

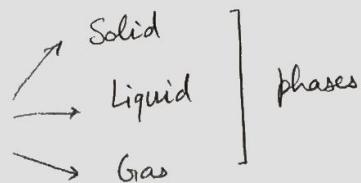
Lecture-1
(09-01-23)

System - think of a large # of particles.

Phases - instead of focusing on microscopic properties, the macroscopic observable properties of a system can be used to characterize their overall properties.

Examples -

Starting from constituent particles as atoms



Starting from constituent particles as electrons
(only referring to charged d.o.f.)

Wigner crystal
Fermi liquid.
Fermi gas

If we are now interested in the spin d.o.f. of electrons (magnetic moments) as fundamental constituents

Ferromagnets, AFM (ordered magnets)
Spin Liquids.
Paramagnets (disordered phase)

Starting with Bosons

BEC
Superfluid
Bose gas

} the distinction b/w the gas & liquid analogous phases is often tricky.

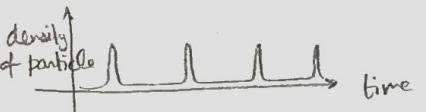
How to distinguish quantum and classical phases of matter?

Depends on what type of degree of freedom is required for the phase to arise.
Identify the correct fundamental constituent particle.

Order vs. Disorder behaviour.

Temporal Spatial	Order	Disorder
Order	Crystal	?
Disorder	Glass (amorphous) solid	Gas

Interesting example of Time crystal



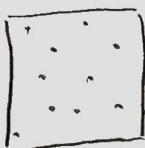
appears & disappears periodically.

Temporal order may be a system fixed in time or can even be time crystal.

Lecture-2
(10-01-23)

The physics of a many-particle system is contained in the Hamiltonian.

Hamiltonian description:



- (i) Kinetic Energy
- (ii) Interaction with a background pot.
- (iii) Inter-particle interactions.

Given only KE, the problem is integrable & easy to solve. (i)

The category of problems with inter-particle interactions is very difficult. (iii)

(ii) → (ii-a) Background fixed. → easy.

→ (ii-b) Background variable. → intermediate difficulty.
(dynamics of background)

For example, in a general solid, the Hamiltonian goes like.

$$H_{\text{solid}} = H_{\text{kin.}}(\text{elec}) + H_{\text{kin.}}(\text{ions}) + H_{\text{int.}}(\text{el.-ion}) + H_{\text{int.}}(\text{el.-el.}) \\ + H_{\text{int.}}(\text{ion-ion})$$

This problem consists of inter-particle interactions b/w same & different particles. ⇒ This is really difficult.

The first step in simplification is realizing that ions can be treated classically.

Ions treated classically + ignoring e^-e^- interactions make the problem much more solvable.

$$H \approx H_{kin}(e^+) + H_{kin}(\text{ion}) + H_{int}(e^- \text{ion})$$



Reduces the problem to the one with a background ion field.

Treating the fixed background is equivalent to solving for the band structure. Essential idea is to reduce the problem to class (ii)

Quantum N-particle systems (identical particles)



N-particles

Physics is described by $\psi(x_1, x_2, \dots, x_N)$

$$|\psi(x_1, x_2, \dots, x_N)|^2 \prod_{i=1}^N dx_i$$

probability of finding N-particles at locations x_1, x_2, \dots, x_N without labelling the particles (since particles are indistinguishable).

Indistinguishability implies the following-

Assume we virtually label the particles. Then under an exchange operation

$$\hat{P}_{j \leftrightarrow k} \psi(x_1, x_2, \dots, x_j, \dots, x_k, \dots, x_n) = e^{i\alpha} \psi(x_1, x_2, \dots, x_k, \dots, x_j, \dots, x_n)$$

"Quantum Mechanics deals with indistinguishability by being non-committal as to which particle is in which state."

Performing the exchange operation again-

$$\hat{P}_{j \leftrightarrow k}^2 \psi(x_1, x_2, \dots, x_j, \dots, x_k, \dots, x_N) = \frac{e^{2i\alpha}}{\lambda^2} \psi(x_1, x_2, \dots, x_j, \dots, x_k, \dots, x_N)$$

$$= \psi(x_1, x_2, \dots, x_j, \dots, x_k, \dots, x_N) \quad \text{since exchanging twice is an } \underline{\text{1}} \text{ operation.}$$

$$\Rightarrow \lambda^2 = e^{2i\alpha} = 1 \quad \Rightarrow \quad \lambda = +1 \quad (\text{Bosons})$$

$$\quad \quad \quad \lambda = -1 \quad (\text{Fermions}).$$

Ref: Fetter & Walecka, Brueks & Flensberg.

\rightarrow non-committal to state of individual particles.

What is a good basis for describing wavefn's $\psi(x_1, x_2, \dots, x_N)$?
Any set of single-particle wavefunctions is good enough for a basis choice of many-particle wavefn.

Single-particle basis: $\{\phi_v(x)\} \quad v \in \mathbb{N}$

Properties -

- $\sum_v \phi_v^*(x) \phi_v(x') = \delta(x-x')$
- $\int dx \phi_{v'}^*(x) \phi_{v'}(x) = \delta_{v,v'}$

Single Particle states as Basis states

Projection of $\phi_{v_1}(x_1)$ along $\psi = \int dx_1 \phi_{v_1}^*(x_1) \psi(x_1, x_2, \dots, x_N)$
 $\sim \langle \phi_{v_1}(x_1) | \psi(x_1, \dots, x_N) \rangle$

$$= A_{N_1} (x_2, x_3, \dots, x_N) \quad \dots, N-1 \text{ particlef.}$$

* This can be inverted by multiplying with $\phi_{V_1}(x_1)$ and summing over V_1

$$\sum_{\nu_1} \int dx_1 \phi_{\nu_1}^*(x_1) \phi_{\nu_1}(\tilde{x}_1) \psi(x_1, \dots x_N) = \sum_{\nu_1} \phi_{\nu_1}(\tilde{x}_1) A_{\nu_1}(x_2, \dots x_N)$$

Analogously, define $A_{v_1 v_2}(x_3, x_4, \dots, x_n)$ from $A_{v_1}(x_2, \dots)$

$$A_{\nu_1 \nu_2}(x_3, x_4, \dots, x_N) = \int dx_2 \phi_{\nu_2}^*(x_2) A_{\nu_1}(x_2, \dots, x_N) \sim \langle \phi_{\nu_2} | \otimes (\langle \phi_{\nu_1} | \psi \rangle)$$

Now inverting like before,

$$\sum_{v_2} \underbrace{\int dx_2 \phi_{v_2}^*(x_2) \phi_{v_2}(\tilde{x}_2)}_{\delta(x_2 - \tilde{x}_2)} A_{v_1}(x_2, \dots, x_n) = \sum_{v_2} \phi_{v_2}(\tilde{x}_2) A_{v_1 v_2}(x_3, \dots, x_n)$$

$$\Rightarrow A_{v_1}(\tilde{x}_2, \dots, x_N) = \sum_{v_2} \phi_{v_2}(\tilde{x}_2) A_{v_1 v_2}(x_3, \dots, x_N)$$

and from eqⁿ (1)

$$\Rightarrow \psi(\tilde{x}_1, \tilde{x}_2, \dots, x_N) = \sum_{v_1, v_2} A_{v_1 v_2}(x_3, \dots, x_N) \phi_{v_1}(\tilde{x}_1) \phi_{v_2}(\tilde{x}_2)$$

$$\Rightarrow \psi(\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_N) = \sum_{v_1, v_2, \dots, v_N} A_{v_1, v_2, v_3, \dots, v_N} \left\{ \prod_{j=1}^N \phi_{v_j}(\tilde{x}_j) \right\} \rightarrow \text{by induction}$$

single-particle states

Any N-particle wavef^m can be written as a (rather-complicated) superposition of product states!

However, even though $\prod_{j=1}^N \phi_{v_j}(x_j)$ is a valid basis, it's not "useful" since they don't satisfy the (anti-) symmetrization requirement of identical particle systems.

Symmetrized Basis:

physically meaningful basis

$$S_{\pm} \left(\prod_{j=1}^N \phi_{v_j}(x_j) \right) = \begin{vmatrix} \phi_{v_1}(x_1) & \dots & \phi_{v_1}(x_N) \\ \phi_{v_2}(x_1) & \dots & \phi_{v_2}(x_N) \\ \vdots & \ddots & \vdots \\ \phi_{v_N}(x_1) & \dots & \phi_{v_N}(x_N) \end{vmatrix}_{\pm} = \langle \tilde{x}|n_{v_1}, n_{v_2}, \dots \rangle$$

$n_v \in \{0, 1\}$ (-)
 $n_v \in \mathbb{Z}^+$ (+)

+ : Bosons, expanded as a permanent. (determinant with all + signs)

- : Fermions, expanded as a usual determinant. (Slater determinant)

For N=2: $\{\phi_v(x)\} \quad v \in \{1, 2\}$

Consider BOSONS.

$$\psi(x_1, x_2) = \sum_{v_1, v_2=1}^2 A_{v_1, v_2} \phi_{v_1}(x_1) \phi_{v_2}(x_2)$$

$$= A_{11} \phi_1(x_1) \phi_1(x_2) + A_{12} \phi_1(x_1) \phi_2(x_2) + A_{21} \phi_2(x_1) \phi_1(x_2)$$

$$+ A_{22} \phi_2(x_1) \phi_2(x_2)$$

By symmetrization argument, $A_{12} = A_{21}$

$$\Rightarrow \psi = A_{11} \phi_1(x_1) \phi_1(x_2) + A_{12} [\phi_1(x_2) \phi_2(x_1) + \phi_1(x_1) \phi_2(x_2)] + A_{22} \phi_2(x_1) \phi_2(x_2)$$

$$\psi(x_2, x_1) = \psi(x_1, x_2)$$

Symmetrized basis states for the N=2 problem -

$$\tilde{\phi} = \begin{vmatrix} \phi_{v_1}(x_1) & \phi_{v_2}(x_1) \\ \phi_{v_1}(x_2) & \phi_{v_2}(x_2) \end{vmatrix}_+ = \phi_{v_1}(x_1)\phi_{v_2}(x_2) + \phi_{v_1}(x_2)\phi_{v_2}(x_1)$$

with $v_1, v_2 \in \{1, 2\}$

Now, instead of using the single-particle basis for expansion, we use the symmetrized / anti-symmetrized basis states -

i.e.

$$\sum_{v_1 \dots v_N} A_{v_1 \dots v_N} \left(\prod_{j=1}^N \phi_{v_j}(x_j) \right) \rightarrow \sum_{v_1 \dots v_N} B_{v_1 \dots v_N} \underbrace{\hat{S}_{\pm} \left(\prod_{j=1}^N \phi_{v_j}(x_j) \right)}_{\substack{\text{single particle} \\ \text{basis.}}} \uparrow$$

Symmetrized /
anti-symmetrized
basis

Lecture - 03
 (11-01-23)

Second quantization: reformulation of Schrödinger eqn. Uses second quantized operators to encode spin statistics instead of cumbersome (anti-)symmetrized state

General wavefn $\psi(x_1, x_2, \dots, x_N)$

In a general N-particle system, the Hamiltonian looks as follows.

$$H = \sum_{k=1}^N T(x_k) \rightarrow \text{kinetic term} \quad x_k \rightarrow \text{co-ord. of } k^{\text{th}} \text{ particle.}$$

$$+ \frac{1}{2} \sum_{k \neq l=1}^N V(x_k, x_l) \rightarrow \text{interaction term.} \\ \text{b/w pairs of particles.}$$

For our N-particle system, the Schrödinger eqn for a time-dependent pdⁿ

$$\text{i}\hbar \frac{\partial}{\partial t} \psi(x_1, x_2, \dots, t) = \hat{H} \psi(x_1, x_2, \dots, x_N, t)$$

Start by expanding ψ in single-particle basis,

$$\psi(x_1, x_2, \dots, x_N, t) = \sum_{v'_1, \dots, v'_N} C(v'_1, v'_2, \dots, v'_N, t) \phi_{v'_1}(x_1) \phi_{v'_2}(x_2) \dots \phi_{v'_N}(x_N) \quad (1)$$

↑
time dependent
in co-effs. ↑ ↑ ↑
single-particle states

Operation A:

Multiply & integrate with $\int dx_1 \dots dx_N \phi_{v_i}(x_1) \dots \phi_{v_N}(x_N)$ → notice the state labels are unprimed here.

• Operation A on LHS -

$$\Rightarrow \text{i}\hbar \frac{\partial}{\partial t} \left(\sum_{v'_1, \dots, v'_N} C(v'_1, \dots, v'_N, t) \underbrace{\langle \phi_{v'_1}(x_1) \dots \phi_{v'_N}(x_N) \rangle}_{\delta v_i, v'_i} \right)$$

$$= \text{i}\hbar \frac{\partial}{\partial t} C(v_1, v_2, \dots, v_N)$$

• Operation A on RHS.

$$\hat{H} = \sum_{k=1}^N \hat{T}(x_k) + \frac{1}{2} \sum_{k \neq l=1}^N \hat{V}(x_k, x_l)$$

Starting with kinetic term of particle "k"-

$$\hat{T}(x_k) \psi = \sum_{v_1' \dots v_N'} C_{v_1' \dots v_N', t} \left[\prod_{j \neq k} \phi_{v_j'}(x_j) \right] \hat{T}(x_k) \phi_{v_k'}(x_k)$$

Applying operation A-

$$= \sum_{v_1' \dots v_N'} C_{v_1' \dots v_N', t} \underbrace{\int \left(\prod_{j \neq k} dx_j \phi_{v_j'}^*(x_j) \phi_{v_j'}(x_j) \right)}_{\delta_{v_j' v_j}} \int dx_k \phi_{v_k'}^*(x_k) \hat{T}(x_k) \phi_{v_k'}(x_k)$$

Since the only sum remaining is over v_k' , relabel $v_k' \rightarrow w$

$$= \sum_w C_{v_1 \dots v_{k-1}, w, v_{k+1} \dots v_N, t} \int dx_k \phi_w^*(x_k) \hat{T}(x_k) \phi_w(x_k)$$

\Rightarrow Sum of all KE terms = $\sum_{k=1}^N \sum_w C_{(v_1 \dots v_{k-1}, w, v_{k+1} \dots v_N, t)} \int dx_k \phi_w^*(x_k) \hat{T}(x_k) \phi_w(x_k)$ ↳ (2)

Similarly, the P.E. term under operation A looks like (relabel $v_k' \rightarrow w$) $v_\ell' \rightarrow \tilde{w}$

Sum of all PE terms = $\frac{1}{2} \sum_{k \neq \ell=1}^N \sum_{w, \tilde{w}} C_{(v_1 \dots v_{k-1}, w, v_{k+1}, \dots, v_{\ell-1}, \tilde{w}, v_{\ell+1} \dots v_N, t)} \int \int dx_k dx_\ell \phi_w^*(x_k) \phi_{\tilde{w}}^*(x_\ell) \hat{V}(x_k, x_\ell)$ $\phi_w(x_k) \phi_{\tilde{w}}(x_\ell)$ ↳ (3)

\Rightarrow i.e. $\partial_t C(v_1 \dots v_N, t) = (2) + (3)$

* We now want $\psi(\dots x_i, \dots x_j, \dots, t) = \pm \psi(\dots x_j, \dots x_i, \dots, t)$

$\Rightarrow \underbrace{C(v_1, v_2, \dots, v_j, \dots, v_k, \dots, v_N, t)}_{\text{(refer to F&W pg.6)}} = \pm C(v_1 \dots v_k, \dots v_j, \dots, v_N, t)$ All the (anti-)symmetry is now put into the coefficients C.

OCCUPATION NUMBER BASIS. (Bosons for now)

Notation for $C(v_1, v_2, \dots, v_N) = C(n_1, n_2, \dots, n_N)$ occupation #s.

Since terms with same occupation #s i.e. n_1 particles in state 1, n_2 in state 2 and so on have the same coeff. (due to symmetrization of coeffs.), we relabel coefficients to $\tilde{C}(n_1, \dots, n_\infty, t)$

$$C(\underbrace{122312}) = +C(132212) \text{ or } C(\underbrace{122312}) = +C(322112)$$

$$\Rightarrow C(v_1, v_2, \dots, v_N, t) = C(\underbrace{111\dots}_{n_1}, \underbrace{222\dots}_{n_2}, \dots, \dots, t) \equiv \tilde{C}(n_1, n_2, \dots, n_\infty, t)$$

Normalization $\int d\tau |\psi|^2 \stackrel{!}{=} 1$

$$\Rightarrow \sum_{v_1, \dots, v_N} |C(v_1, \dots, v_N, t)|^2 \stackrel{!}{=} 1 \rightarrow$$

since many $C(v_1, \dots, v_N)$'s with the same occupation #'s are equal & map to $\tilde{C}(n_1, n_2, \dots, n_\infty, t)$

\therefore The sum over all possible N particles states \Rightarrow there will be repetition of the coefficients with the same occupation # config. However, when summing over ALL the N -particle states, the problem of regrouping these coefficients is equivalent to N objects into boxes with n_1 objects in box 1, n_2 objects in box 2 and so on. And the # of such possibilities is -

$$\text{multinomial coeff.} = \frac{N!}{\prod_{k=1}^{\infty} n_k!}$$

$$\Rightarrow \sum_{v_1, \dots, v_N} |C(v_1, \dots, v_N, t)|^2 \stackrel{!}{=} 1 \rightarrow \sum'_{n_1, n_2, \dots, n_\infty} |\tilde{C}(n_1, n_2, \dots, n_\infty, t)|^2 \cdot \frac{N!}{n_1! n_2! \dots n_\infty!} \stackrel{!}{=} 1$$

where \sum' denotes the restriction $\sum_{i=1}^{\infty} n_i = N$

Redefine the coefficient $f(n_1, n_2, \dots, n_\infty, t) \equiv \left(\frac{N!}{\prod_k n_k!} \right)^{1/2} \tilde{C}(n_1, n_2, \dots, n_\infty, t)$

$$\text{with } \sum_{i=1}^{\infty} n_i = N$$

$$\Rightarrow \sum'_{n_1, n_2, \dots, n_\infty} |f(n_1, n_2, \dots, n_\infty, t)|^2 \stackrel{!}{=} 1$$

Lecture -04

(16-01-2023)

Starting with a many-particle wavefn

$$\psi(x_1, x_2, \dots, x_N, t) = \sum_{v_1, v_2, v_3, \dots, v_N} c(v_1, v_2, \dots, v_N) \prod_j \phi_j$$

$$c(v_1, \dots, \underbrace{v_i, \dots, v_i}_{\text{product over single-particle states}}, \dots, v_N, t) = + c(v_1, \dots, v_i, \dots, v_N, t)$$

→ give the same coeffs \Rightarrow motivated us to move to a new language of occupation basis with $\underbrace{c}_{(v_i, \dots)} \rightarrow \tilde{c}_{(n_i, \dots)}$ for bosons.

∴ We can also write this wavefn in occupation # basis-

$$\psi = \sum_{v_1, \dots, v_N} c(v_1, v_2, \dots, v_N) \prod_j \phi_{v_j}(x_j) = \sum_{n_1, \dots, n_\infty} \tilde{c}(n_1(\vec{v}), n_2(\vec{v}), \dots, n_\infty(\vec{v}), t) \prod_j \phi_{v_j}(x_j)$$

=

Define $\tilde{f} = \left(\frac{N!}{\prod_j n_j!} \right)^{1/2} \tilde{c}$ with $\sum_i n_i = N$

$$\text{Then } |\psi|^2 = 1 \Rightarrow \sum_{n_1, n_2, \dots, n_\infty} |f(n_1, \dots, n_\infty, t)|^2 = 1 \quad \text{with } \sum_{i=1}^\infty n_i = N$$

The original wavefn can now be written as-

$$\psi(x_1, \dots, x_N) = \sum'_{n_1, n_2, \dots, n_\infty} f(n_1, n_2, \dots, n_\infty, t) \left(\frac{\prod_j n_j!}{N!} \right)^{1/2} \sum_{\substack{v_1, v_2, \dots, v_N \\ (n_1, n_2, \dots, n_\infty)}} \phi_{v_1}(x_1) \dots \phi_{v_N}(x_N)$$

From the last lecture,

$$\text{L.H.S.} = i\hbar \partial_t c(v_1, v_2, \dots, v_N, t)$$

$$\text{R.H.S.} = \sum_{k=1}^N \sum_w \left[\begin{array}{l} \text{single-particle} \\ \text{term} \end{array} \right] \langle v_k(x_k) | \hat{T}_k | w(x_k) \rangle c(v_1, v_2, \dots, v_{k-1}, w, v_{k+1}, \dots, v_N, t)$$

• LHS

The $c \rightarrow \tilde{c}$ mapping is many-to-one.

$$\therefore c(v_1, v_2, \dots, v_N, t) \text{ in LHS} = \tilde{c}(n_1, n_2, \dots, n_\infty, t)$$

• RHS

Similarly in RHS

$$c(v_1, v_2, \dots, v_k, w, v_{k+1}, \dots, v_N, t) \rightarrow \tilde{c}(n_1, n_2, \dots, n_{v_k-1}, \dots, n_{w+1}, \dots, n_\infty, t)$$

$$= \sum_{v=1}^{\infty} \sum_w \langle v | \hat{T} | w \rangle n_v \tilde{c}(n_1, n_2, \dots, n_{v-1}, \dots, n_{w+1}, \dots, n_\infty, t)$$

For potⁿ energy interaction,

$$\left[\begin{array}{l} \text{Interaction} \\ \text{Term} \end{array} \right] = \frac{1}{2} \sum_{v, v'} \sum_{w, w'} \langle v v' | \hat{V} | w w' \rangle \left(\begin{array}{c} n_v (n_{v'} - \delta_{v'}) \\ \downarrow \end{array} \right) \tilde{c}(n_1, \dots, n_{v-1}, \dots, n_{w+1}, \dots, n_{w'-1}, \dots, n_\infty, t)$$

multiplicative counting factor

$$\iint dx dx' \phi_v^*(x) \phi_{v'}^*(x') \hat{V} \phi_w(x) \phi_{w'}(x')$$

$$\text{ith } \frac{\partial}{\partial t} \tilde{C}(\dots) = \sum_{i,j} \langle i | \hat{T} | j \rangle n_i \tilde{C}(\dots, n_i-1, \dots, n_j+1, \dots) \\ + \frac{1}{2} \sum_{i,j} \sum_{k,l} \langle i j | \hat{V} | k l \rangle \tilde{C}(\dots, n_i-1, \dots, n_j+1, \dots, n_k-1, \dots, n_l+1, \dots)$$

Finally, we make the switch from $\tilde{C} \rightarrow f$

$$\tilde{C} \equiv f \cdot \left(\frac{\prod_k n_k!}{N!} \right)^{1/2} \quad \text{and multiply both sides by } \left(\frac{N!}{\prod_k n_k!} \right)^{1/2}$$

$$\text{ith } \frac{\partial}{\partial t} f(n_1, \dots, n_{\infty}, t) = \sum_i \langle i | \hat{T} | i \rangle n_i f(\dots) \rightarrow \text{if } i=j$$

$$+ \sum_{i \neq j} \langle i | \hat{T} | j \rangle \sqrt{n_i} \cdot \sqrt{n_j+1} f(\dots, n_i-1, \dots, n_j+1) \rightarrow \text{if } i \neq j$$

+ H.W.

\uparrow
reminds us of
raising & lowering operators!

\uparrow
complete the expression for the \hat{V} term!

Lecture - 05
 (17-01-2023)

Time evolution of each coefficient:

$$\begin{aligned}
 i\hbar \frac{\partial}{\partial t} f(n_1, \dots, n_\infty, t) = & \sum_i \langle i|T|i\rangle n_i f(n_1, \dots, n_\infty, t) \\
 & + \sum_{i \neq j} \langle i|T|j\rangle \sqrt{n_i} \sqrt{n_j+1} f(\dots, n_i-1, \dots, n_j+1, \dots) \\
 & + \sum_{i+j+k+l} \langle ij|V|kl\rangle \sqrt{n_i} \sqrt{n_j} \sqrt{n_k+1} \sqrt{n_l+1} f(\dots, n_i-1, \dots, n_k+1, \dots, n_l+1, \dots) \\
 & + \sum_{i \neq k \neq l} \langle ii|V|kl\rangle \sqrt{n_i} \sqrt{n_i-1} \sqrt{n_k+1} \sqrt{n_l+1} f(\dots, n_i-2, \dots, n_k+1, \dots, n_l+1, \dots)
 \end{aligned}$$

↑ ↑
 annihilating
 two particles from
 state i

+

Let's make use of this interesting creation-annihilation structure.

Basis states: $|n_1, n_2, \dots, n_\infty\rangle$

We desire - • orthonormality $\langle n'_1 n'_2 \dots | n_1 n_2 \dots \rangle = \prod_{i=1}^{\infty} \delta_{n'_i n_i}$
 • completeness $|\psi\rangle = \sum_{n_1, n_2, \dots} c_{n_1 n_2 \dots} |n_1 n_2 \dots \rangle$

We demand operators b_k, b_k^\dagger with the conditions -

$$[b_k, b_{k'}^\dagger] = \delta_{kk'}, \quad [b_k, b_{k'}] = [b_k^\dagger, b_{k'}^\dagger] = 0$$

We now propose we can expand states as-

$$|\psi(t)\rangle = \sum_{n_1, \dots, n_\infty} f(n_1, \dots, n_\infty, t) |n_1, \dots, n_\infty\rangle$$

in eq^n(i)

If we take a product with $|n_1 n_2 \dots\rangle$ & sum over $n_1, n_2 \dots$

$$\text{L.H.S.} \rightarrow i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \left(= i\hbar \frac{\partial}{\partial t} \sum_{n_1, n_2 \dots} f(\dots) |n_1, n_2 \dots\rangle \right)$$

In R.H.S., let's focus on

$$\sum_{i \neq j} \langle i | T | j \rangle \sqrt{n_i} \sqrt{n_j + 1} f(\dots, n_{i-1}, \dots, n_j + 1, \dots)$$

The property of the b_k, b_k^+ operator is as follows-

$$\hat{b}_k |n_k\rangle = \sqrt{n_k} |n_k - 1\rangle \quad] \text{consequence of}$$

$$\hat{b}_k^+ |n_k\rangle = \sqrt{n_k + 1} |n_k + 1\rangle \quad] \text{the operator algebra.}$$

energy
levels
 k

n_k # of particles

$\Rightarrow b_k$ & b_k^+ annihilate or create a particle (respectively) in the occupation number of energy level "k".

$$\sum_{i \neq j} \sum_{n_1, \dots, n_\infty} \langle i | T | j \rangle \sqrt{n_i} \sqrt{n_j + 1} f(\dots, n_{i-1}, \dots, n_j + 1, \dots) |n_1, \dots, n_\infty\rangle$$

do a change of labels

$$n_i = n'_i + 1$$

$$n_k = n'_k \quad \text{for } k \neq i, j$$

$$n_j = n'_j - 1$$

$$\Rightarrow \sum_{i \neq j} \sum_{n'_1, n'_2, \dots, n'_\infty} \langle i | T | j \rangle \sqrt{n'_1 + 1} \sqrt{n'_j + 1} f(n'_1, \dots, n'_\infty) | n'_1, \dots, n'_i + 1, \dots, n'_{j-1}, \dots, n'_\infty \rangle$$

and $\sqrt{n'_i + 1} | n'_i + 1 \rangle = b_i^\dagger | n'_i \rangle$

$$\sqrt{n'_j + 1} | n'_j - 1 \rangle = b_j | n'_j \rangle$$

$$\Rightarrow \sum_{i \neq j} \sum_{n'_1, \dots, n'_\infty} \langle i | T | j \rangle b_i^\dagger b_j f(n'_1, \dots, n'_\infty) | n'_1, \dots, n'_\infty \rangle$$

↑
SECOND
QUANTIZATION
LANGUAGE!

Similarly, this procedure can be followed for other terms.

Therefore, any general two-particle interaction Hamiltonian in the second quantized language looks as follows:

$$\hat{H} = \boxed{\sum_{ij} \langle ij | \hat{T} | ij \rangle \hat{b}_i^\dagger \hat{b}_j + \sum_{ijkl} \langle i j l | \hat{V} | k l \rangle \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_k \hat{b}_l}$$

For bosons: commutator algebra $[b_k, b_{k'}^\dagger] = \delta_{kk'}$

For fermions: anti-commutator algebra $\{b_k, b_{k'}^\dagger\} = \delta_{kk'}$

Free Bosons:

$$\text{First quantized K.E.}, \hat{H} = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m} = \sum_{i=1}^N -\frac{\hbar^2}{2m} \partial_{x_i}^2$$

Nice set of single-particle levels?

$$[\hat{p}_i, \hat{H}] = 0 \Rightarrow \text{momentum } \hat{p}_i \text{ is a good quantum \#.}$$

So, the basis over which we take inner products i.e. the energy spectrum can be labelled by momentum labels.

$$\langle i | \hat{T} | j \rangle = \langle p_i | \hat{T} | p_j \rangle = \frac{\hat{p}_i^2}{2m} S_{ij}$$

$$\Rightarrow \hat{H}_{\text{2nd quantized}} = \sum_{i,j} \langle i | \hat{T} | j \rangle \hat{b}_i^\dagger \hat{b}_j = \sum_i \frac{\hat{p}_i^2}{2m} \hat{b}_i^\dagger \hat{b}_i$$

Same for fermions. (except anti-commutative algebra.)

Let's say we have a set of single particle states

$$\{\phi_i(x)\}_{i=1,\dots,s}$$

Say $N=3$ and these particles are free bosons.

A valid 3 particle state might look like-

$$\Phi(x_1, x_2, x_3) = \alpha \hat{S}^+(\phi_1(x_1) \phi_3(x_2) \phi_5(x_3)) + \beta \hat{S}^+(\phi_1(x_1) \phi_1(x_2) \phi_2(x_3))$$

permanent structures.

$$\begin{aligned}\varepsilon_5 &\longrightarrow \phi_5 \\ \varepsilon_4 &\longrightarrow \phi_4 \\ \varepsilon_3 &\longrightarrow \phi_3 \\ \varepsilon_2 &\longrightarrow \phi_2 \\ \varepsilon_1 &\longrightarrow \phi_1\end{aligned}$$

and we want to compute the exp. value of $\hat{H} = \sum_{i=1}^3 \frac{\hat{p}_i^2}{2m}$ on this state.

$$\langle \hat{H} \rangle = \int dx_1 dx_2 dx_3 \Phi^*(x_1, x_2, x_3) \hat{H} \Phi(x_1, x_2, x_3)$$

Symmetrized wavefn's Φ make this difficult. (^{long} expressions)

The index labelling the levels is $\varepsilon_i = \frac{\hat{p}_i^2}{2m}$.

As discussed, doing this directly is tedious. Let's see if second quantization makes it easy.

Since states $\{\phi_i\}$ are eigenstates of \hat{H} , and $[\hat{H}, \hat{p}_i] = 0$

$$\Rightarrow \hat{H} = \sum_{i,j=1}^s \Phi_i |T| \Phi_j \hat{b}_i^\dagger \hat{b}_j = \sum_{i=1}^s \varepsilon_i \hat{b}_i^\dagger \hat{b}_i$$

In the second quantization language, the previous state can be written as -

$$|\psi\rangle = \alpha|10101\rangle + \beta|21000\rangle \\ = \alpha \hat{b}_1^\dagger \hat{b}_3^\dagger \hat{b}_5^\dagger |10\rangle + \beta \hat{b}_1^\dagger \hat{b}_1^\dagger \hat{b}_2^\dagger |10\rangle$$

$$\langle\psi|\hat{H}|\psi\rangle = [\alpha^* \langle 10101 | + \beta^* \langle 21000 |] \sum_{i=1}^5 b_i^\dagger b_i \varepsilon_i [\alpha|10101\rangle + \beta|21000\rangle] \\ = \langle\psi| (\underbrace{\alpha \varepsilon_1 |10101\rangle}_{\text{+ } \varepsilon_2 \beta |21000\rangle} + \underbrace{2 \beta \varepsilon_1 |21000\rangle}_{\text{+ } \varepsilon_3 \beta |21000\rangle} + \underbrace{\varepsilon_2 \beta |21000\rangle}_{\text{+ } \varepsilon_3 \alpha |10101\rangle} + \underbrace{\varepsilon_3 \alpha |10101\rangle}_{\text{+ } \varepsilon_5 \alpha |10101\rangle}) \\ = [\alpha^* \langle 10101 | + \beta^* \langle 21000 |] \cdot (\alpha(\varepsilon_1 + \varepsilon_3 + \varepsilon_5) |10101\rangle + \beta(2\varepsilon_1 + \varepsilon_2) |21000\rangle) \\ = |\alpha|^2 (\varepsilon_1 + \varepsilon_3 + \varepsilon_5) + |\beta|^2 (2\varepsilon_1 + \varepsilon_2)$$

Let's now look at an example where the KE operator isn't diagonal.

TIGHT BINDING MODEL (electron hopping on a lattice)

$$\hat{H} = -t \sum_i |\psi_i\rangle \langle \psi_{i+1}| + h.c.$$

$$\dots \underset{i}{\circ} \quad \underset{i+1}{\circ} \quad \dots$$

In the second quantization language, \hat{H} becomes -

$$\hat{H} = -t \sum_i [c_i^\dagger c_{i+1} + h.c.] + \varepsilon_0 \sum_i c_i^\dagger c_i$$

$c \rightarrow$ for fermions

tight-binding model
with nearest-neighbour hopping.

$$= (c_1^\dagger \ c_2^\dagger \ \dots \ c_N^\dagger) \begin{pmatrix} \varepsilon_0 & -t & & & 0 & -t \\ -t & \varepsilon_0 & -t & & 0 & \\ & 0 & -t & \varepsilon_0 & -t & 0 \\ & & & \ddots & & \\ -t & 0 & \dots & & -t & \varepsilon_0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

By taking a Fourier transform, this becomes -

$$\hat{H} = \sum_k (-2t \cos(ka) + \varepsilon_0) \tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma}$$

Work this out!

Hint:

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{-ikr_i} \tilde{c}_k$$

$$\frac{1}{N} \sum_i e^{ikr_i} e^{-ik'r_i} = \delta_{kk'}$$

Lecture-07

(23-01-2023)

The most general Hamiltonian in 2nd quantization notation

$$\hat{H} = \sum_{ij} T_{ij} \hat{b}_i^\dagger \hat{b}_j + \sum_{ijkl} V_{ijkl} \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_k \hat{b}_l$$

- 1) For non-interacting Hamiltonians, T_{ij} = fixed
- 2) This class of problems, with T_{ij} being dependent on background potⁿ has T_{ij} variable.
- 3) For a fully interacting system, both T_{ij} & V_{ijkl} are $\neq 0$ and not fixed.

Given the Hamiltonian, our next interest is calculating expectation values. Generally, we are left with vacuum expectations of a string of \hat{b}_i^\dagger 's & \hat{b}_i 's

$$\langle 0 | b_k^\dagger b_e^\dagger b_m^\dagger b_n \dots | 0 \rangle$$

By the defⁿ of vacuum, $\hat{b}_i | 0 \rangle = 0$

∴ We generally prefer all \hat{b} 's on the right.

Normal Ordering. (: :)

Push all the annihilation to the left.

$$: b b^\dagger b^\dagger b : = b^\dagger b^\dagger b b$$

Wick's Theorem.

$$b_k^+ b_e^+ b_m^+ b_n^+ b_s^+ b_t^+ = :b_k^+ b_e^+ b_m^+ b_n^+ b_s^+ b_t^: + :b_k^+ b_e^+ \underbrace{b_m^+ b_n^+}_{} b_s^+ b_t^:$$

+ :b_k^+ b_e^+ b_m^+ b_n^+ b_s^+ b_t^: + \dots \text{ (all single contractions)}

+ \dots \text{ (all double contractions)}

Defn of Wick's contraction

$$\underbrace{b_e^+ b_m^+} = \delta_{em}$$

The essential idea is that uncontracted normal ordered terms will always have a \hat{b} on the left. Therefore, the only contribution to vacuum expectation values is from the fully contracted term. The contraction is always to be done with a \hat{b} on left and \hat{b}^+ to its right.

For fermions, an example -

$$\begin{aligned} \langle 0 | c_k^+ c_m^+ c_t^+ c_s^+ | 0 \rangle &= \langle 0 : c_k^+ \underbrace{c_m^+ c_t^+}_{} c_s^+ : | 0 \rangle + : c_k^+ \underbrace{c_m^+ c_t^+}_{} \underbrace{c_s^+ :}_{\substack{\rightarrow \text{crossing} \\ n=1}} | 0 \rangle \\ &= \delta_{ks} \delta_{mt} + (-1)^n \delta_{kt} \delta_{ms} \\ &= \delta_{ks} \delta_{mt} - \delta_{kt} \delta_{ms} \end{aligned}$$

$n = \#$ of intersection of contraction lines.

$T=0$

quantum averages (ground state exp vals)

What about finite-temp. calculations?

$$\langle \hat{O} \rangle_T = \frac{\text{tr}(e^{-\beta \hat{H}} \hat{O})}{\text{tr}(e^{-\beta \hat{H}})}$$

$$\text{where } \hat{H} = \hat{H}_0 - \mu \hat{N}$$

in the grand canonical ensemble.

Let's take a very simple example of a single state spectrum.

$$\hat{H}_0 = \epsilon b^\dagger b$$



Given μ, T , what is the exp val of

$$\langle \hat{n} \rangle_T = \frac{\text{tr}(\hat{n} e^{-\beta(\hat{H}_0 - \mu \hat{N})})}{\text{tr}(e^{-\beta(\hat{H}_0 - \mu \hat{N})})}$$

Our basis to trace over is the Fock basis $|n_1 n_2 n_3 \dots n_\infty\rangle$

Since we only have a single site (or energy level) here,

\Rightarrow Our basis is $\{|n\rangle\} \quad n \in \mathbb{Z}^+$

$$\langle \hat{n} \rangle = \frac{\sum_n \langle n | e^{-\beta[\epsilon \hat{n}] - \mu(\hat{n})} | \hat{n} | n \rangle}{\sum_n \langle n | e^{-\beta[\epsilon \hat{n}] - \mu(\hat{n})} | n \rangle}$$

$$= \frac{\sum_n e^{-n\beta(\epsilon - \mu)}}{\sum_n e^{-\beta(\epsilon - \mu)n}}$$

$$Z = \sum_n e^{-\beta' n} = 1 + e^{-\beta'} + e^{-2\beta'} + e^{-3\beta'} + \dots \quad \beta' \equiv \beta(\varepsilon - \mu)$$

$$= \frac{1}{1 - e^{-\beta'}} = \frac{e^{\beta'}}{e^{\beta'} - 1}$$

$$\langle \hat{n} \rangle = \frac{1}{\beta Z} \frac{\partial Z}{\partial \mu} = \frac{1}{\beta} \frac{\partial \ln Z}{\partial \mu} = \frac{1}{\beta} \frac{\partial}{\partial \mu} \left[\ln \left(\frac{1}{1 - e^{-\beta(\varepsilon - \mu)}} \right) \right]$$

$$= \frac{1}{\beta} \frac{\partial}{\partial \mu} \left[-\ln (1 - e^{-\beta(\varepsilon - \mu)}) \right] = \left(\frac{1}{\beta} \right) - \frac{1}{1 - e^{-\beta(\varepsilon - \mu)}} \cdot \left(-e^{-\beta(\varepsilon - \mu)} \cdot \beta \right)$$

$$= \frac{e^{-\beta(\varepsilon - \mu)}}{1 - e^{-\beta(\varepsilon - \mu)}} = \frac{1}{\underline{e^{\beta(\varepsilon - \mu)} - 1}} \rightarrow \text{Bose function!}$$

$\therefore \boxed{\langle \hat{n} \rangle_T = \frac{1}{e^{\beta(\varepsilon - \mu)} - 1}}$ for a bosonic single energy system.

F&W
reference

If we had fermions instead,

$$Z = \text{tr} (e^{-\beta(\hat{H} - \mu \hat{n})}) = \sum_{n=0,1} e^{-\beta n (\varepsilon - \mu)}$$

$$= 1 + e^{-\beta(\varepsilon - \mu)}$$

$$\langle \hat{n} \rangle_T = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z = \frac{1}{\beta} \cdot \frac{1}{1 + e^{-\beta(\varepsilon - \mu)}} \cdot e^{-\beta(\varepsilon - \mu)} \cdot \beta$$

$$= \frac{1}{\underline{e^{\beta(\varepsilon - \mu)} + 1}}$$

Lecture - 08

(24/01/2023)

Finite-temp. calculations of expectation values \rightarrow Quantum Stat. Mech.

Let's say we have a string of operators $\hat{G} = b_k^+ b_e^+ b_m^+ b_n$ and we want to calculate a finite-temp. expectation values.

$$\langle b_k^+ b_e^+ b_m^+ b_n \rangle_T = ?$$

$$\text{where } H = \sum_k \epsilon_k b_k^+ b_k$$

$$\text{For bosonic particles, } \langle b_k^+ b_k \rangle_T = n_B(\epsilon_k) = \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1}$$

$$\text{More generally, } \langle b_k^+ b_{k'} \rangle = n_B(\epsilon_k) \delta_{kk'}$$

$$\langle b_k^+ b_{k'}^+ \rangle = 0$$

For $\langle b_k^+ b_e^+ b_m^+ b_n \rangle_T \neq 0$, we firstly must have an equal # of creation & annihilation operations.

$$\langle b_k^+ b_e^+ b_m^+ b_n \rangle_T = \underbrace{\langle b_k^+ b_e^+ b_m^+ b_n \rangle}_{+} + \underbrace{\langle b_k^+ b_e^+ b_m^+ b_n \rangle}_{-}$$

$$\underbrace{b_m^+ b_n}_{+} = \delta_{mn} n_{B/F}$$

$$\underbrace{b_k^+ b_e^+}_{+} = \delta_{ke} (1 \pm n_{B/F})$$

Let's say we now start with a problem & reduce it to a non-interacting Hamiltonian

$$H = \sum_{k,\sigma} (\varepsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma}$$

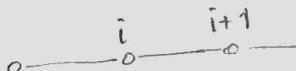
ε_k

How to calculate $\langle \hat{H} \rangle = ?$

$$\begin{aligned} \langle \hat{H} \rangle &= \sum_{k,\sigma} (\varepsilon_k - \mu) \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle = (2s+1) \sum_k \langle c_{k\sigma_0}^\dagger c_{k\sigma_0} \rangle (\varepsilon_k - \mu) \\ &= (2s+1) \sum_k n_F(\varepsilon_k) (\varepsilon_k - \mu) \end{aligned}$$

Essentially, once the Hamiltonian is diagonalized, we can use our tools of a diagonalized non-interacting system on our problem.

Example -



$$H = -t \sum_i (c_i^\dagger c_{i+1} + h.c.) \rightarrow \text{non-diagonal}$$

$$\downarrow c_i = \frac{1}{\sqrt{N}} \sum_k e^{ikr_i} \tilde{c}_k$$

$$H_{\text{diagonal}} =$$

Any such transformation to diagonalize the Hamiltonian must also make sure that the new $\tilde{c}_i^\dagger, \tilde{c}_i$ satisfy the same algebra.

Phases of interacting quantum systems

$$H = \sum_k \epsilon_k c_k^\dagger c_k$$

For most problems, a non-interacting particle system doesn't generally host phases on its own. An exception to this rule is BOSONIC systems, where the effective attraction b/w bosons leads to a BEC.

The simplest example of an interacting problem

Hubbard model: $\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$

↑
same σ , to conserve spin.
we could've had $\sum \sigma, \sigma'$, but
 $s=0$ coupling is negligible.

↑
energy cost
when fermions occupy
the same lattice site.
(\sim Coulomb interaction)

Mean-Field Approximation:

Interaction term: $\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow}$

Substitute $\hat{n}_{i\sigma} = \langle \hat{n}_{i\sigma} \rangle + \delta \hat{n}_{i\sigma}$

$$\hat{n}_{i\sigma} = \langle \hat{n}_{i\sigma} \rangle + \delta \hat{n}_{i\sigma}$$

$$\Rightarrow \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \delta \hat{n}_{i\downarrow} + \langle \hat{n}_{i\downarrow} \rangle \delta \hat{n}_{i\uparrow} + O(\delta^2)$$

$$= \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle (\hat{n}_{i\downarrow} - \langle \hat{n}_{i\downarrow} \rangle)$$

$$+ \langle \hat{n}_{i\downarrow} \rangle (\hat{n}_{i\uparrow} - \langle \hat{n}_{i\uparrow} \rangle)$$

$$= \hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \hat{n}_{i\downarrow} \langle \hat{n}_{i\uparrow} \rangle - \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle$$

\Rightarrow In mean field approximation-

$$\mathcal{H}_{\text{MFT}} = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c.) + U \sum_i (\langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow}) - U \sum_i \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle$$

(25/01/2023)

Mean-field approximation for the Hubbard model:

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c.) + U \sum_i (\langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow})$$

$$-U \sum_i \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle \rightarrow \begin{array}{l} \text{UNRESTRICTED} \\ \text{MEAN-FIELD} \\ (\text{all sort of phases allowed}) \end{array}$$

Now we aren't left with any 4 operator terms. Hamiltonian is essentially a non-interacting system now.

$$H = \sum_{ij} T_{ij} b_i^\dagger b_j$$

However, we don't really know what $\langle \hat{n}_{i\uparrow} \rangle$ or $\langle \hat{n}_{i\downarrow} \rangle$ are. \therefore We don't even know some T_{ij} 's. \Rightarrow We use variational principle, assuming $\langle \hat{n}_{i\uparrow} \rangle$ & $\langle \hat{n}_{i\downarrow} \rangle$ to be parameters & minimize energy w.r.t. these parameters.

$$\begin{array}{c} \hat{n}_{i\uparrow} \\ || \\ \alpha_{i\uparrow} \end{array} \quad \begin{array}{c} \hat{n}_{i\downarrow} \\ || \\ \alpha_{i\downarrow} \end{array}$$

2 parameters per site: $\langle \hat{n}_{i\uparrow} \rangle$ and $\langle \hat{n}_{i\downarrow} \rangle$ $\forall i$

Say the # of sites $N \sim 10^3$

If a fermionic system is non-interacting, we only have a gaseous state. However, introducing the interaction like in the Hubbard model, we can expect to see a magnetically ordered states.

To explore the possibility of a ferromagnetic phase by assuming

$m_i \equiv \langle \hat{n}_{i\uparrow} \rangle - \langle \hat{n}_{i\downarrow} \rangle$ is same for all sites i.e. same magnetization # sites.

So, $a_{i\uparrow} = a_{\uparrow}$ $a_i \rightarrow$ RESTRICTED MEAN-FIELD (only checking for ferromagnetic phase)

$a_{i\downarrow} = a_{\downarrow}$

These restrictions don't necessarily force a ferromagnetic phase. Instead, this "checks" if such a phase even exists.

$$m \equiv \frac{\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle}{2} \Rightarrow \begin{aligned} \langle n_{\uparrow} \rangle &= n + m \\ \langle n_{\downarrow} \rangle &= n - m \end{aligned}$$

On performing a Fourier transform,

$$\mathcal{F}(c_{i\uparrow}^+ c_{i\uparrow}) = \tilde{c}_{k0}^+ \tilde{c}_{k0} \quad \begin{array}{l} \text{Number op. in R-space} \\ \downarrow \\ \text{Number op. in k-space} \end{array}$$

$$\hat{H} = \sum_{k,\sigma} (\varepsilon_k - \mu) \tilde{c}_{k\sigma}^+ \tilde{c}_{k\sigma} + U(n+m) \sum_k \tilde{c}_{k\downarrow}^+ \tilde{c}_{k\downarrow} + U(n-m) \sum_k \tilde{c}_{k\uparrow}^+ \tilde{c}_{k\uparrow}$$

input parameters: t, μ, U

$$\varepsilon_k \equiv -2t(\cos k_x + \cos k_y)$$

unknown parameter: n, m

Method 1: Variational method.

Calculate $\langle \hat{H} \rangle$ and minimize the expectation value w.r.t n & m to get the energies & parameter values in the ground state.

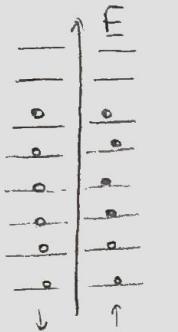
For finite temp., calculate $\langle \hat{H} \rangle_{\text{thermal}}$ & minimize w.r.t n & m .

self-consistency approach -

1. Start with some random values of $\langle \hat{n}_\uparrow \rangle$ & $\langle \hat{n}_\downarrow \rangle$.
2. Calculate $\langle \hat{H} \rangle$ with the new values.
3. Repeat for new $\langle \hat{n}_\uparrow \rangle$ & $\langle \hat{n}_\downarrow \rangle$ terms till $\langle H_{T+1} \rangle - \langle H_T \rangle \ll \epsilon^2$

Let's say our Hamiltonian only has the kinetic term, then -

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) \rightarrow \text{non interacting fermions.}$$

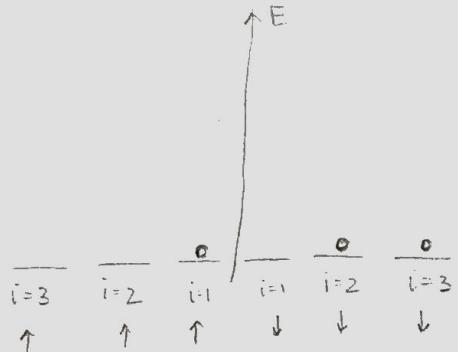


Prefers 2 fermions at each level k .

$$\langle n_{k\uparrow} \rangle - \langle n_{k\downarrow} \rangle = 0$$

Similarly, if we only had the U term, then -

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

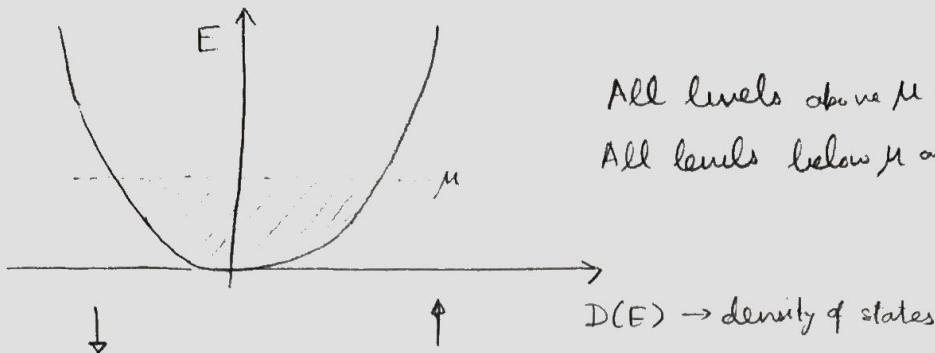


Prefers to put fermions in different sites. 2 fermions on same level/
same site is penalized

$$|\langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle| = 1.$$

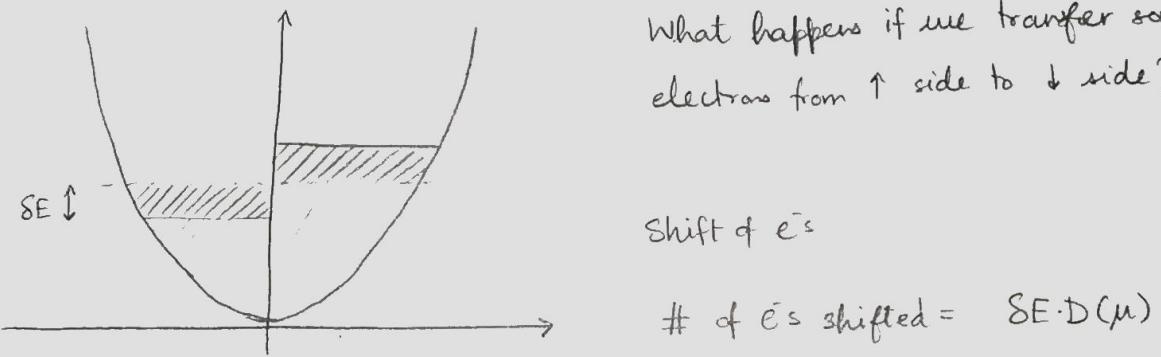
The extreme limits of the problem present competing preferences for filling.

Stoner's criterion:



All levels above μ are unfilled
All levels below μ are filled.

NO FERROMAGNETISM.



This perturbation introduces a change in energy in the U term of \hat{H}

$$\delta E_U = U(n + \delta n)(n - \delta n) - U(n)(n) = -U\delta n^2 < 0$$

⇒ By transferring e⁻s, we favour the U term by reducing energy.

However, if this was the only term, then all e⁻s would've transferred.

But we also have the Kinetic term.

$$\delta E_{\text{kinetic}} = \# \text{ of } e^- \text{'s leaving lower energy & going to a higher energy} \\ = \frac{\delta n \cdot \delta E}{D(\mu)} = \frac{1}{D(\mu)} \delta n^2 > 0$$

∴ Kinetic energy term is penalized if e^- 's go to a higher energy
i.e. they shift the zero magnetization balance.

$$(\delta E)_{\text{total}} = \left[\frac{1}{D(\mu)} - U \right] \delta n^2$$

Stoner's
criterion for
Hubbard model.

$$D(E_F) \cdot U > 1 \rightarrow \text{ferromagnetic state}$$

$$D(E_F) \cdot U < 1 \rightarrow \text{paramagnetic state.}$$

What about an anti-ferromagnetic state?

Lecture - 10

(06/02/2023)

Mean field theory of the Hubbard model.

$$\mu = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} + n_{i\downarrow}$$

To explore the presence of a ferromagnetic phase in HM, we perform a decoupling to explore that particular order parameter. (Last lecture)

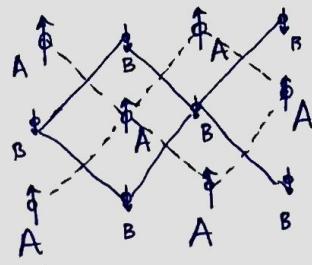
We will now do the same for antiferromagnetism.

We choose the ansatz with alternating up & down spins.



Ferrimagnetic phases.

A linear combination of ferro & antiferro.



$$\hat{H} = -t \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i + h.c.$$

In FM phase, we argued that $n_{i\uparrow} = n_{\uparrow}$ and $n_{i\downarrow} = n_{\downarrow}$

In AFM phase, we call $n_{i\uparrow} = n_{A\uparrow}$, $\begin{cases} i \in A \\ i \in B \end{cases}$

A, B are sublattices.

$$n_{i\downarrow} = n_{B\downarrow} \quad \begin{cases} i \in B \end{cases}$$

$$\begin{aligned} \langle n_{i\uparrow} \rangle &= n + (-1)^{i_x+i_y} m \\ \langle n_{i\downarrow} \rangle &= n - (-1)^{i_x-i_y} m \end{aligned} \quad \text{antiferromagnetic restriction.}$$

$$U \sum_i \hat{n}_{i\uparrow} \cdot \hat{n}_{i\downarrow} \stackrel{\text{approx}}{\approx} U \sum_i (\langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow})$$

$$\Rightarrow U \sum_i ((n + (-1)^{i_x+i_y} m) \hat{n}_{i\downarrow} + (n - (-1)^{i_x+i_y} m) \hat{n}_{i\uparrow})$$

$$= U \underbrace{\sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) n_{\pm}}_{\text{additional chemical pot.}} + U m \underbrace{\sum_i (-1)^{i_x+i_y} c_{i\downarrow}^+ c_{i\downarrow} - (-1)^{i_x+i_y} c_{i\uparrow}^+ c_{i\uparrow}}_{\text{new separated interaction with 2 operator terms.}}$$

AFM $\Rightarrow m \neq 0$ when at equilibrium. (free energy is min.)

Take a Fourier Transform on the entire lattice (always assume PBC)

$$-t \sum_{\langle ij \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.} \longrightarrow \sum_{\mathbf{k}, \sigma} -2t [\cos k_x + \cos k_y] C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma}$$

The same trick doesn't work for our mean field term since the $(-1)^{i_x+i_y}$
 i -dependence prevents us from taking the sum over i inside.

However, let's anyways go ahead with it.

$$(-1)^{i_x+i_y} = e^{i\vec{Q} \cdot \vec{r}_i} \quad \vec{Q} \equiv (\pi, \pi)$$

$$\sum_i e^{i\vec{Q} \cdot \vec{r}_i} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} - e^{+i\vec{Q} \cdot \vec{r}_i} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}$$

$$\hat{c}_{i\sigma} = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\vec{k} \cdot \vec{r}_i} \tilde{C}_{\mathbf{k}, \sigma}$$

$$\hat{c}_{i\sigma}^\dagger = \frac{1}{N} \sum_{\mathbf{k}} e^{i\vec{k} \cdot \vec{r}_i} \tilde{C}_{\mathbf{k}, \sigma}^\dagger$$

$$\sum_i \frac{1}{N} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} e^{i\vec{Q} \cdot \vec{r}_i} e^{i\vec{k} \cdot \vec{r}_i} e^{-i\vec{k}' \cdot \vec{r}_i} \tilde{C}_{\mathbf{k}\uparrow}^\dagger \tilde{C}_{\mathbf{k}'\downarrow}$$

$$\underbrace{\frac{1}{N} \sum_i \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\vec{Q} + \vec{k} - \vec{k}') \cdot \vec{r}_i} \tilde{C}_{\mathbf{k}}^\dagger \tilde{C}_{\mathbf{k}'\downarrow}}_{N \delta(\vec{k} + \vec{Q} - \vec{k}')} =$$

$$\tilde{C}_{\vec{k}\downarrow}^\dagger \tilde{C}_{\vec{k} + \vec{Q}\downarrow}^\dagger$$

↑ Kronecker

$$\Rightarrow H = -\epsilon_k \sum_{k,\sigma} \tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma} + U_m \sum_k (\tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k+Q,\downarrow} - \tilde{c}_{k+Q,\uparrow}^\dagger \tilde{c}_{k,\downarrow}) + -(\mu^* - U_n) \sum_k (\tilde{c}_{k\uparrow}^\dagger \tilde{c}_{k\downarrow} + \tilde{c}_{k\uparrow}^\dagger \tilde{c}_{k\downarrow})$$

But we still have a $\vec{k} - \vec{k} + \vec{Q}$ coupling! Not yet diagonal.

$$\sum_k (\tilde{c}_{k\uparrow}^\dagger \tilde{c}_{k+Q,\uparrow}^\dagger \tilde{c}_{k,\downarrow} \tilde{c}_{k+Q,\downarrow}^\dagger)$$

$$\begin{pmatrix} \epsilon_k + U_n - \mu, -U_m, 0, 0 \\ -U_m, \epsilon_{k+Q} + U_n - \mu, 0, 0 \\ 0, 0, \epsilon_k + U_n - \mu, +U_m \\ 0, 0, +U_m, \epsilon_{k+Q} + U_n - \mu \end{pmatrix} \begin{pmatrix} \tilde{c}_{k,\uparrow} \\ \tilde{c}_{k+Q,\uparrow} \\ \tilde{c}_{k,\downarrow} \\ \tilde{c}_{k+Q,\downarrow} \end{pmatrix}$$

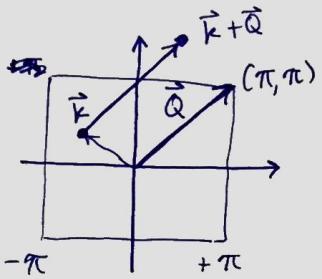
↑ block diagonal.

$$\epsilon_k = -2t(\cos k_x + \cos k_y)$$

of lattice sites in R space = # of points in k-space (BZ)

In R space, Hamiltonian of a N=10 site problem will be 20x20
(additional 2x terms due to spin) \Rightarrow 2N eigenvalues.

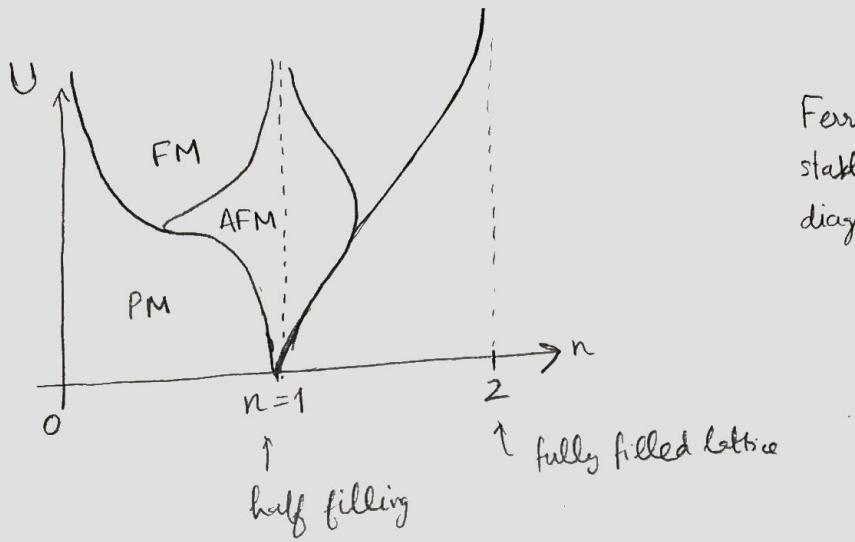
But our k-space Hamiltonian is giving us 4N eigenvalues.



since $\vec{k} + \vec{Q}$ can go outside the B.Z., we only sum over half of the \vec{k} points. Summing over just half of the k -values is enough since $\vec{k} + \vec{Q}$ cover the other half of them.

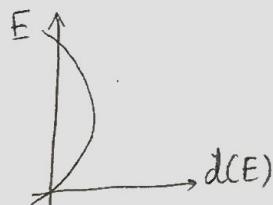
Lecture-11
 (07-02-2023)

Phase diagram of the Hubbard model under the mean field approximation in the restricted form for PM, FM, AFM

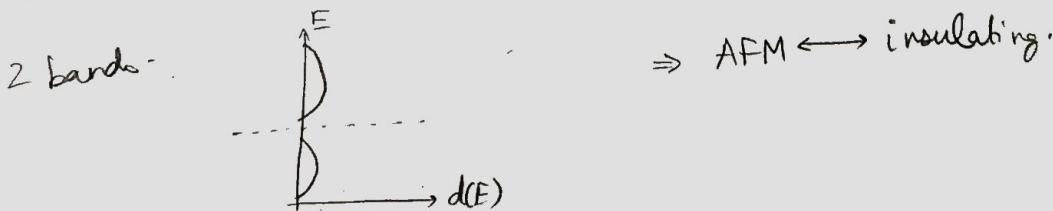


In the absence of interactions ($U=0$), the particles are free to move around the system is extended, which corresponds to a metallic state

$$\therefore \text{PM} \longleftrightarrow \text{metallic. } U=0 \xrightarrow{\quad} \text{PM} \xrightarrow{\quad} \text{PM}$$



However, in AFM, the unit cell of the lattice \neq unit cell of magnetic order as we have two sub lattices which causes the original BZ to split into



Spin-Structure Factor: measures the FT of the spin-pattern
(using neutron diffraction)

Tells us about periodicity in the nature of magnetic ordering.

$$S_{\vec{q}} = \sum_{ij} \vec{s}_i \cdot \vec{s}_j e^{i(\vec{r}_i - \vec{r}_j) \cdot \vec{q}}$$

locations at which peaks occur.

For a system with all spin↑

$$\begin{matrix} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \end{matrix}$$

$$\begin{aligned} S_{\vec{q}} &= \sum_{ij} \underbrace{\vec{s}_i \cdot \vec{s}_j}_{\substack{\parallel \\ 1}} e^{i(\vec{r}_i - \vec{r}_j) \cdot \vec{q}} \\ &= \sum_{ij} e^{i(\vec{r}_i - \vec{r}_j) \cdot \vec{q}} = \delta_{\vec{q}, \vec{0}} \Rightarrow \text{peak at } \vec{q} = \vec{0} \end{aligned}$$

For an antiferromagnetic system

$$\begin{matrix} \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ \downarrow & \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \end{matrix}$$

$$\begin{aligned} S_{\vec{q}} &= \sum_{ij} \underbrace{\vec{s}_i \cdot \vec{s}_j}_{\substack{\parallel \\ \text{alternates b/w } \pm 1}} e^{i(\vec{r}_i - \vec{r}_j) \cdot \vec{q}} \\ &= \sum_{ij} \dots \\ &= S_{\vec{q}, \vec{Q}} \text{ with } \vec{Q} = (\pi, \pi) \end{aligned}$$

↑↑↑↑↑↑↑↑
↓↓↓↓↓↓↓↓
↑↑↑↑↑↑↑↑

AFM

$$S_F = \sum_{ij} \vec{S}_i \cdot \vec{S}_j e^{i(\vec{r}_i - \vec{r}_j) \cdot \vec{q}}$$

$$= \delta_{\vec{q}, \vec{Q}} \quad \text{with } \vec{Q} = (0, \pi)$$

In general, we can look for arbitrary ordering $\vec{Q} = (q_x, q_y)$. These are single \vec{Q} -states with a single peak.

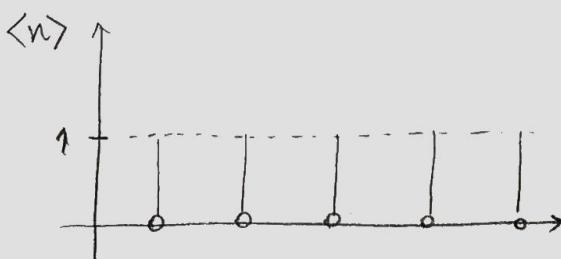
For ferrimagnet, we get peaks at $\vec{q} = (0, 0)$ AND $\vec{q} = (\pi, \pi)$ both. This is the simplest example of multi- \vec{Q} states.

THESE ARE ALSO CALLED SPIN-DENSITY WAVES. (ALTERNATING/MODULATING PATTERN)

Apart from magnetic ordering, we can also have a look at a different order parameter in our problem. One such order parameter is average particle number.

$$\langle \hat{n}_i \rangle = \frac{\langle \hat{n}_{i\uparrow} \rangle + \langle \hat{n}_{i\downarrow} \rangle}{2}$$

In the $U=0$ limit (no interactions, only pure hopping)



Expectation value in a N-particle state.

The particle is equally likely to be at each site.

Extended Hubbard model

$$\hat{H}_{EHM} = \hat{H}_{HM} + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

In the EHM, charge density waves are stable. This is because the V term wants \hat{n}_i, \hat{n}_j to be as low as possible.



These are all conventional-ordered phases. (can write a Landau free-energy function for a given order parameter).

Lecture - 12

(08-02-2023)

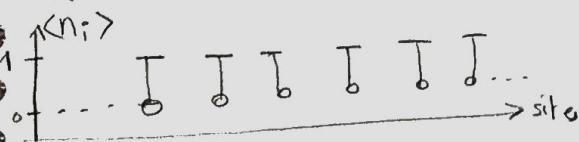
We discussed different kinds of orders in the HM.

Example of local order averages - $\langle \vec{m}_i \rangle, \langle n_i \rangle$

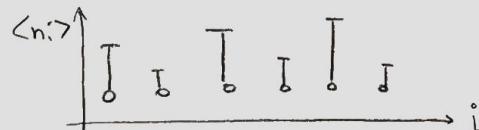
\uparrow magnetization \downarrow density + e^-

ORDERING OF CHARGE DENSITY

For non-interacting model,



In interacting EHM,

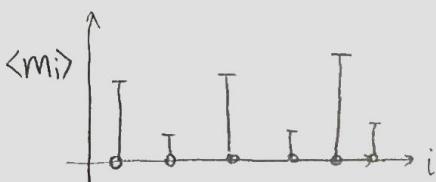


CHARGE-DENSITY WAVES

$n_{\vec{q}}$

ORDERING OF MAGNETIZATION.

Analogous to charge-density wave, the ordering where we have a modulation in avg. magnetization.



SPIN-DENSITY WAVES.



SPIRAL STATES ($\text{single } \vec{Q} \text{ state}$)

SUPERCONDUCTIVITY IN THE HUBBARD MODEL.

(new local variable
regd. to characterize phases)

$$\hat{H} = -t \sum_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - M \sum_{i,\sigma} \hat{n}_{i\sigma}$$

ATTRACTIVE HUBBARD
MODEL

electron phonon coupling??

$$\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} = \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \sim \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rightarrow kill 2 particles$$

$+ \langle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rangle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rightarrow creates 2 particles$

$$-t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{j\sigma}) = (c_{i\uparrow}^\dagger \quad c_{i\downarrow}^\dagger) \begin{pmatrix} -t & 0 \\ 0 & -t \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{pmatrix} \rightarrow \text{diagonal or block-diagonal}$$

How to even write the interaction term as a matrix??

Let's start with a single energy level

— E_0

$$\begin{aligned} H &= E_0 c^\dagger c = E_0 (1 - c c^\dagger) \\ &= \frac{1}{2} [E_0 c^\dagger c - E_0 c c^\dagger] + \frac{E_0}{2} \end{aligned}$$

For fermions, $c c^\dagger + c^\dagger c = 1$

particle-hole transformation

$$\begin{aligned} c &\leftrightarrow h^\dagger \\ c^\dagger &\leftrightarrow h \end{aligned}$$

$$\Rightarrow h^\dagger h + h h^\dagger = 1$$

$$\text{and } H = \frac{1}{2} [E_0 c^\dagger c - E_0 h^\dagger h] + \frac{E_0}{2}$$

Given the vacuum $|0\rangle$,

$$c^\dagger |0\rangle = 0, \quad h^\dagger h |0\rangle = 1$$

$$\Rightarrow H|0\rangle = \frac{1}{2} [0 - \varepsilon_0] + \frac{\varepsilon_0}{2} = 0 \quad \text{as expected.}$$

$$(c^\dagger \quad h^\dagger) \begin{pmatrix} \varepsilon_0/2 & 0 \\ 0 & -\varepsilon_0/2 \end{pmatrix} \begin{pmatrix} c \\ h \end{pmatrix} = (c^\dagger \quad c) \begin{pmatrix} \varepsilon_0/2 & 0 \\ 0 & -\varepsilon_0/2 \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

We have retained the particle (\hat{c}) and hole (\hat{h}) description simultaneously.

Using this motivation for the Hubbard model interaction term-

$$(c_{i\uparrow}^\dagger \quad c_{i\downarrow}^\dagger \quad c_{i\uparrow} \quad c_{i\downarrow}) \begin{pmatrix} -\mu & 0 & 0 & -U\Delta_i \\ 0 & -\mu & +U\Delta_i & 0 \\ \hline 0 & U\Delta_i^* & \mu & 0 \\ -U\Delta_i^* & 0 & 0 & \mu \end{pmatrix} \begin{pmatrix} c_{i\uparrow}^\dagger \\ c_{i\downarrow}^\dagger \\ c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$$

where $\Delta_i \equiv \langle c_{i\uparrow} c_{i\downarrow} \rangle$

Eigen states of such a matrix would be a linear combination

$$\sim \alpha c^\dagger + \beta c$$

↑ ↑
particle exists particle doesn't

If $\alpha = \beta$
 $\Rightarrow (c + c^\dagger)$

MAJORANA
FERMIONS.

Δ_i acts now like a new local order parameter.

↑

Pairing amplitude.

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) - U\Delta \sum_i (c_{i\uparrow}^+ c_{i\downarrow}^+ + h.c.)$$

$\Delta_i = \underline{\Delta} + i$ and $\Delta \in \mathbb{R}$.

We use the BCS assumption that

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\vec{k} \cdot \vec{r}_i} \tilde{c}_{k\sigma}$$

$$\begin{aligned} \sum_i c_{i\uparrow}^+ c_{i\downarrow}^+ &= \frac{1}{N} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \sum_i e^{i(\vec{k} + \vec{k}') \cdot \vec{r}_i} \tilde{c}_{k\uparrow}^+ \tilde{c}_{k'\downarrow} \\ &= \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \left(\frac{1}{N} \sum_i e^{i(\vec{k} + \vec{k}') \cdot \vec{r}_i} \right) \tilde{c}_{k\uparrow}^+ c_{k'\downarrow} \\ &= \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \delta_{\vec{k}, -\vec{k}'} \tilde{c}_{k\uparrow}^+ \tilde{c}_{k'\downarrow} \\ &= \sum_{\mathbf{k}} \tilde{c}_{k\uparrow}^+ \tilde{c}_{k\downarrow} \end{aligned}$$

$$\Rightarrow -U\Delta \sum_i (c_{i\uparrow}^+ c_{i\downarrow}^+ + h.c.) = -U\Delta \sum_{\mathbf{k}} (\tilde{c}_{k\uparrow}^+ \tilde{c}_{-k\downarrow} + h.c.)$$

Lecture-13

(13-02-2023)

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) - U \underbrace{\sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}_{\text{pairing term}}$$

Mean field approx. for pairing term.

$$-U \sum_i \Delta_i^* c_{i\uparrow}^+ c_{i\downarrow} + \Delta_i^* c_{i\uparrow} c_{i\downarrow}$$

$$\text{where } c_{i\uparrow}^+ c_{i\uparrow} c_{i\downarrow}^+ c_{i\downarrow} \rightarrow \langle c_{i\uparrow}^+ c_{i\downarrow} \rangle c_{i\uparrow} c_{i\downarrow} + \langle c_{i\downarrow} c_{i\uparrow} \rangle c_{i\uparrow}$$

In momentum space,

$$H = \sum_{k, \sigma} (\varepsilon_k - \mu) c_{k\sigma}^+ c_{k\sigma} - U \Delta \sum_k [c_{k\uparrow}^+ c_{-k\downarrow}^+ + h.c.]$$

where we use the ferromagnetic assumption $\Delta_i^* = \Delta_i = \Delta$

We do realize that our H isn't really diagonal.

$$(c_{k\uparrow}^+ c_{-k\downarrow}^+ c_{k\downarrow}^+ c_{-k\uparrow}) \begin{pmatrix} \varepsilon_k - \mu & -U\Delta & 0 & 0 \\ U\Delta^* & -[\varepsilon_{-k} - \mu] & 0 & 0 \\ 0 & 0 & \varepsilon_k - \mu & +U\Delta \\ 0 & 0 & +U\Delta^* & -[\varepsilon_{-k} - \mu] \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^+ \\ c_{k\downarrow} \\ c_{-k\uparrow}^+ \end{pmatrix}$$

$$A_{ij} c_{-k\downarrow}^+ c_{-k\uparrow}^+ = -A_{ij} c_{-k\downarrow}^+ c_{k\downarrow} = -A_{ij} (c_{k\downarrow}^+ c_{k\downarrow})|_{k=-k}$$

If we were to diagonalize the \vec{k} -space Hamiltonian, we would get $2N$ energy eigenvalues.

in \vec{k} -space

But if we use the pairing term idea by introducing particles & holes,
 (k) $(-k)$,
we get $4N$ energy eigenvalues (one duplicate for each level).

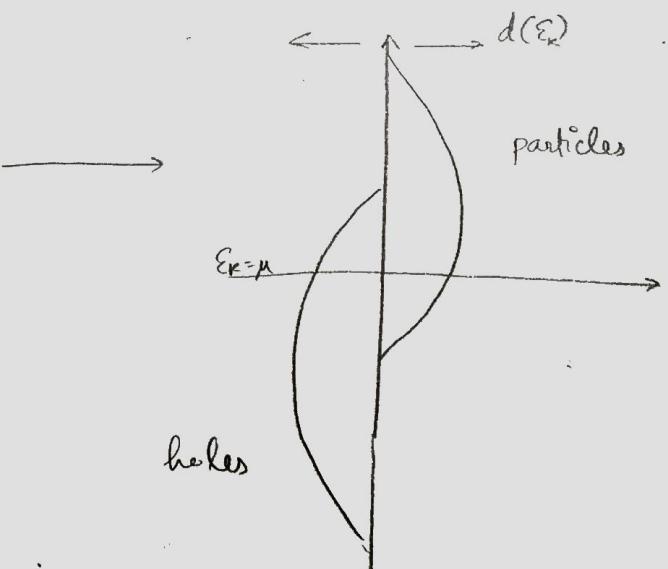
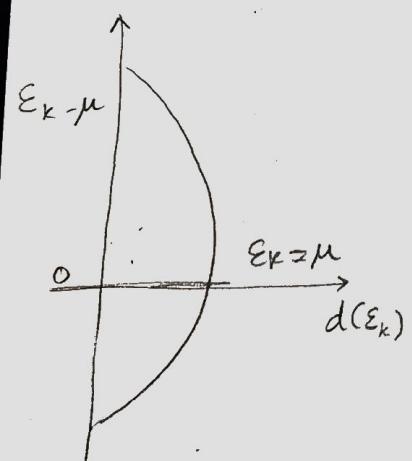
$$\psi_k = \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^+ \\ c_{k\downarrow} \\ c_{-k\uparrow}^+ \end{pmatrix} \rightarrow \text{our elements don't really have the creation & annihilation operators of same site/momenta appearing together.}$$

$$E_k = \pm \sqrt{(E_k - \mu)^2 + |U\Delta|^2} \rightarrow \text{eigenvalues of the full Hamiltonian}$$

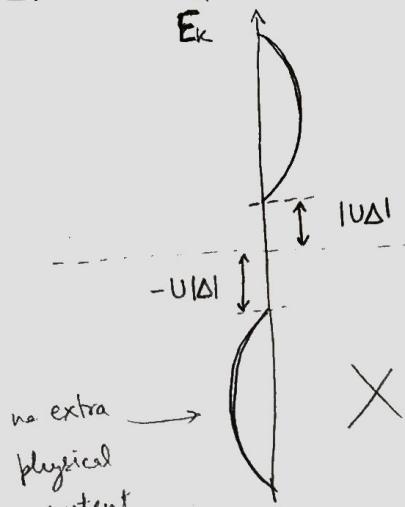
Before pairing

$$\Delta = 0$$

For mathematical convenience



After pairing



$\downarrow d(E_k)$

vacuum state \equiv superconducting state

$| \Psi_{sc} \rangle = \text{vacuum of quasi-particles}$

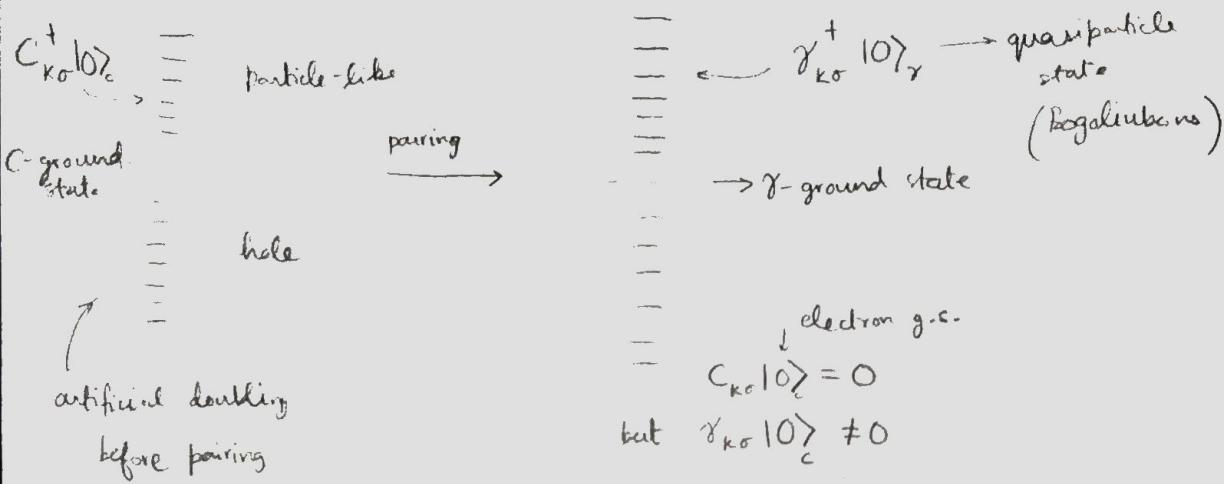
(similar to Dirac vacuum of all-filled negative E levels.)

Lecture - 14

(14-02-2023)

References for superconductivity in Hubbard model:

- Jian-Xin Zhu "Bogoliubov - de Gennes method and its application"



Bogoliubov transformation

$$c_{k\uparrow} = u_k^* \gamma_{k\uparrow} + v_k \gamma_{-k\uparrow}^+$$

$$c_{-k\downarrow}^+ = -v_k^* \gamma_{k\uparrow} + u_k \gamma_{-k\downarrow}^+$$

We want the same anti-commutation relations for γ -operators as well.

$$\text{i.e. } \{\gamma_{k\sigma}, \gamma_{k'\sigma'}^+\} = \delta_{kk'} \delta_{\sigma\sigma'}$$

$$\{\gamma_{k\sigma}, \gamma_{k'\sigma'}\} = 0 = \{\gamma_{k\sigma}^+, \gamma_{k'\sigma'}^+\}$$

Conditions on u_k, v_k ? $\Rightarrow \boxed{|u_k|^2 + |v_k|^2 = 1}$

$$\begin{pmatrix} C_{k\uparrow} \\ + \\ C_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k^* & v_k \\ -v_k^* & u_k \end{pmatrix} \cdot \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^+ \end{pmatrix}$$

$$U = \begin{pmatrix} u_k^* & v_k \\ -v_k^* & u_k \end{pmatrix} \Rightarrow U^{-1} = U^\dagger = \begin{pmatrix} u_k & -v_k \\ v_k^* & u_k^* \end{pmatrix}$$

$$\therefore \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^+ \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} C_{k\uparrow} \\ + \\ C_{-k\downarrow} \end{pmatrix}$$

The original Hamiltonian looked like-

$$\hat{H} = \sum_{k,\sigma} \varepsilon_k C_{k\sigma}^\dagger C_{k\sigma} - \sum_k [\Delta_k C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger + h.c.]$$

Substituting with $c \rightarrow \gamma$ gives terms of the type $\gamma^+ \gamma$, $\gamma^+ \gamma^+$, $\gamma \gamma$.

To diagonalize the Hamiltonian, we'll end up imposing another condition i.e.

$$\underbrace{(\text{coeff. of } \gamma^+ \gamma^+)}_{=0}$$

$$\Rightarrow \boxed{2\varepsilon_k u_k v_k - \Delta_k u_k^2 + \Delta_k^* v_k^2 = 0}$$

After some algebra, we arrive at the condition that

$$|U_k|^2 = \frac{1}{2} \left(1 + \frac{\varepsilon_k}{E_k} \right) \quad E_k \equiv \sqrt{\varepsilon_k^2 + \Delta_k^2}$$

$$|V_k|^2 = \frac{1}{2} \left(1 - \frac{\varepsilon_k}{E_k} \right)$$

The states near $\varepsilon_k = 0$ have the most major effect on quasiparticles being a comparable combination of particle-like and hole states.

γ

$$\sim -C_{k\uparrow} + C_{-k\downarrow}^+$$

Now,

$$\gamma_{k\uparrow} = U_k C_{k\uparrow} - V_k C_{-k\downarrow}^+ \quad \text{How to connect } |0\rangle_c \text{ to } |\alpha\rangle_r?$$

$$\gamma_{-k\downarrow}^+ = V_k^* C_{k\uparrow} + U_k^* C_{-k\downarrow}^+$$

Now let's say we operate all possible γ 's on $|0\rangle_c$

$$\gamma_{k_1\uparrow} \gamma_{-k_1\downarrow} \gamma_{k_2\uparrow} \gamma_{-k_2\downarrow} \dots \gamma_{k_3\uparrow} \dots |0\rangle_c$$

However, applying just one more γ will imply a repetition of γ and $\gamma\gamma=0$

$$\Rightarrow \gamma_{k'\sigma'} [\gamma_{k_1\uparrow} \gamma_{-k_1\downarrow} \gamma_{k_2\uparrow} \gamma_{-k_2\downarrow} \dots |0\rangle_c]$$

$$\Rightarrow |0\rangle_\gamma \equiv \left(\prod_k \gamma_{k\uparrow} \gamma_{-k\downarrow} \right) |0\rangle_c$$

$$|0\rangle_g = \prod_k \left(u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \right) |0\rangle_c$$

Schrieffer wavefunction.

$$b_k^\dagger = c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$$

Lecture-15
 (16-02-2023)

$$|\Psi_{BCE}\rangle = |0\rangle_y = \prod_k (u_k + v_k c_{k\uparrow}^+ c_{-k\downarrow}^+) |0\rangle$$

How does this lead to current without dissipation?

Coherent states: Eigenstates of annihilation operators

$$\text{In QM, } \hat{b}|a\rangle = a|a\rangle \Rightarrow |a\rangle = e^{ab^\dagger} |0\rangle$$

$$|a\rangle = e^{ab^\dagger} |0\rangle \sim \underline{\quad} + \underline{\quad} + \underline{\quad} + \underline{\quad} + \underline{\quad} + \dots$$

superposition of bosons in increasing # in the same state with diff prefactors

$$\begin{aligned} |a\rangle &= e^{ab^\dagger} |0\rangle = \sum_{n=0}^{\infty} \frac{(ab^\dagger)^n}{n!} |0\rangle = \sum_{n=0}^{\infty} \frac{a^n}{\sqrt{n!}} \underbrace{\frac{(b^\dagger)^n}{\sqrt{n!}}}_{|n\rangle} |0\rangle \\ &= \sum_{n=0}^{\infty} \frac{a^n}{\sqrt{n!}} |n\rangle \end{aligned}$$

To prove that this is a coherent state,

$$\begin{aligned} \hat{b}|a\rangle &= \sum_{n=0}^{\infty} \frac{a^n}{\sqrt{n!}} \hat{b}|n\rangle = \sum_{n=1}^{\infty} \frac{a^n}{\sqrt{n!}} \sqrt{n} |n-1\rangle \\ &= a \sum_{n=1}^{\infty} \frac{a^{n-1}}{\sqrt{(n-1)!}} |n-1\rangle = a \sum_{n'=0}^{\infty} \frac{a^{n'}}{\sqrt{n'!}} |n'!\rangle = a|a\rangle \end{aligned}$$

$$\langle \alpha | \alpha \rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} e^{i\alpha m^2} = e^{|\alpha|^2} \neq 1$$

The coherent states don't have the property $\langle \alpha | \alpha' \rangle \neq 0$ also because they are just two arbitrary states $\in \mathcal{H}$.

Writing $\alpha = |\alpha| e^{i\phi}$,

Action of $(-i\partial_\phi)$ on the coherent state?

$$\begin{aligned} -i \frac{\partial}{\partial \phi} \sum_{n=0}^{\infty} \frac{|\alpha|^n e^{in\phi}}{\sqrt{n!}} |n\rangle &= -i \sum_{n=0}^{\infty} |\alpha|^n (in) \frac{e^{in\phi}}{\sqrt{n!}} |n\rangle \\ &= \sum_{n=0}^{\infty} n \cdot \frac{|\alpha|^n e^{in\phi}}{\sqrt{n!}} |n\rangle = \sum_{n=0}^{\infty} \frac{n \alpha^n |n\rangle}{\sqrt{n!}} \\ &= 0|0\rangle + 1|\alpha e^{i\phi}|1\rangle + 2 \frac{|\alpha|^2 e^{2i\phi}}{\sqrt{2!}} |2\rangle + 3 \frac{|\alpha|^3 e^{3i\phi}}{\sqrt{3!}} |3\rangle + \dots \end{aligned}$$

looks like a \hat{n} operator.

$$\hat{n} \equiv -i \frac{\partial}{\partial \phi}$$

↑
like a momentum
operator.

The phase of the α and the number operator are related!

Coming back to superconductivity,

$P_k^+ \equiv c_{k\uparrow}^+ c_{-k\downarrow}^+$. What does this operator do?

- $[P_k^+, P_{k'}^+] = [c_{k\uparrow}^+ c_{-k\downarrow}^+, c_{k'\uparrow}^+ c_{-k'\downarrow}^+]$
 $= \underbrace{c_{k\uparrow}^+ c_{-k\downarrow}^+ c_{k\uparrow}^+ c_{-k\downarrow}^+}_{=0} - c_{k\uparrow}^+ c_{-k\downarrow}^+ c_{k\uparrow}^+ c_{-k\downarrow}^+$
 $= c_{k'\uparrow}^+ c_{-k'\downarrow}^+ c_{k\uparrow}^+ c_{-k\downarrow}^+ - c_{k'\uparrow}^+ c_{k\downarrow}^+ c_{k\uparrow}^+ c_{-k\downarrow}^+ = 0$
- $[P_k, P_k^+] = [c_{-k\downarrow} c_{k\uparrow}, c_{k\uparrow}^+ c_{-k\downarrow}^+]$
 $= c_{-k\downarrow} c_{k\uparrow} c_{k\uparrow}^+ c_{-k\downarrow}^+ - \underbrace{c_{k\uparrow}^+ c_{-k\downarrow}^+ c_{-k\downarrow} c_{k\uparrow}}_{(n_{-k\downarrow})}$
 $= 1 - \hat{n}_{k\uparrow} - \hat{n}_{-k\downarrow}$

Now, the BCS state can be written in terms of new coherent states, which we present as follows-

$$|\psi_{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^+ c_{-k\downarrow}^+) |0\rangle \approx \prod_k (1 + g_k c_{k\uparrow}^+ c_{-k\downarrow}^+) |0\rangle$$

Pseudo-fermionic operator: $\tilde{b}^+ = \sum_k g_k P_k$

We can now prove that $|\psi_{BCS}\rangle = |\alpha\rangle = e^{\alpha \tilde{b}^+} |0\rangle$

$$e^{\alpha \tilde{b}^\dagger} |0\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} (\tilde{b}^\dagger)^n |0\rangle$$

$$(P_k^+)^2 = (C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger)^2 = C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger = -(C_{k\uparrow}^\dagger)^2 (C_{-k\downarrow}^\dagger)^2 = 0$$

$$\Rightarrow (P_k^+)^n = 0$$

and $e^{\alpha \tilde{b}^\dagger} |0\rangle \sim \sum_{n=0}^{\infty} \frac{\alpha^n \prod_k}{n!} e^{\alpha g_k P_k^+} |0\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \prod_k (1 + \alpha g_k P_k^+) |0\rangle$

$\Rightarrow |\psi_{BCS}\rangle$ is a coherent state of \tilde{b}^\dagger !

Allows for a macroscopic wavefn of N-particles.

Current in a superconductor

Start with a tight-binding model:

$$\hat{H} = -\tilde{t} \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i^\dagger)$$

How should a current operator look like for a tight-binding Hamiltonian?

First guess? $\frac{d}{dt} \hat{n}_i = i[H, \hat{n}_i]$



obtain a continuity eqn.

Lecture-16

(20 - 02 - 2022)

For the standard tight-binding model-

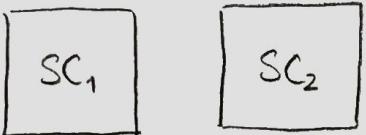
$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.)$$

then the current operator can be obtained via the continuity eqn of charge $c^\dagger c$.

$$\hat{j} = -it \sum_{\langle ij \rangle} [c_i^\dagger c_j - c_j^\dagger c_i]$$

Current flow b/w superconductors?

SIS junction-



For a 2-site e^- problem, c_{10}^\dagger c_{20}^\dagger \Rightarrow

Similarly, by BCS theory, the total state of a SIS junction is given by coherent ground state.

$$\psi_L = \psi e^{i\theta_L} \quad \psi_R = \psi e^{i\theta_R}$$

The phase "difference"

$\theta_L - \theta_R$ is measurable.

$$H \sim -t [\psi_L^\dagger \psi_R + \psi_R^\dagger \psi_L]$$

The current flow b/w these superconductors is -

$$\hat{j}_s = -it [\psi_L^+ \psi_R - \psi_R^+ \psi_L] = -it [\psi^+ \psi e^{i(\theta_R - \theta_L)} - \psi^+ \psi e^{-i(\theta_R - \theta_L)}]$$
$$= -it \psi^+ \psi [e^{i\Delta\theta} - e^{-i\Delta\theta}] = \underline{2t \psi^+ \psi \sin(\theta_R - \theta_L)}$$

d.c. Josephson effect.

A phase difference b/w wavefn's of SC_1 & SC_2
causes a flow in current!

What, if we in addition, also apply a potential difference b/w SC_1 & SC_2 ?

Modification in the Hamiltonian due to the potⁿ diff-

$$\begin{array}{cc} SC_1 & SC_2 \\ (V_L) & (V_R) \end{array}$$

$$\hat{H}'_L = -2eV_L \hat{n}_L , \quad \hat{H}'_R = -2eV_R \hat{n}_R$$

Say we start with the superconductors in the state $\psi_L + \psi_R$, and
then we apply a potential.

$$i \frac{d\hat{\theta}_L}{dt} = [\hat{\theta}_L, \hat{H}'_L] = -2eV_L [\hat{\theta}_L, \hat{n}_L]$$

$$\text{Since } \hat{n}_L = -i \partial_{\theta_L}$$

$$i\hbar \frac{d}{dt} \hat{\theta}_L = \left[\hat{\theta}_L, \frac{d}{d\theta_L} \right] \cdot (-2ieV_L t) \Rightarrow \frac{d\theta_L}{dt} = -2eV_L \frac{t}{\hbar}$$

$$\Rightarrow \boxed{\frac{d}{dt} (\theta_L - \theta_R) = -\frac{2e}{\hbar} (V_L - V_R)}$$

the phase difference varies & the rate of change of $\Delta\theta$ is proportional to ΔV .

$$\Delta\theta = -\frac{2e}{\hbar} \Delta V \cdot t + \Delta\theta_0$$

\Rightarrow The Josephson current now looks like -

$$\dot{j}_s = 2t \sqrt{+} \sin \left(-\frac{2e}{\hbar} \Delta V \cdot t \right) \rightarrow \text{periodic response.}$$

a.c. Josephson effect!

Order of magnitude calculation

$$\Delta V = 10 \mu V \quad (\text{small voltage})$$

$$\omega = \frac{2e}{\hbar} \Delta V \Rightarrow f = \frac{e}{\hbar} \cdot \frac{\Delta V}{\pi} \approx 5 \text{ GHz.}$$

Lecture - 17

(21-02-2022)

last lecture on
conventional ordered phases
(S (spin), N (charge) = Δ (pairing amp.))

London equations (1935)

From Drude theory,

$$j_s = n_s e v$$

↑
density
& charge carriers

$$\Rightarrow \frac{\partial \vec{j}_s}{\partial t} = n_s e \frac{\partial \vec{v}}{\partial t} = \frac{n_s e^2 \vec{E}}{m}$$

accn $\frac{e\vec{E}}{m}$

The scattering of electrons is what introduces the resistance.

what about $\frac{\partial}{\partial t} (\vec{\nabla} \times \vec{j}_s)$?

$$\frac{\partial}{\partial t} (\vec{\nabla} \times \vec{j}_s) = \frac{ne^2}{m} \vec{\nabla} \times \vec{E} = -\frac{ne^2}{m} \frac{\partial_t \vec{B}}{m}$$

$$\Rightarrow \frac{\partial}{\partial t} \left[\vec{\nabla} \times \vec{j}_s + \frac{ne^2}{m} \vec{\nabla} \times \vec{A} \right] = 0$$

$$\Rightarrow \frac{\partial}{\partial t} \vec{\nabla} \times \left(\vec{j}_s + \frac{ne^2}{m} \vec{A} \right) = 0$$

Since circulating superconducting currents can't exist, the only physical solⁿ is to have .

$$\vec{j}_s + \frac{ne^2}{m} \vec{A} = 0 \Rightarrow \boxed{\vec{j}_s = -\frac{ne^2}{m} \vec{A}}$$

↑
true in the London gauge.

$$\vec{\nabla} \cdot \vec{A} = 0$$

$$\hat{n} \cdot \vec{A} = 0$$

Also leads to a simple explanation of Meissner effect.

$$\vec{\nabla} \times \vec{B} = \mu_0 \vec{j}_s + (\text{ignore for now}) = -\mu_0 \frac{n e^2}{m} \vec{A}$$

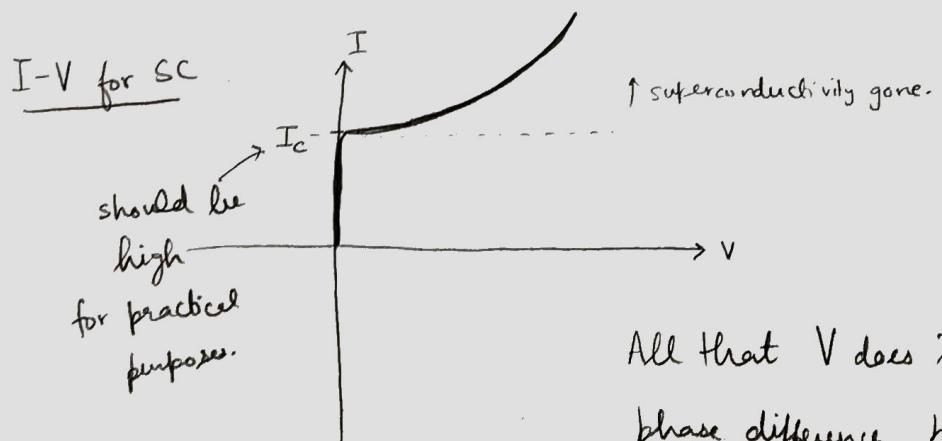
$$\vec{\nabla} \times (\vec{\nabla} \times \vec{B}) = -\mu_0 \frac{n e^2}{m} \vec{\nabla} \times \vec{A}$$

$$\Rightarrow \vec{\nabla}^2 \vec{B} = +\mu_0 \frac{n e^2}{m} \vec{B} \Rightarrow B_i \sim B_0 e^{-\alpha r_i}$$

London penetration depth $\equiv \lambda_L = \sqrt{\frac{m}{\mu_0 n e^2}}$

The proportionality of \vec{j}_s to \vec{A} makes sense in BCS theory as well because j_s in BCS theory $\propto \sin(\Delta\theta \cdot t) \approx \Delta\theta \cdot t \propto \phi \vec{A} \cdot d\vec{l} \cdot t$

The phase of the wavefunction is directly related to \vec{A} !



All that V does is introduce a phase difference b/w ends of a superconductor.

$$\vec{E} = -\vec{\nabla} V - \frac{\partial \vec{A}}{\partial t}$$

Lecture - 18
 (22-02-23)

TOPOLOGICAL PHASES OF MATTER.

Consider a single-particle system: $\hat{H}(t), |\psi(t)\rangle$

The eigenvalue eqn for the Hamiltonian is $\hat{H}(t) |\psi(t)\rangle = E(t) |\psi(t)\rangle$

Discretizing time & separating into many parts, $H(t) \rightarrow \{H(t_1), H(t_2), \dots, H(t_N)\}$

$$\Rightarrow \hat{H}(t_i) |\psi(t_i)\rangle = E(t_i) |\psi(t_i)\rangle \quad \text{for } i=1, \dots, N$$

(separated into many time-independent eqns)

To find the solution to the TDSE,

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$$

We propose an ansatz-

$$|\psi(t)\rangle = c(t) e^{-i\hbar \int_0^t dt' E(t')} |\phi(t)\rangle$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} |\psi\rangle = i\hbar \left[\dot{c}(t) e^{-i\hbar \int_0^t dt' E(t')} |\phi(t)\rangle + c(t) \left(\frac{-i}{\hbar} E(t) \right) e^{-i\hbar \int_0^t dt' E(t')} |\phi(t)\rangle \right]$$

(LHS)

$$(RHS) = c(t) e^{-i\hbar \int_0^t dt' E(t')} E(t) |\phi(t)\rangle$$

On rearranging, we get

$$\dot{c}(t) |\phi(t)\rangle = -c(t) |\dot{\phi}(t)\rangle$$

$$\Rightarrow \dot{c}(t) = -c(t) \langle \phi(t) | \dot{\phi}(t) \rangle$$

Integrating both sides, we get

$$c(t) = c_0 e^{-\int_0^t dt' \langle \phi(t') | \dot{\phi}(t') \rangle}$$

∴ The wavefunction ansatz can now be written as -

$$|\psi(t)\rangle = c_0 e^{i\gamma_c} e^{-i\hbar \int_0^t dt' E(t')} |\phi(t)\rangle$$

$$\text{where } \gamma_c = i \int_0^t dt' \langle \phi(t') | \dot{\phi}(t') \rangle$$

GEOMETRIC / BERRY
PHASE!

Consider now $\hat{H}(t) \equiv \hat{H}(\vec{R}(t))$

$$\Rightarrow \gamma_c = i \int_0^t dt' \langle \phi(\vec{R}(t')) | \dot{\phi}(\vec{R}(t)) \rangle$$

$$\text{Also, } \frac{d\phi(\vec{R}(t'))}{dt'} = \sum_{i=1}^n \frac{\partial \phi}{\partial R_i} \cdot \frac{dR_i}{dt'} = \vec{\nabla}_{\vec{R}} \phi \cdot \frac{d\vec{R}(t)}{dt}$$

$$\Rightarrow \gamma_c = i \int_{\vec{R}_i}^{\vec{R}_f} d\vec{R} \cdot \underbrace{\langle \phi(\vec{R}) | \vec{\nabla}_{\vec{R}} \phi(\vec{R}) \rangle}_{\text{Berry Vector potential}}$$

Berry Vector potential

\therefore Hamiltonians can be classified based on a non-zero value of γ_c in a closed-loop!

As an example, a 1D Hilbert space can't exhibit a non-trivial γ_c .

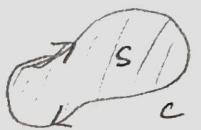
Lecture - 19

(27-02-2023)

Geometric phase around a closed loop

$$\gamma_c^{(n)} = \oint_C d\vec{R} \cdot \vec{A}_n(\vec{R})$$

where Berry vector potential $\vec{A}_n(\vec{R}) = i \langle \phi_n(\vec{R}) | \vec{\nabla}_{\vec{R}} \phi_n(\vec{R}) \rangle$



$$\Rightarrow \gamma_c^{(n)} = \int_S \vec{\Omega}_n \cdot d\vec{s} \quad \text{where } \vec{\Omega}_n \equiv \vec{\nabla}_{\vec{R}} \times \vec{A}_n(\vec{R})$$

↑
Berry curvature for eigenstate n.

What if we instead do an integral over the entire surface?

If we had a strict analogy with electromagnetism, $\oint_S d\vec{S} \cdot \vec{A}_n = 0$.

However, in our problem, generally -

$$\oint_S d\vec{S} \cdot \vec{\Omega}_n \neq 0 \rightarrow \text{topologically non-trivial phase.}$$

$$\oint_S d\vec{S} \cdot \vec{\Omega}_n = 0 \rightarrow \text{topologically trivial phase.}$$

Some other expressions -

$$\circ \langle \phi_m(\vec{R}) | \vec{\nabla}_R \phi_n(\vec{R}) \rangle = \frac{\langle \phi_m(\vec{R}) | \vec{\nabla} H | \phi_n(\vec{R}) \rangle}{E_n - E_m}$$

$$\circ \vec{\Omega}_n = i \sum_{m \neq n} \frac{\langle \phi_n(\vec{R}) | \vec{\nabla}_R H | \phi_m(\vec{R}) \rangle}{(E_n - E_m)^2} \times \langle \phi_m(\vec{R}) | \vec{\nabla}_R H | \phi_n(\vec{R}) \rangle$$

General form of Hamiltonians in Bloch-basis -

$$\hat{H} = \sum_{\vec{k}} \hat{h}(\vec{k}) = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^{\dagger} c_{\vec{k}}$$

If $\epsilon(\vec{k})$ is a number, it is a single band Hamiltonian \rightarrow 1D fl.

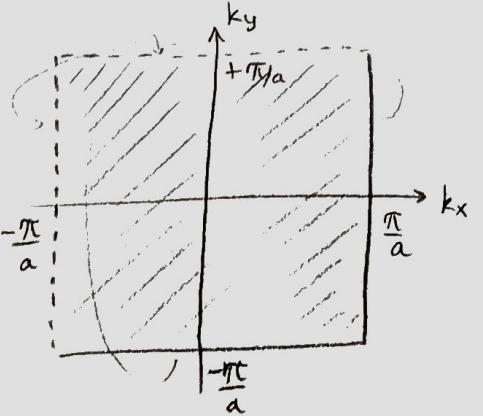
However, for $n \geq 2$ band structure, $\epsilon(\vec{k})$ is a matrix \rightarrow nD fl.

Here, \vec{k} acts like the parameter \vec{R} .

Our main interest lies in finding $\oint_S \vec{\Omega} \cdot d\vec{s} \neq 0$.

For a solid-state problem, $\rightarrow \oint_S \vec{\Omega}^n(\vec{k}) \cdot d\vec{s} \neq 0$

The closed surface integral now corresponds to an integral over the Brillouin zone due to the periodicity of a B.Z.



In n-D, the B.Z. is a nD torus.

This integral over B.Z. is similar to conductance expression

$$\sigma_{ij} \propto \oint_{BZ} V_i V_j \left(-\frac{\partial f}{\partial \epsilon} \right) d^2k$$

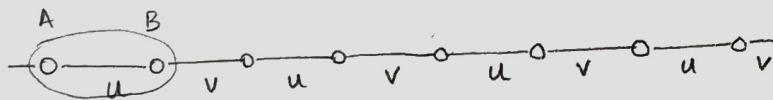
(Also gave a neat explanation of integer QHE)

$$\oint \vec{\Omega}^n(\vec{k}) \cdot d\vec{k} = 2\pi v_n$$

↳ Chern number (TKNN index)

and $\sum_n v_n = 0$

SSH model. (Su - Schrieffer - Heeger)



$$\hat{H} = u \sum_i (c_{iA}^\dagger c_{iB} + h.c.) + v \sum_i (c_{iB}^\dagger c_{i+1,A} + h.c.)$$

$$= \sum_k \begin{pmatrix} c_{kA}^\dagger & c_{kB}^\dagger \end{pmatrix} \begin{pmatrix} 0 & (u+v e^{ik}) \\ (u+v e^{-ik}) & 0 \end{pmatrix} \begin{pmatrix} c_{kA} \\ c_{kB} \end{pmatrix}$$



$$A_\pm = i \langle \phi^\pm | \partial_k \phi^\pm \rangle$$

Firstly, we need the eigenstates of this Hamiltonian in the k -space.

$$|\phi^+\rangle = \begin{pmatrix} x^+ \\ y^+ \end{pmatrix}, \quad |\phi^-\rangle = \begin{pmatrix} x^- \\ y^- \end{pmatrix}$$

$$A^+ = i \begin{pmatrix} (x^+)^* & (y^+)^* \end{pmatrix} \begin{pmatrix} \partial_k x^+ \\ \partial_k y^+ \end{pmatrix} \rightarrow \text{depends on the gauge (scaling) of the eigenvectors.}$$

However $\int_{-\pi}^{\pi} A^+ dk$ is an invariant.

Lecture-20
 (28-02-2023)

SSH model

$$\hat{H} = \sum_k \begin{pmatrix} C_{kA}^+ & C_{kB}^+ \end{pmatrix} \begin{pmatrix} 0 & u + v e^{-ik} \\ u + v e^{+ik} & 0 \end{pmatrix} \begin{pmatrix} C_{kA} \\ C_{kB} \end{pmatrix}$$

This problem is identical to the problem of spin- $\frac{1}{2}$ in magnetic field.

$$\hat{H} = \vec{B} \cdot \vec{\sigma} = \sum \left(\begin{array}{cc} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{array} \right) \left(\begin{array}{c} \sigma_x \\ \sigma_y \end{array} \right)$$

⇒ For the SSH model,

$$B_z = 0, \quad B_x(k) = u + v \cos k, \quad B_y(k) = v \sin k.$$

The eigenvalues of this matrix are $\pm \sqrt{B_x^2 + B_y^2 + B_z^2} = \pm |\vec{B}(k)|$

And the eigenvectors are of the form $\begin{pmatrix} \sin \theta/2 e^{-i\varphi} \\ \pm \cos \theta/2 \end{pmatrix}$

where $\vec{B} = |\vec{B}(k)| \hat{n} = |\vec{B}(k)| \cdot (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$

$\Rightarrow \theta = \frac{\pi}{2}$ simply because $B_z = 0$. and $\varphi = \arctan \left(\frac{B_y}{B_x} \right)$

\Rightarrow eigenvectors are $\frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi} \\ \pm 1 \end{pmatrix}$

$$\Rightarrow \varphi_{(k)} = \arctan \left(\frac{v \sin k}{u + v \cos k} \right) \quad \text{and eigen} \vec{v} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi_{(k)}} \\ \pm 1 \end{pmatrix} \text{ with eigenvalues } \pm |\vec{B}(k)|$$

$$A^+ = \frac{i}{2} \left(e^{i\varphi} + 1 \right) \begin{pmatrix} -i e^{-i\varphi_k} \partial_k(\varphi_k) \\ 0 \end{pmatrix}$$

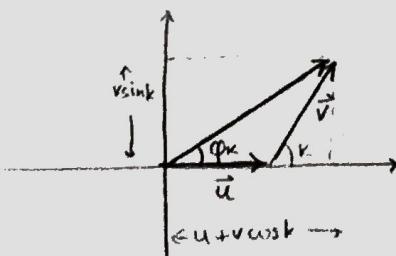
$$= \frac{1}{2} \frac{d\varphi_k}{dk} = \frac{1}{2} \frac{d}{dk} \left[\arctan \left(\frac{v \sin k}{u + v \cos k} \right) \right]$$

However A isn't a meaningful quantity. It is the Berry phase which is physically relevant.

$$\gamma_c = \oint_C dk A = \int_{-\pi}^{\pi} dk \frac{d\varphi_k}{dk} = \underbrace{\int_{\varphi(k=-\pi)}^{\varphi(k=+\pi)} d\varphi_k}_{\oint d\varphi_k} = \varphi(k=+\pi) - \varphi(k=-\pi)$$

If we were to interpret $B_x + iB_y$ as a complex #, then

$$B_x = u + v \cos k, \quad B_y = v \sin k.$$



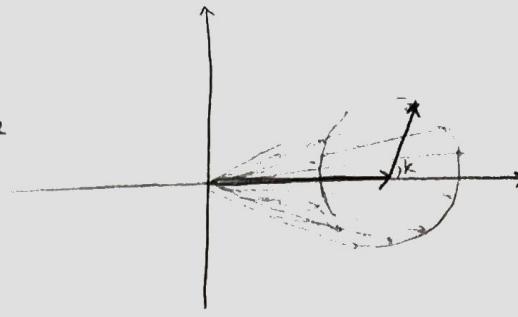
$\varphi_k = \text{phase of the complex } B_x + iB_y$

For $u > v$

On integrating over all the
k values,

$$\int d\varphi_k = 0$$

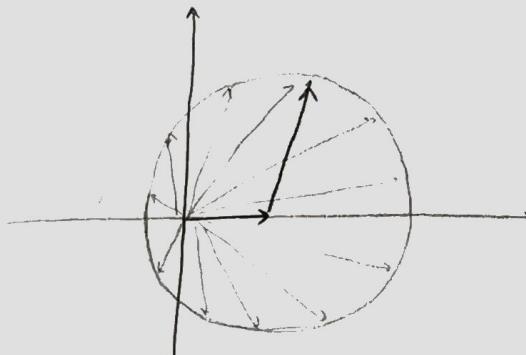
All φ_k 's cancel out.



For $u < v$

on integrating over all
values of k-values,

$$\int d\varphi_k = 2\pi$$



In conventional phases, there is a local variable which determines the ordering phase of the system.

However, topological phases are characterized completely by the structure of eigenvectors & eigenvalues of the problem in k-space.

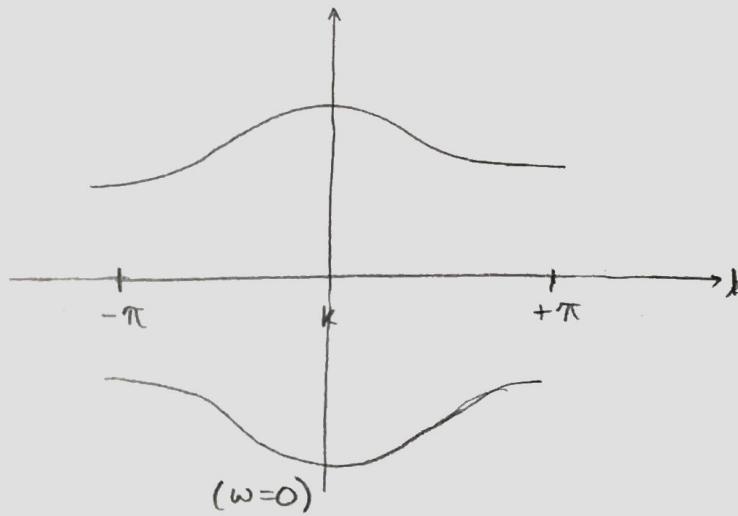
$$E^\pm(k) = \pm \sqrt{u^2 + v^2 + 2uv \cos k}$$

Let's analyze the band structure.

$$k=0 \Rightarrow (u+v)$$

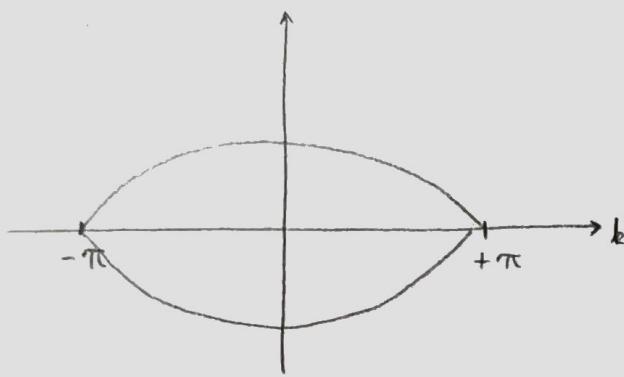
$$k=\pm\pi \Rightarrow |u-v|$$

- $u > v$



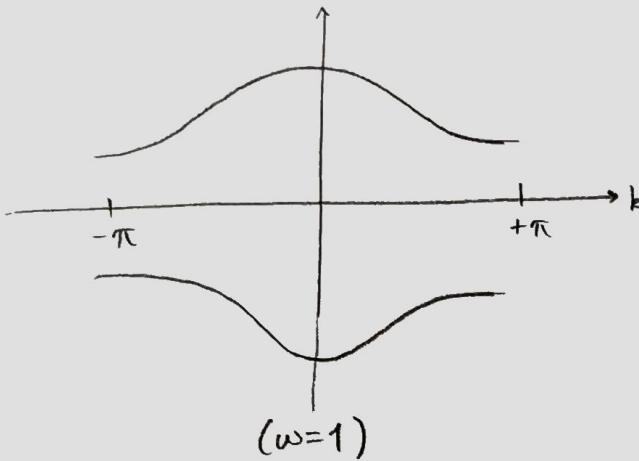
The band will look the same regardless of $u > v$ or $v > u$.

- $u = v$



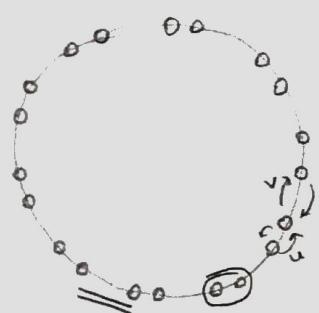
However for $u=v$, we have band gap closing at $\pm\pi$.

- $u < v$



Any topological phase transition is characterized by the closing of the band gap in the dispersion relation. Robert measure of a topological transition in non-interacting systems.

In the momentum space calculations, we have a periodic boundary condition \Rightarrow we have a periodic SSTI chain.



However, choosing different unit cells (\circ or $\circ\circ$) can cause an interchange in topological trivial or non-trivial phase. This is unphysical i.e. dependence of topological phase on what unit cell you choose.

\Rightarrow Any physical system which shows topological phase transitions must have open boundaries.

Bulk-Boundary correspondance (topological properties of the system appear on the boundary)

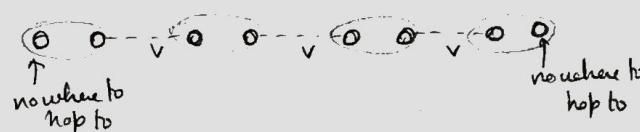


Cases:

(1) $v=0$ $\Rightarrow E = \pm u$ for each unit cell with bonding + antibonding eigenvalues



(2) $u=0$ $\Rightarrow E = \pm v$ in bulk, $0, 0$ for boundary



If the system is in a topologically non-trivial phase, the effect will show up as boundary modes in the system.

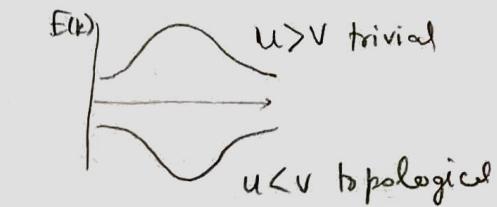
Lecture - 21

(20 - 03 - 2023)

Reminder: In SSH,

- $v=0, \Rightarrow E = \pm u$
- $u=0, \Rightarrow E = \pm v, 0, 0$

\downarrow
edge states



"Bulk-Boundary correspondence"

Topology in superconductors:

Kitaev's p -wave chain-

$$\hat{H} = -t \sum_i [c_i^\dagger c_{i+1} + h.c.] - \mu \sum_i c_i^\dagger c_i + \Delta \sum_i [c_i^\dagger c_{i+1}^\dagger + h.c.]$$

* doesn't have S index unlike attractive BHM. (works with just \uparrow or just \downarrow)

* no same-site interaction unlike attractive BHM.

\uparrow
interaction term

Let's try to diagonalize the Hamiltonian by taking the F.T.

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{-ikr_i} \tilde{c}_k$$

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{k'} e^{+ik'r_i} \tilde{c}_{k'}^\dagger$$

$$\sum_i (c_i^\dagger c_{i+1} + h.c.) \rightarrow 2 \sum_k \cos(k) c_k^\dagger c_k$$

$$\sum_i c_i^\dagger c_i \rightarrow \sum_k c_k^\dagger c_k$$

$$c_i^+ = \frac{1}{\sqrt{N}} \sum_k e^{+ikr_i} \tilde{c}_k^+$$

$$c_{i+1}^+ = \frac{1}{\sqrt{N}} \sum_{k'} e^{+ik'r_i} \tilde{c}_{k'}^+$$

$$\sum_i c_i^+ c_{i+1}^+ = \left(\frac{1}{N} \sum_{k, k'} \sum_i e^{ikr_i} e^{ik'r_i} \right) e^{ik'} \tilde{c}_k^+ \tilde{c}_{k'}^+ = \sum_k e^{-ik} \tilde{c}_k^+ \tilde{c}_{-k}^+$$

$$\sum_i c_{i+1}^+ c_i^+ = \left(\frac{1}{N} \sum_{k, k'} \sum_i e^{ikr_i} e^{ik'r_i} \right) e^{ik} \tilde{c}_k^+ \tilde{c}_{k'}^+ = \sum_k e^{ik} \tilde{c}_k^+ \tilde{c}_{-k}^+$$

$$\text{Now, } \sum_i c_i^+ c_{i+1}^+ + h.c. = \frac{1}{2} \sum_i [c_i^+ c_{i+1}^+ - c_{i+1}^+ c_i^+ + h.c.] \\ \pm \sum_k (\text{isink}) c_k^+ c_{-k}^+ + h.c.$$

$$\Rightarrow \hat{H} = \sum_k (-2t \cos k - \mu) \tilde{c}_k^+ \tilde{c}_k + \Delta \sum_k (\text{isink}) c_k^+ c_{-k}^+ + h.c.$$

We write the Hamiltonian in the "Number spinor" basis (combination of particles & holes)

$$(c_k^+ \quad c_{-k}) \begin{pmatrix} \frac{1}{2}(-2t \cos k - \mu) & i\Delta \text{sink} \\ -i\Delta \text{sink} & \frac{1}{2}(2t \cos k + \mu) \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^+ \end{pmatrix}$$

From our earlier discussion, any 2×2 matrix can be identified with

$$-\vec{B} \cdot \vec{\sigma}.$$

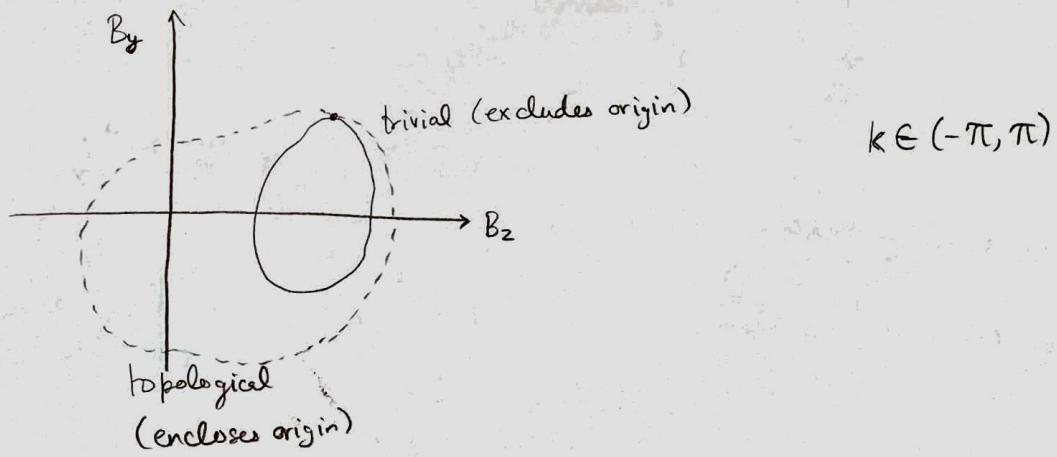
$$\begin{aligned} B_x &= 0 \\ B_y &= +\Delta \sin k \\ B_z &= +t \cos k + \frac{\mu}{2} \end{aligned} \quad \left. \begin{array}{l} \text{ } \\ \text{ } \\ \text{ } \end{array} \right\} \vec{B} \text{ lives in a plane} \Rightarrow \text{introduce the idea of "winding numbers"} \quad \text{!}$$

So, the vector in the y - z plane is - $B_y = \Delta \sin k$, $B_z = t \cos k + \frac{\mu}{2}$

Does this model show any topological phase transitions?

$$\text{Define } Z \equiv B_y + i B_z = (\Delta \sin k) + i \left(t \cos k + \frac{\mu}{2} \right)$$

Just like the SSH model, the Berry phase = $\oint d\phi_k = \text{winding \#}$. So we can use a similar analysis.



$$\text{At } k=0, Z = i \left(t + \frac{\mu}{2} \right)$$

$$\text{At } k=\pi, Z = i \left(\frac{\mu}{2} - t \right)$$

↑
only becomes negative if $t > \frac{\mu}{2}$

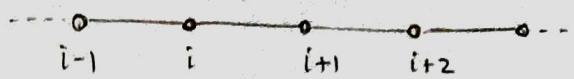
i.e. goes to the left of the origin.

\therefore The topological phase exists when

$$t > \frac{|\mu|}{2} \rightarrow \text{check!}$$

Majorana fermions (a major feature of Kitaev's model)

$$\hat{C} \equiv \hat{\gamma}_1 + i\hat{\gamma}_2$$



c_i, c_{i+1}

We can write $c_j = \frac{1}{2} (\gamma_{j,1} + i\gamma_{j,2})$ \Rightarrow $\begin{cases} \gamma_{j,1} = c_j + c_j^\dagger \\ \gamma_{j,2} = i(c_j^\dagger - c_j) \end{cases}$

$$c_j^\dagger = \frac{1}{2} (\gamma_{j,1} - i\gamma_{j,2})$$

Important property: $\gamma_{j,1}^\dagger = \gamma_{j,1}$
 $\gamma_{j,2}^\dagger = \gamma_{j,2}$

$$\{\gamma_i, \gamma_i^\dagger\} = 2$$

For normal fermions, $c_i c_i = 0$

But for Majorana fermions, $\gamma_{i,1} \gamma_{i,1} = 1$

Lecture - 22

(21-03-2023)

Reminder:

Kitaev's p-wave chain



$$\hat{H} = -t \sum_i (c_i^+ c_{i+1} + h.c.) + \Delta \sum_i c_i^+ c_{i+1}^+ + h.c. - \mu \sum_i c_i^+ c_i$$

Propose, $c_i = \frac{1}{2} (\gamma_{i,1} + i\gamma_{i,2})$ $\gamma_i^\dagger = \gamma_i$ Majorana operators.

$$c_i^+ = \frac{1}{2} (\gamma_{i,1} - i\gamma_{i,2})$$

Let's now consider the particular limit - $\mu=0, \Delta=-t$

Use $\{\gamma, \gamma'\} = 0$

$$\hat{H} = -t \sum_i \left[\frac{1}{4} (\gamma_{i,1} - i\gamma_{i,2})(\gamma_{i+1,1} + i\gamma_{i+1,2}) + h.c. \right]$$

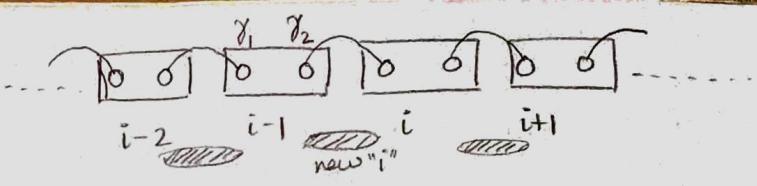
$$+ t \sum_i \left[\frac{1}{4} (\gamma_{i,1} - i\gamma_{i,2})(\gamma_{i+1,1} - i\gamma_{i+1,2}) + h.c. \right]$$

$$(\gamma_{i,1} - i\gamma_{i,2})(\gamma_{i+1,1} + i\gamma_{i+1,2}) = -\cancel{\gamma_{i,1}\gamma_{i+1,1}} + i\gamma_{i,1}\gamma_{i+1,2} + i\gamma_{i,2}\gamma_{i+1,1} \\ + \cancel{\gamma_{i,2}\gamma_{i+1,2}}$$

+

$$(\gamma_{i,1} - i\gamma_{i,2})(\gamma_{i+1,1} - i\gamma_{i+1,2}) = \cancel{\gamma_{i,1}\gamma_{i+1,1}} - i\gamma_{i,1}\gamma_{i+1,2} - i\gamma_{i,2}\gamma_{i+1,1} \\ - \cancel{\gamma_{i,2}\gamma_{i+1,2}}$$

Check = $\gamma_{i,2}\gamma_{i+1,1} (+it)$



Remember, for $|t\mu| < 2t \Rightarrow$ topologically non-trivial phase.

Since $\mu=0$, we are in a topologically non-trivial phase.

Our aim is to see the effect of Majorana fermions on the edge modes.

Define,

$$\gamma_{i+1,1} = \tilde{c}_i + \tilde{c}_i^\dagger$$

$$\gamma_{i,2} = i(\tilde{c}_i^\dagger - \tilde{c}_i)$$

The new i label of \tilde{c} doesn't represent the site. We instead half-shift it.

$$\hat{H} = it \sum_i \gamma_{i,2} \gamma_{i+1,1}$$

$\downarrow \tilde{c}$ transformation.

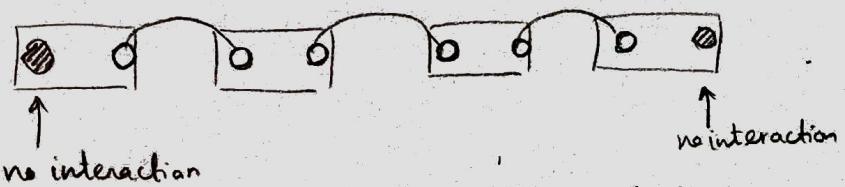
$$\hat{H} = it \sum_i i (\tilde{c}_i^\dagger - \tilde{c}_i)(\tilde{c}_i + \tilde{c}_i^\dagger)$$

$$-\tilde{c}_i \tilde{c}_i^\dagger = 1 + \tilde{c}_i^\dagger \tilde{c}_i$$

$$= -t \sum_i [\tilde{c}_i^\dagger \tilde{c}_i + \tilde{c}_i^\dagger \tilde{c}_i^{\dagger 0} - \tilde{c}_i \tilde{c}_i^0 - \tilde{c}_i \tilde{c}_i^\dagger]$$

$$= -t \sum_i [2\tilde{c}_i^\dagger \tilde{c}_i - 1]$$

Problem at the edge: In a real system, we have open boundaries.



Zero energy Majorana modes!

Why is this called a "p-wave" chain?

Symmetry property of superconducting pairing term

||

Symmetry property of superconducting ground state.

{
S-wave
p-wave
d-wave

For example, in BCS, $\Delta \underset{i}{\sum} c_{i\uparrow}^+ c_{i\downarrow}^+ = \Delta \left[\frac{c_{i\uparrow}^+ c_{i\downarrow}^+}{2} - \frac{c_{i\downarrow}^+ c_{i\uparrow}^+}{2} \right] \rightarrow$ singlet order

Since spin order is antisymmetric, then the spatial part must be symmetric
 $l=0, 2, 4, \dots$
(s-wave, d-wave, ---)

In our Kitaev's chain

$\Delta \underset{i}{\sum} c_{i\uparrow}^+ c_{i\uparrow}^+ \Rightarrow$ spatial part must be antisymmetric $l=1, 3, 5, \dots$
↑
triplet spin order
(p-wave, f-wave, ---)

Symmetry classification of topological order

Say our Hamiltonian

$$H = \sum_{ij} c_i^\dagger h_{ij} c_j$$

$$\text{Defining } \psi^+ \equiv (c_1^\dagger c_2^\dagger \dots c_N^\dagger) \Rightarrow H = \psi^+ h \psi$$

Now if we insert a set of unitaries in b/w -

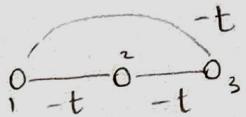
$$H = \underbrace{\psi^+}_{\tilde{\psi}^+} U^+ \underbrace{U h U^+}_{\tilde{h}} \underbrace{U \psi}_{\tilde{\psi}} = \tilde{\psi}^+ \tilde{h} \tilde{\psi}$$

$$\text{Operation on the Hamiltonian} \Rightarrow \tilde{h} = U h U^+$$

If $\tilde{h} = h$, then U is a symmetry of the Hamiltonian. This also means

$$[h, U] = 0 !$$

As an example, let's take a 3-site hopping problem



$$H = (c_1^\dagger c_2^\dagger c_3^\dagger) \begin{pmatrix} 0 & -t & -t \\ -t & 0 & -t \\ -t & -t & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

- Let's now consider a translation operator:

$$T_1 : \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} c_2 \\ c_3 \\ c_1 \end{pmatrix}$$

↑ shift by 1.

Let's check if this is a symmetry of h .

$$\begin{aligned} T_1^+ h T_1 &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -t & -t \\ -t & 0 & -t \\ -t & -t & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} -t & -t & 0 \\ 0 & -t & -t \\ -t & 0 & -t \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -t & -t \\ -t & 0 & -t \\ -t & -t & 0 \end{pmatrix} = h \end{aligned}$$

Since $T_1^+ h T_1 = h \Rightarrow T_1$ is a symmetry of the Hamiltonian.

- Inversion operation: $I: x \rightarrow -x$

$$I \hat{x} I^{-1} = -\hat{x}$$

infact, $I \hat{p} I^{-1} = -\hat{p}$ because $\hat{p} \sim \partial_x \rightarrow -\partial_x$

What about the commutator?

$$I [x, p] I^{-1} = I \underset{I^{-1}I}{\underset{\uparrow}{x}} p I^{-1} - I p \underset{I^{-1}I}{\underset{\uparrow}{x}} I^{-1}$$

$$= (I x I^{-1})(I p I^{-1}) - (I p I^{-1})(I x I^{-1})$$

$$\begin{array}{cccc} " & & & \\ -x & -p & -p & -x \end{array}$$

$$= x p - p x = \underline{\underline{i\hbar}}$$

Since $I \rightarrow I^{-1}$ doesn't perform a conjugation, $\Rightarrow I = \text{unitary}$.

time reversal

$$T : t \rightarrow -t$$

$$T \times T^{-1} = x$$

$$T \wp T^{-1} = -\wp$$

$$T[x\wp]T^{-1} = -[x, \wp] = -i\hbar \hat{p} \Rightarrow [T i T^{-1} = -i]$$

T is s.t. if we apply it to a matrix, it conjugates that matrix. This is a non-unitary symmetry of the Hamiltonian.

T can also be written as a combination of a unitary and conjugation

$$T = U_T K$$

\uparrow \uparrow
unitary conj

For these operations to be symmetries of the Hamiltonian,

$$THT^{-1} \stackrel{!}{=} H$$

$$H = \psi^\dagger h \psi$$

$$\Rightarrow [U_T h U_T^{-1} = h^*]$$

so that the conjugation cancels it.

Some more interesting points-

$$\hat{I}^2 = 1$$

$$\hat{T}^2 = \pm 1$$

\rightarrow depends on spin.

Since angular momentum $\sim \mathbf{x} \cdot \hat{\mathbf{p}}$, and spin \sim angular momentum,

the operation of time reversal -

$$\hat{T} \vec{S} \hat{T}^{-1} = -\vec{S}$$

The unitary part U_T of the operation is like a rotⁿ by π and the other part is conjugate

$$\therefore U_T = e^{-i\pi \vec{S} \cdot \hat{n}} = e^{-i\frac{\pi}{2} \vec{\sigma} \cdot \hat{n}} = \cos\left(\frac{\pi}{2}\right) \vec{\sigma} \cdot \hat{n} - i \sin\left(\frac{\pi}{2}\right) \vec{\sigma} \cdot \hat{n}$$

$$U_T = -i \vec{\sigma} \cdot \hat{n}$$

$$\Rightarrow \hat{T} = -i \vec{\sigma} \cdot \hat{n} k$$

So, for the time reversal symmetry -

The chart looks like -

T
0
+1
-1

T isn't a symmetry of H

T is a symmetry & squares to +1

T is a symmetry & squares to -1

Lecture - 24

(23-03-2023)

Let's say our time-reversal operator \hat{T} is a symmetry.

$$[\hat{T}, \hat{H}] = 0$$

If we now have energy eigenstates $\hat{H}|\psi\rangle = E|\psi\rangle$

$$\Rightarrow \hat{H}(\hat{T}|\psi\rangle) = \hat{T}(\hat{H}|\psi\rangle) = E(\hat{T}|\psi\rangle)$$

Let's say now that we have a time reversal symmetry squaring to -1.

$$\hat{T}^2 = -1$$

Kramer's theorem: if $\hat{T}^2 = -1$ and \hat{T} is a symmetry of \hat{H} , then $|\psi\rangle$ and $\hat{T}|\psi\rangle$ are orthogonal states! → half-integral spin

Proof: Evaluate $\langle \hat{T}\psi | \hat{T}\phi \rangle$

\hat{T} is in the form $\hat{T} = U_T k$

$$\hat{T}|\psi\rangle = U_T k |\psi\rangle \quad \text{and} \quad \langle \psi | \hat{T} = \langle \psi | (U_T k)^\dagger$$

$$\text{so, } \langle \hat{T}\psi | \hat{T}\phi \rangle = \langle \psi | (U_T k)^\dagger (U_T k) | \phi \rangle$$

$$= \sum_{ij\epsilon} [(U_{ij} k \psi_j)^* (U_{ie} k \phi_e)] = \sum_{ij\epsilon} [U_{ij}^* \psi_j k U_{ie} k \phi_e]$$

?

$$k^2 = 1$$

$$= \langle \phi | \psi \rangle$$

Now that $\langle \hat{T}\psi | \hat{T}\phi \rangle = \langle \phi | \psi \rangle$

Now say $| \phi \rangle = \hat{T} | \psi \rangle$. $\Rightarrow \langle \hat{T}\psi | \hat{T}^2\phi \rangle = \langle \hat{T}\psi | \phi \rangle$

$$\Rightarrow \langle \hat{T}\psi | \phi \rangle = - \langle \hat{T}\psi | \psi \rangle \Rightarrow \boxed{\langle \hat{T}\psi | \psi \rangle = 0}$$

Hence, the eigenstates $\hat{T} | \psi \rangle$ and $| \psi \rangle$ are orthogonal. ■

In k -space, the Hamiltonians can be written in the form-

$$H = \sum_{k,\alpha,\beta} \psi_{k,\alpha}^+ \underbrace{h^{\alpha\beta}(\vec{k})}_{\uparrow} \psi_{k,\beta}$$

in most cases, time reversal affects h directly.

Let's analyze the effect of time reversal on creation & annihilation.

$$\hat{T} \hat{c}_i \hat{T}^{-1} = c_i$$

(some sort of a spatial operator.)

What should then be the effect on \tilde{c}_k ?

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{-ikr_i} \tilde{c}_k$$

$$\Rightarrow \hat{T} c_i \hat{T}^{-1} = c_i = \frac{1}{\sqrt{N}} \sum_k \left(\hat{T} e^{-ikr_i} \tilde{c}_k \hat{T}^{-1} \right)$$

$$= \frac{1}{\sqrt{N}} \sum_k \left[\hat{T} e^{-ikr_i} \hat{T}^{-1} \cdot \hat{T} \tilde{c}_k \hat{T}^{-1} \right] = \frac{1}{\sqrt{N}} \sum_k \left[e^{+ikr_i} \hat{T} \tilde{c}_k \hat{T}^{-1} \right]$$

\downarrow
 $i \rightarrow -i$
 $= e^{+ikr_i}$

Putting $\vec{k} \rightarrow -\vec{k}$ on defⁿ of c_i

$$\hat{T} c_i \hat{T}^{-1} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{+ikr_i} \underbrace{\hat{T} \tilde{c}_{\vec{k}} \hat{T}^{-1}} \stackrel{?}{=} c_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{ikr_i} \underbrace{\tilde{c}_{-\vec{k}}}$$

$$\Rightarrow \boxed{\hat{T} \tilde{c}_{\vec{k}} \hat{T}^{-1} = \tilde{c}_{-\vec{k}}}$$

If we apply the $\hat{T} \rightarrow \hat{T}^{-1}$ operation on the original Hamiltonian

$$\begin{aligned} \hat{T} H \hat{T}^{-1} &= \sum_{\alpha, \beta, k} \hat{T} \left[c_{k, \alpha}^+ h^{\alpha \beta}(\vec{k}) c_{k, \beta} \right] \\ &\stackrel{?}{=} \hat{H} \end{aligned}$$

$$= \sum_{\alpha, \beta, k} \left[(\hat{T} c_{k, \alpha}^+ \hat{T}^{-1}) (\hat{T} h^{\alpha \beta}(\vec{k}) \hat{T}^{-1}) (\hat{T} c_{k, \beta} \hat{T}^{-1}) \right]$$

$$\stackrel{k \rightarrow -k}{=} \sum_{\alpha, \beta, k} \left[c_{k, \alpha}^+ (\hat{T} h^{\alpha \beta}(-\vec{k}) \hat{T}^{-1}) c_{k, \beta} \right]$$

$$\text{and } \hat{H} = \sum_{\alpha, \beta, k} \left[c_{k, \alpha}^+ h^{\alpha \beta}(\vec{k}) c_{k, \beta} \right]$$

$$\Rightarrow \hat{T} h^{\alpha \beta}(-\vec{k}) \hat{T}^{-1} = h^{\alpha \beta}(\vec{k})$$

$$\text{or } \boxed{\hat{T} h(\vec{k}) \hat{T}^{-1} = h(-\vec{k})}$$

Example: Check if $\hat{H} = \vec{\sigma} \cdot \vec{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$

Now $\hat{T} \vec{B} \hat{T}^{-1} = \vec{B}$ since it's a magnetic field.

For spin- $\frac{1}{2}$ particles, $\hat{T} = -i \vec{\sigma} \cdot \hat{n} k = -i \sigma_y k$ since we usually choose to flip about z-axis.

$$\hat{T} \hat{\mu} \hat{T}^{-1} = \hat{T} [\vec{\sigma} \cdot \vec{B}] \hat{T}^{-1} = (-i \sigma_y k) [\sigma_x B_x + \sigma_y B_y + \sigma_z B_z] (i \sigma_y k)$$

$$= -i \sigma_y \left[\begin{matrix} \sigma_x^* B_x & \sigma_y^* B_y & \sigma_z^* B_z \\ \sigma_x & -\sigma_y & \sigma_z \end{matrix} \right] k i \sigma_y k$$

$$= -i \sigma_y \left[\begin{matrix} \sigma_x B_x & -\sigma_y B_y & +\sigma_z B_z \\ \sigma_x & \sigma_y & \sigma_z \end{matrix} \right] (i \sigma_y) k^2$$

$$= [B_x \sigma_y \sigma_x - \sigma_y^2 B_y + B_z \sigma_y \sigma_z] \sigma_y$$

$$= [-B_x \sigma_x \sigma_y - B_y \sigma_y \sigma_y - B_z \sigma_z \sigma_y] \sigma_y$$

$$= [-B_x \sigma_x - B_y \sigma_y - B_z \sigma_z] \underbrace{\sigma_y^2}_1 = -\hat{H}$$

$$\Rightarrow \hat{T} \hat{\mu} \hat{T}^{-1} = -\hat{H}$$

Particle-Hole symmetry (charge conjugation symmetry): \hat{P} (or \hat{C})

Operation

$$c_i \rightarrow c_i^\dagger$$

$$c_j^\dagger \rightarrow c_j$$

What happens to a Hamiltonian $H = \sum_{ij} c_i^\dagger h_{ij} c_j$ under particle-hole operation?

Condition: $\hat{C} \hat{H} \hat{C}^{-1} = \hat{H}$

$$\hat{C} \hat{H} \hat{C}^{-1} = \sum_{ij} \hat{C} \underbrace{c_i^\dagger}_{\hat{c}_i} \hat{C}^{-1} \hat{C} h_{ij} \hat{C}^{-1} \underbrace{\hat{c}_j}_{c_j^\dagger} \hat{C}^{-1}$$

$$= \sum_{ij} c_i \hat{C} h_{ij} \hat{C}^{-1} c_j^\dagger$$

↓
 how can this be $= \sum_{ij} c_i^\dagger h_{ij} c_j$??

If $\hat{C} h_{ij} \hat{C}^{-1} = -h_{ji}$

$$CHC^{-1} = \sum_{ij} -c_i h_{ji} c_j^\dagger = \sum_{ji} c_j^\dagger h_{ji} c_i = \hat{H}$$

also, $\hat{C}^2 = \mathbb{1} \Rightarrow$

\hat{C}
0
-1
+1

$$\Rightarrow \hat{C} = U_C k$$

Since $\{U_C, h\} = 0$

\Rightarrow if $| \psi \rangle$ is a state with energy E , then $\hat{C}| \psi \rangle$ has an energy equal to $-E$.

$$h| \psi \rangle = E| \psi \rangle \Rightarrow h[\hat{C}| \psi \rangle] = -E[\hat{C}| \psi \rangle]$$

Chiral symmetry (sublattice symmetry): \hat{C} (or \hat{S})

$$\hat{S} \equiv \hat{C} \hat{T} = U_C k U_T k = U_C U_T^* k^2 \underset{k}{\parallel} = U_C U_T^*$$

Since we only have unitaries, i.e. $\hat{S} = U_C U_T^* \Rightarrow \hat{S}^2 = 1$

10-fold classification of topological materials

\hat{T}
0
-1
+1

\hat{C}
0
-1
1

\hat{S}
0
1

$$3 \times 3 - 1 + 2$$

$\uparrow \uparrow \uparrow$
 $T C$

→ add these two possibilities
remove the 0,0 case
because it can give 2 possibilities

Class	\hat{T}	\hat{C}	\hat{S}	$d=1$	$d=2$	$d=3$
A	0	0	0	0	$\mathbb{Z} \xrightarrow{\text{QHE}}$	0
AIII	0	0	1	\mathbb{Z} (integer)	0	\mathbb{Z}
AI	1	0	0	0	0	0
BDI	1	1	1	\mathbb{Z}	0	0
D	0	1	0	\mathbb{Z}_2	\mathbb{Z}	0
DIII	-1	1	1	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
AII	-1	0	0	0	\mathbb{Z}_2	\mathbb{Z}_2
CII	-1	-1	1	$2\mathbb{Z}$ (even)	0	\mathbb{Z}_2
C	0	-1	0	0	$2\mathbb{Z}$	0
CI	1	-1	1	0	0	$2\mathbb{Z}$

0 → no symmetry

→ SSH

→ Kitaev p-wave

topological classification classes.

In momentum space,

- As derived before $\hat{T} h(\vec{k}) \hat{T}^{-1} = h(-\vec{k})$ implies the Hamiltonian is symmetric under time reversal.
- Similarly, for charge conjugation symmetry, $\hat{C} h(\vec{k}) \hat{C}^{-1} = -h(-\vec{k})$
- For parity symmetry, $\hat{S} h(\vec{k}) \hat{S} = -h(\vec{k})$

For the SSH model, $h(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$ is the general form of Hamiltonian

For SSH, $d_2(k) = 0$

$$d_x(k) = u + v \cos k \Rightarrow h = \begin{pmatrix} 0 & u+v e^{ik} \\ u+v e^{-ik} & 0 \end{pmatrix}$$

$$d_y(k) = v \sin k.$$

① Since we don't have any spin the SSH model, we don't have to worry about any rot's, so, $\hat{T} = i\vec{\sigma} \cdot \hat{n} k \rightarrow \hat{T} = k$

Under \hat{T} , $\hat{T} h(k) \hat{T}^{-1} = k \underbrace{h(k)}_{k} k = h(-k) k^2 = h(-k)$

② For charge conjugation, $h(k) = C_{KA}^+ C_{KB} (u + v e^{ik})$

$$+ C_{KB}^+ C_{KA} (u + v e^{-ik})$$

$$\hat{C} (C_{KA}^+ C_{KB}^+) \begin{pmatrix} 0 & u+v e^{ik} \\ u+v e^{-ik} & 0 \end{pmatrix} \begin{pmatrix} C_{KA} \\ C_{KB} \end{pmatrix} \cdot \hat{C}^{-1}$$

$$= - (C_{KA}^+ C_{KB}^+) \begin{pmatrix} 0 & u+v e^{-ik} \\ u+v e^{ik} & 0 \end{pmatrix} \begin{pmatrix} C_{KA} \\ C_{KB} \end{pmatrix} = -h(-k)$$

③ Sublattice symmetry

$$\hat{S} = \sigma^z \quad \text{This is a symmetry of SSH.}$$

In fact, if we have a Hamiltonian $h(k) = \vec{d}(k) \cdot \vec{\sigma} + d_0 \mathbb{1}$,

then $\sigma_z \cdot h(k) \cdot \sigma_z = -h(k) \quad \text{iff} \quad d_0 = d_z = 0.$ (which SSH automatically follows)

Lecture-26

(28-03-2023)

Consider a general Hamiltonian of the type $h(\vec{k})$ which is 2×2 . We can write this matrix in the basis $\begin{pmatrix} c_{kA}^+ & c_{kB}^+ \end{pmatrix}$

The most general Hamiltonian is given by $h(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma} + d_0(\vec{k}) \sigma_0$

(1) Time Reversal symmetry:

Since we do not have a spin index, the action of time reversal is just complex conjugation.

$$\hat{T} h(\vec{k}) \hat{T}^{-1} = h^*(\vec{k})$$

$$\hat{T} h(\vec{k}) \hat{T}^{-1} = h^*(\vec{k}) = d_x(\vec{k}) \sigma_x - d_y(\vec{k}) \sigma_y + d_z(\vec{k}) \sigma_z + d_0(\vec{k}) \sigma_0$$

How can this be equal to $h(-\vec{k})$, i.e., TRS?

$$h(-\vec{k}) = d_x(-\vec{k}) \sigma_x + d_y(-\vec{k}) \sigma_y + d_z(-\vec{k}) \sigma_z + d_0(-\vec{k}) \sigma_0$$

$$\Rightarrow \text{For } h^*(\vec{k}) \stackrel{!}{=} h(-\vec{k}) \Rightarrow d_x(-\vec{k}) \stackrel{!}{=} d_x(\vec{k}) \rightarrow \text{even}$$

$$d_y(-\vec{k}) \stackrel{!}{=} -d_y(\vec{k}) \rightarrow \text{odd}$$

$$d_z(-\vec{k}) \stackrel{!}{=} d_z(\vec{k}) \rightarrow \text{even}$$

$$d_0(-\vec{k}) = d_0(\vec{k}) \rightarrow \text{even.}$$

(2) Charge conjugation symmetry.

$$\hat{\mu} = \sum (c_{ka}^+ c_{kb}^+) \begin{pmatrix} h(\vec{k}) \end{pmatrix} \begin{pmatrix} c_{ka} \\ c_{kb} \end{pmatrix}$$

$$\hat{H} = \sum c_{ka}^+ c_{ka} [d_0(\vec{k}) + d_2(\vec{k})] + c_{ka}^+ c_{kb} [d_x(\vec{k}) - i d_y(\vec{k})] \\ + c_{kb}^+ c_{kb} [d_0(\vec{k}) - d_2(\vec{k})] + c_{kb}^+ c_{ka} [\text{h.c.}]$$

$$= (1 - c_{ka} c_{ka}^+) (d_0(k) + d_2(k)) + (1 - c_{kb} c_{kb}^+) (d_0(k) - d_2(k)) \\ - c_{kb} c_{ka}^+ [d_x(k) - i d_y(k)] - c_{ka} c_{kb}^+ [d_x(k) + i d_y(k)]$$

$$= (c_{ka} \quad c_{kb}) \begin{pmatrix} & \\ & \end{pmatrix} \begin{pmatrix} c_{ka}^+ \\ c_{kb}^+ \end{pmatrix}$$

Since \hat{C} (charge conjugation) interchanges $c \leftrightarrow c^+$, we've shown $h(\vec{k})$ is symmetric under charge conjugation if $d_0 = 0$.

But $\hat{C} h(\vec{k}) \hat{C}^{-1} = -h(-\vec{k})$ for charge conjugation symmetry

$$\Rightarrow d_x(k) = d_x(-k) \rightarrow \text{even}$$

$$d_y(-k) = -d_y(k) \rightarrow \text{odd}$$

$$d_z(k) = d_z(-k) \rightarrow \text{even.}$$

(3) Chiral symmetry.

$$\hat{S} h(\vec{k}) \hat{S}^{-1} = -h(\vec{k}) \Rightarrow \{\hat{S}, h(\vec{k})\} = 0$$

which means that the eigenvalues appear in the $\pm \varepsilon$ pair.

If $d_0 \neq 0$, the eigenvalues are $d_0 \pm \varepsilon \Rightarrow \underline{\underline{d_0}} \stackrel{!}{=} 0$ for chiral symmetry.

Assuming $\hat{S} = \sigma_2$

$$\begin{aligned} \sigma_2 [d_x \sigma_x + d_y \sigma_y + d_z \sigma_z] \sigma_2 &= [-d_x \sigma_x \sigma_2 - d_y \sigma_y \sigma_2 + d_z \sigma_z \sigma_2] \sigma_2 \\ &= [-d_x \sigma_x - d_y \sigma_y + d_z \sigma_z] \frac{\sigma_2^2}{1} \end{aligned}$$

$$\text{For } \sigma_2 h(\vec{k}) \sigma_2 = -h(\vec{k}) \Rightarrow \underline{\underline{d_z}} \stackrel{!}{=} 0$$

CHEZN INSULATOR: Class A: $T=0, C=0, S=0$ (\mathbb{Z} at $d=2$)

$$(c_{ia}^\dagger \ c_{ib}^\dagger) \equiv c_i^\dagger \rightarrow \text{spinor}$$

Then our Hamiltonian becomes

$$\hat{H} = -t \sum_i \left[c_i^\dagger \left(\frac{\sigma_z - i\sigma_x}{2} \right) c_{i+\hat{x}} + c_i^\dagger \left(\frac{\sigma_z - i\sigma_y}{2} \right) c_{i+\hat{y}} + \text{h.c.} \right]$$

$$+ M \sum_i c_i^\dagger \sigma_z c_i$$

By performing a Fourier Transform,

$$h(\vec{k}) = d(\vec{k}) \cdot \vec{\sigma}$$

where the components of $d(\vec{k})$ are of the form

$$d_x(\vec{k}) = t \sin k_x \rightarrow \text{odd}$$

$$d_y(\vec{k}) = t \sin k_y \rightarrow \text{odd}$$

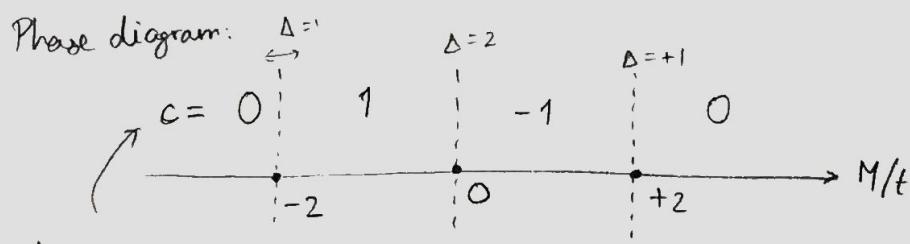
$$d_z(\vec{k}) = M - t \cos k_x - t \cos k_y \xrightarrow[X=0]{} \text{even}$$

\Rightarrow This Hamiltonian doesn't respect T, C, S. None of them.

Energy eigenvalues $E = \pm |\vec{d}(\vec{k})|$

Gap closing? If we consider $\frac{M}{t}$ as an effective parameter, then
we have gap closings at-

- $(M/t) = +2, (0,0)$
- $(M/t) = 0, (0,\pi) \text{ and } (\pi,0)$
- $(M/t) = -2, (\pi,\pi)$



Chern
#

For a 2-band problem, the Chern number is given by

$$C = \frac{1}{4\pi} \int d^2k \quad \hat{d}_k \cdot (\partial_{k_x} \hat{d}_k \times \partial_{k_y} \hat{d}_k)$$

B2

Lecture - 27
 (29/03/2023)

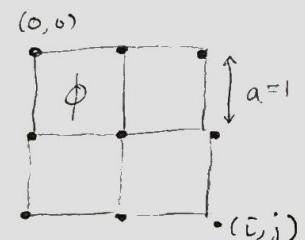
Quantum Hall Effect:

$$\vec{p} \xrightarrow{\text{minimal coupling}} \vec{p} - e\vec{A} \Rightarrow \frac{\vec{p}^2}{2m} \rightarrow \frac{(\vec{p} - e\vec{A})^2}{2m}$$

Let's start the discussion with a square lattice

$$\hat{H} = -t \sum_{(i,j)} \left[C_{(i,j)}^\dagger C_{(i+1,j)} + C_{(i,j)}^\dagger C_{(i,j+1)} + h.c. \right]$$

↑
sum over
all sites



$$\phi = Ba^2 = B$$

The rule for performing the minimal coupling in the second quantization lattice model is given by Peierls' substitution.

$$t_{\vec{k}, \vec{l}} \longrightarrow t_{\vec{k}, \vec{l}} \exp \left[-i \frac{2\pi}{\phi_0} \int_{\vec{k}}^{\vec{l}} \vec{A} \cdot d\vec{l} \right]$$

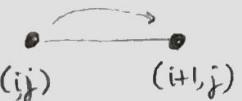
↑
hopping parameter
b/w site \vec{k} & \vec{l} .
elementary unit of flux.

Say we now consider the case where flux per plaquette $\phi = \frac{\phi_0}{2}$.

Also, Peierls' substitution is gauge dependent, but the same gauge should be fixed & substitutions.

Let's say we choose $\vec{A} = (0, \phi x, 0)$

For the horizontal hopping



$$\int_{(i,j)}^{(i+1,j)} \vec{A} \cdot d\hat{x} = \int_{(i,j)}^{(i+1,j)} (0, \phi_x, 0) \cdot (dx, 0, 0) = 0$$

$$\Rightarrow t_{(i,j), (i+1,j)} \rightarrow t_{(i,j), (i+1,j)} e^{\frac{-i2\pi}{\Phi_0} \cdot 0} = 1 \Rightarrow \text{same.}$$

For vertical hopping

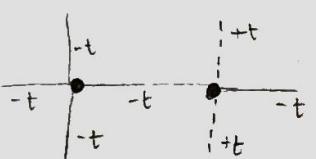
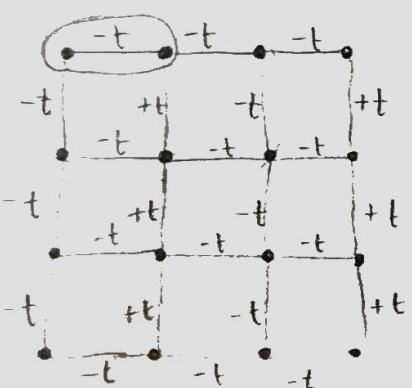


$$\int_{(i,j)}^{(i,j+1)} \vec{A} \cdot d\hat{y} = \int_{(i,j)}^{(i,j+1)} \phi_x \cdot dy = \phi_x \Big|_i \cdot (j+1-j) = \phi_x \Big|_i = \phi_i \equiv \phi_r$$

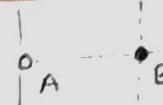
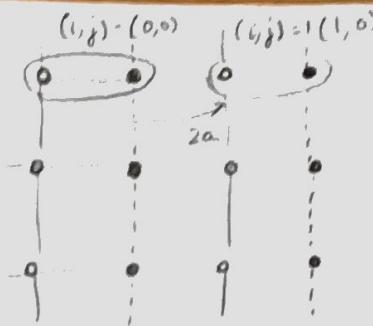
$$\Rightarrow t_{(i,j), (i,j+1)} \rightarrow t_{(i,j), (i,j+1)} e^{-i2\pi \frac{\phi}{\Phi_0} r_i}$$

$$= t_{(i,j), (i,j+1)} e^{-i\pi r_i} = t_{(i,j), (i,j+1)} \underline{(-1)^i}$$

new unit cell



repeating structure



$$r_{i+1} = r_i + 2a$$

$$r_{j+1} = r_j + a$$

$$\hat{H} = -t \sum_{(i,j)} \left[c_{(i,j)A}^\dagger c_{(i,j)B} + c_{(i,j)B}^\dagger c_{(i+1,j)A} + h.c. \right]$$

$$-t \sum_{(i,j)} \left[c_{(i,j)A}^\dagger c_{(i,j+1)A} - c_{(i,j)B}^\dagger c_{(i,j+1)B} + h.c. \right]$$

$$c_{(i,j)A} \xrightarrow{\text{F.T.}} C_{kA}$$

$$C_{iA}^\dagger = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{+i\vec{k} \cdot \vec{r}_i} \tilde{C}_{kA}^\dagger$$

$$C_{iB}^\dagger = \frac{1}{\sqrt{N}} \sum_{\vec{k}'} e^{-i\vec{k}' \cdot \vec{r}_i} \tilde{C}_{k'B}^\dagger$$

$$C_{iB}^\dagger = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} \tilde{C}_{kB}^\dagger$$

$$C_{i+\hat{x},A}^\dagger = \frac{1}{\sqrt{N}} \sum_{\vec{k}'} e^{-ik_x' 2a} e^{-i\vec{k}' \cdot \vec{r}_i} \tilde{C}_{k'A}^\dagger$$

$$\sum_i \tilde{C}_{iA}^\dagger \tilde{C}_{iB}^\dagger + \tilde{C}_{iB}^\dagger \tilde{C}_{i+\hat{x},A}^\dagger = \sum_{\vec{k}, \vec{k}'} e^{i(\vec{k} - \vec{k}') \cdot \vec{r}_i} C_{kA}^\dagger C_{k'B}^\dagger$$

$$\sum_i (C_{kA}^\dagger \quad C_{k'B}^\dagger) \begin{pmatrix} -2t \cos k_y & -t(1 + e^{-2ik_x}) \\ -t(1 + e^{2ik_x}) & +2t \cos k_y \end{pmatrix} \begin{pmatrix} C_{kA} \\ C_{k'B} \end{pmatrix}$$

The $h(\vec{k})$ matrix can again be written as -

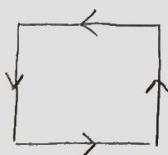
$$h(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$$

Time reversal symmetry is surprisingly preserved for this Hamiltonian despite the presence of a magnetic field. (Check!)

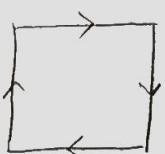
$$t_{\vec{k}, \vec{e}} \rightarrow t_{\vec{k}, \vec{e}} e^{-i \frac{2\pi}{\Phi_0} \int \vec{A} \cdot d\vec{l}}$$

$$\Rightarrow \prod_{e \in \square} t_e \Rightarrow \underbrace{\prod_{e \in \square} t_e}_{t^4} \cdot \underbrace{\prod_{e \in \square} e^{-i \frac{2\pi}{\Phi_0} \int \vec{A} \cdot d\vec{l}}}_\text{total flux}$$

Here, $t^4 \rightarrow t^4 (-1)^3 (+1) = (-1) t^4 = \underbrace{e^{+i\pi}}_{\text{magnetic flux around plaquette}} t^4$


$$= e^{-i\pi} t^4$$

$\therefore \pi$ -fluxes are very special.


$$= e^{+i\pi} t^4$$

Example What if $\phi = \phi_0/3$?

$$t_e \rightarrow t_e e^{-i\frac{2\pi}{\Phi} \phi \cdot r_i} = t_e \left(e^{-i\frac{2\pi}{3}}\right)^{r_i}$$

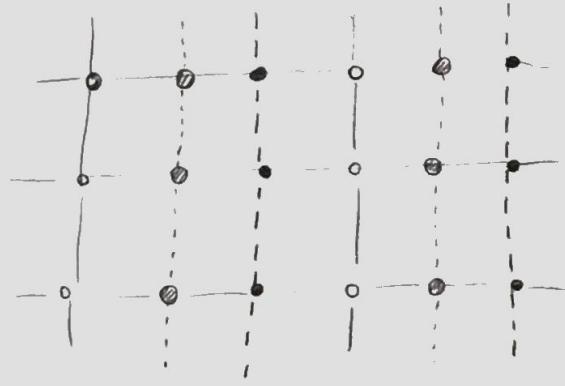
$$t_{r_i=0} = t_0 = t = t_3 = t_6 = t_{3n}$$

$$t_{r_i=1} = t_1 = t e^{-i\frac{2\pi}{3}} = t_4 = t_7 = t_{3n+1} \quad n \in \mathbb{Z}^+$$

$$t_{r_i=2} = t_2 = t e^{-i\frac{4\pi}{3}} = t_5 = t_8 = t_{3n+2}$$

$$\begin{array}{c} \square \\ \text{---} \\ \text{---} \\ \text{---} \end{array} = e^{-i2\pi/3}$$

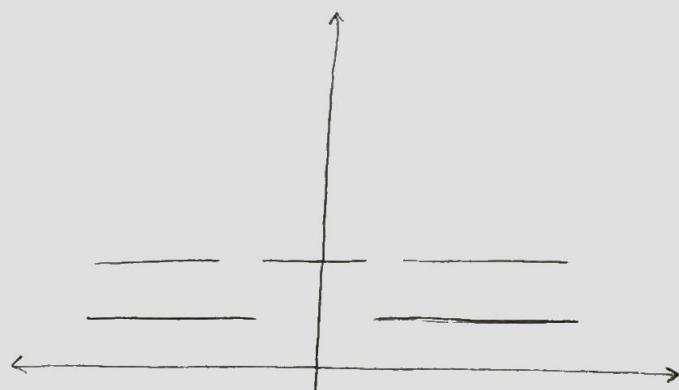
$$\begin{array}{c} \square \\ \text{---} \\ \text{---} \\ \text{---} \end{array} = e^{+i2\pi/3}$$



For $\phi = \phi_0/2$,

$$\begin{array}{c} \square \\ \text{---} \\ \text{---} \\ \text{---} \end{array} = \begin{array}{c} \square \\ \text{---} \\ \text{---} \\ \text{---} \end{array}$$

Hofstadter Butterfly (1976)

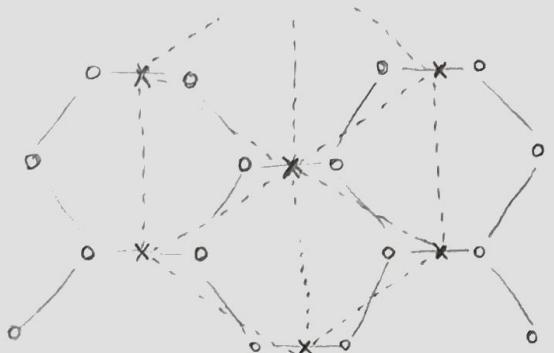


Lecture - 28

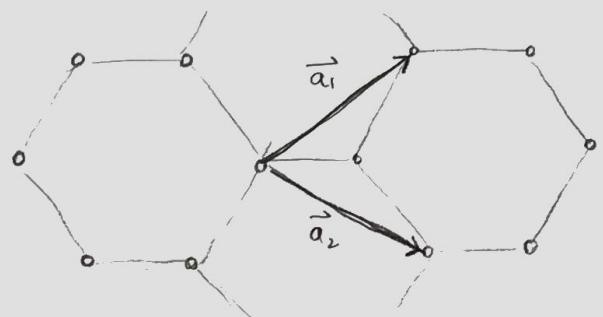
(30-03-2023)

Haldane's Honeycomb lattice model (PRL 1987)
(QHE without \vec{B} field)

Graphene as a proxy for honeycomb lattice - tight binding model?



$$\hat{H} = -t_1 \sum_{\langle i,j \rangle} [c_i^\dagger c_j + h.c.]$$



$$\vec{a}_1 = \frac{a}{2} (3, \sqrt{3})$$

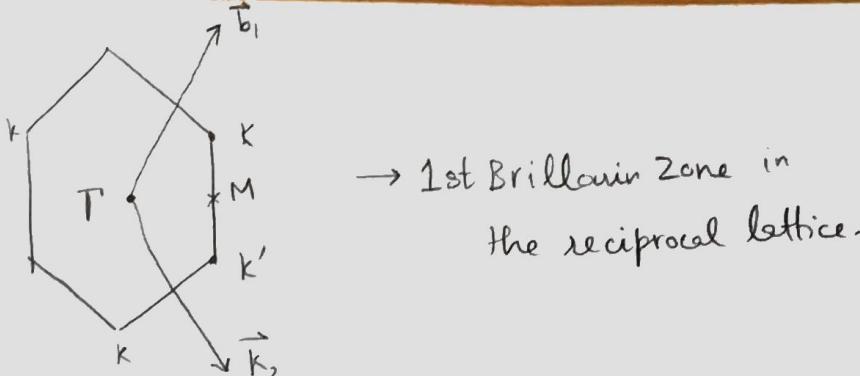
$$\vec{a}_2 = \frac{a}{2} (3, -\sqrt{3})$$

The reciprocal space lattice vectors are now
 $\vec{b}_1 = \frac{2\pi}{3a} (1, \sqrt{3})$
 $\vec{b}_2 = \frac{2\pi}{3a} (1, -\sqrt{3})$

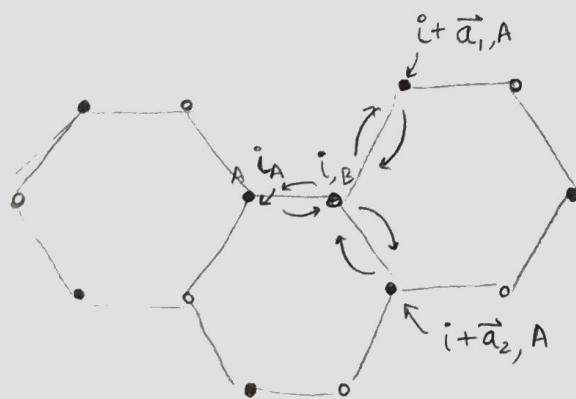
→ triangular

The Wigner-Seitz cell then is a hexagon





→ 1st Brillouin zone in
the reciprocal lattice.



$$\hat{H} = -t_1 \sum_i \left[C_{iA}^\dagger C_{iB} + C_{iB}^\dagger C_{i+\vec{\alpha}_1, A} + C_{iB}^\dagger C_{i+\vec{\alpha}_2, A} + h.c. \right]$$

$$\sum_i C_{iA}^\dagger C_{iB} = -t_1 \sum_K C_{KA}^\dagger C_{KB}$$

$$-t_1 \sum_i C_{iB}^\dagger C_{i+\vec{\alpha}_{1,2}, A} = -t_1 \sum_K C_{KB}^\dagger C_{KA} e^{-i\vec{k} \cdot \vec{\alpha}_{1,2}}$$

$$\Rightarrow \hat{H} = -t_1 \sum_K \left[C_{KA}^\dagger C_{KB} \left(1 + e^{-i\vec{k} \cdot \vec{\alpha}_1} + e^{-i\vec{k} \cdot \vec{\alpha}_2} \right) \right] + h.c.$$

$$h(\vec{k}) = \begin{pmatrix} 0 & 1 + e^{-i\vec{k} \cdot \vec{\alpha}_1} + e^{-i\vec{k} \cdot \vec{\alpha}_2} \\ -t_1 \begin{pmatrix} 1 + e^{i\vec{k} \cdot \vec{\alpha}_1} + e^{i\vec{k} \cdot \vec{\alpha}_2} & 0 \end{pmatrix} \end{pmatrix}$$

$$\Rightarrow dx = -t_1 [1 + \cos(\vec{k} \cdot \vec{\alpha}_1) + \cos(\vec{k} \cdot \vec{\alpha}_2)], dy = -t_1 [\sin(\vec{k} \cdot \vec{\alpha}_1) + \sin(\vec{k} \cdot \vec{\alpha}_2)]$$

Here, $d_0 = d_2 = 0$

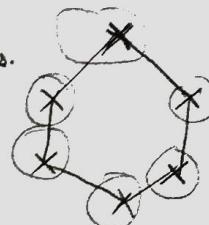
$$d_x(-k) = d_x(k) \rightarrow \text{has all the } \hat{T}, \hat{C}, \hat{S} \text{ symmetries.}$$

$$d_y(-k) = -d_y(k)$$

Dispersion relation for this problem is given by

$$\epsilon_{\pm}(k) = \pm t_1 \sqrt{3 + 2\cos(\sqrt{3}k_y a) + 4\cos(\sqrt{3}k_y \frac{a}{2})\cos\left(3k_x \frac{a}{2}\right)}$$

Gap closes at all the corner pts of the 1st Brillouin zones.



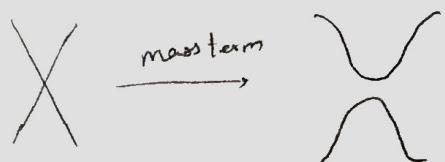
The low energy Hamiltonian of graphene is obtained

by expanding the H about the end pts. $\vec{k} = \vec{k}_{\text{corner}} + \delta\vec{k}$

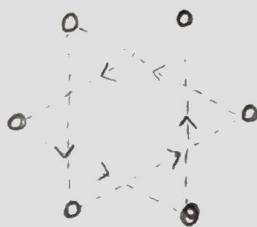
How to break the symmetries of graphene system?

Adding a mass term of the form $M \sigma_2 \begin{pmatrix} M & \\ & -M \end{pmatrix}$ makes

sites A & B inequivalent, and introduces a mass gap (without any topological prop.)



Haldane's idea: Consider second nearest neighbour hopping as well with antidiagonal hopping term $i t_2$.



This next nearest neighbour hopping only contributes diagonal entries.

since we have $t_2(e^{i\vec{k} \cdot \vec{\delta}} + e^{-i\vec{k} \cdot \vec{\delta}}) \rightarrow it_2 e^{i\vec{k} \cdot \vec{\delta}} - it_2 e^{-i\vec{k} \cdot \vec{\delta}}$, we get $\sin(\vec{k} \cdot \vec{\delta})$ type terms in diagonal.

Finally, the Hamiltonian we get looks like

$$h(\vec{k}) = h_0(\vec{k}) + M\sigma_z + 2t_2 \sum_i \sigma_z \underbrace{\sin(\vec{k} \cdot \vec{a}_i)}_{d_2(k)} \\ d_2(k) = -d_2(-k)$$

Breaks all of \hat{T} , \hat{C} and \hat{S} symmetries

Practical question: how to generate hoppings of the type it_2 .

Quantum Hall effect models:

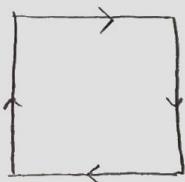
Recall:

Pearls substitution $t_{ij} = t e^{-i \frac{2\pi}{\Phi_0} \int_j^i \vec{A} \cdot d\vec{l}}$

Haldane model explores the Quantum Anomalous Hall Effect (QAHE) where it appears without a magnetic field.

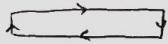
We will now discuss the Quantum Spin Hall effect (QSHE).

Kane-Mele model = 2 copies of the Haldane model.



2D e⁻ gas with B field
gives edge states (no back scattering)

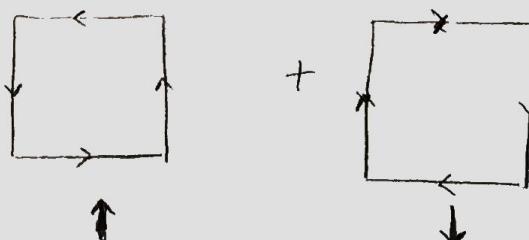
If the size is reduced significantly

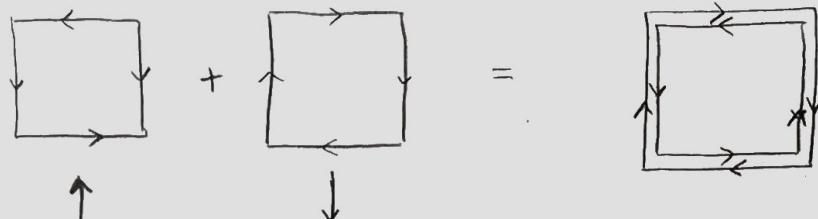


the edge states have the opposite current channel available since it is available in its vicinity.

∴ The Hall current decays exponentially as we go deeper into the sample.

Let us now say we have two copies of QHE and edge modes for diff. spin species.





$$\sigma_{xy}^{\uparrow} + \sigma_{xy}^{\downarrow} = 0$$

The charge Hall current cancels out.

What about the "spin" conductivity?



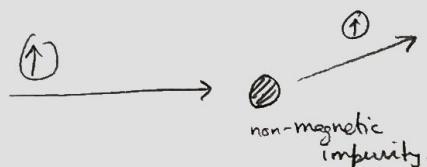
The opposite direction & opposite spin of current cancels the negative signs and

therefore the spin Hall conductivity actually adds up.

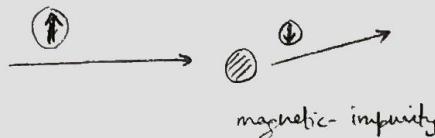
$$\sigma_{xy}^S \neq 0$$

But now that we have counter propagating current modes very close, why is the back scattering not a problem here?

Spin preserving scattering



spin flip scattering



As long as spin flip scattering doesn't occur, the scattering modes don't cancel each other.

In fact, adding spin \uparrow and spin \downarrow copies ends up restoring the time reversal symmetry with $T^2 = -1$.

Further, $| \phi \rangle$ and $\hat{T} | \phi \rangle$ are a Kramer's pair (orthogonal to each other) and hence they don't back-scatter off each other.

Spin-Orbit coupling.

$$\vec{L} \cdot \vec{s} \xrightarrow{\text{time reversal}} (-\vec{L}) \cdot (-\vec{s}) = \vec{L} \cdot \vec{s}$$

Here we are "restoring" TRS in Haldane's model.

$$d_x(\vec{k}) = -t_1 [1 + \cos(\vec{k} \cdot \vec{a}_1) + \cos(\vec{k} \cdot \vec{a}_2)]$$

$$d_y(\vec{k}) = -t_1 [\sin(\vec{k} \cdot \vec{a}_1) + \sin(\vec{k} \cdot \vec{a}_2)]$$

$$d_z(\vec{k}) = m - 2t_2 \sum_i \sin(\vec{k} \cdot \vec{a}_i)$$

By adding another copy of Haldane's model in the opposite spin species, we will enlarge the Hilbert space.

$$h(\vec{k}) = \begin{pmatrix} h_{\text{Haldane}}(\vec{k}) & 0_{2 \times 2} \\ 0_{2 \times 2} & h_{\text{Haldene}}^*(-\vec{k}) \end{pmatrix}$$

↑ time-reversed pattern.

Haldane didn't have spin in his model. But in a spin model, with a spin-orbit coupling, we don't have to add the complex hopping term which is present in Haldane model and the term arises naturally.

The C-atoms have weak spin-orbit coupling, \therefore graphene doesn't show the spin Hall effect. We need to go to heavier elements which form a Honeycomb lattice.

However, not just the Honeycomb lattice supports this QSH-E. The Bernevig-Hughes-Zhang (BHZ) model explores similar physics on a square lattice

$$h(\vec{k}) = d_0(\vec{k}) \mathbb{I} + \vec{d}(\vec{k}) \cdot \vec{\sigma}(\vec{k})$$

$$d_0(\vec{k}) = C - D(k_x^2 + k_y^2)$$

$$d_x(\vec{k}) = Ak_x$$

$$d_y(\vec{k}) = Ak_y$$

$$d_z(\vec{k}) = M - B(k_x^2 + k_y^2)$$

$$\text{where } H = \begin{pmatrix} h(\vec{k}) & 0_{2x2} \\ 0_{2x2} & h^*(-\vec{k}) \end{pmatrix}$$

↑
explicit construction of
TRS in the model.

$$\text{Since we are in the } (\hat{T} \hat{C} \hat{S}) = (-1 0 0)$$

$$(T^2 = -1)$$

symmetry, we have a class AII model.

We have a \mathbb{Z}_2 symmetry class.

The BHZ hamiltonian is actually a small \vec{k} limit of a more general model

$$d_x(\vec{k}) = t \sin k_x$$

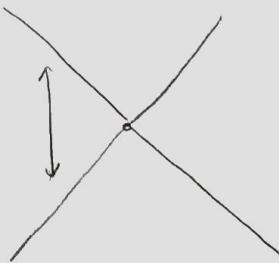
$$d_y(\vec{k}) = t \sin k_y$$

$$d_z(\vec{k}) = m - t \cos k_x - t \cos k_y$$

All of these models are examples of GAPPED TOPOLOGICAL PHASES.

Gapped topological phase.

The gap could be trivial or topological.



Topological gapped phases \rightarrow Topological insulators.

Any measurable quantities appear in open boundary conditions (Buk-Boundary correspondence)

Weyl semimetals

Immerison symmetry $I \ h(\vec{k}) I^{-1} = h(-\vec{k})$

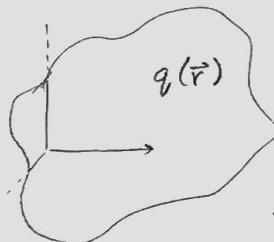
$$\epsilon_{\vec{k}} = \epsilon_{-\vec{k}}$$

Electric polarization

Time reversal symmetry: $T h(\vec{k}) T^{-1} = h(-\vec{k}) \xrightarrow{\text{also}} \epsilon_{\vec{k}} = \epsilon_{-\vec{k}}$

Difficult to trace back presence of electric polarization.

Given a classical charge distribution



$$\text{dipole moment } \vec{d} = \int_V q(\vec{r}) \vec{r} dV$$

Zero (neutral) charge distribⁿ \rightarrow unique solⁿ.

If lower moment = 0, higher moments = const?

Dipole moment in quantum mechanics.

Say there's an electron with a given wavefn ψ living in the background of ions (charge distribⁿ).
Ions \rightarrow treated classically

$$QM \rightarrow q(\vec{r}) = -e |\psi(\vec{r})|^2$$

$$\Rightarrow \vec{d}_{QM} = -e \int d^3r \psi^*(\vec{r}) \vec{r} \psi(\vec{r}) = -e \langle \psi | \vec{r} | \psi \rangle$$

Going to k -space

Block wavefn's

$$-\epsilon \int_{BZ} u_n^*(\mathbf{k}) \times(\mathbf{k}) u_n(\mathbf{k}) dk$$

$$u_n(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}$$

$$= -e \int_{BZ} u_n^*(\mathbf{k}) i \frac{\partial}{\partial \mathbf{k}} u_n(\mathbf{k}) dk$$

↪ Berry potential!

Vanderbilt { Electric
Resta { polarizability

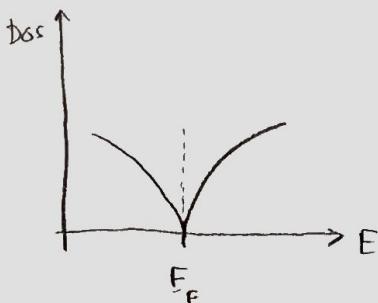
$$\vec{A}_n(\vec{k}) \equiv \langle u_n(\vec{k}) | i \vec{\nabla}_{\vec{k}} | u_n(\vec{k}) \rangle$$

Eigenvalue structure of energies isn't enough to guess absence or presence of electric polarizability. We need to calculate topological gfs like Berry potential!

Semi-metals.

- (1) No gap in the spectrum (definitely not an insulator).
(2) Zero density of state at E_{Fermi} .

semiconductor
~insulators
for a theorist with
a small band gap.



All the properties of a metal are governed by the states at the Fermi level.

For a d -dim system \rightarrow Fermi surface has almost $d-2$ dim's

FOR SEMI-METALS!

Example - Graphene at $E=0$

Dirac Semimetals

For a graphene lattice, the Hamiltonian can be written as

$$h(\vec{k}) = k_x \sigma_x + k_y \sigma_y \Rightarrow \varepsilon(\vec{k}) = \pm |\vec{k}|$$

↪ join at $\vec{k}=0$

However, if we add a perturbation to the $h(\vec{k})$

$$h(\vec{k}) + \text{perturbation} = k_x \sigma_x + k_y \sigma_y + m \sigma_z$$

↑
adds a gap!

Weyl Semimetal

$$h(\vec{k}) = \sigma_x k_x + \sigma_y k_y + \sigma_z k_z$$

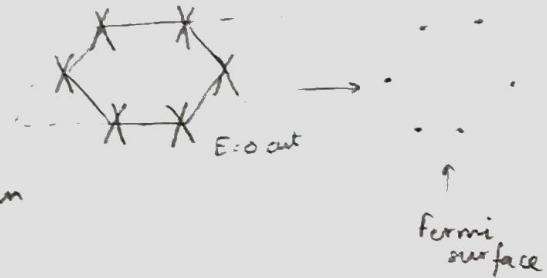
$$\varepsilon = \pm |\vec{k}|$$

Adding a perturbation $+ m \sigma_z$

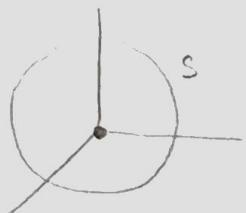
$$\Rightarrow \varepsilon = \pm |\vec{k}'| \text{ where } \vec{k}' \equiv (k_x, k_y, k_z + m)$$

∴ The mass term does NOT create a gap!

The $\vec{k}=0$ point is topologically protected.



Let us now calculate the chem number over a sphere S which contains our *special* point $\vec{k}=0$
gapless



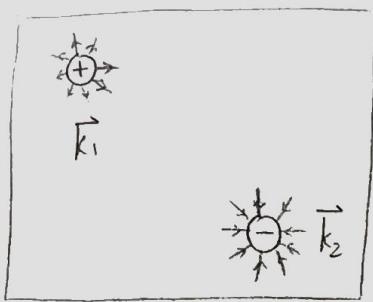
$$\frac{1}{2\pi} \int_S \vec{\Omega}_n(\vec{k}) \cdot d\vec{s} = n_W \quad (\text{~}\sim \text{Gauss law})$$

↑
Weyl charge

∴ The gapless pt. $\vec{k}=0$ contains something qualitatively very similar to a topological charge! Such points are called Weyl points!

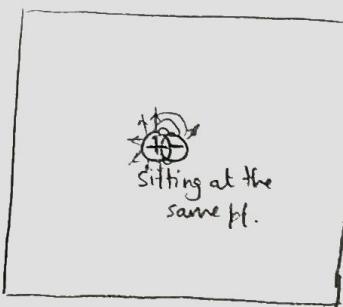
Nielsen-Ninomiya Theorem: The net sum of all Weyl charges over all \vec{k} Weyl points is equal to 0.

WEYL SEMIMETALS



k-space

DIRAC SEMIMETALS



k-space

$n_W = 0 \rightarrow$ Dirac semimetals

$n_W \neq 0 \rightarrow$ Weyl semimetals.

Dirac metals in general have both time reversal & inversion symmetry. Therefore, we can obtain a Weyl semimetal by breaking these 2 symmetries -

(1) Breaking time reversal

(2) Breaking inversion symmetry