BERRY PHASE & TOPOLOGY

Another look.

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Adiabatic evolution and Geometry of Hilber Space

Remember to explore geometry of Hilber space we need to move inside it. Linear algebra is easy but the extra twist comes from COMPLEX NATURE of H.S.
Lets move in the H.S by following a porticular eigenstate but very slowly or adiabatically.

e.g. $\bar{R}(t)$ can be $\bar{P}(t)$

Consider a hamiltonian $H(t) = H(\bar{R}(t))$ $\bar{R} = (R_1, \ldots R_D)$ a set of parameters.
we can think of $\bar{R}$ as a vector in in the D-dim space. No relation to real space!

For each $\bar{R}$ we have a set of eigenstates of $H(\bar{R})$:

$$H(\bar{R}) |n(\bar{R})\rangle = \epsilon_n(\bar{R}) |n(\bar{R})\rangle$$

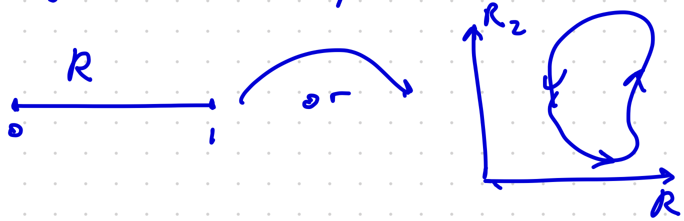
For simplicity, let's also assume ϵ_n is descrete and non-degenerate

The <u>adiabatic theorem</u> tells us:

if it $\rightarrow |\psi_n(t=0)\rangle = |n[\bar{R}(t=0)]\rangle$
initially
in the n^{th} eigenstate it will remain in the n^{th} state as long as the system evolves very slowly in time.

$$|\psi_n(t)\rangle = C_n(t)\,|n[\tilde{R}(t)]\rangle$$

So the path in the parameter space can define the path in the hilbert space.



Since time evolution is a unitary transformation $C_n(t)$ should be a pure phase $\quad U^\dagger U = 1$

e.g. $C_n(t) = e^{i E_n t/\hbar}$

or if H depends on $t \Rightarrow$

$$C_n = \underbrace{e^{i\gamma_n(t)}}\; e^{-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'}$$

this phase will turn out to be <u>very important</u>, it accounts for some extra aspects not captured by the 2^d factor.

After that we plugging it into

$$i\hbar \frac{\partial}{\partial t}|\psi_n(t)\rangle = H(\bar{R}(t))\,|\psi_n(t)\rangle$$

$$\langle \psi_n(t)|x| \quad i\hbar \frac{\partial}{\partial t}\left(e^{i\gamma_n(t)} e^{-i/\hbar \int_0^t dt' \epsilon_n(t')} \right)|n\rangle$$

$$= H e^{i\gamma_n(t)} e^{-i/\hbar \cdots} |n\rangle \implies$$

$$\frac{\partial}{\partial t}\gamma_n(t) = i\langle n(R(t))|\frac{\partial}{\partial t}|n(R(t))\rangle$$

$$\text{or} \quad \gamma_n(t) = i\int_0^t dt' \langle n(\bar{R}(t'))|\frac{\partial}{\partial t'}|n(R(t'))\rangle$$

Problem 1*

Can you show this?! →

$$\boxed{\equiv \oint_C \vec{A}^n(R)\cdot d\bar{R}}$$

where $\bar{A}^n(R) = i\langle n(R)|\frac{\partial}{\partial R}|n(R)\rangle$ is called the <u>Berry connection</u>

This factor also known as a <u>geometric phase</u> which depends only on the path C and not on dynamics. e.g. consider you drive home from Rutgers and watch odometer. The final number is <u>independent</u> of how <u>fast</u> you drive but <u>depends on the route</u> you select.

Problem 2*: Show that if $\langle n(\bar{R})|n(\bar{R})\rangle = 1$ and $\frac{\partial}{\partial \bar{R}}\langle n(\bar{R})|n(\bar{R})\rangle = 0$, $\bar{A}^n(R)$ and γ_n are REAL.

Also we need to emphasize that γ_n is Gauge independent:

a new gauge

$$|n(R)\rangle = e^{i\xi(R)}\,|n(R)\rangle \Rightarrow$$

$$A^n(R) = i\langle n(R)|\frac{\partial}{\partial R}|n(R)\rangle = i\langle n(R)|\,e^{-i\xi(R)}\frac{\partial}{\partial R}e^{i\xi(R)}\,|n(R)\rangle = \overset{-1}{\cancel{i}}\,\langle n(R)|\,\cancel{e^{-i\xi}}\,i\,\cancel{e^{i\xi}}\,\frac{\partial\xi}{\partial R}|n\rangle$$

$$+\; i\langle n|\,\cancel{e^{-i\xi}}\,\cancel{e^{i\xi}}\,\frac{\partial}{\partial R}|n(R)\rangle = -\langle n|\frac{\partial\xi}{\partial R}|n\rangle$$

$$+\;\underbrace{i\langle n|\frac{\partial}{\partial R}|n\rangle}_{A(R)} = A(R) - \frac{\partial}{\partial R}\xi(R)$$

real $A(R) = i\langle n|\frac{\partial}{\partial R}|n\rangle$

$$\Rightarrow \gamma_n \longrightarrow \gamma_n + \xi(\bar{R}(t=0)) - \xi(\bar{R}(t))$$

$$\gamma_n = \int_0^t \dots$$

So we think that γ can be always gauged away

but ....

If we move in a close loop something new will happen: $R(t=0) = R(t=t_{final})$

$$\Rightarrow H(t_0) = H(t_{final})$$

In this case $\xi(t_0) - \xi(t_{final}) = 0$

and $\gamma_n = \oint \bar{A}^n(R)\cdot d\bar{R}$ is gauge independent

and known as Berry phase

It also looks like a vector $\bar{A}^n(R)$ potential in E & M

$$\oint \bar{A}^n \cdot dR =$$

"magnetic flux" in the parameter space

It also means we can introduce a local field $\omega^n_{\mu\nu}(R)$ which is called Berry curvature:

$$\boxed{\omega_{\mu\nu}(R) = \partial_{R_\mu} A^n_\nu(R) - \partial_{R_\nu} A^n_\mu(R)}$$

$(\nabla \times A)$ this is anti-symmetric tensor of rank-2

similar to $F_{\mu\nu}$ in E & M

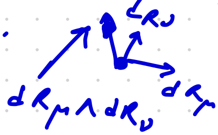
Let's use Stoke's theorem $\oint \bar{F} \cdot dR = \oiint_S \nabla \times F \cdot dS$

$$\gamma_n = \oint \bar{A}^n(R) \cdot dR = \frac{1}{2} \oiint dR_\mu \wedge dR_\nu \, \omega^n_{\mu\nu}(R)$$

this is to avoid double summation

Diff. geometry $dR_\mu \wedge dR_\nu$

a surface are of a parallelogram formed by 2 vectors multiplied.



$dR_\mu \wedge dR_\nu = -dR_\nu \wedge dR_\mu$

Also, in 3D b/c $\omega_{\mu\nu}$ is the rank-2 anti-symmetric tensor

it can be represented by the 3 componets, as a result we can write it as

Read Levi-Civita in Wikipedia!

$$b^\delta = \frac{1}{2} \epsilon^{\delta\mu\nu} \omega_{\mu\nu}$$

ϵ (is Levi-Civita) symbol

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Or $\bar{b}^n = \nabla_R \times \bar{A}^n = i \langle \nabla_R n(R) | \times | \nabla_R n(R) \rangle$

$A^n(R) = i \langle n(R) | \frac{\partial}{\partial R} | n(R) \rangle$ ∇_R

and by analogy to the vector potential in EM

$$\boxed{\gamma_n = \oiint_S \bar{b}^n \cdot ds}$$

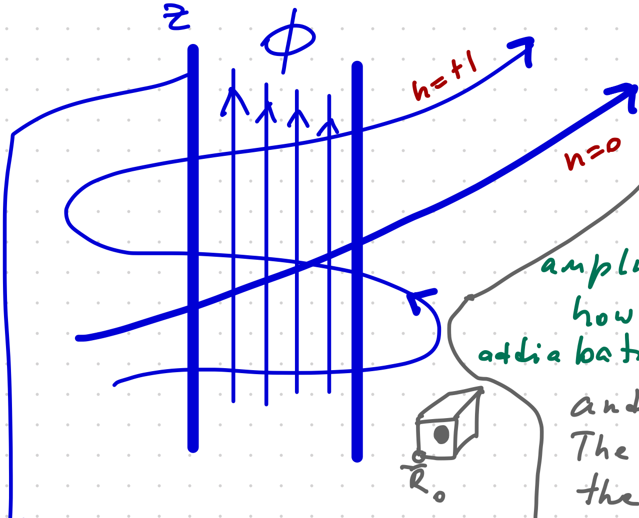
Problem 3: Show that from $\omega^n_{\mu\nu} = \partial_{R_\mu} A_\nu(R) - \partial_{R_\nu} A^n_\mu(R) \Rightarrow$

$$\omega^n_{\mu\nu} = i \left[\langle \partial R_\mu n(R) | \partial_{R_\nu} n(R) \rangle - \langle \partial_{R_\nu} n(\bar{R}) | \partial_{R_\mu} n(R) \rangle \right]$$

Thus the Berry phase is $\equiv$ Aharonov - Bohm phase

The origin of the Berry phase is the physical magnetic flux confined in the physical flux tube

Berry phase & Aharonov - Bohm effect.



Comment for Fig:
Since each line has different length they will have different amplitudes. You may wonder how can we transport electron adiabatically? Place in in the box and turn the corner adiabat. The finite size provides the gap to preserve the adiabatic transport

barrier
no charge particle enters the cylindr $\rightarrow$ no Lorents force!
no effect on particle motion in classical mechanics

but even though $\Phi = 0$ outside of the cylender, $\bar{A}$ is not

$\bar{\nabla} \times \bar{A} = 0$ is everywhere so we can ignore it but

if we move along a close loop which winds around the tube

$$\oint d\bar{r} \cdot A(r) = n\,\Phi$$

TOPOLOGICAL invariant

Global effect:
One way to see it is to consider a Feynman path int:

$$e^{\frac{i}{\hbar} S(\bar{r})} \quad \text{where} \quad S(r) = \int_0^t dt\, \mathcal{L}(\dot{r}, r)$$

$\mathcal{L}$ Lagrangian

in the presence of vector potential

$$\mathcal{L} \rightarrow \mathcal{L} + (-e)\, A(\bar{r}) \cdot \dot{r}$$

Thus $S = \int_0^t d\tau\, \mathcal{L} + (-e)\int A(r)\cdot \frac{dr}{\cancel{d\tau}}\,\cancel{d\tau} \rightarrow$

$$e^{i\theta} = e^{\frac{i(-e)}{\hbar}\int d\bar{r}\cdot A(\bar{r})}$$

which is for closed loop $= n\Phi$ is the topological invariant.

Next we want to show that adiabatic moving of the e^- around the tube gets a <u>Berry phase $\equiv$ Aharonov-Bohm phase</u>

$$\text{i.e.}\quad \theta = \frac{i(-e)}{\hbar}\oint dr\cdot A(r) = -n\, 2\pi\, \Phi/\Phi_0$$

Φ_0 is the flux quantum =

$\Phi_0 = 2.067\cdot 10^{-15}\,\mathrm{Wb}$

To do adiabatic transport we place e^- into a finite size cage (i.e. H should have excitation gap)

$$H = \frac{1}{2m_e}\left(\bar{p} + \frac{e}{c}A(r)\right)^2 + V(r-\bar{R}_0)$$

any strongly confining potential will work.

Also we assume that $\nabla\times A = 0$

$$\bar{A}(\bar{r}) = \frac{\Phi}{2\pi}\nabla\chi(r) \quad \text{with} \quad \oint dr\,\bar{A} = \frac{\Phi_0}{2\pi}\oint dr\cdot\nabla\chi(r) = n\Phi$$

one of the possible choices for $\chi(r) = \frac{\Phi}{\Phi_0}\varphi(r)$

Let us assume that our system is in the ground state described by $\xi_0(r-\bar{R}_0)$ when $\bar{A}=0$ but in the presence of the flux the solution becomes:

$$\psi(\bar{r}) = e^{-i\chi_{R_0}(r)}\,\xi_0(\bar{r}-\bar{R}_0)$$

here is before $\chi_{R_0}(r) \equiv \frac{2\pi}{\Phi_0}\int_{R_0}^{r} dr'\cdot A(r')$

Note, here we evaluate the integral in some path inside the box.

Since $\nabla\times A$ (outside the box) $=0$

$\chi(r)$ is defined insite the box.

R_0

Since $\psi(r)$ is global gauge invariant i.e. $\psi\to\psi e^{i\theta}$

Also θ can be a function of R_0 but not r.

Different choices of $\theta(R_0)$ correspond gauge for Berry connection in the parameter space.

A different choice of $\chi_{R_0}(\bar{r})$ corresponds to different electromagnetic gauge.

Now we choose the gauge as such $\psi(R_0+\bar{\Delta})$ is real, $\xi_0(\Delta)>0$ some point inside the box

$$\psi(\bar{r}) = e^{i\theta(R_0)}\, e^{-i\chi_{R_0}(r)}\,\xi_0(\bar{r}-\bar{R}_0)$$

to fulfill this we simply can take

$$i\theta(\bar{R}_0) = +\,i\chi_{\bar{R}_0}(\bar{r}+\bar{\Delta})$$

Using $\nabla_{\bar{R}_0}\theta(R_0) = \nabla_{R_0}\chi_{R_0}(\bar{R}_0+\bar{\Delta}) = \frac{2\pi}{\Phi_0}\left[A(R_0+\Delta)-A(R_0)\right]$

$A(r) = \frac{\Phi_0}{2\pi}\nabla\chi(r)$

We find that Berry connection

$$\bar{A}(R_0) = i\langle\psi|\nabla_{R_0}|\psi\rangle =$$

$$= i\langle\psi|\nabla_{R_0}|\psi\rangle = i\left\{ e^{-i\theta} e^{+i\chi_0} \underset{\hat{\ }\text{real function}}{\xi_0(r-R_0)}\, \nabla_{R_0} e^{+i\theta} e^{-i\chi_0} \xi_0(r-R_0)\right\} =$$

$$= \cancel{e^{-i\theta}}\,\cancel{e^{i\chi_0}}\,\xi_0\,(i)\,\cancel{e^{i\theta}}\,\nabla\theta\,\cancel{e^{-i\chi_0}}\,\xi_0 \quad +$$

$$\cancel{e^{-i\theta}}\,\cancel{e^{i\chi_0}}\,\xi_0\,\cancel{e^{i\theta}}\,(-i)\,\cancel{e^{-i\chi_0}}\,\nabla\chi_0\,\xi_0 \quad +$$

$$\cancel{e^{-i\theta}}\,\cancel{e^{i\chi_0}}\,\xi_0\,\cancel{e^{i\theta}}\,\cancel{e^{-i\chi_0}}\,\nabla\xi_0$$

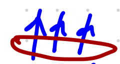
$$= \underbrace{i^2}_{-1}\,\overset{=1}{\xi_0^2}\,\nabla\theta \;+\; \underbrace{i(-i)}_{+1}\,\overset{=1}{\xi_0^2}\,\underbrace{\nabla\chi_0}_{=A\cdot\frac{\Phi_0}{2\pi}} \;+\; i\xi_0\nabla\xi_0$$

$$\uparrow$$

$$-\frac{2\pi}{\Phi_0}\left[\bar{A}(\bar{R}_0+\bar{\Delta}) - \bar{A}(\bar{R}_0)\right] + i\int d\bar{r}^3\, \xi_0(\bar{r}-\bar{R}_0)\nabla_{R_0}\xi_0(\bar{r}-\bar{R}_0) = -\frac{2\pi}{\Phi_0}\bar{A}(R_0+\Delta) + \frac{i}{2}\underbrace{\int dr^3\, \nabla_r\, \xi_0^2(r-R_0)}_{=0 \text{ at the boundary of the box}}$$

$$= -\frac{2\pi}{\Phi_0}\bar{A}(R_0+\Delta)$$

Lets slowly vary $\bar{R}_0$ in a loop such that $R_0+\Delta$ makes a circle around the



flux tube with winding number +1

$$\gamma = \oint d\bar{R}_0\cdot A(R_0) = -\frac{2\pi}{\Phi_0}\underbrace{\oint d\bar{R}_0\cdot\bar{A}(R_0+\Delta)}_{\Phi_{flux}}$$

$$= \underset{\substack{\uparrow\\ \text{negative charge}}}{-}\frac{2\pi}{\Phi_0}\Phi$$

Berry phase in graphene

Cond-mat manuscript 1309.6714

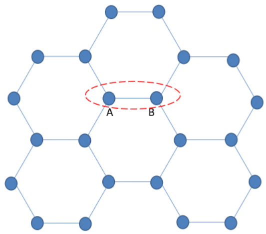


FIG. 1. Crystal structure of graphene.

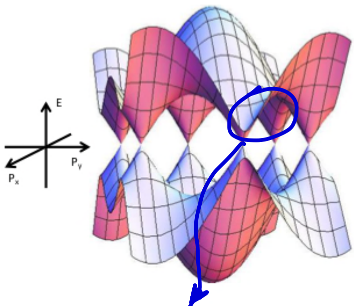
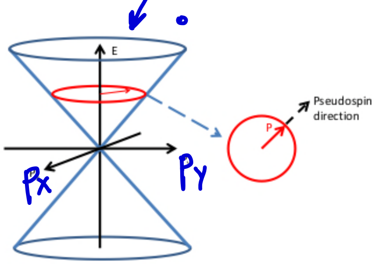


FIG. 2. Band structure of graphene.



Tight-Binding hamiltonian:

$$H = v\begin{pmatrix} \underset{=\varepsilon_A}{0} & p_x - ip_y \\ p_x + ip_y & \underset{=\varepsilon_B}{0}\end{pmatrix}, \quad v \cong 10^6\ \frac{m}{s}$$

crystal momentum near $k \approx 0$

on-site energy

hopping from $A \to B$

$$H\psi = E\psi \qquad \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = E\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \to$$

$$\begin{Bmatrix} + \text{ conduction} \\ - \text{ valence} \end{Bmatrix} \qquad E = \pm v p \quad \text{and}$$

$$\psi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm e^{i\varphi}\end{pmatrix} e^{i\vec{p}\cdot\vec{r}/\hbar}$$

$$p = p_x \cos\varphi \qquad p = p_x \sin\varphi$$

this vector is called pseudospin

Let's calculate Berry phase.

Here we have p as a parameter changing adiabatically accross the circle. To force p into the circle:

Generally, to force the motion of p we apply B, perpendicular to the graphene phane.

Let's rewrite the eigenstate ψ in the symmetric gauge:

$$\psi = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi/2} \\ \pm e^{i\phi/2} \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}.$$

full circle $\varphi \to 2\pi$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\pi} \\ \pm e^{i\pi} \end{pmatrix} e^{ip\cdot r/\hbar} =$$

$$= \frac{1}{\sqrt{2}} \underbrace{e^{i\pi}}_{=-1} \begin{pmatrix} \overbrace{e^{-2\pi i}}^{=1} \\ \pm 1 \end{pmatrix} e^{ip\cdot r/\hbar} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mp 1 \end{pmatrix} e^{ip\cdot r}$$

Lets calculate B.P.

$$\theta = -i \oint_C \langle\psi(\mathbf{p}(t))|\frac{\partial}{\partial t}|\psi(\mathbf{p}(t))\rangle dt.$$

$$\theta = -i \oint_C dt[\frac{1}{2}\begin{pmatrix}1, & e^{-i\phi}\end{pmatrix}\begin{pmatrix} 0 \\ i\frac{\partial\phi}{\partial t}e^{i\phi}\end{pmatrix} + \underbrace{i\frac{\partial \mathbf{p}}{\partial t}\cdot\mathbf{r}/\hbar}_{0} + \underbrace{i\mathbf{p}\cdot\frac{\partial \mathbf{r}}{\partial t}/\hbar}_{0}].$$

b/c of the integration over the close loop

$$\theta = \oint_C dt(\partial\phi/\partial t)/2 = \pi.$$

But if we use

$$\psi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{i\phi} \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar},$$

We can also calculate B.P. from the pseudospin pov.

From:

$$H = v(p_x\sigma_x + p_y\sigma_y),$$ we can write down the direction of the pseudospin vector as

Problem: Show

$$\langle\psi|\sigma_x|\psi\rangle = \cos\phi, \quad \langle\psi|\sigma_y|\psi\rangle = \sin\phi \quad \text{and} \quad \langle\psi|\sigma_z|\psi\rangle = 0.$$

this by using symmetric gage ψ and the definition of $\vec{\sigma}$

So clearly $\vec{p}$ is in the x-y plane (see Fig in p.11)

we also know that rotation of the spin by angle ϕ given by this operator

$$e^{-i\phi S_z/\hbar} = e^{-i\phi\sigma_z/2}.$$

when rotated by 2π is equavalent of given a 'sign' (-1) which is the same as $e^{i\pi} = -1$, or rotation by the π phase.

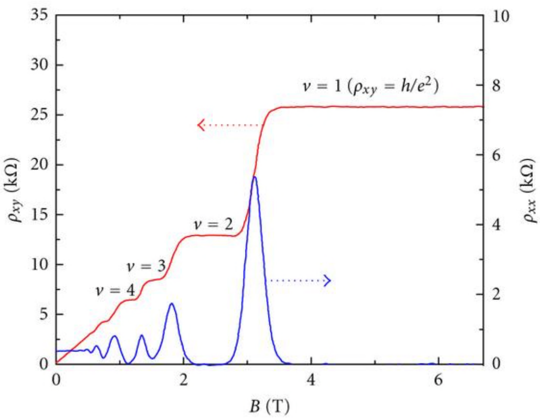
CONNECTION to quantum Hall in graphene

Connection between B.P. and IQHE.

Going back to our starting discussion on IQHE. We concluded that

$E_n = \hbar\omega_c(\underline{\underline{n}} + 1/2)$

and $E = 1/2\,\hbar\omega_c$ is the "0" point energy



<u>But</u> in graphene

$E_n = \sigma\sqrt{2eB\hbar\,\underline{\underline{n}}}$

without the "0" p. energy

Let me demonstrate that it's a direct consequence of the B.P. = π

Let's try to derive the Landau level semiclassically following Onsager.

When electron is in the mag. field any orbit radius is allowed. But Bohr-Sommerfeld rule tells us it must satisfy $\oint d\bar{r}\cdot\bar{p} = 2\pi n\cdot\hbar$

$n = 1, 2, 3 \dots$

For an electron in the magnetic field

$\bar{p} = \hbar\bar{k} - e\bar{A} \Rightarrow$

$\oint (\hbar\bar{k} - e\bar{A})\cdot r\,dr = 2\pi n\hbar \Rightarrow (\hbar\oint dr\cdot k - e\oint dr\cdot A)/\hbar = 2\pi n$

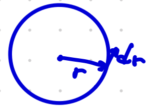
recall $\hbar \dot{k} = -e\dot{r} \times B \Rightarrow \hbar k = -e r \times B +$ + const

"Lorentz force"

from this we can write down:

1st term: $\left(\underbrace{\oint dr \cdot (-e r \times B)} - e \oint dr \cdot A \right) / \hbar = 2\pi n$

$= -eB \oint dr \times r = 2e\Phi$ — flux of the orbit under B



it's from $a \cdot (b \times c) = (a \times b) \cdot c$

2d term: $-e \oint dr \cdot A \overset{\text{Stock's theorem}}{=} -e \oiint ds \cdot \nabla \times A = -e\Phi$, all together

$\left(2e\Phi - e\Phi\right)/\hbar = 2\pi n$

$\dfrac{e\Phi}{\hbar} = 2\pi n \Rightarrow \boxed{\Phi = nh/e} = n\Phi_0$

note, this cond. is in real space

Φ_0 — flux quantum

Few notes:

1) By the way in Bohr - Sommerfeld quantization there is no zero energy term so we include it by artificially adding it like this

$$\left(\hbar \int dr \cdot k - e \int dr \cdot A\right)/\hbar = 2\pi\left(n + \frac{1}{2}\right)$$

$\frac{1}{2}$ — this is so called Maslov index

and it captures how the fully quantum mech. behavior.

2) Free 2D electron gas with the dispersion $E = \frac{p^2}{2m}$ moves along a circle with $\omega_c = \frac{eB}{mc}$ (Larmor radius)

Since the energy is a motion integral in the momentum space the trajectory $p = \sqrt{2mE}$

In the momentum space we can write

$$\frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \hbar\omega_c = \hbar\frac{eB}{c} \Rightarrow$$

$$\pi k^2 = \frac{2\pi eB}{\hbar}$$

Consider the same quantization for graphene As momentum of an electron is forced into a loop in addition to

$\oint dr\cdot k$ and $e\int dr\cdot A/\hbar$ we

have $\underbrace{B.P. = \pi}$ or

$$\left(\hbar\oint dr\cdot k - e\oint d\bar{r}\cdot A\right)/\hbar + \pi = 2\pi\left(n+1/2\right)$$

cancels the Maslov index!

So since $B.P. = \pi$ kills $2\pi\cdot 1/2 = \pi$

we ended up withe the same condition

$\pi k^2 = 2\pi neB/\hbar$

Since the dispersion for Dirac electrons is

$\underline{E = v\hbar k}$ we get

$\hbar k = \sqrt{2neB\hbar}$ and

$$E = v\cdot\sqrt{2eB\hbar n}$$

From this we can conclude in graphene <u>the absence</u> of the zero Landau level is the consequence of the Berry phase π!

THE END