FYS 4480 September 30

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \underbrace{\sum_{ai} a_a^\dagger a_i |\Phi_0\rangle C_i^a}_{1p1h}$$

$$+ \underbrace{\sum_{\substack{ab\\ij}} C_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle}_{2p2h} + \cdots$$

$$+ \cdots \quad NpNh$$

$$= \sum_{PH} C_H^P |\Phi_H^P\rangle$$

$$PH \to i \qquad |\Phi_H^P\rangle \to |\Phi_i\rangle$$

$$C_H^P = C_i$$

$$\sum_j C_j H_{ij} = \lambda C_i$$

$$\langle\Phi_i|\Phi_j\rangle = \delta_{ij} = \delta_{ij}$$

$$H_{ij} = \langle\Phi_i|H|\Phi_j\rangle$$

$$\langle\Phi_c|\hat{H}|\Phi_i^a\rangle = \langle i|\hat{f}|a\rangle$$

$$\langle\Phi_0|H|\Phi_{ij}^{ab}\rangle = \langle ij|\hat{v}|ab\rangle_{AS}$$

$$
\begin{array}{c|cccccc}
 & |\Phi_0\rangle \ (0p0h) & 1p1h & 2p2h & 3p3h & \cdots & NpNh \\
\hline
\langle\Phi_0| & \times & \times & \times & 0 & 0 \cdots & 0 \\
1p1h & \times & \times & \times & \times & 0 \cdots & 0 \\
2p2h & \times & \times & \times & \times & \times & 0 \\
3p3h & 0 & \times & \times & \times & \times & \times \\
4p4h & 0 & 0 & \times & & & \\
\vdots & \vdots & \vdots & 0 & & & \\
 & & & 0 & & & \\
 & & & \vdots & & & \\
NpNh & 0 & 0 & & & &
\end{array}
$$

$$
\times \underbrace{\begin{bmatrix} c_0 \\ c_{1p1h} \\ c_{2p2h} \\ \vdots \\ \vdots \end{bmatrix}}_{C} = \lambda \begin{bmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}
$$

$$HC = \lambda C$$

non-practical of solving

$$HC = \lambda C$$

$$(H-\lambda)C = 0$$

$$(H-\lambda)\underbrace{\sum_{PH} C_H^P |\Phi_H^P\rangle}$$

$$(\hat{H}-E)|\Psi_0\rangle$$

$$\langle\Phi_0| \times (\hat{H}-E)|\Psi_0\rangle$$

$$c_0\langle\Phi_0|(\hat{H}-E)|\Phi_0\rangle +$$

$$\sum_{ai} c_i^a \langle\Phi_0|\hat{H}-E|\Phi_i^a\rangle$$

$$+ \sum_{\substack{ab\\ij}} \langle\Phi_0|\hat{H}-E|\Phi_{ij}^{ab}\rangle c_{ij}^{ab}$$

$$+ 0 = 0$$

intermediate normalization

$$\langle\Psi_0|\Phi_0\rangle = 1 = C_0$$

$$\underbrace{\langle\Phi_0|\hat{H}|\Phi_0\rangle}_{E_0^{Ref}} + \sum_{ai} c_i^a \underbrace{\langle\Phi_0|\hat{H}|\Phi_i^a\rangle}_{\langle i|f|a\rangle}$$

$$+ \sum_{\substack{ab \\ ij}} c_{ij}^{ab} \underbrace{\langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle}_{\langle ij | \hat{v} | ab \rangle_{AS}}$$

$$= E$$

$$\underbrace{\Delta E}_{\text{correlation energy}} = E - E_0^{ref}$$

$$= \sum_{ai} c_i^a \langle i | \hat{f} | a \rangle$$

$$+ \sum_{\substack{ab \\ ij}} c_{ij}^{ab} \langle ij | \hat{v} | ab \rangle_{AS}$$

next row

$\langle \Phi_i^a |$ × 2nd row

$$\langle \Phi_i^a | \hat{H} - E | \Phi_0 \rangle +$$

$$\sum_{bj} c_j^b \langle \Phi_i^a | \hat{H} - E | \Phi_j^b \rangle .$$

$$+ \sum_{\substack{bc \\ jk}} C_{jk}^{bc} \langle \Phi_i^a | \hat{H} - E | \Phi_{jk}^{bc} \rangle$$

$$+ \sum_{\substack{bcd \\ jkl}} C_{jkl}^{bcd} \langle \Phi_i^a | H - E | \times | \Phi_{jkl}^{bcd} \rangle$$

$$= 0$$

$$\underbrace{\langle \Phi_i^a | \hat{H} | \Phi_0 \rangle}_{\langle i | f | a \rangle}$$

$$+ \langle \Phi_i^a | \hat{H} | \Phi_i^a \rangle C_i^a$$

$$+ \sum_{\substack{bj \\ \neq ai}} \langle \Phi_i^a | \hat{H} | \Phi_j^b \rangle C_j^b$$

$$+ \sum_{\substack{bc \\ jk}} \langle \Phi_i^a | \hat{H} | \Phi_{jk}^{bc} \rangle C_{jk}^{bc}$$

$$+ \sum_{\substack{bcd \\ jkl}} \langle \Phi_i^a | \hat{H} | \Phi_{jkl}^{bcd} \rangle C_{jk}^{bcd}$$

$$= E\, C_i^a$$

$\langle \Phi_{ij}^{ab} |$ x third row

$$= \langle ij | \hat{v} | ab \rangle_{AS}$$

$$+ \sum_{kc} \langle \Phi_{ij}^{ab} | \hat{H} | \Phi_k^c \rangle C_k^c$$

2p2h 1p1h

$$+ C_{ij}^{ab} \langle \Phi_{ij}^{ab} | \hat{H} | \Phi_{ij}^{ab} \rangle$$

$$+ \sum_{\substack{kl \\ cd \\ \neq ab \\ ij}} C_{kl}^{cd} \langle \Phi_{ij}^{ab} | \hat{H} | \Phi_{kl}^{cd} \rangle$$

$$+ \sum_{\substack{cde \\ klm}} C_{klm}^{cde} \langle \Phi_{ij}^{ab} | \hat{H} | \Phi_{klm}^{cde} \rangle$$

2p2h − 3p3h

$$+ \text{2p2h} - \text{4p4h} = E\, C_{ij}^{ab}$$

Solved iteratively

$$C_i^a(0) \neq 0 \qquad C_{ij}^{ab}(0) \neq 0$$

$$C_{ijk}^{abc}(0) \ldots = 0$$

<u>2nd row</u>

$$\langle i|f|a\rangle + \langle \Phi_i^a|H|\Phi_i^a\rangle C_i^a$$

$$= E\, C_i^a$$

$$= E_0^{ref} + \langle a|f|a\rangle - \langle i|f|i\rangle$$

$$\langle i|\hat{f}|a\rangle + \left(\langle a|\hat{f}|a\rangle - \langle i|f|i\rangle\right)$$

$$\times\, C_i^a = \Delta E\, C_i^a$$

$$\langle a|f|a\rangle = \underbrace{\langle a|h_0|a\rangle}_{\varepsilon_a}$$

$$+ \sum_j \langle aj|\cancel{v}|aj\rangle_{AS} -$$

$$= \tilde{\varepsilon}_a$$

$$\langle i|f|a\rangle = \tilde{\varepsilon}_i$$

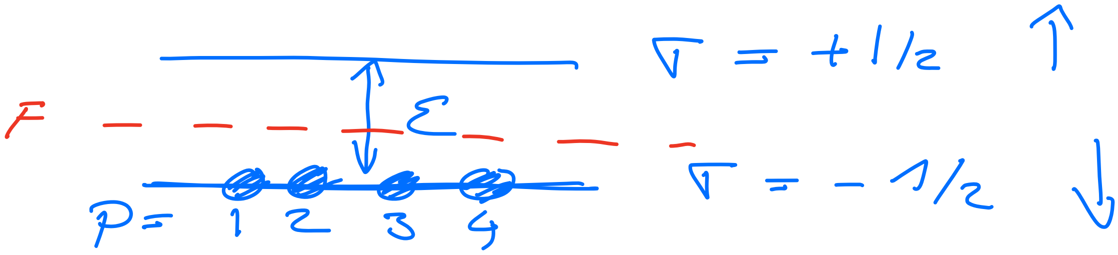
$$\Delta E = 0 \quad \Rightarrow$$

$$C_i^a(0) = \frac{\langle i|f|a\rangle}{\tilde{\varepsilon}_i - \tilde{\varepsilon}_a}$$

$$\Delta E = \sum_{ai} \frac{|\langle i|f|a\rangle|^2}{\tilde{\varepsilon}_i - \tilde{\varepsilon}_a} + \sum_{\substack{ab\\ij}} C_{ij}^{ab} \langle ij|v|ab\rangle_{AS}$$

$$C_{ij}^{ab} = \frac{\langle ij|v|ab\rangle}{\tilde{\varepsilon}_i + \tilde{\varepsilon}_j - \tilde{\varepsilon}_a - \tilde{\varepsilon}_b}$$

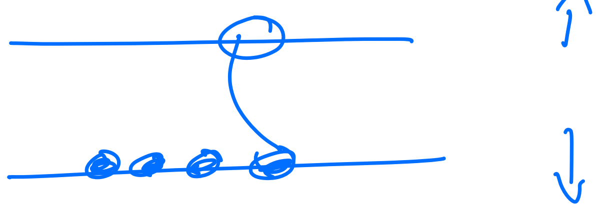
Example: Lipkin model



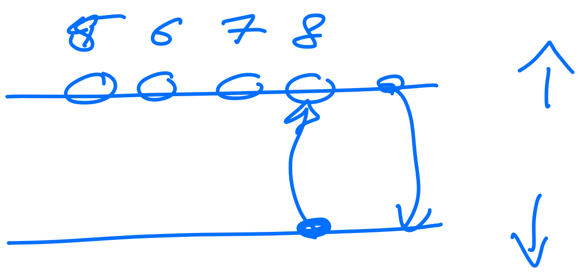
$N=4$

$$|\Phi_0\rangle = a_1^+ a_2^+ a_3^+ a_4^+ |0\rangle$$

$|\phi_1\rangle$



p



$$H = \frac{1}{2}\varepsilon \sum_{\sigma p} \sigma\, a^+_{p\sigma} a_{p\sigma}$$

$$+ \frac{1}{2} V \sum_{\sigma p p'} a^+_{\sigma p} a^+_{\sigma p'} a_{-\sigma p'} a_{-\sigma p}$$

$$+ \frac{1}{2} W \sum_{\sigma p p'} a^+_{p\sigma} a^+_{p'-\sigma} a_{p'\sigma} a_{p-\sigma}$$

$J^2,\ J_z,\ N,\ J_+\ J_-$

$$H_0 = \varepsilon J_z$$

$$J_z = \sum_{p\sigma} \sigma \, a^\dagger_{p\sigma} a_{p\sigma}$$

$$\hat{H} = \varepsilon J_z + \frac{1}{2} V \left(J_+^2 + J_-^2\right)$$

$$+ \frac{W}{2}\left(J_+ J_- + J_- J_+ - \hat{N}\right)$$

$$\hat{N} = \sum_{p\sigma} a^\dagger_{p\sigma} a_{p\sigma}$$

$|\Phi_0\rangle$; $\quad J_z = -2 \quad J = 2$

$J = 2 \quad J_z = -2, -1, 0, 1, 2$

$$|J J_z\rangle = |2 -2\rangle$$

$$|2 -1\rangle$$

$$J_\pm |J J_z\rangle = C^{\pm}_{J_z} |J J_z \pm 1\rangle$$

$$= \sqrt{J(J+1) \mp M(M+1)} \; |J J_z \pm 1$$

$$\langle J J_z' | H | J J_z \rangle \qquad [H, J^2] = 0$$

$$= \varepsilon J_z \, \delta_{J_z' J_z}$$

$$+ \frac{V}{2} \Big\{ C^{+}_{J_z} C^{+}_{J_z+1} \, \delta_{J_z' J_z+1} + C^{-}_{J_z} C^{-}_{J_z-1} \, \delta_{J_z' J_z-1} \Big\}$$

$$+ \frac{W}{2} \Big\{ C^{+}_{J_z-1} C^{-}_{J_z} \, \delta_{J_z J_z'} + C^{+}_{J_z} C^{-}_{J_z-1} \, \delta_{J_z J_z'} + N \, \delta_{J_z J_z'} \Big\} \Rightarrow$$

$a_5^+ a_6^+ a_7^+ a_8^+ |0\rangle$

$J_z = +2$ $\quad$ n $\quad$ 4

$$\mathbb{H} = \begin{bmatrix} 2\varepsilon & 0 & \sqrt{6}\,V & 0 & 0 \\ 0 & \varepsilon + 3W & 0 & 3V & 0 \\ 0 & 0 & 4W & 0 & \sqrt{6}\,V \\ 0 & 0 & 0 & -\varepsilon + 3W & 0 \\ 0 & 0 & 0 & & -2\varepsilon \end{bmatrix}$$

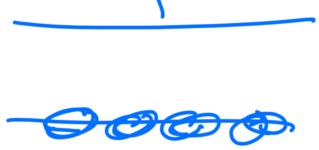
$J_z = -2$

$\varepsilon = 2 \qquad V = -1/3 \qquad W = -1/4$

$E_0 = -4.21$

$|\Psi_0\rangle = c_0 |\Phi_0\rangle + c_1 |\Phi_1\rangle + \dots$

$c_4 |\Phi_4\rangle$



$c_0 = 0.97$

$c_4 = 0.03$

$c_1 = c_3 = 0$

$c_2 = 0.25$

$|\Psi_0\rangle \simeq c_0 |\Phi_0\rangle$