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Exercise 5

a) S.p. states φ_λ $(\lambda = 1, \ldots, A)$, new basis ψ_a $(a = 1, \ldots, A)$

$$\psi_a = \sum_\lambda C_{a\lambda} \varphi_\lambda$$ where $C_{a\lambda}$ are elements of a unitary matrix

New basis is orthogonal

$$\langle \psi_b | \psi_a \rangle = \sum_\lambda \sum_{\lambda'} C^*_{b\lambda'} C_{a\lambda} \underbrace{\langle \varphi_{\lambda'} | \varphi_\lambda \rangle}_{\delta_{\lambda'\lambda}}$$

$$= \sum_\lambda C^*_{b\lambda} C_{a\lambda} = \delta_{ab}$$ using property of unitary matrices

b) $$|\Psi\rangle^{AS} = \frac{1}{\sqrt{A!}} \sum_P (-)^P P \prod_{i=1}^{A} \psi_i$$

$$= \frac{1}{\sqrt{A!}} \sum_P (-)^P P \prod_{i=1}^{A} \left(\sum_\lambda C_{i\lambda} \varphi_\lambda \right)$$

$$= \frac{1}{\sqrt{A!}} \sum_{P_i} (-)^{P_i} P_i \prod_{i=1}^{A} \sum_\lambda (-)^{P_\lambda} P_\lambda \prod_{\lambda=1}^{A} C_{i\lambda} \varphi_\lambda$$ since more than one ptcl cannot occupy a single state

e.g. for $A = 2$:

$$\Psi_a^{AS} = \frac{1}{\sqrt{2}} \left(|a\rangle|b\rangle - |b\rangle|a\rangle \right) = \frac{1}{\sqrt{2}} \Big((c_1^a|1\rangle + c_2^a|2\rangle)(c_1^b|1\rangle + c_2^b|2\rangle) - (c_1^b|1\rangle + c_2^b|2\rangle)(c_1^a|1\rangle + c_2^a|2\rangle) \Big)$$

$$= \Big(\cancel{c_1^a c_1^b |1\,1\rangle} + c_1^a c_2^b |1\,2\rangle + c_2^a c_1^b |2\,1\rangle + \cancel{c_2^a c_2^b |2\,2\rangle} - \cancel{c_1^b c_1^a |1\,1\rangle} - c_1^b c_2^a |1\,2\rangle - c_2^b c_1^a |2\,1\rangle - \cancel{c_2^b c_2^a |2\,2\rangle} \Big)$$

$$\left(c_1^a c_2^b - c_1^b c_2^a\right)|1\ 2\rangle + \left(c_2^a c_1^b - c_2^b c_1^a\right)|2\ 1\rangle$$

$$\underbrace{\left(c_1^a c_2^b - c_1^b c_2^a\right)}_{\det C}|1\ 2\rangle - \underbrace{\left(c_2^b c_1^a - c_2^a c_1^b\right)}_{\det C}|2\ 1\rangle$$

$$\det(C) \doteq \begin{vmatrix} c_1^a & c_2^a \\ c_1^b & c_2^b \end{vmatrix} = c_1^a c_2^b - c_1^b c_2^a$$

So, $\Psi_a^{As} = \det C \ \varphi_\lambda^{As}$

c) Since C is unitary, $CC^\dagger = C^\dagger C = \mathbb{1}$

$$|\det(C)|^2 = \det(C)\det(C^\dagger) = \det(CC^\dagger) = \det(\mathbb{1}) = 1$$

$\therefore$ $|\det(C)| = 1$ and so $\det(C) = e^{i\delta}$

Exercise 6

A-particle Slater determinants $|\varphi_0\rangle$ $|\varphi_i^a\rangle$ $|\varphi_{ij}^{ab}\rangle$

One body operator $\hat{F} = \sum_{i=1}^{A} \hat{f}(x_i)$

Two body operator $\hat{G} = \sum_{i<j}^{A} \hat{g}(x_i\, x_j)$, $\hat{g}(x_i\, x_j) = \hat{g}(x_j\, x_i)$

a) $$\langle \varphi_0 | \hat{F} | \varphi_0 \rangle = \frac{1}{A!} \sum_{i=1}^{A} \langle i | \hat{f} | i \rangle \cdot \cancel{A!}$$

$$\langle \varphi_0 | \hat{G} | \varphi_0 \rangle = \sum_{i>j}^{A} \langle i\, j | g | i\, j \rangle - \langle i\, j | g | j\, i \rangle$$

since $\hat{g}(x_i\, x_j) = \hat{g}(x_j\, x_i)$

b) $$\langle \varphi_0 | \hat{F} | \varphi_i^a \rangle = \sum_{j}^{A} \langle i | f_j | a \rangle \left(\frac{1}{A!} \right)$$

since when $\langle i |$ is not "linked" to $|a\rangle$ (in other words) when i and a are not in the same slot, it is guaranteed that one of the other slots will introduce an inner product between orthogonal s.p. states

e.g. for $A=2$

$$\langle \varphi_0^{A=2} | \hat{F} | \varphi^{A=2\;a}_{\;\;2} \rangle = \cancel{\langle 1\, 2 | f_m | 1\, a \rangle} - \cancel{\langle 1\, 2 | f_m | a\, 1 \rangle} - \cancel{\langle 2\, 1 | f_m | 1\, a \rangle} + \langle 2\, 1 | f | a\, 1 \rangle$$

$a \neq 2, 1$

$$+ \langle 1\, 2 | f_n | 1\, a \rangle - \cancel{\langle 1\, 2 | f_n | a\, 1 \rangle} - \cancel{\langle 2\, 1 | f_n | 1\, a \rangle} + \cancel{\langle 2\, 1 | f | a\, 1 \rangle}$$

$$= \frac{1}{2} \left(\langle 2 | f | a \rangle + \langle 2 | f | a \rangle \right)$$

since the ptcls are identical, we set $f_m = f_n = f$

next page →

$\langle \Phi_0 | \hat{G} | \Phi_i^a \rangle$

- as with the one-body case, whenever $\langle i|$ is not involved in a matrix element with $|a\rangle$, the term will be 0 since there will be an inner product between orthogonal states due to the fact that $|a\rangle$ has replaced $|i\rangle$ only on the right of the operator

$$\hookrightarrow 2\langle i\, j | g | a\, m\rangle - 2\langle i\, j | g | m\, a\rangle \delta_{jm}$$

- factor of 2 since $g(x_i\, x_j) = g(x_j\, x_i)$
- for the same reason as point #1, we must have $j = m$

$$2\langle i\, j | g | a\, j\rangle - 2\langle i\, j | g | j\, a\rangle$$

- sum over states $i > j$

$$\langle \Phi_0 | \hat{G} | \Phi_i^a \rangle = \frac{2}{A!}\sum_{i>j} \langle ij | g | a j\rangle - \langle ij | g | j a\rangle$$

c) $\langle \Phi_0 | \hat{F} | \Phi_{ij}^{ab} \rangle = 0$ since f_0 connects only $\langle i|$ and $|a\rangle$ via $\langle i | f_0 | a\rangle$ or $\langle j|$ and $|b\rangle$ via $\langle j | f_0 | b\rangle$ the remaining "mis matches" between the left and right will make each term 0

$$\langle \Phi_0 | \hat{G} | \Phi_{ij}^{ab} \rangle = 2\langle i\, j | g | a\, b\rangle - 2\langle i\, j | g | b\, a\rangle$$

the only surviving term is when the replacement terms $|a\, b\rangle$ meet the terms they replace $\langle i\, j|$

$\longrightarrow$

$$\langle \Phi_0 | \hat{G} | \Phi_{ijk}^{abc} \rangle = 0$$

since $\hat{G}$ can connect, at most, 2 s.p. states there will be an $|a\rangle$ $|b\rangle$ or $|c\rangle$ matched with a bra from the original set of s.p. states in each term causing each term to be 0.

d) For a two body Hamiltonian, the expectation value

$$\langle \Psi_i | \hat{H} | \Psi_i \rangle \quad \text{where } \Psi_i = \sum_{\lambda=0}^{\infty} C_{i\lambda} \Phi_\lambda^{AS}$$

will only involve terms where Φ_λ on the right differs from $\Phi_{\lambda'}$ on the left by no more than 2 s.p. states