Quantum Mechanics II
Exercise 8

Exercise 8.1 Charge Density and Current Density Operators

In this exercise we consider some of the most fundamental properties of electromagnetism in quantum mechanics, such as gauge invariance and the continuity equation.

a) We will first consider a system of chargeless particles for which we define the operators

$$\hat{\rho}(\mathbf{r}) := \delta(\mathbf{r} - \hat{\mathbf{r}}) \tag{1}$$

$$\hat{\mathbf{j}}(\mathbf{r}) := \frac{1}{2m}\Big(\hat{\mathbf{p}}\,\hat{\rho}(\mathbf{r}) + \hat{\rho}(\mathbf{r})\,\hat{\mathbf{p}}\Big)\,, \tag{2}$$

where $\hat{\rho}(\mathbf{r})$ represents the particle density and $\hat{\mathbf{j}}(\mathbf{r})$ the current density.

Show that for a given (normalizable) state ψ, the following relations hold:

$$\text{(i)}:\quad \langle\,\hat{\rho}(\mathbf{r})\,\rangle_\psi = |\psi(\mathbf{r})|^2\,, \tag{3}$$

$$\text{(ii)}:\quad \langle\,\hat{\mathbf{j}}(\mathbf{r})\,\rangle_\psi = \frac{\hbar}{2mi}\Big[\overline{\psi}(\mathbf{r})\boldsymbol{\nabla}\psi(\mathbf{r}) - \psi(\mathbf{r})\boldsymbol{\nabla}\overline{\psi}(\mathbf{r})\Big] \tag{4}$$

b) Now we want to turn our interest to charged particles. As a first step, we consider a single charged particle controlled by the scalar potential $V(\mathbf{r},t)$ and couple it the electromagnetic field. This system can conveniently be described by the Hamiltonian

$$\hat{\mathcal{H}}(t) = \frac{1}{2m}\Big(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}(\hat{\mathbf{r}})\Big)^2 + V(\hat{\mathbf{r}},t)\,, \tag{5}$$

where the coupling to the vector potential $\mathbf{A}(\mathbf{r})$ is performed by "minimal substitution", $\hat{\mathbf{p}} \to \hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{r}})/c$.

Show that the particle density operator $\hat{\rho}(\mathbf{r})$ and the operator $\hat{\mathbf{J}}(\mathbf{r})$,

$$\hat{\mathbf{J}}(\mathbf{r}) := \hat{\mathbf{j}}(\mathbf{r}) - \frac{e}{mc}\mathbf{A}(\mathbf{r})\,\hat{\rho}(\mathbf{r})\,, \tag{6}$$

satisfy the continuity equation in the Heisenberg-picture (subscript "H"):

$$\frac{\partial}{\partial t}\,\hat{\rho}_H(\mathbf{r},t) + \boldsymbol{\nabla}\cdot\hat{\mathbf{J}}_H(\mathbf{r},t) = 0 \tag{7}$$

Note that in general the current density is *defined* through the continuity equation, i.e. given the density of a system, one expresses its time derivative by the divergence of a vector field. This vector field then *defines* the current density of this system. Consequently, we can identify the operator $\hat{\mathbf{J}}(\mathbf{r})$ with the current density of the system. The first part of the current density (6) is known as the "paramagnetic" current density while the second part denotes the "diamagnetic" part.

c) From classical electrodynamics we know that the electromagnetic field comes with a gauge degree of freedom. In this part of the exercise, we want to consider the corresponding gauge transformation in quantum mechanics.

Show that the matrix elements $\langle\psi\,|\,\hat{\mathbf{J}}(\mathbf{r})\,|\,\varphi\rangle$ are invariant with respect to gauge transformations

$$\mathbf{A}(\mathbf{r}) \longmapsto \mathbf{A}(\mathbf{r}) + [\boldsymbol{\nabla}\chi(\mathbf{r})] \;, \qquad \phi(\mathbf{r}) \longmapsto \phi(\mathbf{r})\, e^{ie\chi(\mathbf{r})/\hbar c} \;, \tag{8}$$

where ϕ stands for both ψ and φ and $\chi(\mathbf{r})$ is an arbitrary scalar function.

What is the difference between gauge transformations in classical electrodynamics and in quantum mechanics?

Hints for Exercise 8.1:

b) In the Heisenberg-picture, an arbitrary operator $\hat{O}_H$ is given by

$$\hat{O}_H(\mathbf{r}, t) = \hat{U}^\dagger(t)\, \hat{O}(\mathbf{r})\, \hat{U}(t) \;, \tag{9}$$

where $\hat{U}(t)$ defines the time-evolution operator. $\hat{O}_H$ follows the equation of motion

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \hat{O}_H(t) = [\hat{O}_H(t), \hat{\mathcal{H}}_H(t)] + i\hbar \left(\frac{\mathrm{d}}{\mathrm{d}t} \hat{O}_S(t) \right)_H \;. \tag{10}$$

Use $\hat{U}(t)$ to express the equation of motion for $\hat{\rho}_H(\mathbf{r}, t)$ in terms of Schrödinger-picture operators.

c) First relate the off-diagonal matrix elements $\langle\psi|\hat{O}|\varphi\rangle$ to a sum of diagonal matrix elements $\langle\psi \pm \varphi|\hat{O}|\psi \pm \varphi\rangle$ and $\langle\psi \pm i\varphi|\hat{O}|\psi \pm i\varphi\rangle$. Hence, it is sufficient to show the statement for diagonal matrix elements.

Exercise 8.2 Quantum Dot Coupled to an Electromagnetic Field

A quantum dot is a small (nano-scale) structure with quantized electronic excitations that are confined to the range of the quantum dot. Usually, quantum dots are implemented in semiconductors and consist of "potential islands" where a single (or sometimes very few) electron is localized.
We will describe a quantum dot as a spherically symmetric three-dimensional harmonic oscillator of frequency ω_d. In this picture, every state can be written as a superposition (tensor product) of states of three independent one-dimensional harmonic oscillators,

$$|\mathbf{n}\rangle \equiv |n_x, n_y, n_z\rangle \equiv |n_x\rangle \otimes |n_y\rangle \otimes |n_z\rangle \;. \tag{11}$$

The energy E_N of such a state $|\mathbf{n}\rangle$, given by $E_N = \hbar\,\omega_d\,(n_x + n_y + n_z + 3/2)$, only depends on $N = n_x + n_y + n_z$. Therefore, the excited states, $N > 0$, are highly degenerate. We assume the quantum dot initially to be set up in the ground state and couple it to a polarized, monochromatic electromagnetic radiation field (not quantized), given by the vector potential

$$\mathbf{A}(\mathbf{r}, t) = \frac{1}{L^{3/2}} \left[\, A\,\mathbf{e}\; e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t} + A^*\,\mathbf{e}^*\; e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega t} \right] \;. \tag{12}$$

Here A is the amplitude, $\mathbf{e}$ the polarization vector, L^3 the volume of the whole system (*not the volume of the quantum dot*) and $\mathbf{k} = (0, 0, k)$ the wave number.

We assume that the transition probability of the system into one of the excited states $|\mathbf{n}\rangle$ is given by Fermi's golden rule,

$$\Gamma_{(\mathbf{0})\rightarrow(\mathbf{n})} = \frac{2\pi}{\hbar}\,\delta(E_n - E_0 - \hbar\omega)\,\frac{e^2}{L^3c^2}\,|A|^2\,\left|\langle\mathbf{n}|\,\hat{\mathbf{j}}(-\mathbf{k})\cdot\mathbf{e}\,|\mathbf{0}\rangle\right|^2 \ , \tag{13}$$

where $\hat{\mathbf{j}}(\mathbf{k})$ represents the paramagnetic current density (cf. Exercise 8.1) in momentum space, i.e.

$$\hat{\mathbf{j}}(\mathbf{k}) = \int \mathrm{d}^3r\, e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{\mathbf{j}}(\mathbf{r}) = \frac{1}{2}\left[\frac{\hat{\mathbf{p}}}{m}\,e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} + e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}\,\frac{\hat{\mathbf{p}}}{m}\right] \ . \tag{14}$$

a) Compute the matrix elements $\langle\mathbf{n}|\,\hat{\mathbf{j}}(-\mathbf{k})\cdot\mathbf{e}\,|\mathbf{0}\rangle$ and distinguish between the three types of polarization:

   (i) $\mathbf{e} = \mathbf{e_X} = (1,0,0)$ *linear polarization in x direction*

   (ii) $\mathbf{e} = \mathbf{e_Y} = (0,1,0)$ *linear polarization in y direction*

   (iii) $\mathbf{e} = \mathbf{e}_\pm = (1,\pm i,0)/\sqrt{2}$ *circular polarization (left- / right-handed)*

b) Show that the total absorption rate $\Gamma(\omega)$ of the quantum dot as a function of the frequency ω, which is defined as the sum over the partial absorption rates, is given by

$$\begin{aligned}\Gamma(\omega) &:= \sum_{n_x,n_y,n_z}\Gamma_{(\mathbf{0})\rightarrow(\mathbf{n})}\\ &= \frac{e^2\pi}{L^3c^2m\hbar}|A|^2\sum_{n_z}\delta\left(n_z+1-\frac{\omega}{\omega_d}\right)\left(\frac{\omega^2}{\omega_d\omega_m}\right)^{\frac{\omega}{\omega_d}-1}\Gamma\left[\frac{\omega}{\omega_d}\right]^{-1}e^{-\frac{\omega^2}{\omega_d\omega_m}} \ ,\end{aligned} \tag{15}$$

   where we introduced $\omega_m = 2c^2m/\hbar$ and $k = \omega/c$.

Hints for Exercise 8.2:

a) It may be useful to express $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ in terms of the creation and annihilation operators of the states $|n_i\rangle$.

   Use the Baker-Campbell-Hausdorff formula,

$$\exp\left\{\hat{A}+\hat{B}\right\} = \exp\left\{\hat{A}\right\}\,\exp\left\{\hat{B}\right\}\,\exp\left\{-\frac{1}{2}\left[\hat{A}\,,\,\hat{B}\right]\right\} \ , \tag{16}$$

   which holds if $[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{B},\hat{A}]] = 0$.

b) Use the relation

$$n! = \Gamma\left[n+1\right] \ . \tag{17}$$