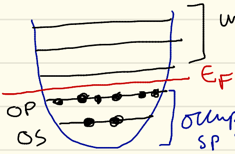
## * Particle - Hole Picture

* For N-body systems, it is useful to switch to basis states labeled as deviations (i.e, excitations of) from some reference N-body Slater Det. $|\Phi\rangle$ rather than states w/ N - $a^\dagger$ acting on $|0\rangle$ where all N-particles explicitly active




] unoccupied sp. states (particle states)

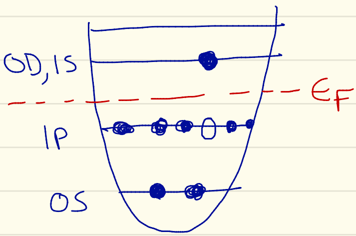
occupied sp states (hole states)

$$|\Phi\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle$$

Important! Many different labeling conventions exist! Here, I will stick to

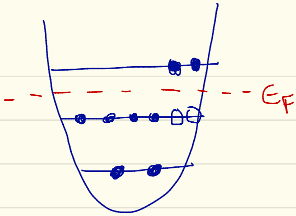
$$\boxed{\begin{array}{ll} a, b, c, \ldots & = \text{particle states} \\ i, j, k, \ldots & = \text{hole states} \\ r, s, t, \ldots & = \text{unrestricted} \end{array}}$$

1 particle - 1 hole (ph) excitations: $|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi\rangle$



2p-2h excitations: $|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_i a_b^\dagger a_j |\Phi\rangle$

$= a_a^\dagger a_b^\dagger a_j a_i |\Phi\rangle$




$$\Rightarrow \mathbb{1}_{\mathcal{F}_N} = |\Phi\rangle\langle\Phi| + \sum_{a,i} |\Phi_i^a\rangle\langle\Phi_i^a| + \sum_{\substack{a<b \\ i<j}} |\Phi_{ij}^{ab}\rangle\langle\Phi_{ij}^{ab}| + \cdots + \sum_{\substack{a<b<\cdots< \\ i<j<\cdots}} |\Phi_{ij\cdots}^{ab\cdots}\rangle\langle\Phi_{ij\cdots}^{ab\cdots}|$$

Re-define creation/annihilation operators $(a, a^\dagger) \longrightarrow (b, b^\dagger)$

$$a_a^\dagger = b_a^\dagger \qquad a_i = b_i^\dagger$$
$$a_a = b_a \qquad a_i^\dagger = b_i$$

Why is this useful?

① $\{a_r, a_s^\dagger\} = \delta_{rs} \longrightarrow \{b_r, b_s^\dagger\} = \delta_{rs}$

i.e., canonical transf.

i.e., mathematically just like $|\alpha_1\alpha_2\cdots\alpha_N) = a_{\alpha_1}^\dagger \cdots a_{\alpha_N}^\dagger |0)$

$a_\alpha |0) = 0$

etc.

② $b_r |\Phi\rangle = 0$

$\langle\Phi| b_r^\dagger = 0$

③ $|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi\rangle = b_a^\dagger b_i^\dagger |\Phi\rangle$

etc...

# Normal Order w/respect to $|\Phi\rangle$

$$\{B_1 B_2 \cdots B_n\} \equiv (-1)^P \, b^\dagger_{P1} \cdots b_{Pn}$$

<u>Notation</u>: to distinguish N-ordering w.r.t. $|\Phi\rangle$ from N-ordering w.r.t $|0\rangle$, I will use $\{\cdots\}$ instead of $N[\cdots]$. // ✱ ✱

<u>ex</u>: $\{b_i b^\dagger_j\} = -b^\dagger_j b_i$

$$\{b_i b^\dagger_a b^\dagger_j b_b\} = b^\dagger_a b^\dagger_j b_i b_b = -b^\dagger_a b^\dagger_j b_b b_i \quad \text{etc}$$

<u>Note</u>: Often, we don't even bother going thru the notational step of $(a, a^\dagger) \rightarrow (b, b^\dagger)$

e.g., the previous 2 examples $\{b_i b^\dagger_j\} = \{a^\dagger_i a_j\} = -a_j a^\dagger_i$

$$\{b_i b^\dagger_a b^\dagger_j b_b\} = \{a^\dagger_i a^\dagger_a a_j a_b\} = a^\dagger_a a_j a^\dagger_i a_b$$

i.e., the curly brackets are sufficient context that we push all $a^\dagger_i + a_a$ to the right and all $a_i + a^\dagger_a$ to the left when N-ordering wrt $|\Phi\rangle$

<u>Contractions wrt $|\Phi\rangle$</u>:

$$\overbracket{B_q B_r} \equiv B_q B_r - \{B_q B_r\}$$

$$\overbracket{b_q b_r} = \overbracket{b^\dagger_q b^\dagger_r} = \overbracket{b^\dagger_q b_r} = 0$$

$$\overbracket{b_q b^\dagger_r} = \delta_{qr}$$

$$\overbracket{B_q B_r} \equiv B_q B_r - \{B_q B_r\}$$

$$\overbracket{b_q b_r} = \overbracket{b_q^\dagger b_r^\dagger} = \overbracket{b_q^\dagger b_r} = 0$$

$$\overbracket{b_q b_r^\dagger} = \delta_{qr}$$

* <u>In terms of the $a^\dagger, a$ -operators,</u>

$$\overbracket{b_q^\dagger b_r} = \delta_{qr} \implies \overbracket{a_a a_b^\dagger} = a_a a_b^\dagger - \{a_a a_b^\dagger\} = a_a a_b^\dagger + a_b^\dagger a_a = \delta_{ab}$$

$$\overbracket{a_i^\dagger a_j} = a_i^\dagger a_j - \{a_i^\dagger a_j\} = a_i^\dagger a_j + a_j a_i^\dagger = \delta_{ij}$$

we can write this more compactly w/ no restriction on the indices

$$\boxed{\begin{aligned} &\overbracket{a_q^\dagger a_r} = \delta_{qr} n_q \qquad && \text{where } n_q = \begin{cases} 1 & \text{if } q \text{ occupied in } |\Phi\rangle \\ 0 & \text{else} \end{cases} \\ &\overbracket{a_q a_r^\dagger} = \delta_{qr} \bar{n}_q && \\ &\overbracket{a_q a_r} = \overbracket{a_q^\dagger a_r^\dagger} = 0 && \bar{n}_q = 1 - n_q \end{aligned}}$$

<u>Wick's theorem wrt $|\Phi\rangle$</u>

$$A_1 \cdots A_n = \{A_1 \cdots A_n\}$$

$$+ \{\overbracket{A_1 A_2} \cdots A_n\} + \{\overbracket{A_1 A_2 \cdots A_n}\} + \text{all single contractions}$$

$$\langle \Phi | A_1 \cdots A_n | \Phi \rangle = \sum_{\substack{\text{fully} \\ \text{contracted}}}$$

$$+ \{\overbracket{A_1 A_2} \overbracket{A_3 A_4} \cdots A_n\} + \text{all double contractions}$$

$$+ \cdots$$

$$+ \{\overbracket{A_1 A_2} \overbracket{A_3 A_4} \overbracket{\cdots A_n}\} + \text{all fully contracted}$$

Ex: find $\langle \Phi | \hat{H} | \Phi \rangle$

$$\langle \Phi | \hat{T} | \Phi \rangle = \sum_{q,r} T_{qr} \langle \Phi | a_q^\dagger a_r | \Phi \rangle = \sum_{qr} T_{qr} \langle \Phi | a_q^\dagger a_r | \Phi \rangle$$

$$= \sum_{qr} T_{qr} n_q \delta_{qr}$$

$$= \sum_q T_{qq} n_q = \sum_{i=1}^{N} T_{ii}$$

$$\langle \Phi | \hat{V} | \Phi \rangle = \frac{1}{4} \sum_{qrst} \langle qr | v | st \rangle \Big( \langle \Phi | a_q^\dagger a_r^\dagger a_t a_s | \Phi \rangle + \langle \Phi | a_q^\dagger a_r^\dagger a_t a_s | \Phi \rangle \Big)$$

$$n_q n_r \delta_{rt} \delta_{qs} \qquad\qquad - \delta_{qt} \delta_{rs} n_q n_r$$

$$= \frac{1}{4} \sum_{qr} \Big( \langle qr | v | qr \rangle - \langle qr | v | rq \rangle \Big) n_q n_r$$

$$+ \langle qr | v | qr \rangle$$

$$= \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle$$

Example: N-ordered H (wrt $|\Phi\rangle$)

$$\hat{H} = \sum_{qr} T_{qr} a_q^\dagger a_r + \frac{1}{4} \sum_{qrst} V_{qrst} a_q^\dagger a_r^\dagger a_t a_s$$

already in N-order wrt $|0\rangle$. It is useful to put it in N-order wrt $|\Phi\rangle$.

* just apply Wick's theorem (wrt $|\Phi\rangle$)

$$T = \sum_{qr} T_{qr}\, a_q^\dagger a_r = \sum_{qr} T_{qr}\left(\{a_q^\dagger a_r\} + a_q^\dagger a_r\right) = \sum_{i} T_{ii} + \sum_{q,r} T_{qr}\{a_q^\dagger a_r\}$$

$$\Rightarrow \quad T = \langle\Phi|T|\Phi\rangle + \hat{T}_N \quad ①$$

(here, N stands for N-ordered NOT # of particles!)

$$\hat{V} = \frac{1}{4}\sum_{qrst} V_{qrst}\, a_q^\dagger a_r^\dagger a_t a_s$$

$$= \frac{1}{4}\sum_{qrst} V_{qrst}\Big(\{q^\dagger r^\dagger t s\} + \{q^\dagger r^\dagger t s\} + \{q^\dagger r^\dagger t s\}$$

$$+ \{q^\dagger r^\dagger t s\} + \{q^\dagger r^\dagger t s\}$$

$$+ \{q^\dagger r^\dagger t s\} + \{q^\dagger r^\dagger t s\}\Big)$$

$$\hat{V} = \langle\Phi|\hat{V}|\Phi\rangle + \sum_{qs}\{q^\dagger s\}\left(\sum_{i=1}^{N} V_{qisi}\right) + \frac{1}{4}\sum_{qrst} V_{qrst}\{q^\dagger r^\dagger t s\} \quad ②$$

Combining ① & ②: $$\hat{H} = E_{ref} + \sum_{qr} f_{qr}\{a_q^\dagger a_r\} + \frac{1}{4}\sum_{qrst} V_{qrst}\{a_q^\dagger a_r^\dagger a_t a_s\}$$

$$= E_{ref} + \hat{f}_N + \hat{V}_N = E_{ref} + \hat{H}_N$$

$$E_{ref} = \langle\Phi|H|\Phi\rangle$$

$$f_{qr} = T_{qr} + \sum_{i=1}^{N} V_{qiri}$$

* Especially useful as approximate treatment of 3N forces

Realistic nuclear hamiltonians have 3NF's

$$H = \sum_{q,r} T_{qr}\, a_q^\dagger a_r + \frac{1}{4}\sum V_{qrst}\, a_q^\dagger a_r^\dagger a_t a_s + \underbrace{\frac{1}{36}\sum W_{qrstuv}\, a_q^\dagger a_r^\dagger a_s^\dagger a_v a_u a_t}_{\text{complicates calculations (memory, more expensive operations)}}$$

* Can N-order H wrt $|\Phi\rangle$

$$H = E_{ref} + \hat{f}_N + \hat{\Gamma}_N + \hat{W}_N$$

0-body (#)

1-body $\sum_{qr} f_{qr}\{q^\dagger r\}$

2-body $\frac{1}{4}\sum \Gamma_{qrst}\{q^\dagger r^\dagger t s\}$

3-body $\frac{1}{36}\sum W_{qrstuv}\{q^\dagger r^\dagger s^\dagger v u t\}$

<u>Key Point</u>: Dominant parts of $\hat{W}$ subsumed in $E_{ref}$, $f_{qr}$, & $\Gamma_{qrst}$

e.g. $\Gamma_{qrst} = V_{qrst} + \sum_i W_{qristi}$ $\qquad a^\dagger a^\dagger a^\dagger a a a$

$$f_{qr} = T_{qr} + \sum_i V_{qiri} + \frac{1}{2}\sum_{ij} W_{qijrij}$$

=> Excellent approximation $\hat{H} \approx E_{ref} + \hat{f}_N + \hat{\Gamma}_N$

no more expensive than "traditional" calculations that ignore 3N completely, yet it implicitly includes dominant 3N contributions

# Derivation of HF equations

* Want to find best variational estimate of gs E within the restricted class of trial wf's that are simple Slater determinants

$$E_{gs} \leq E^{HF} = \min_{|\Phi\rangle \in \text{Slater det}} \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$|\Phi\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle$$

the s.p. states $a_i^\dagger |0\rangle = |i\rangle$ are the a-priori unknown HF basis

reminder: I use the convention $a, b, c, \ldots$ = particles
$i, j, k \ldots$ = holes
$q, r, s \ldots$ = unrestricted

* Expand HF basis in some fixed s.p. basis (e.g., HO basis)

$$\underset{\text{HF basis}}{|q\rangle} = \sum_\alpha \underset{\text{HO basis}}{|\alpha\rangle} \langle \alpha | q \rangle = \sum_\alpha |\alpha\rangle D_{\alpha q}$$

$$\Rightarrow a_q^\dagger = \sum_\alpha C_\alpha^\dagger D_{\alpha q} \qquad \sum_\alpha D_{\alpha q} D^*_{\alpha q'} = \delta_{qq'} \quad (DD^\dagger = D^\dagger D = 1)$$

$$a_q = \sum_\alpha C_\alpha D^*_{\alpha q}$$

$$C_\alpha^\dagger = \sum_q a_q^\dagger D^*_{\alpha q} \quad \text{and} \quad C_\alpha = \sum_q a_q D_{\alpha q}$$

* recall, any Unitary transf. amongst the N-lowest (i.e., hole states) orbitals Only changes $|\Phi\rangle$ by a phase

$$|\Phi'\rangle = \prod_{i=1}^{N}\left(\sum_{j=1}^{N} U_{ij} a_j^\dagger\right)|0\rangle = \sum_{j_1}\cdots\sum_{j_N} U_{1j_1} U_{2j_2}\cdots U_{Nj_N}\, a_{j_1}^\dagger a_{j_2}^\dagger \cdots a_{j_N}^\dagger |0\rangle$$

$$= \underbrace{\mathrm{Det}\,U}_{\substack{\text{irrelevant} \\ \text{phase since } UU^\dagger = 1}} \cdot |\Phi\rangle$$

Therefore, there is no 1-to-1 correspondence between the basis $|i\rangle$ & the S.D. $|\Phi\rangle$

* However, there is a 1-to-1 correspondence between $|\Phi\rangle$ and its 1-body density matrix

$$\rho_{\alpha\beta} = \langle \Phi | c_\beta^\dagger c_\alpha | \Phi \rangle$$

$$= \sum_q \sum_r D_{\beta q}^* D_{\alpha r} \underbrace{\langle \Phi | a_q^\dagger a_r | \Phi \rangle}_{\delta_{qr}\, n_r}$$

$$= \sum_q D_{\beta q}^* D_{\alpha q} n_q = \sum_i D_{\beta i}^* D_{\alpha i}$$

$$\Rightarrow \rho_{\alpha\beta} = \langle \Phi | c_\beta^\dagger c_\alpha | \Phi \rangle = \sum_{i=1}^{N} \langle \alpha | i \rangle \langle i | \beta \rangle$$

$$\boxed{\Rightarrow \rho_{\alpha\beta} = \langle \Phi | c_\beta^\dagger c_\alpha | \Phi \rangle = \sum_{i=1}^{N} \langle \alpha | i \rangle \langle i | \beta \rangle}$$

$\Rightarrow$ equivalently, $\rho_{\alpha\beta} = \langle \alpha | \hat{\rho} | \beta \rangle$ $\quad \hat{\rho} = \sum_{i=1}^{N} |i\rangle\langle i|$

and

$\hat{\rho}^2 = \hat{\rho}$ projector in sp space onto the subspace spanned by occupied orbitals $|i\rangle$

* As we already showed, there is 1-to-1 correspondence between a Slater $|\Phi\rangle$ & its $\hat{\rho}$-operator

* Also, recall that all Slater dets. have $\hat{\rho}^2 = \hat{\rho}$

$\Downarrow$

$$E_{gs} \leq E^{HF} = \underset{|\Phi\rangle \in \text{Slater}}{\text{Min}} E[\Phi] = \underset{|\Phi\rangle \in \text{Slater det}}{\text{Min}} \langle \Phi | H | \Phi \rangle$$

doing this variation over all Slater dets.

equivalent to

Varying $\hat{\rho}$ subject to constraint $\hat{\rho}^2 = \hat{\rho}$

Express $E[\Phi] = \langle \Phi | H | \Phi \rangle$ in terms of 1-body density matrix

$$E[\Phi] = \sum_{\alpha\beta} T_{\alpha\beta} \underbrace{\langle \Phi | c_\alpha^\dagger c_\beta | \Phi \rangle}_{A} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \underbrace{\langle \Phi | c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma | \Phi \rangle}_{B}$$

$$A = \langle \Phi | c_\alpha^\dagger c_\beta | \Phi \rangle = \langle \Phi | c_\alpha^\dagger c_\beta | \Phi \rangle = \rho_{\beta\alpha}$$

$$B = \langle \Phi | c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma | \Phi \rangle + \langle \Phi | c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma | \Phi \rangle$$

$$+\rho_{\delta\beta}\rho_{\gamma\alpha} \qquad\qquad -\rho_{\gamma\beta}\rho_{\delta\alpha}$$

$$\Rightarrow E[\rho] = \sum_{\alpha\beta} T_{\alpha\beta} \rho_{\beta\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \underbrace{V_{\alpha\beta\gamma\delta} \left( \rho_{\delta\beta}\rho_{\gamma\alpha} - \rho_{\gamma\beta}\rho_{\delta\alpha} \right)}_{\text{re-label dummy indices}}$$

$$\boxed{E[\rho] = \sum_{\alpha\beta} T_{\alpha\beta} \rho_{\beta\alpha} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \rho_{\delta\beta} \rho_{\gamma\alpha}}$$

# Variation of the $E[\rho]$

$$\delta E = E[\hat{\rho}+\delta\hat{\rho}] - E[\hat{\rho}]$$

What kind of variations $\delta\hat{\rho}$ can we make to stay in Slater determinant space for $|\Phi\rangle$?

Restricting to Slater det. $|\Phi\rangle \iff (\hat{\rho}+\delta\hat{\rho})^2 = (\hat{\rho}+\delta\hat{\rho})$ [i.e, has to remain projector as we search over $\hat{\rho}$]

$$\Rightarrow (\hat{\rho}+\delta\hat{\rho})^2 = \cancel{\hat{\rho}^2}^{\,\hat{\rho}} + \hat{\rho}\,\delta\hat{\rho} + \delta\hat{\rho}\,\hat{\rho} + \mathcal{O}(\delta\rho^2)$$

$$\Rightarrow (\hat{\rho}+\delta\hat{\rho})^2 = \cancel{\hat{\rho}} + \hat{\rho}\,\delta\hat{\rho} + \delta\hat{\rho}\,\hat{\rho} = \cancel{\hat{\rho}} + \delta\hat{\rho}$$

$$\boxed{\delta\hat{\rho}\,\hat{\rho} = (1-\hat{\rho})\,\delta\hat{\rho}} \quad \otimes$$

Now, let $(1-\hat{\rho}) \equiv \hat{\sigma}$ $\quad \left( \hat{\rho}+\hat{\sigma} = 1, \ \hat{\rho}^2 = \hat{\rho}, \ \hat{\sigma}^2 = \hat{\sigma}, \ \hat{\rho}\hat{\sigma} = 0 \right)$

M. $\otimes$ by $\hat{\rho}$ from left: $\quad \hat{\rho}\,\delta\hat{\rho}\,\hat{\rho} = \cancel{\hat{\rho}\hat{\sigma}}^{\,0}\,\delta\hat{\rho}$

M. $\otimes$ by $\hat{\sigma}$ from right: $\quad \delta\hat{\rho}\,\cancel{\hat{\rho}\hat{\sigma}}_{\,0} = \hat{\sigma}\,\delta\hat{\rho}\,\hat{\sigma}$

Thus we find that $\hat{\rho}\,\delta\hat{\rho}\,\hat{\rho} = \hat{\sigma}\,\delta\hat{\rho}\,\hat{\sigma} = 0$

$$\Rightarrow \boxed{\delta\rho_{ab} = \delta\rho_{ij} = 0 \quad \text{(hh + pp variations vanish)}}$$

$\Rightarrow$ Only variations of the ph sector $\delta\rho_{ai}, \delta\rho_{ia} \neq 0$

So then, $\delta E = E[\rho + \delta\rho] - E[\rho] = \sum_{\alpha\beta} \frac{\delta E}{\delta \rho_{\alpha\beta}} \delta\rho_{\alpha\beta} = 0$

$$\frac{\delta E}{\delta \rho_{\alpha\beta}} = \frac{\delta}{\delta \rho_{\alpha\beta}} \left[ \sum_{\xi\sigma} T_{\xi\sigma} \rho_{\sigma\xi} + \frac{1}{2} \sum_{\mu\nu\sigma\xi} V_{\mu\nu\sigma\xi} \rho_{\nu\xi} \rho_{\mu\sigma} \right]$$

$$= T_{\alpha\beta} + \sum_{\mu\sigma} V_{\mu\alpha\sigma\beta} \rho_{\mu\sigma} \equiv h^{HF}_{\alpha\beta}$$

$$\delta E = 0 = \sum_{\alpha\beta} h^{HF}_{\alpha\beta} \delta\rho_{\alpha\beta}$$ (basis indep, so write it in HF basis where we know only $\delta\rho_{ai}, \delta\rho_{ia}$ non-zero)

$$= \sum_{qr} h^{HF}_{qr} \delta\rho_{qr}$$

$$= \sum_{a,i} h^{HF}_{ai} \delta\rho_{ai} = 0$$

Since $\delta\rho_{ai}$ arbitrary, this implies

$$h^{HF}_{ai} = 0 = h^{HF}_{ia}$$ (particle/hole states not mixed)

$$\boxed{h^{HF}_{ai} = T_{ai} + \sum_{j=1}^{N} V_{ajij} = 0}$$

* recalling that $\hat{\rho} = \sum_{i=1}^{N} |i\rangle\langle i|$

$$\hat{\sigma} = \sum_{a=N+1}^{\infty} |a\rangle\langle a| = 1 - \hat{\rho}$$

$$\Rightarrow \hat{\rho}\, h^{HF} (1-\hat{\rho}) = 0$$

$$\Rightarrow \hat{\rho}\, h^{HF} - h^{HF}\hat{\rho} = 0$$

$\hat{\rho}$ + $h^{HF}$ simultaneously diagonalizeable

$$h^{HF} = \left[\begin{array}{c|c} \hat{\rho} h^{HF} \hat{\rho} & 0 \\ \hline 0 & \hat{\sigma} h^{HF} \hat{\sigma} \end{array}\right]$$

particle + hole blocks can be diagonalized separately

$\Rightarrow$ Go ahead and diagonalize $\hat{\rho}$ + $\hat{h}^{HF}$ simultaneously

$$\boxed{\begin{array}{ll} \hat{\rho}\,|q\rangle = n_q |q\rangle & n_q = \begin{cases} 1 & q < N \\ 0 & q > N \end{cases} \\ h^{HF}|q\rangle = \varepsilon_q |q\rangle & \end{array}}$$

$$h^{HF}|q\rangle = \varepsilon_q |q\rangle \quad (*)$$

* Now expand unknown $|q\rangle = \sum_\alpha |\alpha\rangle D_{\alpha q}$

Some known fixed basis (eg - HO)

* Then eq. (*) becomes

$$\boxed{\sum_\beta \langle\alpha|h^{HF}|\beta\rangle D_{\beta q} = \varepsilon_q D_{\alpha q} \\ \text{where } \langle\alpha|h^{HF}|\beta\rangle = \langle\alpha|T|\beta\rangle + \sum_{\mu\nu}\langle\alpha\mu|V|\beta\nu\rangle \rho_{\mu\nu}}$$

Requires iterative sol'n since $h^{HF}$ depends on the eigenfunctions $D_{\beta q}$ via

$$\rho_{\mu\nu} \equiv \sum_{i=1}^{N}\langle\mu|i\rangle\langle i|\nu\rangle = \sum_{i=1}^{N} D_{\mu i} D^*_{\nu i}$$

Schematic Sol'n Strategy: ① Guess initial $\rho^{(0)}_{\mu\nu}$ (e.g., take the fixed $|\alpha\rangle$ basis as the initial guess for HF states $\Rightarrow \rho^{(0)}_{\mu\nu} = \delta_{\mu\nu} n_\mu$)

② Build $\langle\alpha|h^{HF}|\beta\rangle$

③ diagonalize $\Rightarrow D^{(1)}_{\alpha q}$

+ build $\rho^{(1)}_{\mu\nu} = \sum_i D^{(1)}_{\mu i} D^{(1)*}_{\nu i}$

+ $h^{(1)}_{\alpha\beta}$

iterate till things don't change

Total $E_{HF}$ : $= \langle \Phi | H | \Phi \rangle$

$$\boxed{E^{HF} = \sum_i T_{ii} + \frac{1}{2} \sum_{ij} \langle ij | V | ij \rangle}$$

$|i\rangle$ are the converged, self consistent orbits from $h^{HF}|i\rangle = \varepsilon_i |i\rangle$

* but $\langle i | h^{HF} | i \rangle = \varepsilon_i = T_{ii} + \sum_j \langle ij | V | ij \rangle$

$$\Downarrow$$

$$\boxed{\begin{aligned} E^{HF} &= \sum_{i=1}^{N} \varepsilon_i - \frac{1}{2} \sum_{ij} \langle ij | V | ij \rangle \\ &= \frac{1}{2} \left( \sum_i \left( T_{ii} + \varepsilon_i \right) \right) \end{aligned}}$$

## How it looks in $|\vec{r},\sigma\rangle$ basis

$$h_{\alpha\beta} = t_{\alpha\beta} + \sum_{\mu\nu} \langle \alpha\mu|V|\beta\nu\rangle \rho_{\mu\nu}$$

here, $|\alpha\rangle \to |\vec{r},\sigma\rangle$

HF basis

$$\rho_{\mu\nu} \to \rho(\vec{r}\sigma, \vec{r}'\sigma') = \sum_{i=1}^{A} \langle \vec{r}\sigma|i\rangle\langle i|\vec{r}'\sigma'\rangle$$

* For a local, spin-indep. V: $(\vec{r}_1\sigma_1 \vec{r}_2\sigma_2|V|\vec{r}_3\sigma_3\vec{r}_4\sigma_4)$

$$= V(\vec{r}_1-\vec{r}_2)\,\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\,\delta(\vec{r}_1-\vec{r}_3)\delta(\vec{r}_2-\vec{r}_4)$$

$\Big\}$ Some algebra

Convert $\sum_\beta h^{HF}_{\alpha\beta} D_{\beta q} = \varepsilon_q D_{\alpha q}$ to coordinate space:

$$\left(-\frac{\nabla^2}{2m} + U_H(\vec{r})\right)\phi_q(\vec{r}\sigma) + \sum_{\sigma'}\int d\vec{r}'\, U_F(\vec{r}\sigma,\vec{r}'\sigma')\,\phi_q(\vec{r}'\sigma') = \varepsilon_q \phi_q(r\sigma)$$

$U_H(\vec{r})$ = "Hartree potential" $= \int d\vec{r}'\, V(\vec{r}-\vec{r}')\,\rho(\vec{r}')$ $\quad \rho(\vec{r}') = \sum_{i,\sigma} \phi_i^*(\vec{r}\sigma)\phi_i(\vec{r}\sigma)$

$U_F(\vec{r}\sigma,\vec{r}'\sigma')$ = "Fock" or "Exchange potential" $= -V(\vec{r}-\vec{r}')\,\rho(\vec{r}\sigma,\vec{r}'\sigma')$

$$\rho(\vec{r}\sigma,\vec{r}'\sigma') = \sum_i \phi_i^*(\vec{r}'\sigma')\phi_i(\vec{r}\sigma)$$

* Non-local Fock term makes life hard.

How might we simplify? We could use that $V(\vec{r}_1-\vec{r}_2)$ is short range (unlike Coulomb potential) for NN interactions

$$V(\vec{r}) \approx g_0\delta(\vec{r}) + g_2\nabla^2\delta(r) + \cdots$$

e.g., $V(r) \approx g\,\delta(\vec{r})$

$$\Rightarrow U_H(\vec{r}) \simeq g\,\rho(\vec{r})$$

$$\Rightarrow U_F(\vec{r}\sigma,\vec{r}\sigma') = -g\,\delta(\vec{r}-\vec{r}')\,\rho(\vec{r}\sigma,\vec{r}\sigma') = -g\,\delta(\vec{r}-\vec{r}')\,[\underbrace{\rho(\vec{r})}_{\sum_i \phi_i^*(\vec{r}\sigma)\phi_i(\vec{r}\sigma')}]_{\sigma\sigma'},$$

$\Rightarrow$ HF 1-body eqn. is now local! (We'll see more of this when we learn about Skyrme forces)

$$E^{HF}[\rho(\vec{r},\vec{r}')] \longrightarrow E^{HF}[\rho(\vec{r})]$$

## * Preview of a more satisfactory way to get rid of non-locality

a quick overview of the density matrix expansion method (DME)

* It's too naive to take $V(\vec{r}_1-\vec{r}_2) \approx g\,\delta(\vec{r}_1-\vec{r}_2)$. Why?

$$V(\vec{r}) \propto \frac{e^{-m_\pi r}}{r} \quad (m_\pi \simeq 140\,\text{MeV}) \xrightarrow[\text{trans.}]{\text{Fourier}} V(\vec{q}) \propto \frac{1}{\vec{q}^{\,2}+m_\pi^2} \quad \otimes$$

Claim: $V(r) \simeq g_0\,\delta(\vec{r}) + g_2 \nabla^2 \delta(\vec{r}) + \cdots \Longleftrightarrow V(\vec{q}) \simeq V(0) + \frac{V''(0)}{2!} q^2 + \cdots$

Can taylor expand $\otimes$ only if $q < m_\pi$

* avg. $k_F$ in medium/heavy nucleus $\gtrsim 200$ MeV, which is $\gg m_\pi$.

$\therefore$ Not really correct to say $V(\vec{r}) \approx g\,\delta(\vec{r}) + \cdots$

DME: Is it possible to map $E^{HF}[\rho(\vec{r},\vec{r}')] \to E^{HF}[\rho(\vec{r})]$?
I.e., to make it depend on local qty's like $\rho(\vec{r})$, $\nabla^2\rho(\vec{r})$, etc.?

$$E = \langle\Phi|T|\Phi\rangle + \underbrace{\frac{1}{2}\iint d\vec{r}_1 d\vec{r}_2\, \rho(\vec{r}_1) V(\vec{r}_1-\vec{r}_2)\rho(\vec{r}_2)}_{\text{Hartree energy (depends on } \rho(\vec{r}) \text{ already)}} - \underbrace{\frac{1}{2}\iint d\vec{r}_1 d\vec{r}_2\, \rho^2(\vec{r}_1,\vec{r}_2)\, V(\vec{r}_1-\vec{r}_2)}_{\text{Fock or exchange energy depends on non-local } \rho(\vec{r},\vec{r}')}$$

Idea of DME: $\rho(\vec{r}_1,\vec{r}_2) = \rho(\vec{R}+\frac{\vec{r}}{2}, \vec{R}-\frac{\vec{r}}{2}) \approx \sum_n C_n(r)\, \mathcal{O}_n(R)$

- where $\mathcal{O}_n(R)$ is shorthand for local quantities, things like $\rho(\vec{R})$, $\nabla^2\rho(\vec{R})$, $\underset{\text{KE density}}{\tau(R)}$, $\underset{\text{spin-orbit current density}}{\vec{J}(R)}$, $\underset{\text{spin density}}{\vec{S}(R)}$

Fock energy $\Rightarrow$ $\langle V\rangle_F \simeq \sum_{n,m}\int d\vec{R}\, \mathcal{O}_n(\vec{R})\mathcal{O}_m(\vec{R}) \times \underbrace{\int d\vec{r}\, V(\vec{r})C_n(r)C_m(r)}_{= g_{nm}}$

Now we've mapped the non local original expression into a form

$\langle V\rangle_F \sim \int d\vec{R}\, \mathcal{E}(\vec{R})$ (i.e., integral over a local energy density
$\mathcal{E}(R) = \sum_{n,m} g_{nm}\, \mathcal{O}_n(R)\mathcal{O}_m(R)$)