PHY982 Exercise 5 & 6 Hao Lin

- Exercise 5

a) $|\psi_a\rangle = \sum_\lambda C_{a\lambda}|\phi_\lambda\rangle$

$\langle\psi_b| = \sum_{\lambda'} C^*_{b\lambda'}\langle\phi_{\lambda'}|$

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

$$= \sum_{\lambda\lambda'} C_{a\lambda}C^*_{b\lambda'}\delta_{\lambda',\lambda} = \sum_\lambda C_{a\lambda}C^*_{b\lambda}$$

Let $\mathcal{U}$ be the unitary transformation matrix. If we identify $C_{a\lambda} = (\mathcal{U})_{a\lambda}$, then $(\mathcal{U}^+)_{\lambda b} = (\mathcal{U})^*_{b\lambda} = C^*_{b\lambda}$.

$$\langle\psi_b|\psi_a\rangle = \sum_\lambda C_{a\lambda}C^*_{b\lambda} = \sum_\lambda (\mathcal{U})_{a\lambda}(\mathcal{U}^+)_{\lambda b}$$

$$= (\mathcal{U}\mathcal{U}^+)_{ab} = (\mathbb{1})_{ab} = \delta_{a,b}.$$

The new basis is therefore orthonormal.

b) $C = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1A} \\ C_{21} & & \ddots & \vdots \\ \vdots & & \ddots & \vdots \\ C_{A1} & \cdots & \cdots & C_{AA} \end{pmatrix}$ $\quad \overline{\Phi}(\phi_\lambda) = \begin{pmatrix} \phi_1(\vec{x}_1) & \phi_1(\vec{x}_2) & \cdots & \phi_1(\vec{x}_A) \\ \phi_2(\vec{x}_1) & & \ddots & \vdots \\ \vdots & & & \vdots \\ \phi_A(\vec{x}_1) & \cdots & \cdots & \phi_A(\vec{x}_A) \end{pmatrix}$

$$\overline{\Phi}(\psi_a) = \begin{pmatrix} \psi_1(\vec{x}_1) & \psi_1(\vec{x}_2) & \cdots & \psi_1(\vec{x}_A) \\ \psi_2(\vec{x}_1) & & \ddots & \vdots \\ \vdots & & \ddots & \vdots \\ \psi_A(\vec{x}_1) & \cdots & \cdots & \psi_A(\vec{x}_A) \end{pmatrix}$$

$$= \begin{pmatrix} \sum_\lambda C_{1\lambda}\phi_\lambda(\vec{x}_1) & \cdots & \sum_\lambda C_{1\lambda}\phi_1(\vec{x}_A) \\ \vdots & \ddots & \vdots \\ \vdots & & \vdots \\ \sum_\lambda C_{A\lambda}\phi_\lambda(\vec{x}_1) & \cdots & \sum_\lambda C_{A\lambda}\phi_\lambda(\vec{x}_A) \end{pmatrix}$$

$\{\overline{\Phi}(\psi_a)\}_{ij} = \sum_\lambda C_{i\lambda}\phi_\lambda(\vec{x}_j) = \sum_\lambda \{C\}_{i\lambda}\{\overline{\Phi}(\phi_\lambda)\}_{\lambda j}$ for all i and j

$\Rightarrow \overline{\Phi}(\psi_a) = C\,\overline{\Phi}(\phi_\lambda) \Rightarrow \underline{\det\{\overline{\Phi}(\psi_a)\} = \det(C)\det\{\overline{\Phi}(\phi_\lambda)\}}$.

c) ~~C is a unitary matrix.~~

$\det(C^\dagger) = \det(C)^*$.

Since $C^\dagger C = \mathbb{1}$, $\det(C^\dagger C) = \det(C^\dagger)\det(C)$

$= |\det(C)|^2 = 1$.

$\Rightarrow \det(C) = e^{i\alpha}$ for some real α.

Recalling that $\det(\Phi(\psi_a)) = \det(C)\det(\Phi(\phi_\lambda))$, we have

$$\det(\Phi(\psi_a)) = e^{i\alpha}\det(\Phi(\phi_\lambda))$$

• Exercise 6

a) $\langle \Phi_0 | \hat{F} | \Phi_0 \rangle$

$= A! \langle \hat{A}\Phi_{HF} | \hat{F} | A\Phi_{HF} \rangle$ with $|\Phi_{HF}\rangle := |\psi_1(\vec{x}_1)\rangle |\psi_2(\vec{x}_2)\rangle \cdots |\psi_A(\vec{x}_A)\rangle$

$= A! \langle \Phi_{HF} | \hat{F}\hat{A} | \Phi_{HF} \rangle$

$= \langle \Phi_{HF} | \sum_{i=1}^{A} \hat{f}(x_i) | \Phi_{HF} \rangle = \sum_{i=1}^{A} \langle \psi_i | f | \psi_i \rangle$.

$\langle \Phi_0 | \hat{G} | \Phi_0 \rangle$

$= A! \langle \Phi_{HF} | \hat{G}\hat{A} | \Phi_{HF} \rangle$

interchange i & j

$= \sum_{i>j}^{A} \left(\langle \Phi_{HF} | \hat{g}(x_i, x_j) | \Phi_{HF} \rangle - \langle \Phi_{HF} | \hat{g}(x_i, x_j) \hat{P}_{ij} | \Phi_{HF} \rangle \right)$

$= \sum_{i>j}^{A} \left(\langle ij | \hat{g} | ij \rangle - \langle ij | \hat{g} | ji \rangle \right)$

$\cancel{= \frac{1}{2} \sum_{i,j}^{A} \left(\langle ij | \hat{g} | ij \rangle - \langle ij | \hat{g} | ji \rangle \right)}$.

b) $\langle \Phi_0 | \hat{F} | \Phi_i^a \rangle = A! \langle \Phi_{HF}^0 | \hat{F}\hat{A} | \Phi_{HF}^{i\to a} \rangle$

$= \langle \psi_i | \hat{f} | \psi_a \rangle$.

with $|\Phi_{HF}^{i\to a}\rangle$ being the product with $\psi_i(\vec{x}_i)$ replaced by $\psi_a(\vec{x}_i)$.

$$\langle \Phi_0 | \hat{G} | \Phi_i^a \rangle = A! \langle \Phi_{HF}^0 | \hat{G} \hat{A} | \Phi_{HF}^{i \to a} \rangle$$

$$= \sum_{j \neq i} \left(\langle ij | \hat{g} | aj \rangle - \langle ij | \hat{g} | ja \rangle \right)$$

c) $\langle \Phi_0 | \hat{F} | \Phi_{ij}^{ab} \rangle = 0$, because a one-body operator can "connect" only one single particle state, while the given bra and ket states differ by at least 2 single particle states.

$$\langle \Phi_0 | \hat{G} | \Phi_{ij}^{ab} \rangle = \langle ij | \hat{g} | ab \rangle - \langle ij | \hat{g} | ba \rangle.$$

$\langle \Phi_0 | \hat{G} | \Phi_{ijk}^{abc} \rangle = 0$ because a two-body operator can connect two different states only.

d) $\langle \Psi_i | \hat{H} | \Psi_i \rangle = \sum_{\lambda \lambda'} c_{i\lambda}^* c_{i\lambda'} \langle \Phi_\lambda | \hat{H} | \Phi_{\lambda'} \rangle$

$\langle \Phi_\lambda | \hat{H} | \Phi_{\lambda'} \rangle$ may contribute only if Φ_λ and $\Phi_{\lambda'}$ differ by no more than two single particle states.