TFY4210, Quantum theory of many-particle systems, 2015: Tutorial 3

1. Second-quantized form of some single-particle operators.

Consider a system of electrons.

(a) The total momentum operator is in first quantization given by

$$\boldsymbol{P} = \sum_{j=1}^{N} \frac{\hbar}{i} \nabla_j. \tag{1}$$

Find the second-quantized representation of $\boldsymbol{P}$ expressed using the momentum-spin $(\boldsymbol{k}, \sigma)$ single-particle basis.

(a) The spin operator for an electron is in first quantization given by

$$\boldsymbol{s} = \frac{\hbar}{2}\boldsymbol{\tau}, \quad \text{with} \quad \boldsymbol{\tau} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}, \tag{2}$$

i.e. the x-, y, and z components of $\boldsymbol{\tau}$ are the respective Pauli matrices. Show that the second-quantized representation of $\boldsymbol{S} = \sum_{j=1}^{N} \boldsymbol{s}_j$, expressed using some single-particle basis (μ,σ) where μ here represents quantum numbers not related to spin, is given by

$$\boldsymbol{S} = \frac{\hbar}{2} \sum_{\mu} \left\{ c^\dagger_{\mu\downarrow} c_{\mu\uparrow} + c^\dagger_{\mu\uparrow} c_{\mu\downarrow}, i(c^\dagger_{\mu\downarrow} c_{\mu\uparrow} - c^\dagger_{\mu\uparrow} c_{\mu\downarrow}), c^\dagger_{\mu\uparrow} c_{\mu\uparrow} - c^\dagger_{\mu\downarrow} c_{\mu\downarrow} \right\}. \tag{3}$$

2. Cancellation of the $\boldsymbol{q} = 0$ term in the jellium model of interacting electrons.

In the lectures we showed that the second-quantized representation of the Coulomb electron-electron interaction energy is

$$H_{\text{el}-\text{el}} = \frac{1}{2\Omega} \sum_{\boldsymbol{q}} \sum_{\boldsymbol{k},\sigma} \sum_{\boldsymbol{k}',\sigma'} v_{\boldsymbol{q}} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma} \tag{4}$$

where $v_{\boldsymbol{q}}$ is the Fourier transform of the Coulomb interaction. At first sight the presence of a $\boldsymbol{q} = 0$ term in $H_{\text{el}-\text{el}}$ would appear problematic since $v_{\boldsymbol{q}} \propto 1/q^2$ (as will be seen in (b) below). A real system, however, must be charge neutral to be stable, so there must also be positive charges present that compensate the negative ones and thus also give contributions to the Coulomb interaction energy of the system, and this will cancel the $q = 0$ term in $H_{\text{el}-\text{el}}$. To investigate this in detail in a concrete model, consider a system consisting of electrons and a background of compensating positive charges, modeled to be fixed in space with a certain density $\rho_+(\boldsymbol{r})$. The total Coulomb interaction energy of the system can then be written as

$$H_I = H_{\text{el}-\text{el}} + H_{\text{b}-\text{b}} + H_{\text{el}-\text{b}} \tag{5}$$

where the three terms on the rhs represent, respectively, the interaction energy of the electrons, of the positive background, and between the electrons and the background. In first quantization we can write

$$H_{\mathrm{el-el}} = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\sum_{i\neq j}^{N}\frac{e^{-\mu|\boldsymbol{r}_i-\boldsymbol{r}_j|}}{|\boldsymbol{r}_i-\boldsymbol{r}_j|}, \tag{6}$$

$$H_{\mathrm{b-b}} = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\int d^3r\int d^3r'\,\frac{\rho_+(\boldsymbol{r})\rho_+(\boldsymbol{r}')e^{-\mu|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{7}$$

$$H_{\mathrm{el-b}} = -\frac{e^2}{4\pi\epsilon_0}\sum_{i=1}^{N}\int d^3r\,\frac{\rho_+(\boldsymbol{r})e^{-\mu|\boldsymbol{r}_i-\boldsymbol{r}|}}{|\boldsymbol{r}_i-\boldsymbol{r}|}, \tag{8}$$

where the case of the Coulomb interaction corresponds to taking $\mu = 0$ in these expressions. The μ-dependent factor has been included to ensure that the $q = 0$ terms are mathematically well defined. It will be shown that they cancel for an arbitrary value of μ. At the end of the calculation, after the thermodynamic limit $\Omega \to \infty$ has been taken (keeping the density N/Ω of electrons fixed), the parameter μ is then taken to 0, recovering the Coulomb case of interest.

Charge neutrality requires that $\int d^3r\ \rho_+(\boldsymbol{r}) = N$. We will in the following consider the so-called *jellium model*, where the background charge is taken to be uniform, i.e. $\rho_+(\boldsymbol{r}) = N/\Omega$.

(a) Show that $H_{\mathrm{b-b}}$ and $H_{\mathrm{el-b}}$ are both constants, given by, respectively,

$$H_{\mathrm{b-b}} = \frac{1}{2}\frac{e^2}{\epsilon_0\mu^2}\frac{N^2}{\Omega}, \tag{9}$$

$$H_{\mathrm{el-b}} = -\frac{e^2}{\epsilon_0\mu^2}\frac{N^2}{\Omega}. \tag{10}$$

Hint: Use translational invariance to shift the origin of integration.

(b) Show that the Fourier transform of the μ-dependent generalization $\frac{e^{-\mu|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}$ of the Coulomb interaction is given by

$$v_{\boldsymbol{q}} = \frac{e^2}{\epsilon_0(q^2+\mu^2)}. \tag{11}$$

(c) Using the second-quantized representation of $H_{\mathrm{el-el}}$ (with $v_{\boldsymbol{q}}$ given by (11)), show that its $q = 0$ term evaluates to

$$\frac{1}{2}\frac{e^2}{\epsilon_0\mu^2}\frac{N^2-N}{\Omega}. \tag{12}$$

Show from this that the interaction Hamiltonian for the Coulomb case reduces to

$$H_{\mathrm{I}} = \frac{1}{2\Omega}\sum_{\boldsymbol{q}\neq 0}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'}\frac{e^2}{\epsilon_0 q^2}c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}c_{\boldsymbol{k}',\sigma'}c_{\boldsymbol{k},\sigma}. \tag{13}$$

(You will need to argue that the second term in (12) can be omitted in the proper limit (first $\Omega \to \infty$, then $\mu \to 0$) because it gives a vanishing contribution to the energy per particle.)