Conservation

Symmetry in an arbitrary translation $x \to x + a$ leads to momentum $\hat{p} = -i\partial_x$ conservation. In a similar way, we will show that the conservation of $-i\partial_\gamma$ leads to conservation of the probability density. We have,

$$-i\partial_\gamma \Psi = -i\,\frac{\Psi e^{i\delta\gamma} - \Psi}{\delta\gamma} = -i\,\frac{(1 + i\delta\gamma)\Psi - \Psi}{\delta\gamma} = \Psi \tag{10}$$

Then, $\langle\Psi| - i\partial_\gamma|\Psi\rangle = \langle\Psi|\Psi\rangle$.

2.2 Appendix 2. Bloch waves invariance under a phase change in the k space

We apply the Hamiltonian operator on $\Psi' = \Psi e^{i\gamma(k)} = e^{ikr}u_{nk}(r)e^{i\gamma(k)}$ to obtain:

$$\hat{H}\Psi' = \left[-\frac{1}{2m}\nabla_r + V(r)\right]\Psi' = e^{i\gamma(k)}\hat{H}\Psi = E_{nk}\Psi'$$

we see then that Ψ' and Ψ represent the same state.

2.3 Appendix 3. The Berry's phase

We write $\Psi_n = e^{-iE_nt/\hbar}e^{i\gamma(r,t)}u_{nR}(r)$ and inject it onto the Schrödinger equation $i\hbar\dot{\Psi} = \hat{H}\Psi$:

$$i\hbar\dot{\Psi} = E_n\Psi - \hbar\dot{\gamma}\Psi + i\,\hbar\,e^{-iE_nt/\hbar}e^{i\gamma(r,t)}\nabla_R u_{nR}(r)\dot{R} \tag{11}$$

$$\hat{H}\Psi = e^{-iE_nt/\hbar}e^{i\gamma(r,t)}\hat{H}u_{nR}(r) = E_n\Psi \tag{12}$$

Then, $\dot{\gamma} = i\,e^{-iE_nt/\hbar}e^{i\gamma(r,t)}\nabla_R u_{nR}(r)\dot{R}$

Left-multiplying by Ψ^* and carrying out integration over r, we find that: $\dot{\gamma} = i\,\langle u_{nR}(r)|\nabla_R\,u_{nR}(r)\rangle\dot{R}$.

In other words,

$$\gamma(C) = \oint_C i\,\langle u_{nR}(r)|\nabla_R\,u_{nR}(r)\rangle\cdot d\mathbf{R} \tag{13}$$

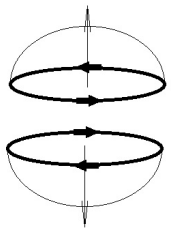
2.4 Appendix 4. Magnetic charge quantization

Let's consider the vector potential $A' = A + \nabla\Lambda$, with $\Lambda = 2q_m \arctan\frac{y}{x}$. Should we use A' instead of A, then, a phase factor $e^{i\Lambda}$ arises multiplying the wave function we derive by using A. Since the tangent y/x corresponds to an undefined angle α or $\alpha + n\pi$, with $n \in Z$ (i.e., α and $\alpha + n2\pi$ correspond to the same point), then, $e^{i\,2q_m n\pi}$ must be unity for any $n \in Z$ and, therefore, also $q_m \in Z$.

2.5 Appendix 5. The vector potential of a magnetic monopole must have singularities

Let's consider an sphere with the monopole at its center and name C to the equatorial line. Next, we compute the magnetic flux through the north cap plus that through the south cap.

$$\begin{aligned}\oiint BdS &= \iint_{D_1} BdS + \iint_{D_2} BdS \\ &= \oint_C Ad\ell + \oint_C A(-d\ell) = 0\end{aligned} \tag{14}$$



The figure shows how in either integration the equator C is travelved in the opposite direction.

The only way to have a net non-zero flux is that A had a singularity. Then, the vector potential in the equator (where we carry out the circulation) is a multi-evaluated function: we can either use $A = \frac{(-y,x,0)}{r^2}$ or $A' = \frac{(y,-x,0)}{r^2}$. As a consequence, we cannot actually use the vector potential to calculate the flux. We must employ the field instead:

$$\oiint \mathbf{B}\mathbf{d}S = \oiint q_m \frac{\mathbf{r}}{r^3}\mathbf{d}S = \int_0^{\pi}\int_0^{2\pi} q_m \sin\theta d\theta d\phi = 4\pi q_m \neq 0 \tag{15}$$

2.6 Appendix 6. Deriving equation 5

Our starting point is: $\gamma_n(C) = \oint_c i\,\langle u_{nR}(r)|\nabla_R u_{nR}(r)\rangle \cdot d\mathbf{R}$. By using Stokes theorem we may turn it into:

$$\gamma_n(C) = \iint_C i\,\nabla_R \times \langle u_{nR}(r)|\nabla_R\, u_{nR}(r)\rangle \cdot d\mathbf{S} \tag{16}$$

We should point out that $\langle u|\nabla u\rangle$ must be a pure imaginary number, due to the fact that $\langle u|u\rangle = 1$ and therefore $\nabla\langle u|u\rangle = 0$. Since $\langle\nabla u|u\rangle + \langle u|\nabla u\rangle = (a+ib) + (a+ib)^* = 2a$, we have that $a = 0$ and then, $\langle\nabla u|u\rangle = ib$. Therefore, $i\,\langle u|\nabla u\rangle = -\mathrm{Im}(\langle \mathrm{u}|\nabla \mathrm{u}\rangle)$.

Next, we calculate:

$$\nabla \times \langle u|\nabla u\rangle = \begin{bmatrix} \vec{\imath} & \vec{\jmath} & \vec{k} \\ \partial_x & \partial_y & \partial_z \\ \langle u|\partial_x u\rangle & \langle u|\partial_y u\rangle & \langle u|\partial_z u\rangle \end{bmatrix} \tag{17}$$

For example, $(\nabla \times \langle u|\nabla u\rangle)_x = \langle\partial_y u|\partial_z u\rangle - \langle\partial_z u|\partial_y u\rangle$.

Taking into account that:

$$\begin{bmatrix} \vec{\imath} & \vec{\jmath} & \vec{k} \\ \langle\partial_x u| & \langle\partial_y u| & \langle\partial_z u| \\ |\partial_x u\rangle & |\partial_y u\rangle & |\partial_z u\rangle \end{bmatrix} = \vec{\imath}(\langle\partial_y u|\partial_z u\rangle - \langle\partial_z u|\partial_y u\rangle) + \vec{\jmath}(\dots) + \vec{k}\,(\dots) \tag{18}$$

we can finally write: $\nabla \times \langle u|\nabla u\rangle = \langle\nabla u| \times |\nabla u\rangle$.

Since $\sum_v |v\rangle\langle v| = 1$ and $\langle u|\nabla u\rangle$ is a pure imaginary number, the product $\langle\nabla u|u\rangle\langle u|\nabla u\rangle$ is real (it has not imaginary component) and we can write:

$$\gamma_n(C) = -\mathrm{Im}\iint \mathrm{d}\mathbf{S}\sum_{\mathrm{m}\neq\mathrm{n}}\langle\nabla \mathrm{u_n}|\mathrm{u_m}\rangle \times \langle \mathrm{u_m}|\nabla \mathrm{u_n}\rangle, \tag{19}$$

due to the fact that $\langle\nabla u| \times |\nabla u\rangle = \sum_v\langle\nabla u|v\rangle\langle v| \times \nabla u\rangle = \sum_v\langle\nabla u|v\rangle \times \langle v|\nabla u\rangle$. We exclude the term $u = v$ as it has not an imaginary component.

On the other hand, $\nabla\hat{H}|u\rangle = \nabla(\hat{H})|u\rangle + \hat{H}|\nabla u\rangle$. Then, $\langle v|\nabla\hat{H}u\rangle = E_u\langle v|\nabla u\rangle = \langle v|\nabla(\hat{H})|u\rangle + E_v\langle v|\nabla u\rangle \rightarrow (E_u - E_v)\langle v|\nabla u\rangle = \langle v|\nabla(\hat{H})|u\rangle$. Consequently,

$$\gamma_n(C) = -\iint V_n(R)\,d\mathbf{S} \tag{20}$$

with

$$V_n(R) = \mathrm{Im}\sum_{\mathrm{m}\neq\mathrm{n}}\frac{\langle \mathrm{u_n}|\nabla_{\mathrm{R}}(\hat{\mathrm{H}})|\mathrm{u_m}\rangle\langle \mathrm{u_m}|\nabla_{\mathrm{R}}(\hat{\mathrm{H}})|\mathrm{u_n}\rangle}{(\mathrm{E_n} - \mathrm{E_m})^2} \tag{21}$$

2.7 Appendix 7

Let's first pay attention to the cross product of complex vectors.
We are interest in the case $v_1 = \langle +|\hat{\sigma}|-\rangle = (1, -i, 0)$, $v_2 = \langle -|\hat{\sigma}|+\rangle = (1, i, 0)$ and $(E_n - E_m)^2 = 4R^2$. We have:

$$\begin{aligned} v_1 \times v_2 &= [(1,0,0) - i\,(0,1,0)] \times [(1,0,0) + i\,(0,1,0)] \\ &= (1,0,0) \times (1,0,0) + (0,1,0) \times (0,1,0) - i\,(0,1,0) \times (1,0,0) + i\,(1,0,0) \times (0,1,0) \\ &= 2\,i\,(0,0,1) \end{aligned} \tag{22}$$

Then, $(F_n)_x = (F_n)_y = 0$, $\mathrm{Im(F_n)_z} = \frac{1}{2}\frac{1}{\mathrm{R^2}}$.

2.8 Appendix 8: Zero flux over the graphene first Brillouin zone

The unit vectors of the graphene direct lattice are $\mathbf{a}_1 = a(\sqrt{3}/2, -1/2)$, $\mathbf{a}_2 = a(0,1)$, with a the cell constant. Then, those of the reciprocal lattice can be calculated to be $\mathbf{b}_1 = (2\pi/a)(2/\sqrt{3}, 0)$ and $\mathbf{b}_2 = (2\pi/a)(1/\sqrt{3}, 1)$. In terms of these last vectors, the K and K' points have the following coordinates $K = (2/3)(\mathbf{b}_1 + \mathbf{b}_2)$, $K' = (1/3)(\mathbf{b}_1 + \mathbf{b}_2)$.

Should we select the energy origin at $\mathbf{k} = 0$, them, the graphene first neighbors Tight Binding Hamiltonian has zero diagonal matrix elements $H_{11} = H_{22} = 0$. The extradiagonal ones read:

$$H_{12} = H_{21}^* = \sum_R e^{i\,\mathbf{k}\cdot\mathbf{R}} \langle \chi_1 | \hat{H} | \chi_{2R} \rangle = \langle \chi_1 | \hat{H} | \chi_2 \rangle (1 + e^{i\,\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\,\mathbf{k}\cdot\mathbf{a}_2})$$

where call t to the integral $\langle \chi_1 | \hat{H} | \chi_2 \rangle$.

In the surroundings of the K point we have:

$$e^{i\,\mathbf{k}\cdot\mathbf{a}_1} = e^{i\mathbf{K}\cdot\mathbf{a}_1} e^{i\mathbf{q}\cdot\mathbf{a}_1} \approx e^{-i\,2\pi/3}(1 + i\,\mathbf{q}\cdot\mathbf{a}_1) = e^{-i\,2\pi/3}(1 + i\,q_x \frac{1}{2} a + i\,q_y a\,\frac{\sqrt{3}}{2})$$

The last replacement is made under the assumption of representing vector $\mathbf{q}$ on a specific Cartesian coordinate system: since $\mathbf{a}_1$ and $\mathbf{a}_2$ are unit but non-orthogonal vectors, we choose axis x along the unit vector resulting of the sum $\hat{x} = \mathbf{a}_1 + \mathbf{a}_2 = (\sqrt{3}/2, 1/2)$. The y axis is selected along the vector resulting from the subtraction $\mathbf{a}_1 - \mathbf{a}_2 = (\sqrt{3}/2, -3/2)$. This subtraction vector has not unity norm and then we normalize it: $\hat{y} = (1/2, -\sqrt{3}/2)$. Next, we write $\mathbf{q} = q_x\hat{x} + q_y\hat{y}$.

In a similar way, we calculate $e^{i\,\mathbf{k}\cdot\mathbf{a}_2}$, that allows to write $H_{12} = \frac{\sqrt{3}at}{2}(q_x - i\,q_y) = \hbar\,v_F\,q_-$.

The same procedure yields $H'_{12} = -\frac{\sqrt{3}at}{2}(q_x + i\,q_y) = -\hbar\,v_F\,q_+$ in the K' surroundings.

Therefore, in the surroundings of K,

$$H = \hbar v_f \begin{pmatrix} 0 & q_- \\ q_+ & 0 \end{pmatrix} = v_f \begin{pmatrix} 0 & k_- \\ k_+ & 0 \end{pmatrix} = v_f\,k \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \tag{23}$$

with eigenvectors $v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix}$, $v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-i\phi} \\ 1 \end{pmatrix}$.

In the surroundings of K' we have:

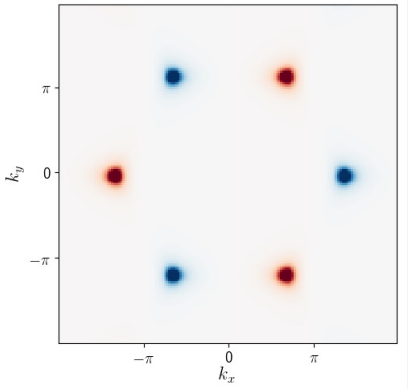
$$H' = -v_f\,k \begin{pmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{pmatrix} \tag{24}$$

with eigenvectors $v'_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi} \\ 1 \end{pmatrix}$, $v'_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{i\phi} \\ 1 \end{pmatrix}$.

By using polar coordinates, $\nabla = (\partial_k, \frac{1}{k}\partial_\phi)$, so that Berry's connexion in the surroundings of K results: $\mathbf{A}_k = -i\,\langle v_1 | \partial_k | v_1 \rangle = 0$, $\mathbf{A}_\phi = -\frac{i}{k}\,\langle v_1 | \partial_\phi | v_1 \rangle = -\frac{1}{2k}$. In the K' surroundings we find out $\mathbf{A}'_k = 0$, $\mathbf{A}'_\phi = \frac{1}{2k}$.

The respective curvatures $\mathbf{F} = \nabla \times \mathbf{A} = (\partial_k \mathbf{A}_\phi - \frac{1}{k}\partial_\phi \mathbf{A}_k)$ result $\mathbf{F} = \frac{1}{2k^2}$ i $\mathbf{F}' = -\frac{1}{2k^2}$. As a consequence, $\int_{1BZ} \mathbf{F} d\mathbf{k} = 0$.

In the figure we show the curvature in the graphene reciprocal lattice unit cell (first Brillouin zone). We can see that it only has an appreciable value around the points K, where it is positive ($\frac{1}{2k^2}$), and K', where it is negative ($-\frac{1}{2k^2}$).



References

[1] M. V. Berry, Proc. R. Soc. Lond. A 392 (1984) 45.

[2] F. D. M. Haldane, Phys. Rev. Lett., 61 (1988) 2015

[3] J. Li, I. Martin, M. Büttiker and A.F. Morpurgo, Phys. Scr. T146 (2012) 014021