Lecture 9 part II

Topological Quantum Mechanics

Q. Why some insulators are interesting
e.g. QHE and the other are trivial
e.g. a piece of plastic?

Consider, QHE: ① $\sigma_{xy} \sim \hbar$. So quantum is important.
② Transport is a motion of charge. In QM charge is related to a conjugate variable of charge.
i.e. like p is conjugate of z.
Invariant under $\phi \to \phi + \delta\phi$ implies the conservation of charge. So perhaps phase of the wave function is the key. Focus on phase. First, is phase of any importance?
A: relative yes, absolute no. ⇒ i.e:
$|\psi\rangle \to |\psi'\rangle = e^{i\varphi}|\psi\rangle \Rightarrow \langle\psi|A|\psi\rangle = \langle\psi'|A|\psi'\rangle$

However, $|\psi\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_2\rangle \Rightarrow$

$$\langle\psi|P|\psi\rangle = \frac{\overbrace{\langle\psi_1|P|\psi_1\rangle}^{}_{\bar{P}\text{ in }\psi_1} + \underbrace{\langle\psi_2|P|\psi_2\rangle}_{\bar{P}\text{ in }\psi_2}}{2} + \frac{\langle\psi_1|P|\psi_2\rangle + \text{conj}}{2}$$

The physical meaning of ← is in the interference

$|\psi'\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{e^{i\varphi}}{\sqrt{2}}|\psi_2\rangle \Rightarrow$

$$\langle\psi'|p|\psi'\rangle = \frac{\langle\psi_1|p|\psi_1\rangle + \langle\psi_2|P|\psi_2\rangle}{\sqrt{2}} + \frac{e^{i\varphi}\langle\psi_1|P|\psi_2\rangle + e^{-i\varphi}\langle\psi_2|P|\psi_1\rangle}{2} =$$

$$= \ldots + \cos\varphi\,\frac{\langle\psi_1|P|\psi_2\rangle + \langle\psi_2|P|\psi_1\rangle}{2}$$

↑ this can be measured!
AND VERY IMPORTANT

~~CENTRAL CHARGE AND QUANTUM GROUP~~

Common use of the phase is in condensed matter.
Phase of Bloch waves: Consider a particle moving in a periodic potential.

$$\left[-\frac{1}{2m}\nabla^2 + V(r)\right]\psi(r) = \epsilon\,\psi(r) \qquad \text{where } V(\bar{r}) = V(\bar{r}+\bar{a})$$

The eigenfunctions of this equations:

$$\psi_{n,k} = U_{n,k}(r)\,e^{ikr} \quad \leftarrow \text{Bloch wave functions}$$

Now what is the phase of the Bloch ~~wafes~~ wave:

As usual in QM, doesn't matter, as it's invariant under <u>global</u> shift in the momentum space.

$\psi_{n,k}(r) = u_{n,k}(r)\, e^{ikr}$ $\quad \psi'_{n,k}(r) = e^{i\varphi}\, u_{n,k}(r)\, e^{ikr}$

is the same.

What's interesting it is also invariant under <u>local</u> shift:

$\psi'_{n,k}(r) = e^{i\varphi(k)}\, u_{n,k}(r)\, e^{ikr}$. Which means that there is no mixing of waves with different k. as time goes on and on.

<u>Let's focus on local phase symmetry:</u>

Lets briefly rewew the concept of gage in real space and then we will switch to the momentum space.

$$i\frac{\partial}{\partial t}\psi(r,t) = -\frac{\nabla^2}{2m}\psi(r,t) + V(r)\psi(r,t) \leftarrow \psi' \equiv e^{i\varphi}\psi(r)$$

$\psi'(r)$ will follow exactly the same equation as $\psi(r)$. And we say the system is <u>invariant under global phase shift.</u> or global phase symmetry.

Remember, each symmetry implies the conservation of something.

e. g. $x \to x+a$ implies $-i\frac{\partial}{\partial x}$ conserved.

so here for $U(1)$ phase symmetry we expect

$-i\frac{\partial}{\partial\varphi}$ is conserved.

Now we switch to the Local $U(1)$ phase symmetry.

i.e $\varphi(r)$ $\quad \psi(r,t) = e^{i\varphi(r,t)}\psi(r,t)$

is Sch. eq. still invariant? NO.

$\frac{\partial}{\partial t} e^{i\varphi} \neq e^{i\varphi}\frac{\partial}{\partial t}$ and $\nabla e^{i\varphi} \neq e^{i\varphi}\nabla$.

But can we make the equation invariant?

Yes if we introduce some "charge particle" trick.

Lets recall the problem of motion of a chaged particle e. We change its $\bar{p} \to \bar{p} + e\bar{A}/c$ and change $\frac{i\partial}{\partial t} \to \frac{i\partial}{\partial t} - e\bar{\Phi}$

$$(i\hbar \frac{\partial}{\partial t} - e\bar{\Phi})\,\psi(r,t) = \left[\frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}A\right)^2\right]\psi(r,t) + V(r)\,\psi(r,t)$$

$$\left(i\hbar\frac{\partial}{\partial t} - e\bar{\Phi} + \hbar\frac{\partial\phi(r,t)}{\partial t}\right)\psi'(r,t) = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}A - \hbar\nabla\phi(r,t)\right)^2\psi(r,t) + V(r)\,\psi(r,t)$$ if we ~~define~~ define

$$\bar{\Phi}' = \bar{\Phi} - \frac{\hbar}{e}\frac{\partial\varphi(r,t)}{\partial t} \quad \text{and} \quad A' = A + \frac{c\hbar}{e}\frac{\partial\phi(r,t)}{\partial r}$$

we get: $$\left(i\hbar\frac{\partial}{\partial t} - e\bar{\Phi}'\right)\psi'(r,t) = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}A'\right)^2\psi(r,t) + V(r)\,\psi(r,t)$$

The change of $\boxed{\begin{array}{l}\bar{\Phi}' \to \bar{\Phi} - \frac{\hbar}{c}\frac{\partial\varphi(r,t)}{\partial t} \\ A' \to A + \frac{c\hbar}{e}\frac{\partial\varphi}{\partial r}\end{array}}$ and

is called the gage transformation, and it keeps physics $\bar{E}$ and $\bar{B}$ the same. More popular way to write it is to absorb $\frac{c\hbar}{e}$ into φ:

$$\boxed{\bar{\Phi} \to \bar{\Phi}' = \bar{\Phi} - \frac{1}{c}\frac{\partial\varphi}{\partial t} \qquad \begin{array}{l} A \to A' = A + \nabla\varphi(r,t) \\ \psi(r,t) \to \psi' = \psi(r,t)\,e^{i\frac{e}{c\hbar}\varphi(r,t)}\end{array}}$$

The local phase invariance is related to the ~~field~~ gage field.

Berry connection and Berry curvature

Lets introduce the Berry connection

$$\bar{A}_n = -i\langle U_{n,k}|\nabla_k|U_{n,k}\rangle$$

As you can immidiatelly see this is a quage field in the momentum space, very similar to the vector potential.

$|U_{n,k}\rangle \to e^{i\varphi_n(k)}|U_{n,k}\rangle$ to make the Bloch f. to be local phase invariant we need to do this:

$$A_n \to A_n' = -i\langle U_{n,k}|e^{-i\varphi_n(k)}\nabla_k e^{i\varphi_n(k)}|U_{n,k}\rangle =$$

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$$|u_{n,k}\rangle \to e^{i\varphi_n(k)}\,|u_{n,k}\rangle$$

$$A_n \to A_n' = -i\,\langle u_{nk}|\,e^{-i\varphi_n(k)}\,\nabla_k\,e^{i\varphi_n(k)}\,|u_{nk}\rangle$$

$$= \underbrace{-i\,\langle u_{nk}|\nabla_k|u_{nk}\rangle}_{=A_n} + \nabla_k\varphi_n(k)\,\langle u_{nk}|u_{nk}\rangle =$$

$$= A_n + \nabla_k\varphi_n(k)$$

So the Berry connection changes like a gage field in the <u>k-space</u>.

<u>BERRY CURVATURE</u>

~~Recall B phase is not observed~~

Recall A is not observable as its value depends on the choice of a gage.

The quantity with a physical meaning is a curl of it, which is a magnetic field B.

$\underline{F_n} = \nabla_k \times A_n = -i\,\epsilon_{ik}\,\partial_{k_i}\langle u_{nk}|\partial_{k_i}|u_{nk}\rangle = \underline{-i\,\epsilon_{ij}\,\langle \partial_{k_i} u_{nk}|\partial_{k_j} u_{nk}\rangle}$. This value of F_n ~~are~~ is known as BERRY CURVATURE which is observable.

POSITION OPERATOR IN LATTICE.

Without lattice: $p = -i\hbar\nabla$ and $r = i\hbar\nabla_p$

what about lattice?

One can prove that for the Bloch waves

$$r = i\partial_k\delta_{n,m} - A_{m,n}$$

where m and n are the Band indices and

$$A_{m,n} = -i\,\langle u_{m,k}|\nabla_k|u_{nk}\rangle$$

Note if $m=n$ it turns into the Berry connection.

if separation between bands large we can zoom in to one band and ignore many other.

$$\begin{cases} r = i\partial_k - A_n \\ p = -i\partial_r - \frac{e}{c}A \end{cases}$$

, comparing to the momentum of a charge e

For Bloch waves the conjugate require the gauge field. Berry connection is such a field.

Berry curvature and the Hall effect.

see Haldane, Phys. Rev. Lett. 93, 206602 (2004)

In the presence of E and B

$$\frac{dp}{dt} = F = eE + ev\times B$$

$$\frac{dr}{dt} = \nabla_p \epsilon(p) + \frac{dp}{dt}\times[\nabla_p \times A(p)]$$

$$\frac{dr}{dt} = \nabla_p \epsilon(p) + (eE + ev\times B)\times[\nabla_p\times A(p)]$$

next I will replace p by k $p=\hbar k$

$$\frac{dr}{dt} = \frac{1}{\hbar}\{\nabla_k \epsilon(k) + (eE + ev\times B)\times[\nabla_k \times A(k)]\}$$

Recall $\nabla_k \times A(k) = F(k)\bar{e}_z$ where $\bar{e}_z$ is along z.

$$\frac{dr}{dt} = \frac{1}{\hbar}\{\nabla_k \epsilon(k) + (eE + ev\times B)\times[\nabla_k\times A(k)]\} = \frac{1}{\hbar}[\nabla_k \epsilon(k) +$$
$$+ (eE\times e_z + ev\times B\times e_z)F(k)]$$

If all electrons have the same velocity: $j = env = \frac{eNv}{A}$

But in reality for particles with different k velocities are different so $Nv = \sum_{n,k} v_{n,k}$ ← all occupied states.

$$j = \frac{e}{A}\sum v_{n,k} = \frac{e}{A}\sum_{n,k}\frac{dr}{dt} = \frac{e}{A}\sum_{n,k}\frac{1}{\hbar}[\nabla_k \epsilon_n(k) +$$
$$(e\bar{E}\times e_z + ev\times B\times e_z)F_n(k)]$$

The Hall effect comes from $eE\times e_z$ as it's the only term which generates $v \perp E$. And we can ignore all other terms, when we compute Hall conductivity. For Hall current $\perp E$

$$j_H = \frac{e}{A}\sum_{n,k}\frac{1}{\hbar} eE\times e_z F_n(k) = e^2 E\times e_z \frac{1}{A}\sum_{nk} F_n(k)$$

~~For totaly field bands~~

$$\sigma_{xy} = \frac{j_H}{E} = \frac{e^2}{\hbar}\frac{1}{A}\sum_{n,k} F_n(k)$$

For complitely field bands

$$\sum_{n,k} F_n(k) = A\int_{BZ}\frac{d^2k}{(2\pi)^2} F_n(k) \Rightarrow$$

$$\boxed{\sigma_{xy} = \frac{j_H}{E} = \frac{e^2}{\hbar}\frac{1}{A}\sum_{nk} F_n(k) = \frac{e^2}{\hbar}\left[\sum_n \int_{BZ} d^2k \frac{F_n(k)}{2\pi}\right.}$$

Notice this is when all bands are fully occupied!

Dirac quantization, Gauss-Bonnet theorem

From math point of view B, Berry curvature $\mathcal{F}_n$ and the Gassian curvature k are the same!
So for simplicity we will use B to calculate

- $\oiint B\, ds$ and show it's quantized.

$$\oiint B \cdot ds = \oiint B_n\, dS = \frac{c\hbar}{2qe} \cdot n$$

, n = integer magnetic charge which measure the # of magnetic monopoles inside M.

- $\oiint k\, dS = 2\pi \chi_M$, χ_M is even integer, known as the Euler characterisic, which measure the topological nature of the manifold M

- $\oiint_{BZ} \mathcal{F}\, dk = 2\pi C$ quantized, C is an intger called as the TKNN invariant or the Chern number

MAGNETIC MONOPOLE AND DIRAC quantization

(see M. Nakahara, Geometry, topology and physics, IOP)

For electric charge : $q_e = \oiint_M E \cdot dS$, $\nabla \cdot E = \rho$
For magnetic field: $q_m = \oiint_M B \cdot dS$, $q_m = 0$ b/c $\nabla \cdot B = 0$
But if there is a magnetic monopole!

$$B = q_m \frac{e_r}{r^2} = q_m \frac{r}{r^3} = q_m \frac{(x, y, z)}{(x^2+y^2+z^2)^{3/2}}$$

$\nabla \times A = B$. The value of A is not unique, but they are connected by a gauge transformation.

$$A = q_m \frac{(y, -x, 0)}{r(r-z)} \Rightarrow \nabla \times A = q_m \nabla \times \frac{(y, -x, 0)}{r(r-z)} =$$

$$q_m (\partial_x\ \partial_y\ \partial_z) \times \frac{(y, -x, 0)}{r(r-z)} = \cdots\cdots = q_m \frac{(x, y, z)}{(x^2+y^2+z^2)^{3/2}}$$

And it's singular at $z = r$.
In fact we can prove that no matter what there will be always one singular point.
The point is A is NON singular but non observable all observables are singular.
Moreover for the gauge $A = q_m \frac{(-y, x, 0)}{r(r+z)}$ has a pole $z = -r$ (south pole)

$$\begin{cases} A_N = q_m \dfrac{(-y, x, 0)}{r(r+z)} \\ A_S = q_m\, (y, -x, 0)/r(r-z) \end{cases}$$

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At the equator the vector potential is multivalued

i.e. $A_N = A_S + 2q_m \frac{(-y,x,0)}{(r-z)(r+z)}$; at $z=0$ $A_N = A_S + 2q_m \frac{(-y,x,0)}{r^2}$

$= A_N + 2q_m \nabla\varphi$

$$\phi \to \Phi' = \Phi - \frac{\partial\Lambda(r,t)}{c\,\partial t}$$

$A \to A' = A + \nabla\Lambda(r,t)$, $\psi(r,t) \to \psi'(r,t) = \psi(r,t)\, e^{i\frac{q_e}{c\hbar}\Lambda}$

Here $\Lambda(r,t) = 2q_m\varphi$

$$\psi_N(r,t) = \psi_S(r,t)\, e^{i\frac{q_e}{c\hbar}\Lambda} = \psi_S\, e^{i\frac{2q_m q_e}{c\hbar}\varphi}$$

also we know φ and $\varphi + 2\pi$ are the same point.

φ: $\psi_N(r,t) = \psi_S(r,t)\, e^{i\frac{2q_m q_e}{c\hbar}\varphi}$

and $\varphi + 2\pi$: $\psi_N(r,t) = \psi_S(r,t)\, e^{i\frac{2q_m q_e}{c\hbar}(\varphi+2\pi)}$

to have both equations valid $\frac{2q_m q_e}{c\hbar} = n$

$\psi_N = \psi_S\, e^{in(\varphi+2\pi)} = \psi_S\, e^{in\varphi}$

$$\boxed{q_m = \frac{c\hbar}{2q_e}n}$$

Why charge is quantized?

Nobody knows.

Going back to the Hall conductivity

$$\underline{\underline{\sigma_{xy}}} = \frac{e^2}{\hbar}\left[\sum_{n,\,k\in\text{fully occupied}} \int_{BZ} d^2k\, \frac{F_n(k)}{2\pi}\right] = \underline{\underline{\frac{e^2}{\hbar}n}}$$

END OF L9.