

Exercise 8.1 Charge Density and Current Density Operators

- a) (i) We simply express the expectation value $\langle \hat{\rho}(\mathbf{r}) \rangle_\psi$ as an integration over the entire coordinate space by using the special form of the unity operator,

$$\mathbb{I} = \int d\mathbf{r}' |\mathbf{r}'\rangle \langle \mathbf{r}'|, \quad (1)$$

as well as the definition

$$\langle \mathbf{r} | \psi \rangle \equiv \psi(\mathbf{r}). \quad (2)$$

Then with $\hat{\rho}(\mathbf{r}) \equiv \delta(\mathbf{r} - \hat{\mathbf{r}})$ we have

$$\begin{aligned} \langle \hat{\rho}(\mathbf{r}) \rangle_\psi &\equiv \langle \psi | \hat{\rho}(\mathbf{r}) | \psi \rangle \\ &= \int d\mathbf{r}' \langle \psi | \mathbf{r}' \rangle \langle \mathbf{r}' | \delta(\mathbf{r} - \hat{\mathbf{r}}) | \psi \rangle \\ &= \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') \langle \psi | \mathbf{r}' \rangle \langle \mathbf{r}' | \psi \rangle = |\psi(\mathbf{r})|^2. \end{aligned} \quad (3)$$

- (ii) One can do the same for $\langle \hat{\mathbf{j}}(\mathbf{r}) \rangle_\psi$,

$$\begin{aligned} \langle \hat{\mathbf{j}}(\mathbf{r}) \rangle_\psi &= \frac{1}{2m} \int d\mathbf{r}' \left(\langle \psi | \hat{\mathbf{p}} | \mathbf{r}' \rangle \langle \mathbf{r}' | \delta(\mathbf{r} - \hat{\mathbf{r}}) | \psi \rangle \right. \\ &\quad \left. + \langle \psi | \delta(\mathbf{r} - \hat{\mathbf{r}}) | \mathbf{r}' \rangle \langle \mathbf{r}' | \hat{\mathbf{p}} | \psi \rangle \right) \\ &= \frac{1}{2m} \left(i\hbar [\nabla \bar{\psi}(\mathbf{r})] \psi(\mathbf{r}) - i\hbar \bar{\psi}(\mathbf{r}) [\nabla \psi(\mathbf{r})] \right). \end{aligned} \quad (4)$$

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

$$\hat{O}_H(\mathbf{r}, t) = \hat{U}^\dagger(t) \hat{O}(\mathbf{r}) \hat{U}(t), \quad (5)$$

where $\hat{U}(t)$ is the unitary time evolution operator corresponding to the Hamiltonian $\hat{\mathcal{H}}(t)$. We know that Heisenberg-picture operators follow the Heisenberg equation of motion,

$$i\hbar \frac{d}{dt} \hat{O}_H(t) = [\hat{O}_H(t), \hat{\mathcal{H}}_H(t)] + i\hbar \left(\frac{d}{dt} \hat{O}_S(t) \right)_H. \quad (6)$$

The potential term $V(\hat{\mathbf{r}}, t)$ of the Hamiltonian commutes with the density and thus drops out of the commutator.

Thus, we can write

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\rho}_H(\mathbf{r}, t) &= \hat{U}(t)^\dagger \frac{i}{\hbar} [\hat{H}(t), \delta(\mathbf{r} - \hat{\mathbf{r}})] \hat{U}(t) \\ &= \hat{U}(t)^\dagger \frac{i}{2\hbar m} \left\{ \left[\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}), \delta(\mathbf{r} - \hat{\mathbf{r}}) \right] \cdot \left(\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}) \right) \right. \\ &\quad \left. + \left(\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}) \right) \cdot \left[\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}), \delta(\mathbf{r} - \hat{\mathbf{r}}) \right] \right\} \hat{U}(t) \end{aligned}$$

Now we have to evaluate the commutator

$$\left[\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}), \delta(\mathbf{r} - \hat{\mathbf{r}}) \right]. \quad (7)$$

First note that the $e\mathbf{A}(\hat{\mathbf{r}})/c$ term drops out because it does only depend on $\hat{\mathbf{r}}$ which commutes with $\rho(\hat{\mathbf{r}})$. The remaining commutator can be evaluated within coordinate space representation of the operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$.

$$\begin{aligned} [\hat{\mathbf{p}}, \delta(\mathbf{r} - \hat{\mathbf{r}})] &\sim \left[\frac{\hbar}{i} \nabla_{\mathbf{x}}, \delta(\mathbf{r} - \mathbf{x}) \right] \\ &= \left(\frac{\hbar}{i} [\nabla_{\mathbf{x}} \delta(\mathbf{r} - \mathbf{x})] + \frac{\hbar}{i} \delta(\mathbf{r} - \mathbf{x}) \nabla_{\mathbf{x}} \right) - \frac{\hbar}{i} \delta(\mathbf{r} - \mathbf{x}) \nabla_{\mathbf{x}} \\ &= \frac{\hbar}{i} [\nabla_{\mathbf{x}} \delta(\mathbf{r} - \mathbf{x})] \\ &= -\frac{\hbar}{i} [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{x})] \\ &\sim -\frac{\hbar}{i} [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}})] \end{aligned} \quad (8)$$

Note that the gradient only acts on the delta distribution and not on anything else, indicated by the rectangular brackets. Thus, we find

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\rho}_H(\mathbf{r}, t) &= -\hat{U}(t)^\dagger \frac{1}{2m} \left\{ [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}})] \cdot \left(\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}) \right) \right. \\ &\quad \left. + \left(\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}) \right) \cdot [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}})] \right\} \hat{U}(t) \\ &= -\hat{U}(t)^\dagger \frac{1}{2m} \left\{ [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}})] \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}})] \right\} \hat{U}(t) \\ &\quad + \hat{U}(t)^\dagger \frac{e}{mc} \mathbf{A}(\hat{\mathbf{r}}) \cdot [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}})] \hat{U}(t) \\ &= -\hat{U}(t)^\dagger \nabla_{\mathbf{r}} \mathbf{j}(\mathbf{r}) \hat{U}(t) \\ &\quad + \hat{U}(t)^\dagger \frac{e}{mc} \mathbf{A}(\hat{\mathbf{r}}) \cdot [\nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}})] \hat{U}(t), \end{aligned} \quad (9)$$

where we have used the definition of the current operator, Eq. (5) and (6) on the exercise sheet.

Here we have to be very careful how to interpret the last term. In the end we want to relate this expression to the divergence of $\hat{\mathbf{J}}(\mathbf{r})$. By comparing (9) with the definition of the current operator, we note that we have to transform $\mathbf{A}(\hat{\mathbf{r}})$ into $\mathbf{A}(\mathbf{r})$ which can be done by using the intriguing identity of the delta function¹:

$$f(\mathbf{r}') \nabla_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}') = f(\mathbf{r}) (\nabla_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}')) + \delta(\mathbf{r} - \mathbf{r}') (\nabla_{\mathbf{r}} f(\mathbf{r})) \quad (11)$$

¹This can be shown by using an arbitrary Schwartz-space function $\phi(\mathbf{r})$

$$\begin{aligned} \int d\mathbf{r} \left\{ f(\mathbf{r}') \nabla_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}') \right\} \phi(\mathbf{r}) &= - \int d\mathbf{r} \left\{ f(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') \right\} \nabla_{\mathbf{r}} \phi(\mathbf{r}) \\ &= - \int d\mathbf{r} \left\{ f(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \right\} \nabla_{\mathbf{r}} \phi(\mathbf{r}) \\ &= + \int d\mathbf{r} \left\{ f(\mathbf{r}) (\nabla_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}')) + \delta(\mathbf{r} - \mathbf{r}') (\nabla_{\mathbf{r}} f(\mathbf{r})) \right\} \phi(\mathbf{r}). \end{aligned} \quad (10)$$

The argument is valid for any test function ϕ and, hence, the terms in curly brackets are equal. Note that we have used a scalar function $f(\mathbf{r}')$ for simplicity. The argument naturally generalizes for vectors $\mathbf{f}(\mathbf{r}')$ by applying for every term of the scalar product $\mathbf{f}(\mathbf{r}') \cdot \nabla_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}')$ individually.

With this we can continue to evaluate the second term in (9):

$$\begin{aligned}
\hat{U}(t)^\dagger \frac{e}{mc} \mathbf{A}(\hat{\mathbf{r}}) \cdot \nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}}) \hat{U}(t) &= \hat{U}(t)^\dagger \left\{ \frac{e}{mc} \mathbf{A}(\mathbf{r}) \cdot \nabla_{\mathbf{r}} \delta(\mathbf{r} - \hat{\mathbf{r}}) \right. \\
&\quad \left. + \frac{e}{mc} \delta(\mathbf{r} - \hat{\mathbf{r}}) \nabla_{\mathbf{r}} \cdot \mathbf{A}(\mathbf{r}) \right\} \hat{U}(t) \\
&= \hat{U}(t)^\dagger \nabla_{\mathbf{r}} \cdot \left(\frac{e}{mc} \mathbf{A}(\mathbf{r}) \delta(\mathbf{r} - \hat{\mathbf{r}}) \right) \hat{U}(t) \\
&= -\hat{U}(t)^\dagger \nabla_{\mathbf{r}} \cdot \left(-\frac{e}{mc} \mathbf{A}(\mathbf{r}) \delta(\mathbf{r} - \hat{\mathbf{r}}) \right) \hat{U}(t) \quad (12)
\end{aligned}$$

Using Eqs. (9) and (12) we have found

$$\begin{aligned}
\frac{\partial}{\partial t} \hat{\rho}_H(\mathbf{r}, t) &= -\hat{U}(t)^\dagger \nabla_{\mathbf{r}} \cdot \left\{ \mathbf{j}(\mathbf{r}) - \left(-\frac{e}{mc} \mathbf{A}(\mathbf{r}) \delta(\mathbf{r} - \hat{\mathbf{r}}) \right) \right\} \hat{U}(t) \\
&= -\nabla_{\mathbf{r}} \cdot \hat{\mathbf{J}}_H(\mathbf{r}, t) \quad (13)
\end{aligned}$$

In the last calculation, the operators have to be interpreted as operator-valued distributions.

From this result it follows that for a charged particle, $\hat{\mathbf{J}}(\mathbf{r})$ and *not* $\hat{\mathbf{j}}(\mathbf{r})$ corresponds to the current operator of the system. The same result can be found if one introduces the coupling to the vector potential $\mathbf{A}(\mathbf{r})$ in terms of “minimal substitution” (the replacement $\hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{r}})/c$) in the definition of the current density operator of the chargeless particle in part (a).

- c) With some simple algebra, we can relate off-diagonal matrix elements of some operator \hat{O} to its diagonal matrix elements in some other basis,

$$\begin{aligned}
4\langle \psi | \hat{O} | \phi \rangle &= \langle \psi + \phi | \hat{O} | \psi + \phi \rangle - \langle \psi - \phi | \hat{O} | \psi - \phi \rangle \\
&\quad - i\langle \psi + i\phi | \hat{O} | \psi + i\phi \rangle + i\langle \psi - i\phi | \hat{O} | \psi - i\phi \rangle. \quad (14)
\end{aligned}$$

In consequence, it is sufficient to study diagonal matrix elements.

It is now convenient to use the relations derived in part (a) of this exercise.

We first compute expectation value of the paramagnetic part ($\propto \hat{\mathbf{j}}$) of the total current operator $\hat{\mathbf{J}}(\mathbf{r}) = \hat{\mathbf{j}}(\mathbf{r}) - \mathbf{A}(\mathbf{r})\hat{\rho}(\mathbf{r})e/mc$. After a gauge transformation, we find

$$\begin{aligned}
&\langle e^{ie\chi(\mathbf{r})/\hbar c} \psi | \hat{\mathbf{j}}(\mathbf{r}) | e^{ie\chi(\mathbf{r})/\hbar c} \psi \rangle \\
&= \frac{\hbar}{2mi} \left[e^{-ie\chi(\mathbf{r})/\hbar c} \bar{\psi}(\mathbf{r}) \nabla (e^{ie\chi(\mathbf{r})/\hbar c} \psi(\mathbf{r})) - e^{-ie\chi(\mathbf{r})/\hbar c} \psi(\mathbf{r}) \nabla (e^{-ie\chi(\mathbf{r})/\hbar c} \bar{\psi}(\mathbf{r})) \right] \\
&= \frac{\hbar}{2mi} [\bar{\psi}(\mathbf{r}) \nabla \psi(\mathbf{r}) - \psi(\mathbf{r}) \nabla \bar{\psi}(\mathbf{r})] + \frac{\hbar}{2mi} \frac{2ie}{\hbar c} |\psi(\mathbf{r})|^2 \nabla \chi(\mathbf{r}) \\
&= \langle \psi | \hat{\mathbf{j}}(\mathbf{r}) | \psi \rangle + |\psi(\mathbf{r})|^2 \frac{e}{mc} \nabla \chi(\mathbf{r}). \quad (15)
\end{aligned}$$

For the second (diamagnetic) term ($\propto \mathbf{A}(\mathbf{r})\hat{\rho}(\mathbf{r})$), we find after a gauge transfor-

mation

$$\begin{aligned}
\langle e^{i\mathbf{e}\chi(\mathbf{r})/\hbar c}\psi | \left(\mathbf{A}(\mathbf{r}) + [\nabla\chi(\mathbf{r})] \right) \hat{\rho}(\mathbf{r}) \frac{e}{mc} | e^{i\mathbf{e}\chi(\mathbf{r})/\hbar c}\psi \rangle \\
= \frac{e}{mc} \left(\mathbf{A}(\mathbf{r}) + [\nabla\chi(\mathbf{r})] \right) \langle e^{i\mathbf{e}\chi(\mathbf{r})/\hbar c}\psi | \hat{\rho} | e^{i\mathbf{e}\chi(\mathbf{r})/\hbar c}\psi \rangle \\
= \frac{e}{mc} \left(\mathbf{A}(\mathbf{r}) + [\nabla\chi(\mathbf{r})] \right) \langle \psi | \hat{\rho} | \psi \rangle \\
= \frac{e}{mc} \mathbf{A}(\mathbf{r}) |\psi(\mathbf{r})|^2 + \frac{e}{mc} [\nabla\chi(\mathbf{r})] |\psi(\mathbf{r})|^2 .
\end{aligned} \tag{16}$$

Now if we subtract (16) from (15), we obtain the matrix elements of the charge-current density operator and we find that the additional terms in (16) and (15) induced by the gauge transformation drop out. Hence, the matrix elements of the current operator remain invariant with respect to gauge transformations.

In contrast to classical electrodynamics, where the physics remains invariant under a gauge transformation of the vector potential, in quantum mechanics the wave function must acquire a phase (in addition to the shift of the vector potential) in order to render the physics gauge invariant. Usually, the phase of the wave function, remains a feature that cannot be observed and one could neglect the difference between gauge transformations in quantum mechanics and classical physics. An exciting case where this difference plays a crucial role is given by the Aharonov-Bohm effect (discussed in QM-I). Here, gauging away the vector potential does not only leave us with an overall phase of the wave function but, due to the special geometry, with a phase difference that indeed is observable.

Exercise 8.2 Quantum Dot Coupled to an Electromagnetic Field

- a) The position and momentum operator are expressed in terms of the creation and annihilation operators of the three harmonic oscillators as follows:

$$\hat{\mathbf{r}} = \sqrt{\frac{\hbar}{2\omega_d m}} (\hat{a}_x + \hat{a}_x^\dagger, \hat{a}_y + \hat{a}_y^\dagger, \hat{a}_z + \hat{a}_z^\dagger) , \tag{17}$$

$$\hat{\mathbf{p}} = -i\sqrt{\frac{\hbar\omega_d m}{2}} (\hat{a}_x - \hat{a}_x^\dagger, \hat{a}_y - \hat{a}_y^\dagger, \hat{a}_z - \hat{a}_z^\dagger) . \tag{18}$$

- (i) We will first consider the case of a linearly polarized electromagnetic field $\mathbf{e} = \mathbf{e}_x = (1, 0, 0)$. For this case we find (note that $[\hat{p}_i, \hat{r}_j] = 0$ if $i \neq j$)

$$\begin{aligned}
\hat{\mathbf{j}}(-\mathbf{k}) \cdot \mathbf{e} &= \frac{1}{2} \left[\frac{\hat{p}_x}{m} e^{ik\hat{r}_z} + e^{ik\hat{r}_z} \frac{\hat{p}_x}{m} \right] \\
&= e^{ik\hat{r}_z} \frac{\hat{p}_x}{m} \\
&= e^{ikr_0(\hat{a}_z^\dagger + \hat{a}_z)} \frac{p_0}{m} (\hat{a}_x - \hat{a}_x^\dagger) \\
&= e^{ikr_0\hat{a}_z^\dagger} e^{ikr_0\hat{a}_z} e^{-\frac{(kr_0)^2}{2}} \frac{p_0}{m} (\hat{a}_x - \hat{a}_x^\dagger)
\end{aligned} \tag{19}$$

where we have defined $r_0 = \sqrt{\frac{\hbar}{2\omega_d m}}$ and $p_0 = -i\sqrt{\frac{\hbar\omega_d m}{2}}$.

We will now begin to evaluate the matrix elements

$$\langle \mathbf{n} | \hat{\mathbf{j}}(-\mathbf{k}) \cdot \mathbf{e} | \mathbf{0} \rangle = \langle n_x, n_y, n_z | \hat{\mathbf{j}}(-\mathbf{k}) \cdot \mathbf{e} | 0, 0, 0 \rangle \tag{20}$$

From the definition of the creation and annihilation operators of the three harmonic oscillators, we immediately find

$$(\hat{a}_x - \hat{a}_x^\dagger) |0, 0, 0\rangle = -|1, 0, 0\rangle, \quad (21)$$

$$e^{ikr_0 \hat{a}_z} |1, 0, 0\rangle = |1, 0, 0\rangle. \quad (22)$$

Hence, we have to evaluate the matrix elements

$$\langle n_x, n_y, n_z | e^{ikr_0 \hat{a}_z^\dagger} |1, 0, 0\rangle = \langle n_x, n_y, n_z | \sum_{n=0}^{\infty} \frac{(ikr_0)^n}{n!} (\hat{a}_z^\dagger)^n |1, 0, 0\rangle \quad (23)$$

$$= \langle n_x, n_y, n_z | \frac{(ikr_0)^{n_z}}{\sqrt{n_z!}} |1, 0, n_z\rangle \quad (24)$$

With this expression, the final result reads

$$\langle \mathbf{n} | \hat{\mathbf{j}}(-\mathbf{k}) \cdot \mathbf{e} | \mathbf{0} \rangle = \begin{cases} -\frac{(ikr_0)^{n_z}}{\sqrt{n_z!}} e^{-\frac{(kr_0)^2}{2}} \frac{p_0}{m} & \text{if } \langle n_x, n_y, n_z | = \langle 1, 0, n_z | \\ 0 & \text{else} \end{cases}$$

- (ii) For polarization in y direction, $\mathbf{e} = \mathbf{e}_Y$, we get the same result by simply exchanging $n_x \leftrightarrow n_y$.
- (iii) In the case of circular polarization, we use the fact that $\mathbf{e}_\pm = (\mathbf{e}_X \pm i\mathbf{e}_Y)/\sqrt{2}$. With the results of (i) and (ii) we get

$$\langle \mathbf{n} | \hat{\mathbf{j}}(-\mathbf{k}) \cdot \mathbf{e} | \mathbf{0} \rangle = \begin{cases} -\frac{1}{\sqrt{2}} \frac{(ikr_0)^{n_z}}{\sqrt{n_z!}} e^{-\frac{(kr_0)^2}{2}} \frac{p_0}{m} & \text{if } \langle n_x, n_y, n_z | = \langle 1, 0, n_z | \\ -\frac{\pm i}{\sqrt{2}} \frac{(ikr_0)^{n_z}}{\sqrt{n_z!}} e^{-\frac{(kr_0)^2}{2}} \frac{p_0}{m} & \text{if } \langle n_x, n_y, n_z | = \langle 0, 1, n_z | \\ 0 & \text{else} \end{cases}$$

- b) The total absorption rate is defined as the sum over the partial absorption rates for the individual transitions $|\mathbf{0}\rangle$ to $|\mathbf{n}\rangle$,

$$\begin{aligned} \Gamma(\omega) &= \sum_{n_x, n_y, n_z} \Gamma_{0 \rightarrow (n_x, n_y, n_z)} \quad (25) \\ &= \sum_{n_x, n_y, n_z} \frac{2\pi}{\hbar} \delta(E_n - E_0 - \hbar\omega) \frac{e^2}{L^3 c^2} |A|^2 \left| \langle n_x, n_y, n_z | \hat{\mathbf{j}}(-\mathbf{k}) \cdot \mathbf{e} | 0, 0, 0 \rangle \right|^2. \end{aligned}$$

At first we note that due to the sum over all $|\mathbf{n}\rangle$ the total absorption rate $\Gamma(\omega)$ is the same for all three different types of polarization. It is therefore convenient to consider $\mathbf{e} = \mathbf{e}_X$, linear polarization in x -direction. This lets us evaluate the sum over n_x and n_y extremely simple by setting $n_x = 1$ and $n_y = 0$.

$$\Gamma(\omega) = \sum_{n_z} \frac{2\pi}{\hbar} \delta\left(\hbar\omega_d \left(n_z + 1 - \frac{\omega}{\omega_d}\right)\right) \frac{e^2}{L^3 c^2} |A|^2 \left(\frac{(kr_0)^{2n_z}}{n_z!} e^{-(kr_0)^2} \frac{|p_0|^2}{m} \right) \quad (26)$$

$$= \frac{e^2 \pi}{L^3 c^2 m \hbar} |A|^2 \sum_{n_z} \delta\left(n_z + 1 - \frac{\omega}{\omega_d}\right) \left(\frac{\omega^2}{\omega_d \omega_m}\right)^{\omega_d^{-1}} \Gamma\left[\frac{\omega}{\omega_d}\right]^{-1} e^{-\frac{\omega^2}{\omega_d \omega_m}} \quad (27)$$

where we have used $k = \frac{\omega}{c}$, $\omega_m = \frac{2c^2 m}{\hbar}$ and $n! = \Gamma[n + 1]$.