To obtain the final expression for $\mathbf{A}$ in second quantization we simply express $\mathbf{A}_{\mathbf{k},\lambda}$ in terms of $P_{\mathbf{k},\lambda}$ and $Q_{\mathbf{k},\lambda}$, which in turn is expressed in terms of $a^\dagger_{\mathbf{k},\lambda}$ and $a_{\mathbf{k},\lambda}$:

$$A_{\mathbf{k},\lambda} = A^R_{\mathbf{k},\lambda} + iA^I_{\mathbf{k},\lambda} \to \frac{Q_{\mathbf{k},\lambda}}{2\sqrt{\epsilon_0}} + i\,\frac{P_{\mathbf{k},\lambda}}{2\omega_{\mathbf{k}}\sqrt{\epsilon_0}} = \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}}}\,a_{\mathbf{k},\lambda}, \quad \text{and} \quad A^*_{\mathbf{k},\lambda} \to \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}}}\,a^\dagger_{\mathbf{k},\lambda}. \tag{1.88}$$

Substituting this into the expansion Eq. (1.82) our final result is:

$$\mathbf{A}(\mathbf{r},t) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{k}}\sum_{\lambda=1,2}\sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}}}\Big(a_{k,\lambda}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} + a^\dagger_{k,\lambda}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}\Big)\boldsymbol{\epsilon}_\lambda. \tag{1.89}$$

1.4.3 Operators for kinetic energy, spin, density, and current

In the following we establish the second quantization representation of the four important single-particle operators associated with kinetic energy, spin, particle density, and particle current density.

First, we study the kinetic energy operator T, which is independent of spin and hence diagonal in the spin indices. In first quantization it has the representations

$$T_{\mathbf{r},\sigma'\sigma} = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}}\,\delta_{\sigma',\sigma}, \qquad \text{real space representation,} \tag{1.90a}$$

$$\langle\mathbf{k}'\sigma'|T|\mathbf{k}\sigma\rangle = \frac{\hbar^2k^2}{2m}\delta_{\mathbf{k}',\mathbf{k}}\,\delta_{\sigma',\sigma}, \qquad \text{momentum representation.} \tag{1.90b}$$

Its second quantized forms with spin indices follow directly from Eqs. (1.63) and (1.73)

$$T = \sum_{\mathbf{k},\sigma}\frac{\hbar^2k^2}{2m}a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma} = -\frac{\hbar^2}{2m}\sum_\sigma\int d\mathbf{r}\;\Psi^\dagger_\sigma(\mathbf{r})\Big(\nabla^2_{\mathbf{r}}\Psi_\sigma(\mathbf{r})\Big). \tag{1.91}$$

The second equality can also be proven directly by inserting $\Psi^\dagger(\mathbf{r})$ and $\Psi(\mathbf{r})$ from Eq. (1.74). For particles with charge q a magnetic field can be included in the expression for the kinetic energy by substituting the canonical momentum $\mathbf{p}$ with the kinetic momentum[4] $\mathbf{p} - q\mathbf{A}$,

$$T_{\mathbf{A}} = \frac{1}{2m}\sum_\sigma\int d\mathbf{r}\;\Psi^\dagger_\sigma(\mathbf{r})\Big(\frac{\hbar}{i}\nabla_{\mathbf{r}} - q\mathbf{A}\Big)^2\Psi_\sigma(\mathbf{r}). \tag{1.92}$$

Next, we treat the spin operator $\mathbf{s}$ for electrons. In first quantization it is given by the Pauli matrices

$$\mathbf{s} = \frac{\hbar}{2}\boldsymbol{\tau}, \quad \text{with} \quad \boldsymbol{\tau} = \left\{\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right\}. \tag{1.93}$$

[4] In analytical mechanics $\mathbf{A}$ enters through the Lagrangian: $L = \frac{1}{2}mv^2 - V + q\mathbf{v}\cdot\mathbf{A}$, since this by the Euler-Lagrange equations yields the Lorentz force. But then $\mathbf{p} = \partial L/\partial\mathbf{v} = m\mathbf{v} + q\mathbf{A}$, and via a Legendre transform we get $H(\mathbf{r},\mathbf{p}) = \mathbf{p}\cdot\mathbf{v} - L(\mathbf{r},\mathbf{v}) = \frac{1}{2}mv^2 + V = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + V$. Considering infinitesimal variations $\delta\mathbf{A}$ we get $\delta H = H(\mathbf{A}+\delta\mathbf{A}) - H(\mathbf{A}) = -q\mathbf{v}\cdot\delta\mathbf{A} = -q\int d\mathbf{r}\,\mathbf{J}\cdot\delta\mathbf{A}$, an expression used to find $\mathbf{J}$.

To obtain the second quantized operator we pull out the spin index explicitly in the basis kets, $|\nu\rangle = |\mu\rangle|\sigma\rangle$, and obtain with fermion operators the following vector expression,

$$\mathbf{s} = \sum_{\mu\sigma\mu'\sigma'} \langle\mu'|\langle\sigma'|\mathbf{s}|\sigma\rangle|\mu\rangle\, c^\dagger_{\mu'\sigma'}c_{\mu\sigma} = \frac{\hbar}{2}\sum_{\mu}\sum_{\sigma'\sigma}\langle\sigma'|(\tau^x,\tau^y,\tau^z)|\sigma\rangle\, c^\dagger_{\mu\sigma'}c_{\mu\sigma}, \tag{1.94a}$$

with components

$$s^x = \frac{\hbar}{2}\sum_{\mu}(c^\dagger_{\mu\downarrow}c_{\mu\uparrow} + c^\dagger_{\mu\uparrow}c_{\mu\downarrow}) \quad s^y = i\frac{\hbar}{2}\sum_{\mu}(c^\dagger_{\mu\downarrow}c_{\mu\uparrow} - c^\dagger_{\mu\uparrow}c_{\mu\downarrow}) \quad s^z = \frac{\hbar}{2}\sum_{\mu}(c^\dagger_{\mu\uparrow}c_{\mu\uparrow} - c^\dagger_{\mu\downarrow}c_{\mu\downarrow}). \tag{1.94b}$$

We then turn to the particle density operator $\rho(\mathbf{r})$. In first quantization the fundamental interpretation of the wave function $\psi_{\mu,\sigma}(\mathbf{r})$ gives us $\rho_{\mu,\sigma}(\mathbf{r}) = |\psi_{\mu,\sigma}(\mathbf{r})|^2$ which can also be written as $\rho_{\mu,\sigma}(\mathbf{r}) = \int d\mathbf{r}'\, \psi^*_{\mu,\sigma}(\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r})\psi_{\mu,\sigma}(\mathbf{r}')$, and thus the density operator for spin σ is given by $\rho_\sigma(\mathbf{r}) = \delta(\mathbf{r}'-\mathbf{r})$. In second quantization this combined with Eq. (1.63) yields

$$\rho_\sigma(\mathbf{r}) = \int d\mathbf{r}'\, \Psi^\dagger_\sigma(\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r})\Psi_\sigma(\mathbf{r}') = \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}). \tag{1.95}$$

From Eq. (1.75) the momentum representation of this is found to be

$$\rho_\sigma(\mathbf{r}) = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} a^\dagger_{\mathbf{k}'\sigma}a_{\mathbf{k}\sigma} = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} a^\dagger_{\mathbf{k}+\mathbf{q}\sigma}a_{\mathbf{k}\sigma} = \frac{1}{\mathcal{V}}\sum_{\mathbf{q}}\left(\sum_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}+\mathbf{q}\sigma}\right)e^{i\mathbf{q}\cdot\mathbf{r}}, \tag{1.96}$$

where the momentum transfer $\mathbf{q} = \mathbf{k}'-\mathbf{k}$ has been introduced.

The fourth and last operator to be treated is the particle current density operator $\mathbf{J}(\mathbf{r})$. It is related to the particle density operator $\rho(\mathbf{r})$ through the continuity equation $\partial_t\rho + \nabla\cdot\mathbf{J} = 0$. This relationship can be used to actually define $\mathbf{J}$. However, we shall take a more general approach based on analytical mechanics, see Eq. (1.92) and the associated footnote. This allows us in a simple way to take the magnetic field, given by the vector potential $\mathbf{A}$, into account. By analytical mechanics it is found that variations δH in the Hamiltonian function due to variations $\delta\mathbf{A}$ in the vector potential is given by

$$\delta H = -q\int d\mathbf{r}\, \mathbf{J}\cdot\delta\mathbf{A} \tag{1.97}$$

We use this expression with H given by the kinetic energy Eq. (1.92). Variations due to a varying parameter are calculated as derivatives if the parameter appears as a simple factor. But expanding the square in Eq. (1.92) and writing only the $\mathbf{A}$ dependent terms of the integrand, $-\Psi^\dagger_\sigma(\mathbf{r})\frac{q\hbar}{2mi}[\nabla\cdot\mathbf{A} + \mathbf{A}\cdot\nabla]\Psi_\sigma(\mathbf{r}) + \frac{q^2}{2m}\mathbf{A}^2\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})$, reveals one term where ∇ is acting on $\mathbf{A}$. By partial integration this ∇ is shifted to $\Psi^\dagger(\mathbf{r})$, and we obtain

$$H = T + \sum_\sigma\int d\mathbf{r}\left\{\frac{q\hbar}{2mi}\mathbf{A}\cdot\left[\Big(\nabla\Psi^\dagger_\sigma(\mathbf{r})\Big)\Psi_\sigma(\mathbf{r}) - \Psi^\dagger_\sigma(\mathbf{r})\Big(\nabla\Psi_\sigma(\mathbf{r})\Big)\right] + \frac{q^2}{2m}\mathbf{A}^2\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})\right\}. \tag{1.98}$$

The variations of Eq. (1.97) can in Eq. (1.98) be performed as derivatives and $\mathbf{J}$ is immediately read off as the prefactor to $\delta\mathbf{A}$. The two terms in the current density operator are denoted the paramagnetic and the diamagnetic term, $\mathbf{J}^{\nabla}$ and $\mathbf{J}^{A}$, respectively:

$$\mathbf{J}_\sigma(\mathbf{r}) = \mathbf{J}^{\nabla}_\sigma(\mathbf{r}) + \mathbf{J}^{A}_\sigma(\mathbf{r}), \tag{1.99a}$$

$$\text{paramagnetic}: \quad \mathbf{J}^{\nabla}_\sigma(\mathbf{r}) = \frac{\hbar}{2mi}\Big[\Psi^\dagger_\sigma(\mathbf{r})\Big(\nabla\Psi_\sigma(\mathbf{r})\Big) - \Big(\nabla\Psi^\dagger_\sigma(\mathbf{r})\Big)\Psi_\sigma(\mathbf{r})\Big], \tag{1.99b}$$

$$\text{diamagnetic}: \quad \mathbf{J}^{A}_\sigma(\mathbf{r}) = -\frac{q}{m}\mathbf{A}(\mathbf{r})\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}). \tag{1.99c}$$

The momentum representation of $\mathbf{J}$ is found in complete analogy with that of ρ

$$\mathbf{J}^{\nabla}_\sigma(\mathbf{r}) = \frac{\hbar}{m\mathcal{V}}\sum_{\mathbf{kq}}(\mathbf{k}+\frac{1}{2}\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}+\mathbf{q},\sigma}, \qquad \mathbf{J}^{A}_\sigma(\mathbf{r}) = \frac{-q}{m\mathcal{V}}\mathbf{A}(\mathbf{r})\sum_{\mathbf{kq}}e^{i\mathbf{q}\cdot\mathbf{r}}a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}+\mathbf{q},\sigma}. \tag{1.100}$$

The expression for $\mathbf{J}$ in an arbitrary basis is treated in Exercise 1.2.

1.4.4 The Coulomb interaction in second quantization

The Coulomb interaction operator V is a two-particle operator not involving spin and thus diagonal in the spin indices of the particles. Using the same reasoning that led from Eq. (1.63) to Eq. (1.73) we can go directly from Eq. (1.64) to the following quantum field operator form of V:

$$V(\mathbf{r}_2-\mathbf{r}_1) = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int d\mathbf{r}_1 d\mathbf{r}_2\,\frac{e_0^2}{|\mathbf{r}_2-\mathbf{r}_1|}\Psi^\dagger_{\sigma_1}(\mathbf{r}_1)\Psi^\dagger_{\sigma_2}(\mathbf{r}_2)\Psi_{\sigma_2}(\mathbf{r}_2)\Psi_{\sigma_1}(\mathbf{r}_1). \tag{1.101}$$

Here we have introduced the abbreviation $e_0^2 = e^2/4\pi\epsilon_0$.We can also write the Coulomb interaction directly in the momentum basis by using Eq. (1.31) and Eq. (1.64) with $|\nu\rangle = |\mathbf{k},\sigma\rangle$ and $\psi_{\mathbf{k},\sigma}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}}e^{i\mathbf{k}\cdot\mathbf{r}}\chi_\sigma$. We can interpret the Coulomb matrix element as describing a transition from an initial state $|\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2\rangle$ to a final state $|\mathbf{k}_3\sigma_1,\mathbf{k}_4\sigma_2\rangle$ without flipping any spin, and we obtain

$$\begin{aligned} V &= \frac{1}{2}\sum_{\sigma_1\sigma_2}\sum_{\substack{\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4}}\langle\mathbf{k}_3\sigma_1,\mathbf{k}_4\sigma_2|V|\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2\rangle\, a^\dagger_{\mathbf{k}_3\sigma_1}a^\dagger_{\mathbf{k}_4\sigma_2}a_{\mathbf{k}_2\sigma_2}a_{\mathbf{k}_1\sigma_1} \\ &= \frac{1}{2}\sum_{\sigma_1\sigma_2}\sum_{\substack{\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4}}\left(\frac{e_0^2}{\mathcal{V}^2}\int d\mathbf{r}_1 d\mathbf{r}_2\,\frac{e^{i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2-\mathbf{k}_3\cdot\mathbf{r}_1-\mathbf{k}_4\cdot\mathbf{r}_2)}}{|\mathbf{r}_2-\mathbf{r}_1|}\right)a^\dagger_{\mathbf{k}_3\sigma_1}a^\dagger_{\mathbf{k}_4\sigma_2}a_{\mathbf{k}_2\sigma_2}a_{\mathbf{k}_1\sigma_1}. \end{aligned} \tag{1.102}$$

Since $\mathbf{r}_2-\mathbf{r}_1$ is the relevant variable for the interaction, the exponential is rewritten as