Exercise Sheet 7

1. *expansion of field operators*

Show that the field operators can be expanded in a complete orthonormal set $\{\varphi_n(x)\}$ as $\hat{\Psi}^\dagger(x) = \sum_n \overline{\varphi_n(x)}\, c_n^\dagger$.

2. *Slater determinants*

Show that $\langle 0|\hat{\Psi}(x_1)\hat{\Psi}(x_2)\hat{\Psi}(x_3)\, c_3^\dagger c_2^\dagger c_1^\dagger|0\rangle = \det \begin{vmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \varphi_3(x_1) \\ \varphi_1(x_2) & \varphi_2(x_2) & \varphi_3(x_2) \\ \varphi_1(x_3) & \varphi_2(x_3) & \varphi_3(x_3) \end{vmatrix}$

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 $n_{\alpha_1,\dots,\alpha_N}(x) = \langle 0|c_{\alpha_1}\cdots c_{\alpha_N}\, \hat{n}(x) c_{\alpha_N}^\dagger\cdots c_{\alpha_1}^\dagger|0\rangle = \sum_n |\varphi_{\alpha_n}(x)|^2$.

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 $\prod_n c_n^\dagger|0\rangle$ and find their eigenenergies.