Plan :

Feb. 19

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- Review harmonic oscillator
  - remind ourselves the creation/annihilation operators

- Quantization of field
  fields = harmonic oscillators

- Second quantization framework
  - Many-body wavefunction in first quantization framework
  - Fock space
  - one-body, two-body operators in 2nd quantization framework

- Diagonalization and Bogoliubov transform.

- Field integral for boson :
  - Feynmann path integral for single particle
  - Path integral for harmonic oscillator (construct from coherent states)
  - Field integral for boson.

next week ?

Harmonic oscillator

The Hamiltonian of HO:

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 . \qquad [\hat{x}, \hat{p}] = i\hbar$$

define creation/annihilation operators:

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} \hat{x} + i \frac{\hat{p}}{\sqrt{m\omega\hbar}} \right) \qquad (1)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} \hat{x} - i \frac{\hat{p}}{\sqrt{m\omega\hbar}} \right)$$

then. $[\hat{a}, \hat{a}^\dagger] = \underline{1}$.

$$H = \hbar\omega \left(\hat{N} + \frac{1}{2} \right), \quad \hat{N} = \hat{a}^\dagger \hat{a} .$$

The eigenvalue of $\hat{N}$ is a good qn.

so we write eigenstates as $|n\rangle$. $\hat{N}|n\rangle = n|n\rangle$.

$n \geq 0$ b.c. $n = \langle n | a^\dagger a | n \rangle = (\langle n | a^\dagger)(a|n\rangle) \geq 0$.

Therefore, the GS is $|0\rangle$, $E_0 = \frac{1}{2}\hbar\omega$.

Next, using $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$, we find

$$\hat{N}(a^\dagger|n\rangle) = (n+1)\, a^\dagger |n\rangle . \Rightarrow a^\dagger|n\rangle \propto |n+1\rangle$$

Higher excitations can be generated by hitting $|0\rangle$ with $\hat{a}^{\dagger}$'s. The eigenvalue n is raised by 1 when hit by $\hat{a}^{\dagger}$.

Similarly, $\hat{a}$ lowers the quantum # n by 1.

If $n \notin \mathbb{Z}$ is allowed, then keep acting $\hat{a}$ on $|n\rangle$ takes the state to negative n, which is impossible.

So the eigenstates are $\{|n\rangle \,|\, n \in \mathbb{Z}\}$

Creation/annihilation operators act on states as follows:

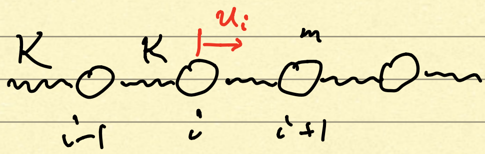
$$a^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$a|n\rangle = \sqrt{n}\,|n\rangle.$$

Quantization of fields.

We will see : field = a collection of harmonic oscillators

Let us consider the collective modes in an elastic string (classical)



Let the displacement at ith site be u_i.

Lagrangian $L = \sum_i \frac{1}{2} m \dot{u}_i^2 - \frac{1}{2} K (u_i - u_{i-1})^2$

Fourier transform: $u_i = \frac{1}{\sqrt{N}} \sum_k u_k e^{ikx_i}$ $\quad N$: # of sites

$$L = \sum_k \frac{1}{2} m |\dot{u}_k|^2 - \frac{1}{2} m \omega_k^2 |u_k|^2 .$$

where we defined $\omega_k = 2\sqrt{\frac{K}{m}} \sin\left(\frac{ka}{2}\right)$. $\quad p_i = \frac{1}{\sqrt{N}} \sum_k p_k e^{ikx_i}$

$$H = \sum_k \frac{|p_k|^2}{2m} + \frac{1}{2} m \omega_k^2 |u_k|^2 . \quad p_i \equiv m \dot{u}_i$$

Quantize: $[\hat{u}_i, \hat{p}_i] = i\hbar$.

$$[\hat{u}_k, \hat{p}_{-k'}] = \frac{1}{N} \sum_{ij} e^{-ikx_i} e^{ik'x_j} [\hat{u}_i, \hat{p}_j]$$

$$= \frac{1}{N} \sum_i e^{i(k'-k)x_i} \cdot i\hbar = i\hbar \delta_{kk'}$$

$$\mathcal{H} \to \sum_k \frac{\hat{p}_k \hat{p}_{-k}}{2m} + \frac{1}{2} m \omega_k^2 \hat{u}_k \hat{u}_{-k}$$

Defining $a_k = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega_k}{\hbar}} u_k + i \sqrt{\frac{1}{m\omega_k \hbar}} p_k \right)$

$$a_k^\dagger = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega_k}{\hbar}} u_{-k} - i \sqrt{\frac{1}{m\omega_k \hbar}} p_{-k} \right) \qquad u_k^\dagger - i p_k^\dagger$$

we find $\mathcal{H} = \sum_k \hbar \omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right)$

where $[a_k, a_k^\dagger] = 1$

$$u_k = \sqrt{\frac{\hbar}{2m\omega_k}} \left(a_k + a_{-k}^\dagger \right)$$

Second Quantization

- Many-body wavefunction in first quantization framework for bosons and fermions.
- Occupation number basis and second quantization
- Write interaction/operators in second quantization framework.
- Diagonalize Hamiltonian.
- Bogoliubov transform.

Wavefunctions in first quantization

Consider a system with N particles.

single-particle Hilbert space $\{\psi_\nu\}$, $\nu = 1, 2 \ldots d$.

d : dim of one-particle Hilbert space

If particles are distinguishable,

The n-particle basis can be chosen as direct product of n copies of single-particle states

Using r_i to label each particle, the basis for many-body wavefunctions can be written as:

$$\psi(r_1, r_2 \ldots r_N) \in \left\{ \begin{matrix} \phi_1(r_1) & \phi_1(r_2) & \cdots & \phi_1(r_N) \\ \phi_2(r_1) & \phi_1(r_2) & \cdots & \phi_1(r_N) \\ & \vdots & & \\ \phi_d(r_1) & \cdots & \cdots & \phi_d(r_N). \end{matrix} \right\} \quad (1)$$

The requirement of identical particle:

Invariance of observables under permutation.

Wfns pick up a phase

$$\Psi(r_1 \dots r_j \dots r_i \dots r_N) = e^{i\theta_{ij}} \Psi(r_1 \dots r_i \dots r_j \dots r_N).$$

The wavefunction goes back to itself when hit by a permutation operator twice. $e^{i2\theta} = 1 \rightarrow e^{i\theta} = \pm 1.$

$\pm$: Boson / Fermion

Therefore, we need to construct a set of basis that satisfies the statistics of boson / fermion

a) **Boson** : $\Psi(r_1, r_2) = \Psi(r_2, r_1)$

so Symmetrize :

e.g. two particles, $d = 2$ $(\uparrow\downarrow)$

$\nu_1 = \uparrow$, $\nu_2 = \downarrow$, $\Psi_{\{\nu_i\}} = \frac{1}{\sqrt{2}}\left(\phi_\uparrow(r_1)\phi_\downarrow(r_2) + \phi_\downarrow(r_1)\phi_\uparrow(r_2)\right)$

$\nu_1 = \nu_2 = \uparrow$, $\Psi_{\{\nu_i\}} = \phi_\uparrow(r_1)\phi_\uparrow(r_2)$

Generally, $\Psi_{\underline{\{\nu_i\}}}(r_1 \cdots r_N) = \frac{1}{\sqrt{N_P}} \sum_P \prod_{i=1}^N \phi_{\nu_{P(i)}}(r_i)$

N_P : # of terms (permutations) in $\Psi_{\{\nu_i\}}$. $N_P = \dfrac{N!}{\prod_{\nu=1}^{d} n_\nu!}$

b) **Fermion** : $\Psi(r_1, r_2) = -\Psi(r_2, r_1)$

so antisymmetrize :

$$\Psi_{\{\nu_i\}}(r_1 \cdots r_N) = \frac{1}{\sqrt{N_P}} \sum_P \prod_{i=1}^N \phi_{\nu_{P(i)}}(r_i) \underbrace{\mathrm{sgn}(P)}_{=(-1)^\sigma}$$

(σ: # of exchanges to get to P)

$N_P = N!$

$$= \frac{1}{\sqrt{N_P}} \begin{vmatrix} \phi_{\nu_1}(r_1) & \cdots & \phi_{\nu_1}(r_N) \\ \vdots & & \vdots \\ \phi_{\nu_N}(r_1) & \cdots & \phi_{\nu_N}(r_N) \end{vmatrix}$$

This way of describing wavefunctions is complicated.

Let's avoid track particle "labels" since they are non-physical.

Instead of asking which state each particle is in,

we now only ask how many particles occupy each state.

Introduce occupation number basis:

$$|n_1 \cdots n_d\rangle, \quad \sum_{\nu=1}^{d} n_\nu = N$$

Called "Fock space" if $N \to \infty$

We can introduce creation/annihilator operators for each single-particle state ν:

For boson:

$$b_\nu |n_1 \cdots n_\nu \cdots n_d\rangle = \sqrt{n_\nu}\, |n_1 \cdots n_\nu - 1, \cdots n_d\rangle$$

$$b_\nu^+ |n_1 \cdots n_\nu \cdots n_d\rangle = \sqrt{n_\nu + 1}\, |n_1 \cdots n_\nu + 1, \cdots n_d\rangle$$

$$[b_\nu, b_{\nu'}^+] = \delta_{\nu\nu'}, \quad \text{other} = 0.$$

For fermion:

$$c_\nu |n_1 \cdots 1_\nu \cdots n_d\rangle = (-1)^{\sum_{i=1}^{\nu-1} n_i} |n_1 \cdots 0_\nu \cdots n_d\rangle$$

$$c_\nu^+ |n_1 \cdots 0_\nu \cdots n_d\rangle = (-1)^{\sum_{i=1}^{\nu-1} n_i} |n_1 \cdots 1_\nu \cdots n_d\rangle$$

$$\{c_\nu, c_{\nu'}^+\} = \delta_{\nu\nu'}, \quad \text{other} = 0.$$

why define this sign? How to understand in 1st quantization?

$$\phi_1(r_1)\,\phi_2(r_2) \cdots \phi_N(r_N) \xrightarrow{c_k^+} \phi_k(r_1)\,\phi_1(r_2)\,\phi_2(r_3) \cdots \phi_{k-1}(r_k) \cdots$$

need $\sum_{i=1}^{\nu-1} n_i$ exchanges to restore the order of $\phi_1(r_1)\,\phi_2(r_2) \cdots \phi_k(r_k) \cdots$

Operators in 2nd quantization

Goal : express operators (whose form is known in 1st quantization) with creation/annihilation operators.

In 1st quantization.

$\sum_i x\,|x(r_i)\rangle\langle x(r_i)|$

one-body : $\hat{F} = \sum_{i=1}^{N} \hat{f}(r_i)$ r_i : particle label.

$\hat{f}(r_i) = \sum_{\mu\mu'} f_{\mu'\mu} |\phi_{\mu'}(r_i)\rangle\langle\phi_\mu(r_i)|$ $f_{\mu'\mu} = \langle\phi_{\mu'}|\hat{f}|\phi_\mu\rangle$

two-body : $\hat{G} = \frac{1}{2}\sum_{i\neq j}^{N} \hat{g}(r_i, r_j)$ $g_{\mu'\nu'\nu\mu} = \langle\phi_{\mu'}(1)\phi_{\nu'}(2)|\hat{g}|\phi_\nu(2)\phi_\mu(1)\rangle$

$\hat{g}(r_i, r_j) = \sum_{\mu'\nu'\nu\mu} g_{\mu'\nu'\nu\mu} |\phi_{\mu'}(r_j)\phi_{\nu'}(r_i))(\phi_\nu(r_i)\phi_\mu(r_j)|$

How to write them in 2nd quantization framework?

Plan: evaluate $\langle\{n'_\nu\}|\hat{F}|\{n_\nu\}\rangle$ in 1st quantization, and compare with $\langle\{n'_\nu\}|\hat{b}^\dagger_{\mu'}\hat{b}_\mu|\{n_\nu\}\rangle$.

For bosons: in 1st quantization framework :

$\langle\{n'_\nu\}|\hat{F}|\{n_\nu\}\rangle$

$= \sum_{lk} f_{lk} \sum_{i=1}^{N} \langle \cdots n_l+1 \cdots n_k-1 \cdots | \phi_l(r_i)\rangle\langle\phi_k(r_i)| \cdots n_l \cdots n_k \cdots\rangle$

count the # of terms (permutations) in $|\{n_\nu\}\rangle$

total # of terms : $N_{tot}(\{n_\nu\}) = \dfrac{N!}{\prod_\nu n_\nu!}$

# of terms where particle-r_i is in the k-state :

$$N_{\phi_k(r_i)}(\{n_\nu\}) = \frac{(N-1)!}{(n_k-1)!\prod_{\nu\neq k} n_\nu!}$$

$$\langle\cdots\rangle = \sum_{lk} f_{lk} \sum_{i=1}^{N} N_{\phi_k(r_i)}(\cdots n_l \cdots n_k \cdots) \frac{1}{\sqrt{N_{tot}(\cdots n_l+1 \cdots n_k-1 \cdots)}} \frac{1}{\sqrt{N_{tot}(\cdots n_l \cdots n_k \cdots)}}$$

$$= \sum_{lk} f_{lk} \, N \cdot \frac{(N-1)!}{n_l! \ldots (n_k-1)! \ldots} \frac{1}{\sqrt{\frac{N! \, N!}{(n_l+1)!(n_k-1)! \, n_l! \, n_k! \ldots}}}$$

$$= \sum_{lk} f_{lk} \sqrt{n_k} \sqrt{n_l+1}$$

This is identical to how $b_l^\dagger b_k$ act on $|\ldots n_l \ldots n_k\rangle$

So one body operator:

$$\hat{F} = \sum_{lk} f_{lk} b_l^\dagger b_k \, , \quad f_{lk} = \langle \phi_l | \hat{f} | \phi_k \rangle$$

Similarly for two-body operator:

$$\langle \{n_\nu'\} | \hat{G} | \{n_\nu\} \rangle$$

$$= \frac{1}{2} \sum_{k'l'lk} g_{k'l'lk} \sum_{i \neq j} \langle n_{k'}+1 \ldots n_{l'}+1 \ldots n_l-1 \ldots n_k-1 | \phi_{k'}(r_i) \phi_{l'}(r_j) \rangle \langle \phi_l(r_j) \phi_k(r_i) | n_{k'}, \ldots n_{l'}, \ldots n_l \ldots n_k \rangle$$

$$= \frac{1}{2} \sum_{k'l'lk} g_{k'l'lk} \frac{(N-2)!}{\ldots n_{k'}! \ldots n_{l'}! \ldots (n_l-1)! \ldots (n_k-1)! \ldots} \, N(N-1) \frac{1}{\sqrt{\frac{N!}{n_{k'}! \, n_{l'}! \, n_l! \, n_k! \ldots}}} \frac{1}{\sqrt{\frac{N!}{(n_{k'}+1)!(n_{l'}+1)!(n_l-1)!(n_k-1)! \ldots}}}$$

$$= \frac{1}{2} \sum_{k'l'lk} g_{k'l'lk} \sqrt{n_{k'}+1} \sqrt{n_{l'}+1} \sqrt{n_l} \sqrt{n_k}$$

So $\hat{G} = \frac{1}{2} \sum_{k'l'lk} g_{k'l'lk} \, b_{k'}^\dagger b_{l'}^\dagger b_l b_k$

For fermions, we don't need to worry about these $\sqrt{n_k}$ factors since they are always 1. But we need to keep track of the order

$$\hat{F}\,|\ldots\phi_l(r_i)\ldots\phi_k(r_j)\ldots\rangle = \langle\phi_{l'}(r_i)\,\phi_{k'}(r_j)|\,\hat{f}\,|\,\phi_k(r_j)\,\phi_l(r_i)\rangle$$

$$|\ldots\phi_{l'}(r_i)\ldots\phi_{k'}(r_j)\ldots\rangle$$

To realize the same operation with $c^{+}c$ operators, we need 4 operators in following order: $c_{l'}^{+}c_{k'}^{+}c_k c_l$

Proof:

$$|\ldots\phi_l(r_i)\ldots\phi_k(r_j)\ldots\rangle \xrightarrow{F} \ldots\ |\ldots\phi_{l'}(r_i)\ldots\phi_{k'}(r_j)\ldots\rangle$$

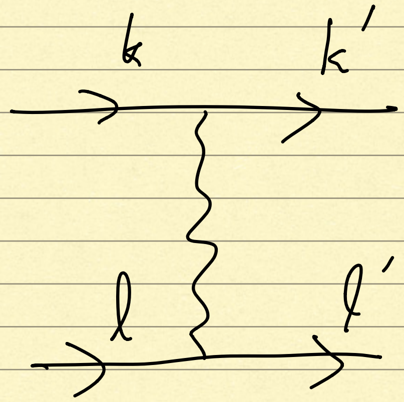
$$\downarrow \qquad\qquad\qquad\qquad \downarrow$$

$$c_l^{+}c_k^{+}|\ldots\rangle \xrightarrow{?} c_{l'}^{+}c_{k'}^{+}|\ldots\rangle$$

$$\left(c_{l'}^{+}c_{k'}^{+}c_k c_l\right)c_l^{+}c_k^{+} = c_{l'}^{+}c_{k'}^{+}$$

So for fermions, $\hat{F} = \frac{1}{2}\sum_{l'k'kl} f_{l'k'kl}\, c_{l'}^{+}c_{k'}^{+}c_k c_l$

corresponding to the following diagram



The End of

Second Quantization

Diagonalizing quadratic Hamiltonian. [copied from class notes]

$$\mathcal{H} = \sum_{ij} H_{ij} \hat{C}_i^\dagger \hat{C}_j \qquad H_{ij} \text{ Hermitian.} \qquad U^\dagger H \overset{\text{unitary matrix}}{U} = \underset{\text{diagonal matrix}}{E}$$

do a unitary transform : $\hat{C}_i = \sum_{il} U_{il} \hat{\alpha}_l$.

$$\hat{H} = \sum_{ijkl} \hat{\alpha}_k^\dagger \underbrace{U_{ik}^*}_{} \underline{H_{ij}}\, \underline{U_{jl}}\, \hat{\alpha}_l \qquad \underline{(U^\dagger)_{ki}}$$

$$= \sum_{kl} \hat{\alpha}_k^\dagger (U^\dagger H U)_{kl} \hat{\alpha}_l = \sum_m E_m \hat{\alpha}_m^\dagger \hat{\alpha}_m$$

Operator algebra is basis independent

$$[\hat{\alpha}_i, \hat{\alpha}_j^\dagger] = \sum_{kl} (U^\dagger)_{ik} [\hat{C}_k, \hat{C}_l^\dagger] U_{lj}$$

$$= i \sum_k (U^\dagger)_{ik} U_{kj} = i (U^\dagger U)_{ij} = i \delta_{ij} .$$

Similar for fermions,

E.g. tight-binding

$$\hat{H} = -J \sum_x C_x^\dagger C_{x+1} + h.c.$$

$$C_x = \frac{1}{\sqrt{N}} \sum_k e^{ikx} C_k$$

$$\mathcal{H} = -\frac{1}{N} J \sum_x \sum_{kk'} e^{-ikx} e^{ik'(x+1)} C_k^\dagger C_{k'} + h.c.$$

$$= -J \sum_k e^{ik} C_k^\dagger C_k + h.c. = -2J \sum_k \cos k \; C_k^\dagger C_k \leftarrow$$

Bogoliubov transform

Physically important systems are usually described by quadratic Hamiltonian.

$U(1)$ symmetry does not necessarily exist

e.g. magnet $\quad H = J_x S_x S_x + J_y S_y S_y$

superfluid: $\quad H_{MF}$ contains $\underline{c^\dagger c^\dagger + cc}$

Consider following toy Hamiltonian:

$$H = \varepsilon (c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda (c_1 c_2 + c_2^\dagger c_1^\dagger)$$

How to diagonalize it?

Try a linear transform.

$$c_1 = u d_1 + v d_2^\dagger, \qquad c_1^\dagger = u d_1^\dagger + v d_2$$

$$c_2 = v d_1^\dagger + u d_2 \qquad c_2^\dagger = v d_1 + u d_2^\dagger \qquad (u, v \in \mathbb{R})$$

satisfies $[d_1, d_2] = [d_1^\dagger, d_2^\dagger] = 0$.

To make $[d_1, d_1^\dagger] = [d_2, d_2^\dagger] = 1$ we need $u^2 - v^2 = 1$

so $\begin{cases} u = \cosh\theta \\ v = \sinh\theta \end{cases}$ $\qquad uv = \frac{1}{2}\sinh 2\theta. \quad u^2 + v^2 = \cosh 2\theta$

In matrix form $\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} = \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$

$$H = (c_1^\dagger \; c_2) \begin{pmatrix} \epsilon & \lambda \\ \lambda & \epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} - \epsilon \leftarrow \text{constant. ignore}$$

$$= (d_1^\dagger \; d_2) \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} \epsilon & \lambda \\ \lambda & \epsilon \end{pmatrix} \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$$

off-diagonal elements: $\underline{2\epsilon uv + \lambda(u^2 + v^2) = 0} \implies \tanh 2\theta = -\frac{\lambda}{\epsilon}$.

$u = \sqrt{\frac{1}{2}(1 + \cosh 2\theta)} = \sqrt{\frac{1}{2}\left(1 + \sqrt{\frac{1}{1 - \tanh^2 2\theta}}\right)} = \sqrt{\frac{1}{2}\left(1 + \frac{\epsilon}{\tilde{\epsilon}}\right)}, \quad v = \sqrt{\frac{1}{2}\left(1 - \frac{\epsilon}{\tilde{\epsilon}}\right)}. \quad \tilde{\epsilon} = \sqrt{\epsilon^2 - \lambda^2}$

diagonal element: $\epsilon(u^2 + v^2) + 2\lambda uv = \sqrt{\epsilon^2 - \lambda^2}$.

$$H = \tilde{\epsilon}(d_1^\dagger d_1 + d_2^\dagger d_2) - \text{const.}$$

Meaning of particle number nonconserving ~~transform~~

In harmonic oscillator :

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

where

$$a = \sqrt{\frac{m\omega}{2\hbar}}\, x + \frac{i}{\sqrt{2m\omega\hbar}}\, p \qquad a' = \sqrt{\frac{m\omega'}{2\hbar}}\, x + \frac{i}{\sqrt{2m\omega'\hbar}}\, p$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\, x - \frac{i}{\sqrt{2m\omega\hbar}}\, p \qquad a'^\dagger = \cdots$$

take $a' a'^\dagger$ with a "wrong" value ω' instead of ω.

— squeezed state. Hermitian, but particle number nonconserving

$$H = \hbar\omega'\left(a'^\dagger a' + \frac{1}{2}\right) + \frac{1}{2} m\left(\omega^2 - \omega'^2\right) \frac{\hbar}{2m\omega} \left(a' + a'^\dagger\right)^2$$

$$= \hbar \frac{\omega^2 + \omega'^2}{2\omega'} a'^\dagger a' + \frac{m\left(\omega^2 - \omega'^2\right)}{4\omega'} \left(a'a' + a'^\dagger a'^\dagger\right)$$

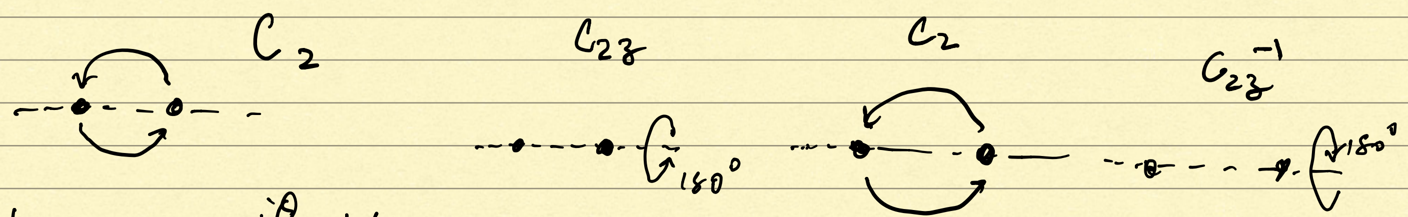
Some explanation for page 7:

The wavefunction goes back to itself when hit by a permutation operator twice. $e^{i2\theta} = 1 \longrightarrow e^{i\theta} = \pm 1$.

Only for dim ≥ 3.

$\pm$: Boson / Fermion

Proof: In $d \geq 3$, we have in-plane rotation C_{2z}



$$C_2 \psi(r_1, r_2) = e^{i\theta} \psi(r_1, r_2)$$

$$C_{2z} C_2 C_{2z}^{-1} = C_2^{-1}$$

$$\Downarrow$$

$$e^{i\theta} = e^{-i\theta} = \pm 1.$$

dim = 2, anyons.
