Exercise Sheet 7 due 25 June 2018

1. *Slater determinants*

Consider the field-operators $\hat\Psi(\vec r\,) = \sum_j \varphi_j(\vec r\,)\, c_j$. Show that

$$\langle 0|\hat\Psi(\vec r_1)\hat\Psi(\vec r_2)\hat\Psi(\vec r_3)\, c_n^\dagger c_m^\dagger c_k^\dagger|0\rangle = \det\begin{vmatrix} \varphi_k(\vec r_1) & \varphi_m(\vec r_1) & \varphi_n(\vec r_1) \\ \varphi_k(\vec r_2) & \varphi_m(\vec r_2) & \varphi_n(\vec r_2) \\ \varphi_k(\vec r_3) & \varphi_m(\vec r_3) & \varphi_n(\vec r_3) \end{vmatrix}$$

2. *field operators*

Prove the anticommutation relations $\{\hat\Psi(\vec r\,), \hat\Psi(\vec r\,')\}$, $\{\hat\Psi^\dagger(\vec r\,), \hat\Psi^\dagger(\vec r\,')\}$, and $\{\hat\Psi(\vec r\,), \hat\Psi^\dagger(\vec r\,')\}$ for the field-operators.

3. *Hamiltonian in second quantization*

In first quantization, the Hamiltonian for N interacting electrons in an external potential $V(\vec r\,)$ is given by

$$H = \sum_{i=1}^{N}\left(-\frac{1}{2}\Delta_{\vec r_i} + V(\vec r_i)\right) + \sum_{i<j}\frac{1}{|\vec r_i - \vec r_j|} = \sum_{i=1}^{N} T(\vec r_i) + \sum_{i<j} U(\vec r_i, \vec r_j)$$

Show that for Slater determinants

$$\Psi_{N;a,b,\dots,n}(\vec r_1, \vec r_2, \dots, \vec r_N) = \frac{1}{\sqrt{N!}}\,\langle 0|\hat\Psi(\vec r_1)\hat\Psi(\vec r_2)\cdots\hat\Psi(\vec r_N) c_n^\dagger \cdots c_b^\dagger c_a^\dagger|0\rangle$$

the matrix elements of the one- and two-body Hamiltonian can be written as

$$\int d^3r_1 d^3r_2 \dots d^3r_N\; \Psi^*_{N;a',b',\dots,n'}(\vec r_1, \vec r_2, \dots, \vec r_N)\, T\, \Psi_{N;a,b,\dots,n}(\vec r_1, \vec r_2, \dots, \vec r_N)$$
$$= \left\langle 0 \left| c_{a'} c_{b'} \cdots c_{n'} \;\left(\sum_{\alpha,\beta} T_{\alpha,\beta}\, c_\alpha^\dagger c_\beta\right)\; c_n^\dagger \cdots c_b^\dagger c_a^\dagger \right| 0 \right\rangle$$

where

$$T_{\alpha,\beta} = \int d^3r\; \phi_\alpha^*(\vec r\,)\, T(\vec r\,)\, \phi_\beta(\vec r\,)$$

and

$$\int d^3r_1 d^3r_2 \dots d^3r_N\; \Psi^*_{N;a',b',\dots,n'}(\vec r_1, \vec r_2, \dots, \vec r_N)\, U\, \Psi_{N;a,b,\dots,n}(\vec r_1, \vec r_2, \dots, \vec r_N)$$
$$= \left\langle 0 \left| c_{a'} c_{b'} \cdots c_{n'} \;\left(\frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} U_{\alpha,\beta,\gamma,\delta}\, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma\right)\; c_n^\dagger \cdots c_b^\dagger c_a^\dagger \right| 0 \right\rangle$$

with

$$U_{\alpha,\beta,\gamma,\delta} = \int d^3r_1 d^3r_2\; \phi_\alpha^*(\vec r_1)\phi_\beta^*(\vec r_2)\, U(\vec r_1, \vec r_2)\, \phi_\gamma(\vec r_1)\phi_\delta(\vec r_2)$$