Systems of Identical Particle

* let $\mathcal{H}$ = Hilbert space of 1-particle system

$\{|\alpha\rangle\}$ = orthonormal basis obeying $\langle\alpha|\beta\rangle = \delta_{\alpha\beta}$, $\sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{1}_{\text{1-body}}$

e.g: for $S=\frac{1}{2}$ particles $|\vec{r},\sigma\rangle$ position/spin basis

$|n\ell m\sigma\rangle$ HO (uncoupled)

$|n(\ell\frac{1}{2})jm\rangle$ HO (coupled)

$$\psi_\alpha(\vec{r},\sigma) = \langle\vec{r},\sigma|\alpha\rangle$$

Notation: $|\vec{x}\rangle \equiv |\vec{r},\sigma\rangle$ $\int d\vec{x} = \sum_\sigma \int d^3r$, etc

* Extend to N-body system: $\mathcal{H}_N = \underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{\text{N-copies}}$

orthonormal basis: $|\alpha_1\alpha_2\cdots\alpha_N) \equiv |\alpha_1\rangle\otimes|\alpha_2\rangle\otimes\cdots\otimes|\alpha_N\rangle$ Note the curved bracket!

$$\sum_{\alpha_1\cdots\alpha_N} |\alpha_1\cdots\alpha_N)(\alpha_1\cdots\alpha_N| = \mathbb{1}_{\mathcal{H}_N}$$

$$(\alpha_1\alpha_2\cdots\alpha_N|\alpha_1'\alpha_2'\cdots\alpha_N') = \langle\alpha_1|\alpha_1'\rangle\langle\alpha_2|\alpha_2'\rangle\cdots\langle\alpha_N|\alpha_N'\rangle$$
$$= \delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}\cdots\delta_{\alpha_N\alpha_N'}$$

$$\psi_{\alpha_1\cdots\alpha_N}(\vec{x}_1,\cdots\vec{x}_N) \equiv (\vec{x}_1\cdots\vec{x}_N|\alpha_1\cdots\alpha_N) = \psi_{\alpha_1}(\vec{x}_1)\,\psi_{\alpha_2}(\vec{x}_2)\cdots\psi_{\alpha_N}(\vec{x}_N)$$

Claim: Un-symmetrized basis $|\alpha_1\cdots\alpha_N)$ OK for N-Distinguishable particles but NOT for identical particle

Symmetrization Postulate for N identical Particle Systems

* 2 types of particles $\left\langle \begin{array}{l} \text{Bosons (spin } 0,1,2,\ldots) \\ \text{Fermions (spin } \frac{1}{2}, \frac{3}{2}, \ldots) \end{array} \right.$ occur in Nature.

* Wf's for N-identical particles are either totally symmetric under exchanges (BOSONS) or totally Anti-Symmetric (FERMIONS) [Cf. Spin-Statistics thm. of QFT]

[Before the spin-Statistics thm in QFT, the founders of QM figured this need for Sym./Anti-Sym. wf's from Zeeman spectra (fermions) + Planck Radiation law (bosons)]

$$\Psi(\vec{r}_{P1}, \vec{r}_{P2}, \ldots \vec{r}_{PN}) = \xi^{P}\, \Psi(\vec{r}_1, \ldots \vec{r}_N) \qquad (P1, P2, \ldots PN) \text{ permutation of } (1, 2, \ldots N)$$

$$\xi = \begin{cases} +1 & \text{Bosons} \\ -1 & \text{Fermions} \end{cases}$$

P = "parity of permutation"
= # of pairwise transpositions to bring $(P1, P2, \ldots PN)$ into $(1, 2, \ldots N)$

* Since most of what we do in NP is to work w/ fermions, let's hereafter do the derivations for fermions + just quote the analogous Boson result

* Antisymmetrizer | Symmetrizer Operator

$$A_N\, |\alpha_1 \alpha_2 \cdots \alpha_N) = \frac{1}{N!} \sum_P (-1)^P\, |\alpha_{P1}\rangle \otimes |\alpha_{P2}) \otimes \cdots \otimes |\alpha_{PN})$$

$$S_N\, |\alpha_1 \alpha_2 \cdots \alpha_N) = \frac{1}{N!} \sum_P |\alpha_{P1}) \otimes |\alpha_{P2}\rangle \otimes \cdots \otimes |\alpha_{PN})$$

Exercise: Show $A_N^2 = A_N$ (i.e., projector)

Exercise: Show for $N = 3$ the $A_3 = (1 + P_{13}P_{12} + P_{23}P_{12})(1 - P_{12})$
i.e., consider $A_3 |\alpha_1 \alpha_2 \alpha_3)$ + show it has appropriate antisymmetry

<u>N-body A.S. basis states</u>:

$$\boxed{\begin{aligned}|\alpha_1\alpha_2\cdots\alpha_N\rangle &= \sqrt{N!}\,A_N|\alpha_1\alpha_2\cdots\alpha_N) \\ &= \frac{1}{\sqrt{N!}}\sum_P(-1)^P\,|\alpha_{P1}\rangle\otimes|\alpha_{P2}\rangle\otimes\cdots\otimes|\alpha_{PN}\rangle\end{aligned}}$$

* Pauli principle "built in" since a given sp label, say α_1, can occur at most once

e.g.: $|\alpha_1\alpha_1\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1\alpha_1) - |\alpha_1\alpha_1)\right) = 0$

$|\alpha_1\alpha_1\alpha_3\rangle = 0$ etc

<u>Completeness</u>: $\displaystyle\sum_{\alpha_1\ldots\alpha_N}|\alpha_1\alpha_2\cdots\alpha_N)(\alpha_1\alpha_2\cdots\alpha_N| = \mathbb{1}_{\mathcal{H}_N}$

M. from left + right by A_N

$$\Rightarrow \sum_{\alpha_1\ldots\alpha_N}A_N|\alpha_1\ldots\alpha_N)(\alpha_1\ldots\alpha_N|A_N = A_N^2 = A_N \equiv \mathbb{1}_{\mathcal{F}_N} \qquad \mathcal{F}_N = A_N\mathcal{H}_N$$

$$\Rightarrow \boxed{\frac{1}{N!}\sum_{\alpha_1\ldots\alpha_N}|\alpha_1\cdots\alpha_N\rangle\langle\alpha_1\ldots\alpha_N| = \mathbb{1}_{\mathcal{F}_N}}$$

N! corrects for the fact that states differing only by permutations of sp labels are physically equivalent since they differ at most by a (−) sign.

e.g.: in N=2 system, $|\alpha_1\alpha_2\rangle$ + $|\alpha_2\alpha_1\rangle$ represent the same physical state since $|\alpha_2\alpha_1\rangle = -|\alpha_1\alpha_2\rangle$

$$\Rightarrow \mathbb{1}_{\mathcal{F}_2} = \frac{1}{2!}\sum_{\alpha_1\alpha_2}|\alpha_1\alpha_2\rangle\langle\alpha_1\alpha_2|$$

$$= \sum_{\alpha_1<\alpha_2}|\alpha_1\alpha_2\rangle\langle\alpha_1\alpha_2|$$

$$\Rightarrow \boxed{\mathbb{1}_{\mathcal{F}_N} = \frac{1}{N!}\sum_{\alpha_1\alpha_2\cdots\alpha_N} |\alpha_1\alpha_2\cdots\alpha_N\rangle\langle\alpha_1\alpha_2\cdots\alpha_N| = \sum_{\alpha_1<\alpha_2<\cdots<\alpha_N} |\alpha_1\alpha_2\cdots\alpha_N\rangle\langle\alpha_1\alpha_2\cdots\alpha_N|}$$

Overlaps of A.S. states

$$\begin{aligned}
\langle\alpha_1\alpha_2\cdots\alpha_N|\alpha_1'\alpha_2'\cdots\alpha_N'\rangle &= N!\,(\alpha_1\alpha_2\cdots\alpha_N|A_N^2|\alpha_1'\alpha_2'\cdots\alpha_N') \\
&= N!\,(\alpha_1\alpha_2\cdots\alpha_N|A_N|\alpha_1'\alpha_2'\cdots\alpha_N') \\
&= \cancel{N!}\,\frac{1}{\cancel{N!}}\sum_P(-1)^P(\alpha_1\alpha_2\cdots\alpha_N|\alpha_{P1}'\alpha_{P2}'\cdots\alpha_{PN}') \\
&= \sum_P(-1)^P\langle\alpha_1|\alpha_{P1}')\langle\alpha_2|\alpha_{P2}'\rangle\cdots\langle\alpha_N|\alpha_{PN}'\rangle \\
&= \sum_P(-1)^P\delta_{\alpha_1\alpha_{P1}'}\delta_{\alpha_2\alpha_{P2}'}\cdots\delta_{\alpha_N\alpha_{PN}'}
\end{aligned}$$

Assuming a standard ordering of the sp quantum #'s (i.e., $\alpha_1<\alpha_2<\cdots<\alpha_N$ + ditto for α_i'), then only the identity permutation contributes

$$\Rightarrow \langle\alpha_1\alpha_2\cdots\alpha_N|\alpha_1'\alpha_2'\cdots\alpha_N'\rangle = \delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}\cdots\delta_{\alpha_N\alpha_N'}$$ <u>for ordered states</u>

Else, if there's no restriction that $\alpha_1<\alpha_2\cdots<\alpha_N$ + $\alpha_1'<\alpha_2'<\cdots<\alpha_N'$, then

$$\begin{aligned}
\langle\alpha_1\alpha_2\cdots\alpha_N|\alpha_1'\alpha_2'\cdots\alpha_N'\rangle &= \sum_P(-1)^P\delta_{\alpha_1\alpha_{P1}'}\delta_{\alpha_2\alpha_{P2}'}\cdots\delta_{\alpha_N\alpha_{PN}'} \\
&= \mathrm{Det}\left[\langle\alpha_i|\alpha_j'\rangle\right] = \begin{vmatrix} \langle\alpha_1|\alpha_1'\rangle & \cdots & \langle\alpha_1|\alpha_N'\rangle \\ \vdots & & \\ \langle\alpha_N|\alpha_1'\rangle & \cdots & \langle\alpha_N|\alpha_N'\rangle \end{vmatrix}
\end{aligned}$$

Normalized AS N-body wf : $\Psi_{\alpha_1\alpha_2\cdots\alpha_N}(x_1,\cdots x_N) = (x_1 x_2 \cdots x_N | \alpha_1 \alpha_2 \cdots \alpha_N\rangle$

"Slater Det"

$$= \frac{1}{\sqrt{N!}} \sum_P (-1)^P (x_1 \cdots x_N | \alpha_{P1} \alpha_{P2} \cdots \alpha_{PN})$$

$$= \frac{1}{\sqrt{N!}} \sum_P (-1)^P \langle x_1 | \alpha_{P1}) \langle x_2 | \alpha_{P2}) \cdots$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \langle x_1|\alpha_1\rangle & \cdots & \langle x_N|\alpha_1\rangle \\ \vdots & \ddots & \vdots \\ \langle x_1|\alpha_N\rangle & & \langle x_N|\alpha_N\rangle \end{vmatrix}$$

* Manipulating these SD's (e.g., computing $\langle V\rangle = \sum_{i<j=1}^{N} \int dx_1 \cdots dx_N \, \Psi^*_{\alpha_1\cdots\alpha_N}(x_1\cdots x_N)\, V(x_i,x_j)\, \Psi_{\alpha_1\cdots\alpha_N}(x_1\cdots x_N)$) is a pain in the neck.

* Luckily, there's a much more elegant way using 2^{nd}-quantization

For Completeness, here are the analogous Bosonic results

Say $\{\alpha_1, \alpha_2, \ldots \alpha_p\}$ distinct states w/ n_1 in α_1, n_2 in α_2, etc., where $N = \sum_\alpha n_\alpha$

$$\Rightarrow |\alpha_1 \alpha_2 \cdots\rangle = \sqrt{\frac{N!}{n_1! n_2! \cdots n_p!}}\, S_N |\alpha_1 \alpha_2 \cdots)$$

extra factor to ensure

$\langle \alpha_1 \alpha_2 \cdots \alpha_N | \alpha_1 \alpha_2 \cdots \alpha_N\rangle = 1$

Arises because permuting the n_1 particles in α_1 gives $n_1!$ physically equivalent states

Boson results (Cont'd)

$$\mathbb{1}_{B_N} = S_N \cdot \left(\sum_{\alpha_1 \ldots \alpha_N} |\alpha_1 \cdots \alpha_N)(\alpha_1 \ldots \alpha_N| \right) S_N = \sum_{\alpha_1 \ldots \alpha_N} \frac{(\Pi_\alpha n_\alpha !)}{N!} |\alpha_1 \ldots \alpha_N\rangle\langle \alpha_1 \ldots \alpha_N|$$

Analogous results for, e.g., Slater Permanent

$$\psi_{\alpha_1 \ldots \alpha_N}(x_1 \ldots x_N) = \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{\Pi_\alpha n_\alpha !}} \sum_P \psi_{\alpha_{P_1}}(x_1) \psi_{P_2}(x_2) \cdots$$

Second Quantization (Fermions 1st, then just quote Boson results)

Fock Space $= \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \cdots$ ($\mathcal{F}_N$ = fermion Hilbert space for N-particles)

$$\mathbb{1}_{FS} = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\alpha_1 \ldots \alpha_N} |\alpha_1 \ldots \alpha_N\rangle\langle \alpha_1 \ldots \alpha_N| = \sum_{N=0}^{\infty} \sum_{\alpha_1 < \alpha_2 \cdots < \alpha_N} |\alpha_1 \ldots \alpha_N\rangle\langle \alpha_1 \ldots \alpha_N|$$

Note: the $N=0$ state called the vacuum & denoted by $|0\rangle$ (or $|\,\rangle$)

Creation/Annihilation Operators

$$\boxed{a^\dagger_\alpha |\alpha_1 \alpha_2 \ldots \alpha_N\rangle \equiv |\alpha \alpha_1 \alpha_2 \ldots \alpha_N\rangle}$$

"Creation" or "Addition" Operator

e.g.: $a^\dagger_\beta |0\rangle = |\beta\rangle$ $\qquad a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma |0\rangle = |\alpha\beta\gamma\rangle$

$a^\dagger_\alpha a^\dagger_\beta |0\rangle = |\alpha\beta\rangle$

$\Rightarrow$ build up all basis states of F.S. by repeated action of creation operators to vacuum. //

One immediate consequence: $|\alpha\beta\rangle = a^\dagger_\alpha a^\dagger_\beta |0\rangle = -|\beta\alpha\rangle = -a^\dagger_\beta a^\dagger_\alpha |0\rangle$

$$\boxed{\begin{gathered} \Rightarrow \{a^\dagger_\alpha, a^\dagger_\beta\} = a^\dagger_\alpha a^\dagger_\beta + a^\dagger_\beta a^\dagger_\alpha = 0 \\ \text{and} \\ \{a_\alpha, a_\beta\} = 0 \end{gathered}}$$

Meaning of adjoint a_α: $a_\alpha |\alpha_1 \alpha_2 \cdots \alpha_N\rangle = \mathbb{1}_{F.S.}\, a_\alpha |\alpha_1 \cdots \alpha_N\rangle$ (assume ordered $\alpha_1 < \alpha_2 \cdots < \alpha_N$)

$$= \sum_{M=0}^{\infty} \sum_{\alpha_1' < \alpha_2' \cdots < \alpha_M'} |\alpha_1' \cdots \alpha_M'\rangle \langle \alpha_1' \cdots \alpha_M' | a_\alpha | \alpha_1 \cdots \alpha_N\rangle$$

but $a^\dagger_\alpha |\alpha_1' \cdots \alpha_M'\rangle = |\alpha \alpha_1' \cdots \alpha_M'\rangle$

$\Rightarrow \langle \alpha_1' \cdots \alpha_M' | a_\alpha = \langle \alpha \alpha_1' \cdots \alpha_M' |$

$$= \sum_{M=0}^{\infty} \sum_{\alpha_1' \cdots \alpha_M'}^{\text{ordered}} |\alpha_1' \cdots \alpha_M'\rangle \underbrace{\langle \alpha \alpha_1' \cdots \alpha_M' | \alpha_1 \cdots \alpha_N\rangle}_{\text{vanishes unless } M = N-1} \quad \otimes$$

$\Rightarrow a_\alpha |\alpha_1 \cdots \alpha_N\rangle \in F_{N-1}$ so a_α is called "annihilation" or "removal" operator.

*Now, $\langle \alpha \alpha_1' \alpha_2' \cdots \alpha_M' |$ not in standard order (unless $\alpha < \alpha_1'$). Say $\alpha_{i-1}' < \alpha < \alpha_i'$

$$|\alpha \alpha_1' \alpha_2' \cdots \alpha_{i-1}' \alpha_i' \cdots \alpha_{N-1}'\rangle = (-1)^{i-1} |\alpha_1' \cdots \alpha_{i-1}' \alpha \alpha_{i+1}' \cdots \alpha_N'\rangle$$

Thus, eqn $\otimes$ becomes: $a_\alpha |\alpha_1 \cdots \alpha_N\rangle = \sum_{\alpha_1' \cdots \alpha_{N-1}'}^{\text{ordered}} |\alpha_1' \cdots \alpha_{N-1}'\rangle (-1)^{i-1} \underbrace{\langle \alpha_1' \cdots \alpha_{i-1}' \alpha \alpha_i' \cdots \alpha_{N-1}' | \alpha_1 \alpha_2 \cdots \alpha_N\rangle}_{= \delta_{\alpha_1'\alpha_1} \delta_{\alpha_2'\alpha_2} \cdots \delta_{\alpha\alpha_i} \delta_{\alpha_i'\alpha_{i+1}} \cdots \delta_{\alpha_{N-1}'\alpha_N}}$

$$= (-1)^{i-1} |\alpha_1 \alpha_2 \cdots \alpha_{i-1} \alpha_{i+1} \cdots \alpha_N\rangle \delta_{\alpha\alpha_i}$$

$$\Rightarrow \boxed{\begin{aligned} a_\alpha |\alpha_1 \cdots \alpha_N\rangle &= (-1)^{i-1} |\alpha_1 \cdots \alpha_{i-1} \alpha_{i+1} \cdots \alpha_N\rangle \quad \text{if } \alpha=\alpha_i \text{ occupied} \\ &= 0 \quad \text{else} \end{aligned}}$$

1 trivial consequence is $a_\alpha |0\rangle = \langle 0| a_\alpha^\dagger = 0$

*We've shown $\{a_\alpha^\dagger, a_\beta^\dagger\} = \{a_\alpha, a_\beta\} = 0$. What about $\{a_\alpha, a_\beta^\dagger\}$?

$$a_\lambda a_\mu^\dagger |\alpha_1 \cdots \alpha_N\rangle = a_\lambda |\mu \alpha_1 \cdots \alpha_N\rangle = \delta_{\lambda\mu} |\alpha_1 \cdots \alpha_N\rangle + \sum_{i=1}^{N} (-1)^i \delta_{\lambda \alpha_i} |\mu \alpha_1 \cdots \alpha_{i-1} \alpha_{i+1} \cdots \alpha_N\rangle \quad (1)$$

and

$$a_\mu^\dagger a_\lambda |\alpha_1 \cdots \alpha_N\rangle = a_\mu^\dagger \sum_{i=1}^{N} (-1)^{i-1} \delta_{\lambda\alpha_i} |\alpha_1 \cdots \alpha_{i-1} \alpha_{i+1} \cdots \alpha_N\rangle = \sum_{i=1}^{N} (-1)^{i-1} \delta_{\lambda\alpha_i} |\mu \alpha_1 \cdots \alpha_{i-1} \alpha_{i+1} \cdots \alpha_N\rangle \quad (2)$$

$$(1) + (2) = \{a_\lambda, a_\mu^\dagger\} |\alpha_1 \cdots \alpha_N\rangle = \delta_{\lambda\mu} |\alpha_1 \cdots \alpha_N\rangle$$

$$\boxed{\begin{aligned} \Rightarrow \{a_\lambda, a_\mu^\dagger\} &= \delta_{\lambda\mu} \\ \{a_\lambda, a_\mu\} &= 0 \\ \{a_\lambda^\dagger, a_\mu^\dagger\} &= 0 \end{aligned}}$$

"Fundamental Anti-Commutation Relations"

All the tedium of properly antisymmetrizing fermion wf's is encoded in the anti-comm. relations

$\Rightarrow$ Maybe show Morten's slides on how 2nd-quant. tailor-made for bit manipulations on a computer.

Change of basis Let $\{|\alpha\rangle\}$ + $\{|i\rangle\}$ be two different complete s.p. bases w/ corresponding $(a^\dagger_\alpha, a_\alpha)$ + $(c^\dagger_i, c_i)$

$$|\alpha\rangle = \sum_i |i\rangle\langle i|\alpha\rangle = \sum_i |i\rangle U_{i\alpha}$$

where $\langle\beta|\alpha\rangle = \delta_{\alpha\beta} = \sum_{ij} U^*_{j\beta} U_{i\alpha} \cancel{\langle j|i\rangle}^{\delta_{ij}} \Rightarrow \sum_i U^*_{i\beta} U_{i\alpha} = \delta_{\alpha\beta}$

$$\Rightarrow |\alpha\rangle = a^\dagger_\alpha|0\rangle = \sum_i c^\dagger_i |0\rangle U_{i\alpha}$$

$$\boxed{a^\dagger_\alpha = \sum_i c^\dagger_i \langle i|\alpha\rangle = \sum_i c^\dagger_i U_{i\alpha}}$$

* Likewise, $\langle\alpha| = \sum_i \langle\alpha|i\rangle\langle i| = \sum_i U^*_{i\alpha}\langle i|$

$$\Downarrow$$

$$\boxed{a_\alpha = \sum_i \langle\alpha|i\rangle c_i = \sum_i c_i U^*_{i\alpha}}$$

* This unitary change of basis is called "Canonical" since Fund. AC relations preserved

i.e. Suppose $\{c_i, c^\dagger_j\} = \delta_{ij}$ etc

$$\Rightarrow \{a_\alpha, a^\dagger_\beta\} = \sum_{ij} U_{i\beta} U^*_{j\alpha} \{c_j, c^\dagger_i\} = \sum_i U_{i\beta} U^*_{i\alpha} = \delta_{\alpha\beta}$$

example: $|\alpha\rangle = |n\ell m \tfrac{1}{2}\sigma\rangle$ $\Rightarrow$ $a^\dagger(\vec{r}\sigma) = \sum_{n\ell m\sigma'} c^\dagger_{n\ell m\sigma'} \langle n\ell m\sigma'|\vec{r}\sigma\rangle$ "Field Operator"

$|i\rangle = |\vec{r},\sigma\rangle$ (often denoted $\psi^\dagger_\sigma(\vec{r})$)

$$= \sum_{n\ell m\sigma'} c^\dagger_{n\ell m\sigma'} R^*_{n\ell}(r) Y^*_{\ell m}(\hat{r}) \chi^*_{\sigma'}(\sigma)$$

2^{nd}-quantization representation of Operators in Fock Space

* 1-body Operator F specified by its M.E.'s in 1-body space

$$F = \sum_{\alpha,\beta} |\alpha\rangle\langle\alpha|F|\beta\rangle\langle\beta|$$

* In N-particle space, $F_N = \sum_{i=1}^{N} F(i)$ $\quad$ (e.g. $T = \sum_i \frac{p_i^2}{2m}$)

$$F(i)|\alpha_1\cdots\alpha_N) = |\alpha_1\rangle\otimes|\alpha_2\rangle\otimes\cdots\otimes\left(F(i)|\alpha_i\rangle\right)\otimes\cdots|\alpha_N\rangle$$ only acts on ith particle

$$= \sum_{\beta_i} \langle\beta_i|F|\alpha_i\rangle \times |\alpha_1\cdots\alpha_{i-1}\beta_i\alpha_{i+1}\cdots\alpha_N)$$

$$\boxed{\Rightarrow F_N|\alpha_1\cdots\alpha_N) = \sum_{i=1}^{N}\sum_{\beta_i} \langle\beta_i|F|\alpha_i\rangle\, |\alpha_1\cdots\alpha_{i-1}\beta_i\alpha_{i+1}\cdots\alpha_N)}$$

To get action of $F_N|\alpha_1\cdots\alpha_N\rangle = F_N A_N|\alpha_1\cdots\alpha_N)\sqrt{N!}$ $\quad$ but $[F_N, A_N] = 0$

$$= \sqrt{N!}A_N\, F_N|\alpha_1\cdots\alpha_N)$$

$$\boxed{F_N|\alpha_1\cdots\alpha_N\rangle = \sum_{i=1}^{N}\sum_{\beta_i} \langle\beta_i|F|\alpha_i\rangle\, |\alpha_1\cdots\alpha_{i-1}\beta_i\alpha_{i+1}\cdots\alpha_N\rangle}$$

Representation in Fock Space: Strategy is to derive result in a basis for which F diagonal, then transform to arbitrary sp basis

let $F|a\rangle = f_a|a\rangle \Rightarrow F = \sum_a f_a|a\rangle\langle a|$

$$F_N|a_1\cdots a_N\rangle = \left(\sum_{i=1}^{N} f_{a_i}\right)|a_1\cdots a_N\rangle$$

<u>Number operator</u> $\hat{n}_b = a_b^\dagger a_b$

$$\hat{n}_b |a_1 \cdots a_N\rangle = a_b^\dagger \sum_{i=1}^{N} (-1)^{i-1} \delta_{a_i b} |a_1 \cdots a_{i-1} a_{i+1} \cdots a_N\rangle$$

$$= \sum_{i=1}^{N} (-1)^{i-1} \delta_{b,a_i} |b\, a_1 \cdots a_{i-1} a_{i+1} \cdots a_N\rangle$$

$$= \sum_{i=1}^{N} (-1)^{i-1} \times (-1)^{i-1} \delta_{b,a_i} |a_1 \cdots a_{i-1} b\, a_{i+1} \cdots a_N\rangle$$

$$= \left(\sum_{i=1}^{N} \delta_{b a_i}\right) |a_1 \cdots a_{i-1} a_i a_{i+1} \cdots a_N\rangle$$

Counts the # of particles (0 or 1 for fermions) in the state b

$$\Rightarrow \hat{N} \equiv \sum_b \hat{n}_b = \sum_b a_b^\dagger a_b$$

$$\Rightarrow \hat{N} |a_1 \cdots a_N\rangle = N |a_1 \cdots a_N\rangle$$

Counts total # of particles

Now, $F_N |a_1 \cdots a_N\rangle = \left(\sum_{i=1}^{N} f_{a_i}\right) |a_1 \cdots a_N\rangle = \sum_a f_a \hat{n}_a |a_1 \cdots a_N\rangle$

$$\Rightarrow \boxed{\hat{F} = \sum_a \langle a|F|a\rangle a_a^\dagger a_a}$$

Fock-space rep. of 1-body operator in diagonal rep. of F

<u>NOTE</u>: $\hat{F}$ contains no reference to N unlike the "1st quantized" way of writing F_N.

* arbitrary basis: let $|a\rangle = \sum_{\alpha} |\alpha\rangle\langle\alpha|a\rangle$

$$\Rightarrow a_a^\dagger = \sum_{\alpha} c_\alpha^\dagger \langle\alpha|a\rangle \Leftrightarrow \sum_a a_a^\dagger \langle a|\alpha\rangle = c_\alpha^\dagger$$

$$\Rightarrow \hat{F} = \sum_a \langle a|F|a\rangle a_a^\dagger a_a = \sum_{a,b} \langle a|F|b\rangle a_a^\dagger a_b$$

$$= \sum_{a,b}\sum_{\alpha,\beta} \langle a|F|b\rangle c_\alpha^\dagger \langle\alpha|a\rangle c_\beta \langle b|\beta\rangle$$

$$\boxed{\hat{F} = \sum_{\alpha,\beta} \langle\alpha|F|\beta\rangle c_\alpha^\dagger c_\beta}$$

* Fock Space rep. of 2-body Operator

* Same idea as 1-body deriv., but a bit more tedious

i.e., 2-body operator on 2-body space given by

$$V = \sum_{\alpha\beta}\sum_{\gamma\delta} |\alpha\beta)(\alpha\beta|V|\gamma\delta)(\gamma\delta|$$

* as before, lets first work in 2-body basis that makes V diagonal

i.e., let $V|ab) = V_{ab}|ab)$

$$\Rightarrow V = \sum_{ab} V_{ab} |ab)(ab|$$

Now, V acting in N-body space

$$V_N \equiv \sum_{i<j} V(i,j) \qquad V(i,j) \text{ acts only on } i \,\&\, j^{th} \text{ particle}$$

$$\Rightarrow V_N |a_1 a_2 \cdots a_N\rangle = V_N \sqrt{N!}\, A_N |a_1 \cdots a_N)$$

$$= \sqrt{N!}\, A_N\, V_N |a_1 \cdots a_N)$$

$$= \sqrt{N!}\, A_N \cdot \sum_{i<j=1}^{N} V_{a_i a_j} |a_1 \cdots a_N) = \sum_{i<j=1}^{N} V_{a_i a_j} |a_1 \cdots a_N\rangle$$

$$\Rightarrow V_N |a_1 a_2 \cdots a_N\rangle = \underbrace{\left(\sum_{i<j=1}^{N} V_{a_i a_j}\right)}_{\text{Sum over all distinct pairs.}} |a_1 \cdots a_N\rangle$$

Need a number operator that counts # of pairs of particles in the states a & b.

Claim: $\hat{P}_{ab} \equiv \hat{n}_a \hat{n}_b - \delta_{ab} \hat{n}_a$ does the job.

$$= a_a^\dagger a_a a_b^\dagger a_b - \delta_{ab} a_a^\dagger a_a$$

$$= a_a^\dagger \cancel{\delta_{ab}} a_b - a_a^\dagger a_b^\dagger a_a a_b - \cancel{\delta_{ab} a_a^\dagger} a_a$$

$$\hat{P}_{ab} = a_a^\dagger a_b^\dagger a_b a_a$$ counts pairs of particles in states a & b

$$\Rightarrow V_N |a_1 \ldots a_N\rangle = \left(\sum_{i<j=1}^{N} V_{a_i a_j}\right) |a_1 \ldots a_N\rangle = \frac{1}{2}\left(\sum_{i\neq j=1}^{N} V_{a_i a_j}\right) |a_1 \ldots a_N\rangle$$

$$= \frac{1}{2}\sum_{a,b} V_{ab} \hat{P}_{ab} |a_1 \ldots a_N\rangle$$

$$\Rightarrow \boxed{\hat{V} = \frac{1}{2}\sum_{ab} V_{ab}\, a_a^\dagger a_b^\dagger a_b a_a}$$

Fock space rep. in diagonal basis

*Again, note that there's no ref. to N!!

* <u>In arbitrary sp basis</u> (same steps as 1-body example)

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta)\, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

order is crucial for fermions!

<u>Exercise</u>: Show we can write $\hat{V}$ also as

$$\hat{V} = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|V|\gamma\delta\rangle\, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \qquad |\gamma\delta\rangle = \frac{1}{\sqrt{2}}\left[|\gamma\delta) - |\delta\gamma)\right]$$

$$= \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \left[(\alpha\beta|V|\gamma\delta) - (\alpha\beta|V|\delta\gamma)\right] c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

Wick's Theorem

<u>ex</u>: $\langle \alpha_1'\alpha_2' | \hat{F} | \alpha_1\alpha_2 \rangle = \sum_{\alpha\beta} F_{\alpha\beta} \langle \alpha_1'\alpha_2' | a^\dagger_\alpha a_\beta | \alpha_1 \alpha_2 \rangle$

$$= \sum_{\alpha\beta} F_{\alpha\beta} \langle 0 | a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} | 0 \rangle$$

One strategy is to use F.A.C.R. to push a's to right where $a|0\rangle = 0$ + $a^\dagger$'s to left where $\langle 0 | a^\dagger = 0$

e.g. $\langle 0 | a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} | 0 \rangle = \langle 0 | a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha [a_\beta, a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}] | 0 \rangle + \cancelto{0}{\langle 0 | a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a_\beta | 0 \rangle}$

$$= \langle 0 | [a_{\alpha_2'} a_{\alpha_1'}, a^\dagger_\alpha] [a_\beta, a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}] | 0 \rangle \quad \otimes$$

Now use a trick $[A,BC] = ABC - BCA = \{A,B\}C - B\{A,C\}$

$$\Rightarrow [a_\beta, a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}] = \delta_{\beta\alpha_1} a^\dagger_{\alpha_2} - a^\dagger_{\alpha_1} \delta_{\beta\alpha_2}$$

$$\Rightarrow [a_{\alpha_2'} a_{\alpha_1'}, a^\dagger_\alpha] = -[a^\dagger_\alpha, a_{\alpha_2'} a_{\alpha_1'}] = -\delta_{\alpha\alpha_2'} a_{\alpha_1'} + a_{\alpha_2'} \delta_{\alpha\alpha_1'}$$

$$\otimes = \langle 0 | [-\delta_{\alpha\alpha_2'} a_{\alpha_1'} + \delta_{\alpha\alpha_1'} a_{\alpha_2'}][\delta_{\beta\alpha_1} a^\dagger_{\alpha_2} - \delta_{\beta\alpha_2} a^\dagger_{\alpha_1}] | 0 \rangle$$

$$= +\delta_{\alpha\alpha_1'}\delta_{\beta\alpha_1}\delta_{\alpha_2'\alpha_2} - \delta_{\alpha\alpha_1'}\delta_{\beta\alpha_2}\delta_{\alpha_2'\alpha_1} - \delta_{\alpha\alpha_2'}\delta_{\beta\alpha_1}\delta_{\alpha_1'\alpha_2} + \delta_{\alpha\alpha_2'}\delta_{\beta\alpha_2}\delta_{\alpha_1'\alpha_1}$$

$$\Rightarrow \langle \alpha_1'\alpha_2' | F | \alpha_1\alpha_2 \rangle = F_{\alpha_1'\alpha_1}\delta_{\alpha_2'\alpha_2} + F_{\alpha_2'\alpha_2}\delta_{\alpha_1'\alpha_1} - F_{\alpha_1'\alpha_2}\delta_{\alpha_2'\alpha_1} - F_{\alpha_2'\alpha_1}\delta_{\alpha_1'\alpha_2}$$

* Straightforward but tedious to use FACR's, especially for more complicated strings of $a\,a^\dagger$'s.

* Statement of Wick's theorem

Normal ordering: let $A_1 A_2 \cdots A_n$ = string of creation + annihilation ops.
(A_i can be either $a_i^\dagger$ or a_i)

$$N[A_1 A_2 \cdots A_n] = (-1)^P a^\dagger_{P_1} a^\dagger_{P_2} \cdots a_{P_{N-1}} a_{P_N}$$

N-product puts all $a^\dagger$'s to the left + all a's to the right

$(-1)^P$ = Signature of permutation that takes
$A_1 A_2 \ldots A_n \longrightarrow a^\dagger_{P_1} a^\dagger_{P_2} \cdots a_{P_N}$

ex: $N[a_i a_j^\dagger] = -a_i^\dagger a_j$

$$N[a_i^\dagger a_j a_k a_\ell^\dagger] = a_i^\dagger a_\ell^\dagger a_j a_k = -a_\ell^\dagger a_i^\dagger a_j a_k = -a_i^\dagger a_\ell^\dagger a_k a_j = +a_\ell^\dagger a_i^\dagger a_k a_j$$

(Not always unique!)

$$\boxed{\text{Key Point: } \langle 0 | N[A_1 A_2 \cdots A_n] | 0 \rangle = 0}$$

* Wick Contractions

$$\boxed{\overline{A_1 A_2} \equiv A_1 A_2 - N[A_1 A_2]}$$

* 4 possible fundamental Contractions

$$\wick{\c a^\dagger_1 \c a^\dagger_2} = a^\dagger_1 a^\dagger_2 - N(a^\dagger_1 a^\dagger_2) = a^\dagger_1 a^\dagger_2 - a^\dagger_1 a^\dagger_2 = 0$$

$$\wick{\c a^\dagger_1 \c a_2} = a^\dagger_1 a_2 - N(a^\dagger_1 a_2) = a^\dagger_1 a_2 - a^\dagger_1 a_2 = 0$$

$$\wick{\c a_1 \c a_2} = a_1 a_2 - N(a_1 a_2) = 0$$

$$\wick{\c a_1 \c a^\dagger_2} = a_1 a^\dagger_2 - N(a_1 a^\dagger_2) = a_1 a^\dagger_2 + a^\dagger_2 a_1 = \{a_1, a^\dagger_2\} = \delta_{12}$$

* Normal Products w/ Contractions

$\wick{\c A_1 \c A_2}$ is just a number. However, it doesn't mean we can just pull it out of N-ordered string. Need to keep track of how many uncontracted or contracted A's you pass as you bring the pair side-by-side.

e.g.: $$N[\wick{\c A_1 A_2 \c A_3}] = -N[\wick{\c A_1 \c A_2} A_3] = -\wick{\c A_1 \c A_2}\, N[A_3]$$

$$N[\wick{\c A_1 A_2 A_3 \c A_4}] = +\wick{\c A_1 \c A_4}\, N[A_2 A_3]$$

$$N[A_1 \wick{\c A_2 \c A_3} A_4] = +\wick{\c A_2 \c A_3}\, N[A_1 A_4]$$

$$N[\wick{\c1 A_1 \c2 A_2 \c1 A_3 \c2 A_4} A_5 \cdots] \quad - \wick{\c A_1 \c A_3}\, \wick{\c A_2 \c A_4}\, N[A_5 \cdots]$$

Statement of Wick's theorem (See the textbooks for a simple but tedious proof)

$$A_1 A_2 \cdots A_n = N(A_1 A_2 \cdots A_n) + \sum_{\substack{\text{single}\\ \text{contractions}}} N(\overbrace{A_1 A_2} A_3 \cdots A_n)$$

$$+ \sum_{\substack{\text{double}\\ \text{contractions}}} N(\overbrace{A_1 \overbrace{A_2 A_3} \cdots A_n})$$

$$+ \cdots$$

$$+ \sum_{\substack{\text{fully}\\ \text{contracted}}} N(\overbrace{A_1 A_2}\,\overbrace{A_3 A_4}\,\overbrace{A_5 A_6} \cdots \overbrace{\cdots A_n})$$

e.g.: $$a_1 a_2^\dagger a_3 a_4^\dagger = N(a_1 a_2^\dagger a_3 a_4^\dagger) + N(a_1 a_2^\dagger \overbrace{a_3 a_4^\dagger}) + N(\overbrace{a_1 a_2^\dagger} a_3 a_4^\dagger)$$

$$+ N(\overbrace{a_1 a_2^\dagger a_3 a_4^\dagger})$$

$$+ N(\overbrace{a_1 a_2^\dagger}\,\overbrace{a_3 a_4^\dagger})$$

Big Win: $$\langle 0 | A_1 A_2 \cdots A_n | 0 \rangle = \sum_{\substack{\text{fully}\\ \text{contracted}\\ \text{terms}}}$$

ex: $\langle \alpha_1' \alpha_2' | \hat{F} | \alpha_1 \alpha_2 \rangle = \sum_{\alpha\beta} F_{\alpha\beta} \langle 0 | a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} | 0 \rangle$

$$\langle 0 | a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} | 0 \rangle = \sum_{\substack{\text{fully} \\ \text{contracted}}} = a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} + a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$$

$$+\,\delta_{\alpha\alpha_1'} \delta_{\beta\alpha_1} \delta_{\alpha_2'\alpha_2} \qquad - \delta_{\alpha\alpha_1'} \delta_{\beta\alpha_2} \delta_{\alpha_2'\alpha_1}$$

$$+ a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} + a_{\alpha_2'} a_{\alpha_1'} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$$

$$-\,\delta_{\alpha\alpha_2'} \delta_{\beta\alpha_1} \delta_{\alpha_1'\alpha_2} \qquad + \delta_{\alpha\alpha_2'} \delta_{\beta\alpha_2} \delta_{\alpha_1\alpha_1'}$$

$$\boxed{\begin{aligned} \Rightarrow \langle \alpha_1' \alpha_2' | \hat{F} | \alpha_1 \alpha_2 \rangle = {} & F_{\alpha_1'\alpha_1} \delta_{\alpha_2'\alpha_2} + F_{\alpha_2'\alpha_2} \delta_{\alpha_1'\alpha_1} \\ & - F_{\alpha_1'\alpha_2} \delta_{\alpha_2'\alpha_1} - F_{\alpha_2'\alpha_1} \delta_{\alpha_1'\alpha_2} \end{aligned}}$$

* As before, but w/ much less effort!