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Exercise 5

a) $\psi_a = \sum_\lambda c_{a\lambda}\varphi_\lambda \Rightarrow |a\rangle = \sum_\lambda c_{a\lambda}|\lambda\rangle$ where $\langle\lambda'|\lambda\rangle = \delta_{\lambda\lambda'}$

$$\langle a'|a\rangle = \left\{\sum_{\lambda\lambda'} c^*_{a'\lambda'} c_{a\lambda} \underbrace{\langle\lambda'|\lambda\rangle}_{\delta_{\lambda\lambda'}}\right\} = \sum_\lambda c^*_{a'\lambda} c_{a\lambda}$$

Because the transformation is unitary, $\sum_k a_{\lambda k} a^*_{\gamma k} = \delta_{\lambda\gamma}$

$$\Rightarrow \langle a'|a\rangle = \sum_\lambda c^*_{a'\lambda} c_{a\lambda} = \delta_{a'a} \Rightarrow \boxed{\langle a'|a\rangle = \delta_{a'a}}$$

i.e. the new basis is orthogonal

b) We know the identity.

$$\begin{vmatrix} \sum_{k=1}^{n} b_{1k}c_{k1} & \cdots & \sum_{k=1}^{n} b_{1k}c_{kn} \\ \vdots & & \vdots \\ \sum_{k=1}^{n} b_{nk}c_{k1} & \cdots & \sum_{k=1}^{n} b_{nk}c_{kn} \end{vmatrix} = \mathrm{Det}(C)\,\mathrm{Det}(B)$$

The slater determinant in the new basis is given by:

$$\Psi = \frac{1}{\sqrt{A!}}\begin{vmatrix} \psi_1(x_1) & \cdots & \psi_1(x_A) \\ \vdots & \ddots & \vdots \\ \psi_A(x_1) & \cdots & \psi_A(x_A) \end{vmatrix} = \frac{1}{\sqrt{A!}}\begin{vmatrix} \sum_\lambda c_{1\lambda}\varphi_\lambda(x_1) & \cdots & \sum_\lambda c_{1\lambda}\varphi_\lambda(x_A) \\ \vdots & \ddots & \vdots \\ \sum_\lambda c_{A\lambda}\varphi_\lambda(x_1) & \cdots & \sum_\lambda c_{A\lambda}\varphi_\lambda(x_A) \end{vmatrix}$$

Slater Determinant in old basis

$$\boxed{\Psi = \mathrm{Det}(C)\cdot\Psi_0}$$

where: $C = \begin{bmatrix} C_{11} & \cdots & C_{1A} \\ \vdots & & \vdots \\ C_{A1} & \cdots & C_{AA} \end{bmatrix}$, $\Psi_0 = \frac{1}{\sqrt{A!}}\begin{vmatrix} \varphi_1(x_1) & \cdots & \varphi_1(x_A) \\ \vdots & \ddots & \vdots \\ \varphi_A(x_1) & \cdots & \varphi_A(x_A) \end{vmatrix}$

c) From (b), $\Psi = \det(\hat{C})\, \Phi_0$

Because $\hat{C}$ is a unitary matrix, $|\det(c)| = 1$.

$\Rightarrow$ $\det(c) = e^{i\kappa}$ where κ is real, so

Ψ is equal to Φ_0 up to some complex constant.

6) (a) $\langle \Phi_0 | F | \Phi_0 \rangle = ?$

$$|\Phi_0\rangle = \frac{1}{\sqrt{A!}} \sum_P (-1)^P \hat{P} \prod_{\lambda=1}^{A} |\alpha_\lambda\rangle \;;\; |\Phi_H\rangle = \prod_{\lambda=1}^{A} |\alpha_\lambda\rangle$$

$$\langle \Phi_0 | F | \Phi_0 \rangle = \langle \Phi_H | \hat{F} A | \Phi_H \rangle$$

$$= \langle \Phi_H | \sum_{\lambda=1}^{A} \hat{f}(x_\lambda) \left\{ \sum_P (-1)^P \hat{P} | \Phi_H \rangle \right\}$$

$$= \langle \alpha_1 | f(x_1) | \alpha_1 \rangle + \dots + \langle \alpha_A | f(x_A) | \alpha_A \rangle$$

all terms $\langle \alpha_\lambda | f(x_\lambda) | \alpha_\gamma \rangle = \delta_{\lambda\gamma}$! b/c basis is orthogonal

$$\boxed{\langle \Phi_0 | F | \Phi_0 \rangle = \sum_{\lambda}^{A} \langle \alpha_\lambda | f(x_\lambda) | \alpha_\lambda \rangle}$$

$$\langle \Phi_0 | \hat{G} | \Phi_0 \rangle = \langle \Phi_H | \sum_{\lambda > \gamma}^{A} g(x_\lambda, x_\gamma) \left\{ \sum_P (-1)^P \hat{P} | \Phi_H \rangle \right\}$$

Consider some element λ, γ

all other terms cancel due to orthogonality

$$\sum_{\lambda > \gamma}^{A} \langle \alpha_\lambda \alpha_\gamma | g(x_\lambda, x_\gamma) \left\{ |\alpha_\lambda \alpha_\gamma\rangle - |\alpha_\gamma \alpha_\lambda\rangle \right\}$$

$$\boxed{\langle \Phi_0 | \hat{G} | \Phi_0 \rangle = \sum_{\lambda > \gamma}^{A} \left\{ \langle \alpha_\lambda \alpha_\gamma | \hat{g} | \alpha_\lambda \alpha_\gamma \rangle - \langle \alpha_\lambda \alpha_\gamma | \hat{g} | \alpha_\gamma \alpha_\lambda \rangle \right\}}$$

b) $\langle \Phi_0 | F | \Phi_i^a \rangle = \langle \Phi_H | \sum_k^A \hat{f}(x_k) \left\{ \sum_P (-1)^P \hat{P} \, |\alpha_1 \ldots \alpha_a \ldots \alpha_A\rangle \right\}$

$$= \langle \alpha_1 \ldots \alpha_i \ldots \alpha_A | \sum_k^A \hat{f}(x_k) \left\{ \sum_P (-1)^P \hat{P} \, |\alpha_1 \ldots \alpha_a \ldots \alpha_A\rangle \right\}$$

All terms with $\langle \alpha_i | \alpha_a \rangle = 0$, so we are left with:

$$\boxed{\langle \Phi_0 | F | \Phi_i^a \rangle = \langle \alpha_i | f(x_i) | \alpha_a \rangle}$$

$\langle \Phi_0 | G | \Phi_i^a \rangle = \langle \Phi_H | \sum_{k>j}^A \hat{g}(x_k, x_j) \left(\sum_P (-1)^P \hat{P} \, |\alpha_1 \ldots \alpha_a \ldots \alpha_A\rangle \right)$

$$= \sum_{k>j}^A \langle \alpha_1 \ldots \alpha_i \ldots \alpha_A | g(x_k, x_j) \left(\sum_P (-1)^P \hat{P} \, |\alpha_1 \ldots \alpha_a \ldots \alpha_A\rangle \right)$$

Any term not containing the matrix element for i & a will drop because $\langle \alpha_i | \alpha_a \rangle = 0$

$$\Rightarrow \boxed{\langle \Phi_0 | G | \Phi_i^a \rangle = \sum_j \left\{ \langle \alpha_i \alpha_j | g(x_i, x_j) | \alpha_a \alpha_j \rangle - \langle \alpha_i \alpha_j | g(x_i, x_j) | \alpha_j \alpha_a \rangle \right\}}$$

c) $\langle \Phi_0 | \hat{F} | \Phi_{ij}^{ab} \rangle = \langle \alpha_1 \ldots \alpha_i, \alpha_j \ldots \alpha_A | \sum_k \hat{f}(x_k) \left\{ \sum_P (-1)^P \hat{P} \, |\alpha_1 \ldots \alpha_a \alpha_b \ldots \alpha_A\rangle \right\}$

$\boxed{\langle \Phi_0 | \hat{F} | \Phi_{ij}^{ab} \rangle = 0}$, because $\langle \alpha_i | \alpha_a \rangle = 0$ & $\langle \alpha_j | \alpha_b \rangle = 0$ and one of these terms is always present.

$$\langle \Phi_0 | \hat{G} | \Phi_{ij}^{ab} \rangle = \langle \alpha_1 \ldots \alpha_i \alpha_j \ldots \alpha_A | \sum_{k>l} g(x_k, x_l) \left\{ \sum_P (-1)^P \hat{P} \, |\alpha_1 \ldots \alpha_a \alpha_b \ldots \alpha_A\rangle \right\}$$

$$\boxed{\langle \Phi_0 | \hat{G} | \Phi_{ij}^{ab} \rangle = \langle \alpha_i \alpha_j | g(x_i, x_j) | \alpha_a \alpha_b \rangle - \langle \alpha_i \alpha_j | g(x_i, x_j) | \alpha_b \alpha_a \rangle}$$

Only these terms contribute. All others include $\langle \alpha_i | \alpha_a \rangle$ or $\langle \alpha_j | \alpha_b \rangle$. Furthermore, $\boxed{\langle \Phi_0 | G | \Phi_{ijk}^{abc} \rangle = 0}$ for this

d) The one-body term will involve A terms. The two body term will include two terms if $A = 2$.

A	# terms	
2	2	$\langle 12 \| \hat{g} \| 12 \rangle - \langle 12 \| \hat{g} \| 21 \rangle$
3	6	$\langle 12 \|$, $\langle 32 \|$, $\langle 31 \|$
4	12	$\langle 12 \|$, $\langle 32 \|$, $\langle 31 \|$, $\langle 43 \|$, $\langle 42 \|$, $\langle 41 \|$
5	20	

The pattern appears to be that for A states we have $A(A-1)$ terms for the two body operator:

$\therefore$ There are $A + A(A-1) = \boxed{A^2 \text{ terms!}}$