Exercise Sheet 7 due 25 June

1. *anticommutators*

For the operators defined by $c^\dagger_\varphi := \int dx\, \varphi(x)\, \hat\Psi^\dagger(x)$ show that $\{c_\alpha,\, c^\dagger_\beta\} = \langle\alpha|\beta\rangle$.

2. *Slater determinants*

Show that $\langle 0|\hat\Psi(x_1)\hat\Psi(x_2)\hat\Psi(x_3)\, c^\dagger_3 c^\dagger_2 c^\dagger_1|0\rangle = \det\begin{vmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \varphi_3(x_1) \\ \varphi_1(x_2) & \varphi_2(x_2) & \varphi_3(x_2) \\ \varphi_1(x_3) & \varphi_2(x_3) & \varphi_3(x_3) \end{vmatrix}$

3. *density operator* $\hat n(x) = \hat\Psi^\dagger(x)\hat\Psi(x)$

i. For an N-electron state with wave-function

$$\Psi(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}}\langle 0|\hat\Psi(x_1)\cdots\hat\Psi(x_N)|\Psi\rangle$$

show that $n(x) = N\int dx_2\cdots dx_N\, |\Psi(x,x_2,\dots,x_N)|^2 = \langle\Psi|\hat\Psi^\dagger(x)\hat\Psi(x)|\Psi\rangle$.

ii. For a Slater determinant $\Phi_{\alpha_1,\dots,\alpha_N}(x_1,\dots,x_N)$ show that the density is given by $n_{\alpha_1,\dots,\alpha_N}(x) = \langle 0|c_{\alpha_1}\cdots c_{\alpha_N}\, \hat n(x) c^\dagger_{\alpha_N}\cdots c^\dagger_{\alpha_1}|0\rangle = \sum_n |\varphi_{\alpha_n}(x)|^2$.

4. *non-interacting Hamiltonian*

Consider the non-interacting N-electron Hamiltonian

$$H(\vec r_1,\dots,\vec r_N) = \sum_{i=1}^{N}\left(-\frac{1}{2}\Delta_i + V(\vec r_i)\right)$$

Rewrite the Hamiltonian in second quantization using the basis of eigenfunctions

$$\left(-\frac{1}{2}\Delta + V(\vec r)\right)\varphi_n(\vec r) = \varepsilon_n\varphi_n(\vec r)$$

Show that the eigenstates of $\hat H$ are the Slater determinants $\prod_n c^\dagger_n|0\rangle$ and find their eigenenergies.