Lecture Fys4480, October 13, 2023

Thouless' theorem

$$|\Phi_0^{HF}\rangle = |c\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle$$

$$|c'\rangle = \exp\left\{ \sum_{ai} C_i^a a_a^\dagger a_i \right\} |c\rangle$$

$$\langle c|c'\rangle \neq 0$$

Reminder from HF + variational calculus

$$|\phi\rangle \to |\phi\rangle + |\delta\phi\rangle \quad \text{(1st quantization)}$$

$$\langle\phi'|\phi\rangle \neq 0 \quad = |\phi'\rangle$$

$$|c\rangle \to |c'\rangle = |c\rangle + |\delta c\rangle$$

$$= |c\rangle + \sum_{ai} \delta C_i^a a_a^\dagger a_i |c\rangle$$

$$\langle \delta c | H | c \rangle = \langle c | H | \delta c \rangle = 0$$

in 2nd quantization

$$\langle a | \hat{f} | i \rangle =$$

$$\langle a | \hat{h}_0 | i \rangle + \sum_j \langle aj | v | ij \rangle_{AS}$$

$$= 0$$

$$\begin{cases} \langle a | f | i \rangle = 0 \\ \langle i | f | i \rangle = \varepsilon_i^{HF} \end{cases}$$

$$\begin{cases} \langle a | f | a \rangle = \varepsilon_a^{HF} \\ \langle i | f | i \rangle = \varepsilon_i^{HF} \end{cases}$$

$$\langle p | q \rangle = \delta_{pq}$$

$$|c'\rangle = \prod_{i \le F} \left[1 + \sum_{a>F} c_i^a a_a^\dagger a_i + \frac{1}{2} \left(\sum_{a>F} c_i^a a_a^\dagger a_i \right)^2 + \dots \right] |c\rangle$$

$$|c'\rangle = \exp\left\{ \sum_{ai} c_i^a a_a^\dagger a_i \right\} |c\rangle$$

$i = 1, 2$

$$|c'\rangle = \exp\left\{ \underbrace{\sum_a c_1^a a_a^\dagger a_1}_{A} + \underset{B}{\sum_a c_2^a a_a^\dagger a_2} \right\} |c\rangle$$

$$\exp(A_1 + B_2) = e^{A_1} e^{B_2} \qquad [A, B] = 0$$

$$[a_a^\dagger a_i, a_b^\dagger a_j] =$$

$$a_a^\dagger a_i a_b^\dagger a_j - a_b^\dagger a_j a_a^\dagger a_i =$$

$$\text{— " —} \quad + a_b^\dagger a_a^\dagger a_j a_i =$$

$$\text{— " —} \quad - a_a^\dagger a_b^\dagger a_j a_i =$$

$$\text{— " —} \quad + a_a^\dagger a_b^\dagger a_i a_j =$$

$$\text{— " —} \quad - a_a^\dagger a_i a_b^\dagger a_j = 0$$

$$|c'\rangle = \prod_{i=1}^{N} \Big(1 + \sum_a c_i^a a_a^\dagger a_i + \frac{1}{2} \sum_{ab,\, i} a_a^\dagger a_i a_b^\dagger a_i + \dots\Big) |c\rangle$$

$$(a_i)^n \quad n > 1$$

$$= \prod_{i=1}^{N} \left(1 + \sum_a c_i^a a_a^\dagger a_{i'}\right) |0\rangle$$

$$= \prod_{i=1}^{N} \left(1 + \sum_a c_i^a a_a^\dagger a_{i'}\right) a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_N}^\dagger |0\rangle$$

$$= \Big[\left(1 + \sum_a c_{i_1}^a a_a^\dagger a_{i_1'}\right) a_{i_1'}^\dagger \Big)$$

$$\times \Big(\left(1 + \sum_a c_{i_2}^a a_a^\dagger a_{i_2'}\right) a_{i_2'}^\dagger \Big)$$

$$\vdots$$

$$\times \Big(\left(1 + \sum_a c_{i_N}^a a_a^\dagger a_{i_N'}\right) a_{i_N'}^\dagger \Big) \Big] |0\rangle$$

$$= \prod_i \underbrace{\left(a_i^\dagger + \sum_a c_i^a a_a^\dagger\right)}_{b_i^\dagger} |0\rangle$$

$$= \prod_i b_i^\dagger |0\rangle$$

Constraint with sum

$$a > F$$

$$|p\rangle = a_p^\dagger |0\rangle$$

$$|\lambda\rangle = \sum_p c_{\lambda p} |p\rangle$$

can we construct a general

SD $|\tilde{c}\rangle = \prod_i \tilde{b}_i^{+}|0\rangle$?

not necessarily $\tilde{b}_i^{+} = b_i^{+}$

$$\tilde{b}_i^{+} = \sum_p f_{ip}\, a_p^{+}$$

$$|\tilde{c}\rangle = |c'\rangle \qquad \langle c|\tilde{c}\rangle \neq 0$$

$$\langle c|\tilde{c}\rangle = \langle 0|\, a_{i_N}\, a_{i_{N-1}} \cdots a_{i_2}\, a_{i_1}$$

$$\times \left(\sum_{p=i_1}^{i_N} f_{i_1 p}\, a_p^{+} \right) \left(\sum_{q=i_1}^{i_N} f_{i_2 q}\, a_q^{+} \right)$$

$$\cdots \left(\sum_{t=i_1}^{i_N} f_{i_N t}\, a_t^{+} \right) |0\rangle$$

$$\boxed{\langle c | \tilde{c} \rangle = 1}$$

$$\Rightarrow \det(f_{ip}) = 1$$

2-particles

$$\langle c | a_2 a_1 \Big[\overbrace{(f_{11} a_1^\dagger + f_{12} a_2^\dagger)}^{f_1^\dagger} \times \underbrace{(f_{21} a_1^\dagger + f_{22} a_2^\dagger)}_{f_2^\dagger} \Big] | 0 \rangle$$

$$\langle c | a_2 a_1 \Big(f_{11} a_1^\dagger \cancel{f_{21} a_1^\dagger} + f_{11} a_1^\dagger f_{22} a_2^\dagger + f_{12} \underline{a_2}^\dagger f_{21} \underline{a_1}^\dagger + f_{12} f_{22} \cancel{a_2^\dagger a_2^\dagger} \Big) \times | 0 \rangle$$

$$= f_{11} f_{22} - f_{12} f_{21} = \begin{vmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{vmatrix}$$

if f has inverse

$$\sum_{i} f_{ik} f^{-1}_{kj} = \delta_{ij}$$

$$\sum_{j} f^{-1}_{ij} f_{jk} = \delta_{ik}$$

$$\sum_{i} f^{-1}_{ki} b^{+}_{i} = \sum_{i} f^{-1}_{ki} \sum_{p=i_1}^{\infty} f_{ip} a^{+}_{p}$$

$$= a^{+}_{k} + \sum_{i} \sum_{p=i_{\cancel{n}+1}}^{\infty} f^{-1}_{ki} f_{ip} a^{+}_{p}$$

$$c_{kp} = \sum_{i \leq F} f^{-1}_{ki} f_{ip}$$

we can redefine

$$a_k^\dagger + \sum_i \sum_{p=i_{N+1}}^{\infty} S_{ki}^{-1} S_{ip}\, a_p^\dagger$$

$$= a_k^\dagger + \sum_{p=i_{N+1}}^{\infty} \tilde{c}_{kp}\, a_p^\dagger$$

$$= a_k^\dagger + \sum_a c_i^a\, a_a^\dagger$$

$$= b_k^\dagger \quad \Rightarrow$$

$$|\tilde{c}\rangle = \prod_i \tilde{b}_i^\dagger |0\rangle = \prod_i b_i^\dagger |0\rangle$$

In First quantization

$$\Phi_c^{HF} = \det(C)\det(\Phi_c)$$

2nd quantization

$$|c\rangle = \mathrm{Exp}\left\{\sum_{ai} c_i^a a_a^\dagger a_i\right\}|0\rangle$$

$$\langle \delta c|H|c\rangle \Rightarrow$$

$$\langle a|g|i\rangle = 0$$

$$\langle ip|h|H|c\rangle = 0$$