Second-quantization representation of the Hamiltonian of an interacting electron gas in an external potential

As a first concrete example of the second quantization formalism, we consider a gas of electrons interacting via the Coulomb interaction, and which may also be subjected to an external potential. The Hamiltonian for the electrons is given by

$$H = T + U + V \tag{1}$$

where T is the kinetic energy operator, U is the external potential (assumed to be spin-independent; it could e.g. be the periodic potential due to the crystal lattice in a crystalline solid), and V is the Coulomb interaction between the electrons. In first quantization,

$$\begin{aligned} T &= -\sum_{i=1}^{N} \frac{\hbar^2}{2m}\nabla_i^2, && (2)\\ U &= \sum_{i=1}^{N} u(\boldsymbol{r}_i), && (3)\\ V &= \sum_{\substack{i,j\\ i\neq j}}^{N} v(\boldsymbol{r}_i,\boldsymbol{r}_j) && (4) \end{aligned}$$

where $u(\boldsymbol{r})$ is the external potential felt by an electron at position $\boldsymbol{r}$ and

$$v(\boldsymbol{r},\boldsymbol{r}') = v(\boldsymbol{r}-\boldsymbol{r}') = \frac{e^2}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{5}$$

We take the system to be a cube of side lengths L and volume $\Omega = L^3$. For convenience we impose periodic boundary conditions in all 3 spatial directions. Thus the point $(x = L, y, z)$ is identified with the point $(x = 0, y, z)$, $(x, y = L, z)$ is identified with $(x, y = 0, z)$ and $(x, y, z = L)$ is identified with $(x, y, z = 0)$.[1]

Let us find the second-quantization representation of H expressed in terms of the momentum-spin (i.e. $\alpha = (\boldsymbol{k},\sigma)$) single-particle basis. The single-particle basis functions are thus eigenfunctions of the momentum operator $\boldsymbol{p}$ and z-component S^z of the spin operator for a single electron, and are given by

$$\phi_\alpha(x) = \phi_{\boldsymbol{k}\sigma}(\boldsymbol{r},s) = \frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\chi_\sigma(s) \tag{6}$$

where[2]

$$\chi_\sigma(s) = \delta_{s\sigma} \tag{7}$$

[1] Please note that the symbol x is used for two different things in these notes: the x coordinate in real space and the total space-spin coordinate $x = (\boldsymbol{r}, s)$; hopefully it should be clear from the context which of the two meanings is intended.

[2] In the standard matrix representation (setting $\hbar = 1$), $S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ with eigenstates $|\uparrow = +1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\downarrow = -1/2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, giving $\chi_\sigma(s) \equiv \langle s|\sigma\rangle = \delta_{s\sigma}$.

with s, σ taking the possible values $\pm 1/2 = \uparrow, \downarrow$. The periodic boundary conditions imply that only wavevectors $\boldsymbol{k}$ on the form

$$\boldsymbol{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \tag{8}$$

with n_i $(i = x, y, z)$ being arbitrary integers, are allowed. For example, the identification of $x = 0$ and $x = L$ gives $\phi(x = 0) = \phi(x = L)$, from which it follows that $1 = e^{ik_x L}$ and thus $k_x = 2\pi n_x / L$ for integer n_x. The eigenfunctions $\{\phi_\alpha(x)\}$ form a complete and orthonormal set. Let us check the orthonormality:

$$\begin{aligned} \int dx\, \phi^*_{\alpha'}(x)\phi_\alpha(x) &= \int d^3r \sum_s \phi^*_{\boldsymbol{k}'\sigma'}(\boldsymbol{r}, s)\phi_{\boldsymbol{k}\sigma}(\boldsymbol{r}, s) \\ &= \underbrace{\frac{1}{\Omega}\int d^3r\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}_{\delta_{\boldsymbol{k}\boldsymbol{k}'}} \underbrace{\sum_s \delta_{\sigma' s}\delta_{\sigma s}}_{\delta_{\sigma\sigma'}} = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\sigma\sigma'} = \delta_{\alpha\alpha'}. \end{aligned} \tag{9}$$

The kinetic energy operator T is a single-particle operator, so its second-quantization representation is given by

$$T = \sum_{\alpha,\alpha'} \langle\alpha'|\frac{\boldsymbol{p}^2}{2m}|\alpha\rangle c^\dagger_{\alpha'} c_\alpha \tag{10}$$

where the matrix element

$$\begin{aligned} \langle\alpha'|\frac{\boldsymbol{p}^2}{2m}|\alpha\rangle &= \int dx\, \phi^*_{\alpha'}(x)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\phi_\alpha(x) \\ &= \sum_s \int d^3r \left(\frac{1}{\sqrt{\Omega}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}}\delta_{s\sigma'}\right)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\left(\frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\delta_{s\sigma}\right) \qquad (11) \\ &= \sum_s \int d^3r \left(\frac{1}{\sqrt{\Omega}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}}\delta_{s\sigma'}\right)\left(\frac{\hbar^2\boldsymbol{k}^2}{2m}\right)\left(\frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\delta_{s\sigma}\right) \\ &= \frac{\hbar^2\boldsymbol{k}^2}{2m} \underbrace{\left(\frac{1}{\Omega}\int d^3r\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}\right)}_{\delta_{\boldsymbol{k}\boldsymbol{k}'}} \underbrace{\left(\sum_s \delta_{s\sigma'}\delta_{s\sigma}\right)}_{\delta_{\sigma\sigma'}} \\ &= \frac{\hbar^2\boldsymbol{k}^2}{2m}\, \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\sigma\sigma'}. \qquad (12) \end{aligned}$$

Thus the matrix elements of the the kinetic energy operator $\boldsymbol{p}^2/2m$ for a single particle are diagonal in this basis. This should be entirely as expected (and is the reason why we chose this basis to begin with): given that the basis functions are eigenfunctions of $\boldsymbol{p}$, they are also eigenfunctions of $\boldsymbol{p}^2/2m$. Putting this result back into (10) gives

$$T = \sum_{\boldsymbol{k}\sigma} \frac{\hbar^2\boldsymbol{k}^2}{2m}\, c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}. \tag{13}$$

Thus the diagonality implies that T becomes just a linear combination of number operators $c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} \equiv \hat{n}_{\boldsymbol{k}\sigma}$.

Similarly, the second-quantized representation of the external potential U, which is also a single-particle operator, becomes

$$U = \sum_{\alpha,\alpha'} \langle \alpha' | u | \alpha \rangle c^\dagger_{\alpha'} c_\alpha \tag{14}$$

where

$$\begin{aligned} \langle \alpha' | u | \alpha \rangle &= \int dx\ \phi^*_{\alpha'}(x) u(\boldsymbol{r}) \phi_\alpha(x) \\ &= \sum_s \int d^3r \left(\frac{1}{\sqrt{\Omega}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}} \delta_{s\sigma'} \right) u(\boldsymbol{r}) \left(\frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \delta_{s\sigma} \right) \qquad (15) \\ &= \frac{1}{\Omega} \underbrace{\int d^3r\, u(\boldsymbol{r}) e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}_{u_{\boldsymbol{k}'-\boldsymbol{k}}} \sum_s \delta_{s\sigma'} \delta_{s\sigma} \\ &= \frac{1}{\Omega} u_{\boldsymbol{k}'-\boldsymbol{k}}\ \delta_{\sigma\sigma'} \qquad (16) \end{aligned}$$

where $u_{\boldsymbol{q}}$ is the Fourier transform of $u(\boldsymbol{r})$. Thus

$$U = \frac{1}{\Omega} \sum_{\boldsymbol{k}\sigma\boldsymbol{k}'\sigma'} u_{\boldsymbol{k}'-\boldsymbol{k}} \delta_{\sigma\sigma'} c^\dagger_{\boldsymbol{k}'\sigma'} c_{\boldsymbol{k}\sigma} = \frac{1}{\Omega} \sum_{\boldsymbol{k}\boldsymbol{q}\sigma} u_{\boldsymbol{q}}\, c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k}\sigma} \tag{17}$$

which describes a scattering process in which an electron is scattered from momentum $\boldsymbol{k}$ to momentum $\boldsymbol{k}+\boldsymbol{q}$. As a special case, note that if $u(\boldsymbol{r}) = u$, i.e. a constant independent of $\boldsymbol{r}$, so that the system is translationally invariant, we have $\frac{1}{\Omega} u_{\boldsymbol{q}} = u\delta_{\boldsymbol{q},0}$, in which case U becomes diagonal in the $(\boldsymbol{k},\sigma)$ basis.

Finally, the second-quantized representation of the electron-electron interaction V, which is a two-particle operator, is

$$V = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta | v | \gamma\delta \rangle c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma, \tag{18}$$

where, writing $\alpha = (\boldsymbol{k}_1, \sigma_1)$, $\beta = (\boldsymbol{k}_2, \sigma_2)$, $\delta = (\boldsymbol{k}_3, \sigma_3)$, and $\gamma = (\boldsymbol{k}_4, \sigma_4)$, we have

$$\begin{aligned} \langle \alpha\beta | v | \gamma\delta \rangle &= \int dx \int dx\, \phi^*_\alpha(x) \phi^*_\beta(x') v(x,x') \phi_\gamma(x) \phi_\delta(x') = \sum_s \int d^3r \sum_{s'} \int d^3r' \\ &\left(\frac{1}{\sqrt{\Omega}} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} \delta_{s\sigma_1} \right) \left(\frac{1}{\sqrt{\Omega}} e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}'} \delta_{s'\sigma_2} \right) v(\boldsymbol{r}-\boldsymbol{r}') \left(\frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}_4\cdot\boldsymbol{r}} \delta_{s\sigma_4} \right) \left(\frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}_3\cdot\boldsymbol{r}'} \delta_{s'\sigma_3} \right) \\ &= \left(\sum_s \delta_{s\sigma_1} \delta_{s\sigma_4} \right) \left(\sum_{s'} \delta_{s'\sigma_2} \delta_{s'\sigma_3} \right) \\ &\quad \cdot \frac{1}{\Omega^2} \int d^3r \int d^3r'\ v(\boldsymbol{r}-\boldsymbol{r}') e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_4)\cdot\boldsymbol{r}} e^{-i(\boldsymbol{k}_2-\boldsymbol{k}_3)\cdot\boldsymbol{r}'} \qquad (19) \end{aligned}$$

Let us define $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$ and change integration variables to $\boldsymbol{R}$ and $\boldsymbol{r}'$. The integrals then factorize as follows:

$$\underbrace{\frac{1}{\Omega} \int d^3R\, v(\boldsymbol{R}) e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_4)\cdot\boldsymbol{R}}}_{\equiv v_{\boldsymbol{k}_1-\boldsymbol{k}_4}} \cdot \underbrace{\frac{1}{\Omega} \int d^3r'\, e^{-i(\boldsymbol{k}_2-\boldsymbol{k}_3+\boldsymbol{k}_1-\boldsymbol{k}_4)\cdot\boldsymbol{r}'}}_{=\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4+\boldsymbol{k}_3-\boldsymbol{k}_2}} \tag{20}$$

where $v_{\boldsymbol{q}}$ is the Fourier transform of $v(\boldsymbol{r})$. Thus

$$\langle\alpha\beta|v|\gamma\delta\rangle = \frac{1}{\Omega}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4+\boldsymbol{k}_3-\boldsymbol{k}_2}v_{\boldsymbol{k}_1-\boldsymbol{k}_4} \tag{21}$$

which gives

$$V = \frac{1}{2\Omega}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4+\boldsymbol{k}_3-\boldsymbol{k}_2}v_{\boldsymbol{k}_1-\boldsymbol{k}_4}c^\dagger_{\boldsymbol{k}_1\sigma_1}c^\dagger_{\boldsymbol{k}_2\sigma_2}c_{\boldsymbol{k}_3\sigma_3}c_{\boldsymbol{k}_4\sigma_4} \tag{22}$$

Doing the summation over $\boldsymbol{k}_1$ and over σ_3 and σ_4 then gives (after renaming $\sigma_1 \equiv \sigma$, $\sigma_2 \equiv \sigma'$)

$$V = \frac{1}{2\Omega}\sum_{\sigma,\sigma'}\sum_{\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} v_{\boldsymbol{k}_3-\boldsymbol{k}_2}\; c^\dagger_{\boldsymbol{k}_4+\boldsymbol{k}_3-\boldsymbol{k}_2,\sigma}c^\dagger_{\boldsymbol{k}_2\sigma'}c_{\boldsymbol{k}_3\sigma'}c_{\boldsymbol{k}_4\sigma}. \tag{23}$$

Let us define new summation variables $\boldsymbol{k}$, $\boldsymbol{k}'$, and $\boldsymbol{q}$ by

$$\boldsymbol{k}_4 \equiv \boldsymbol{k}, \quad \boldsymbol{k}_3 \equiv \boldsymbol{k}', \quad \boldsymbol{k}_2 \equiv \boldsymbol{k}' - \boldsymbol{q}. \tag{24}$$

This gives

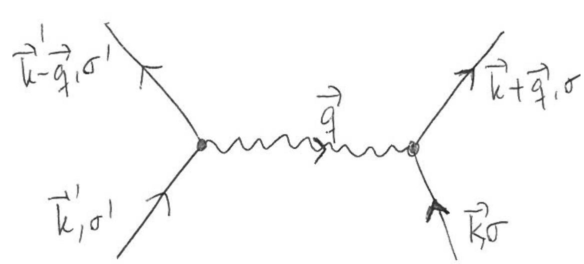
$$\boldsymbol{k}_4 + \boldsymbol{k}_3 - \boldsymbol{k}_2 = \boldsymbol{k} + \boldsymbol{q}, \tag{25}$$

$$\boldsymbol{k}_3 - \boldsymbol{k}_2 = \boldsymbol{q}. \tag{26}$$

Thus

$$V = \frac{1}{2\Omega}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}} \sum_{\substack{\boldsymbol{k},\sigma\\ \boldsymbol{k}',\sigma'}} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma}. \tag{27}$$

This expression describes a scattering process in which two electrons scatter by exchanging momentum $\boldsymbol{q}$. Before the scattering the electrons have momenta $\boldsymbol{k}$ and $\boldsymbol{k}'$, after the scattering the electrons have momenta $\boldsymbol{k}+\boldsymbol{q}$ and $\boldsymbol{k}'-\boldsymbol{q}$. Note that the total momentum $\boldsymbol{k}+\boldsymbol{k}'$ is conserved in the scattering process. This is a consequence of the translational invariance of the interaction, i.e. the fact that it only depends on $\boldsymbol{r}-\boldsymbol{r}'$, not on $\boldsymbol{r}$ and $\boldsymbol{r}'$ separately. Also note that since the Coulomb interaction (5) is spin-independent, the electrons spins are not affected by the scattering process. A diagrammatic representation of the scattering process is shown in the figure.



Mathematically, the scattering is described by the annihilation of the incoming electrons with momentum $\boldsymbol{k}$ and $\boldsymbol{k}'$ and the creation of the outgoing electrons with momentum $\boldsymbol{k}+\boldsymbol{q}$ and $\boldsymbol{k}'-\boldsymbol{q}$.