TFY4210, Quantum theory of many-particle systems, 2016: Solution to tutorial 3

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

(a) The total momentum operator $\boldsymbol{P}$ is a single-particle operator and thus its second-quantized representation is

$$\boldsymbol{P} = \sum_{\alpha,\beta} \left[\int dx\ \phi_\alpha^*(x) \frac{\hbar}{i} \nabla \phi_\beta(x) \right] c_\alpha^\dagger c_\beta. \tag{1}$$

With $x = (\boldsymbol{r}, s)$ and $\beta = (\boldsymbol{k}, \sigma)$ the eigenfunctions in (1) are of the form $\phi_\beta(x) = \phi_{\boldsymbol{k}\sigma}(\boldsymbol{r}, s) = (1/\sqrt{\Omega}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \delta_{s\sigma}$. Thus

$$\begin{aligned}
\int dx\ \phi_\alpha^*(x) \frac{\hbar}{i} \nabla \phi_\beta(x) &= \sum_s \int_\Omega d^3r \left(\frac{1}{\sqrt{\Omega}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}} \delta_{s\sigma'} \right) \frac{\hbar}{i} \nabla \left(\frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \delta_{s\sigma} \right) && (2) \\
&= \sum_s \int_\Omega d^3r \left(\frac{1}{\sqrt{\Omega}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}} \delta_{s\sigma'} \right) \frac{\hbar}{i} i\boldsymbol{k} \left(\frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \delta_{s\sigma} \right) \\
&= \hbar\boldsymbol{k} \left(\frac{1}{\Omega} \int d^3r\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \right) \left(\sum_s \delta_{s\sigma'} \delta_{s\sigma} \right) \\
&= \hbar\boldsymbol{k}\ \delta_{\boldsymbol{k}\boldsymbol{k}'} \delta_{\sigma\sigma'}. && (3)
\end{aligned}$$

Putting this back into (1) gives

$$\boldsymbol{P} = \sum_{\boldsymbol{k}\sigma} \hbar\boldsymbol{k}\ c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma}. \tag{4}$$

(b) The first-quantized form of the total spin operator is $\boldsymbol{S} = \sum_{j=1}^N \boldsymbol{s}_j$. As this is a single-particle operator, its second-quantized form is

$$\boldsymbol{S} = \sum_{\tilde{\mu}\tilde{\mu}'} \langle \tilde{\mu} | \boldsymbol{s} | \tilde{\mu}' \rangle c_{\tilde{\mu}}^\dagger c_{\tilde{\mu}'} = \frac{\hbar}{2} \sum_{\tilde{\mu}\tilde{\mu}'} \langle \tilde{\mu} | \boldsymbol{\tau} | \tilde{\mu}' \rangle c_{\tilde{\mu}}^\dagger c_{\tilde{\mu}'}, \tag{5}$$

where $\{|\tilde{\mu}\rangle\}$ is some chosen single-particle basis. We can write $|\tilde{\mu}\rangle = |\mu\rangle \otimes |\sigma\rangle$ where here $|\sigma\rangle = |\pm\frac{1}{2}\rangle$ is a basis state for the spin degree of freedom and $|\mu\rangle$ is a basis state for the degrees of freedom not related to spin (for concreteness we assume that the quantum numbers μ are discrete). As the spin operator $\boldsymbol{\tau}$ only acts on the spin state, we have

$$\langle \tilde{\mu} | \boldsymbol{\tau} | \tilde{\mu}' \rangle = \langle \mu | \mu' \rangle \langle \sigma | \boldsymbol{\tau} | \sigma' \rangle = \delta_{\mu\mu'} \langle \sigma | \boldsymbol{\tau} | \sigma' \rangle \tag{6}$$

which gives

$$\boldsymbol{S} = \frac{\hbar}{2} \sum_\mu \sum_{\sigma,\sigma'} \langle \sigma | \boldsymbol{\tau} | \sigma' \rangle c_{\mu\sigma}^\dagger c_{\mu\sigma'} = \frac{\hbar}{2} \sum_\mu \sum_{\sigma,\sigma'} \boldsymbol{\tau}_{\sigma\sigma'} c_{\mu\sigma}^\dagger c_{\mu\sigma'}, \tag{7}$$

or, componentwise,

$$S^j = \frac{\hbar}{2}\sum_\mu \sum_{\sigma,\sigma'} \tau^j_{\sigma\sigma'} c^\dagger_{\mu\sigma} c_{\mu\sigma'}. \tag{8}$$

Here we used that the matrix elements of the Pauli matrices are defined as $\tau^j_{\sigma\sigma'} = \langle\sigma|\tau^j|\sigma'\rangle$, i.e. the Pauli matrices are a matrix representation of the spin-1/2 spin operator components (divided by $\hbar/2$) in the basis of eigenstates of the z-component of the spin operator. (The matrix representation of an operator $\hat{O}$ in a basis $\{|a\rangle\}$ is given by a matrix O with matrix elements $O_{ab} = \langle a|\hat{O}|b\rangle$.) Writing out the Pauli matrix components explicitly gives the expression shown in the problem text. For example, for S^y we get

$$\begin{aligned} S^y &= \frac{\hbar}{2}\sum_\mu \sum_{\sigma,\sigma'} \tau^y_{\sigma\sigma'} c^\dagger_{\mu\sigma} c_{\mu\sigma'} \\ &= \frac{\hbar}{2}\sum_\mu (\tau^y_{\uparrow\uparrow} c^\dagger_{\mu\uparrow} c_{\mu\uparrow} + \tau^y_{\uparrow\downarrow} c^\dagger_{\mu\uparrow} c_{\mu\downarrow} + \tau^y_{\downarrow\uparrow} c^\dagger_{\mu\downarrow} c_{\mu\uparrow} + \tau^y_{\downarrow\downarrow} c^\dagger_{\mu\downarrow} c_{\mu\downarrow}) \\ &= \frac{\hbar}{2}\sum_\mu (0 \cdot c^\dagger_{\mu\uparrow} c_{\mu\uparrow} + (-i) \cdot c^\dagger_{\mu\uparrow} c_{\mu\downarrow} + i \cdot c^\dagger_{\mu\downarrow} c_{\mu\uparrow} + 0 \cdot c^\dagger_{\mu\downarrow} c_{\mu\downarrow}) \\ &= \frac{\hbar}{2}\sum_\mu i(c^\dagger_{\mu\downarrow} c_{\mu\uparrow} - c^\dagger_{\mu\uparrow} c_{\mu\downarrow}). \end{aligned} \tag{9}$$

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

Inserting $\rho_+(\boldsymbol{r}) = N/\Omega$ gives

$$H_{\text{b-b}} = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\left(\frac{N}{\Omega}\right)^2 \int d^3r' \int d^3r \, \frac{e^{-\mu|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{10}$$

For finite μ the last integral has a finite value in the limit $\Omega \to \infty$ we are interested in. To evaluate this we change the integration variable from $\boldsymbol{r}$ to $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$ (as we consider $\Omega \to \infty$ the integration limits are not affected). The first integral (over $\boldsymbol{r}'$) simply becomes Ω. Altogether, this gives

$$\begin{aligned} H_{\text{b-b}} &= \frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\frac{N^2}{\Omega}\int d^3R \, \frac{e^{-\mu|\boldsymbol{R}|}}{|\boldsymbol{R}|} = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\frac{N^2}{\Omega} \cdot 4\pi \cdot \int_0^\infty dR \, R^2 \, \frac{e^{-\mu R}}{R} \\ &= \frac{1}{2}\frac{e^2}{\epsilon_0}\frac{N^2}{\Omega} \cdot \frac{1}{\mu^2} \underbrace{\int_0^\infty dx \, x \, e^{-x}}_{1} = \frac{1}{2}\frac{e^2}{\epsilon_0\mu^2}\frac{N^2}{\Omega}. \end{aligned} \tag{11}$$

(The factor 4π came from the angular integration. We introduced a new integration variable $x = \mu R$ and used integration by parts to evaluate the resulting integral.) Similarly,

$$\begin{aligned} H_{\text{el-b}} &= -\frac{e^2}{4\pi\epsilon_0}\frac{N}{\Omega}\sum_i \int d^3r \frac{e^{-\mu|\boldsymbol{r}-\boldsymbol{r}_i|}}{|\boldsymbol{r}-\boldsymbol{r}_i|} \\ &= -\frac{e^2}{4\pi\epsilon_0}\frac{N}{\Omega} \cdot N \underbrace{\int d^3R \frac{e^{-\mu|\boldsymbol{R}|}}{|\boldsymbol{R}|}}_{4\pi/\mu^2} = -\frac{e^2}{\epsilon_0\mu^2}\frac{N^2}{\Omega}. \end{aligned} \tag{12}$$

Therefore

$$H_{\mathrm{b-b}} + H_{\mathrm{el-b}} = -\frac{1}{2}\frac{e^2}{\epsilon_0\mu^2}\frac{N^2}{\Omega}. \tag{13}$$

(b) Choosing the z axis to point along $\boldsymbol{q}$, we have

$$\begin{aligned}
v_{\boldsymbol{q}} &= \int d^3r\; v(\boldsymbol{r})e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{e^2}{4\pi\epsilon_0}\int d^3r \frac{e^{-\mu|\boldsymbol{r}|-i\boldsymbol{q}\cdot\boldsymbol{r}}}{|\boldsymbol{r}|} \\
&= \frac{e^2}{4\pi\epsilon_0}\int_0^{2\pi} d\phi \int_0^{\infty} dr\, r\, e^{-\mu r} \underbrace{\int_{-1}^{1} d(\cos\theta)e^{-iqr\cos\theta}}_{\frac{1}{iqr}(e^{iqr}-e^{-iqr})} \\
&= \frac{e^2}{2iq^2\epsilon_0}\underbrace{\int_0^{\infty} dx\; \left[e^{(-\alpha+i)x} - e^{(-\alpha-i)x}\right]}_{2i/(1+\alpha^2)} \qquad (\alpha \equiv \mu/q) \\
&= \frac{e^2}{\epsilon_0(q^2+\mu^2)}.
\end{aligned} \tag{14}$$

(c) The second-quantized representation of $H_{\mathrm{el-el}}$, using the μ-generalized Coulomb interaction, is

$$H_{\mathrm{el-el}} = \frac{1}{2\Omega}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'}\frac{e^2}{\epsilon_0(q^2+\mu^2)}c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}c_{\boldsymbol{k}',\sigma'}c_{\boldsymbol{k},\sigma}. \tag{15}$$

Its $\boldsymbol{q}=0$ part is

$$\frac{1}{2\Omega}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'}\frac{e^2}{\epsilon_0\mu^2}c^{\dagger}_{\boldsymbol{k},\sigma}\underbrace{c^{\dagger}_{\boldsymbol{k}',\sigma'}c_{\boldsymbol{k}',\sigma'}}_{\hat{n}_{\boldsymbol{k}',\sigma'}}c_{\boldsymbol{k},\sigma} \equiv H^{q=0}_{\mathrm{el-el}}. \tag{16}$$

Using $[\hat{n}_{\boldsymbol{k}'\sigma'}, c^{\dagger}_{\boldsymbol{k}\sigma}] = \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\sigma\sigma'}c^{\dagger}_{\boldsymbol{k}\sigma}$ this can be rewritten

$$\begin{aligned}
H^{q=0}_{\mathrm{el-el}} &= \frac{e^2}{2\Omega\epsilon_0\mu^2}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'}(\hat{n}_{\boldsymbol{k}',\sigma'}c^{\dagger}_{\boldsymbol{k}\sigma} - \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\sigma\sigma'}c^{\dagger}_{\boldsymbol{k}\sigma})c_{\boldsymbol{k}\sigma} \\
&= \frac{e^2}{2\Omega\epsilon_0\mu^2}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'}(\hat{n}_{\boldsymbol{k}',\sigma'}\hat{n}_{\boldsymbol{k}\sigma} - \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\sigma\sigma'}\hat{n}_{\boldsymbol{k}\sigma}) \\
&= \frac{e^2}{2\Omega\epsilon_0\mu^2}(\hat{N}^2 - \hat{N})
\end{aligned} \tag{17}$$

where we used that the total number operator $\hat{N} = \sum_{\boldsymbol{k},\sigma}\hat{n}_{\boldsymbol{k}\sigma}$.

We always here consider many-particle states $|\Psi(N)\rangle$ that are eigenstates of $\hat{N}$. Thus, since

$$H^{q=0}_{\mathrm{el-el}}|\Psi(N)\rangle = \frac{e^2}{2\Omega\epsilon_0\mu^2}(N^2 - N)|\Psi(N)\rangle \tag{18}$$

we can effectively treat $H^{q=0}_{\mathrm{el-el}}$ as a c-number, with the operator $\hat{N}$ replaced by the eigenvalue N, i.e.

$$H^{q=0}_{\mathrm{el-el}} = \frac{1}{2}\frac{e^2}{\epsilon_0\mu^2}\left(\frac{N^2}{\Omega} - \frac{N}{\Omega}\right). \tag{19}$$

Note that the contribution of the second term on the rhs to the energy *per particle* is

$$-\frac{1}{2}\frac{e^2}{\epsilon_0 \mu^2 \Omega} \tag{20}$$

which goes to zero in the proper limit (first $\Omega \to \infty$, then $\mu \to 0$). For this reason we will omit the second term in (19). On the other hand, the first term in (19) cancels $H_{\mathrm{b-b}} + H_{\mathrm{el-b}}$. This gives,

$$\begin{aligned} H_I &= H_{\mathrm{el-el}} + H_{\mathrm{b-b}} + H_{\mathrm{el-b}} = H_{\mathrm{el-el}}^{q\neq 0} \\ &= \frac{1}{2\Omega}\sum_{\boldsymbol{q}\neq 0}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'} \frac{e^2}{\epsilon_0(q^2+\mu^2)} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma} \\ &\to \frac{1}{2\Omega}\sum_{\boldsymbol{q}\neq 0}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'} \frac{e^2}{\epsilon_0 q^2} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma} \end{aligned} \tag{21}$$

where in the last line we have taken the limit $\mu \to 0$ describing the Coulomb interaction (the limit $\Omega \to \infty$, which should be taken first, has been left implicit).