Quantum Optics Assignment 1

Christian Lange

September 1, 2023

1 Typical photon energies

Jupyter notebook used for calculations included at the end of this document.

(a) Photon energies

For a photon with wavelength λ and frequency $f = c/\lambda$, the energy E and momentum p are as follows.

$$E = \hbar\omega = hf \tag{1}$$

$$p = \frac{h}{\lambda} \tag{2}$$

For a photon with wavelength 852 nm, these give

- Photon energy in Joule: 2.33×10^{-19} J
- Photon energy in eV: 1.46 eV
- Frequency of light: 352 THz

The temperature difference of the atom after emission of the photon is obtained through $E = k_B T$. $T = 1.69 \times 10^4$ K

(b) Total energy

We can get the velocity from $E = hf = \frac{1}{2}mv^2$.

- Final velocity: 4.2 km/s

(c) Recoil velocity

The recoil velocity is obtained with $p = \frac{h}{f} = mv$.

- Recoil velocity: 29.5 mm/s
- Recoil energy: 1.66×10^{-29} J

2 Mechanical velocity and electromagnetic fields in quantum mechanics

The vector potential

It is useful to know the following definitions about the vector potential, which I found on Wikipedia. Here, $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic fields.

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{3}$$

$$\mathbf{E} = -\nabla U(\mathbf{r}, t) - \frac{\partial \mathbf{A}}{\partial t} \tag{4}$$

(a) Commutators

Functions of $\mathbf{r}$ commute with $\mathbf{r}$, and likewise with $\mathbf{p}$.

$$[\mathbf{r}, \mathbf{A}(\mathbf{r}, t)] = 0 \tag{5}$$
$$[\mathbf{r}, U(\mathbf{r}, t)] = 0 \tag{6}$$

(b) Calculating the velocity

$$H = \frac{1}{2m} \sum_{i=x,y,z} \left[p_i^2 + q^2 A_i^2 (\mathbf{r}, t) - q p_i A_i (\mathbf{r}, t) - q A_i (\mathbf{r}, t) p_i\right] + qU (\mathbf{r}, t) \tag{7}$$

$$[x, H] = \frac{1}{2m} \sum_{i=x,y,z} \left\{ \left[x, p_i^2\right] - q \left[x, p_i A_i (\mathbf{r}, t)\right] - q \left[x, A_i (\mathbf{r}, t) p_i\right] \right\} \tag{8}$$
$$= \frac{1}{2m} \left\{p_x [x, p_x] + [x, p_x] p_x - q [x, p_x] A_x (\mathbf{r}, t) - q A_i (\mathbf{r}, t) [x, p_x]\right\} \tag{9}$$
$$= \frac{1}{2m} \left\{2i\hbar p_x - 2qi\hbar A_x (\mathbf{r}, t)\right\} \tag{10}$$
$$= \frac{i\hbar}{m} \left\{p_x - q A_x (\mathbf{r}, t)\right\} \tag{11}$$

$$\frac{d}{dt} \langle x \rangle = \frac{1}{i\hbar} \langle [x, H] \rangle + \left\langle \frac{\partial}{\partial t} x \right\rangle \tag{12}$$
$$= \frac{1}{m} \langle p_x - q A_x (\mathbf{r}, t) \rangle \tag{13}$$

Similarly,

$$\frac{d}{dt} \langle y \rangle = \frac{1}{m} \langle p_y - q A_y (\mathbf{r}, t) \rangle \tag{14}$$
$$\frac{d}{dt} \langle z \rangle = \frac{1}{m} \langle p_z - q A_z (\mathbf{r}, t) \rangle \tag{15}$$

so that

$$\langle \mathbf{v} \rangle = \frac{1}{m} \langle \mathbf{p} - q \mathbf{A} (\mathbf{r}, t) \rangle \tag{16}$$

(c) The Force

Based on the result from (b), we can define the velocity operator as follows.

$$\mathbf{v} = \frac{1}{m} \left[\mathbf{p} - q \mathbf{A} (\mathbf{r}, t)\right] \tag{17}$$

We can find the acceleration by a second application of Ehrenfest's theorem.

$$\frac{d}{dt} \langle \mathbf{v} \rangle = \frac{1}{i\hbar} \langle [\mathbf{v}, H] \rangle + \left\langle \frac{\partial}{\partial t} \mathbf{v} \right\rangle \tag{18}$$

There are two things we must be careful of.

1. In general, the velocity operator has explicit time dependence through $\mathbf{A} (\mathbf{r}, t)$, so that we cannot write $\left\langle \frac{\partial}{\partial t} \mathbf{v} \right\rangle = \mathbf{0}$.
2. While it is true that any operator $\mathscr{O}$ commutes with itself $[\mathscr{O}, \mathscr{O}] = 0$, it is not necessarily the case that a vector of operators $\mathbf{O}$ commutes with its square $[\mathbf{O}, \mathbf{O} \cdot \mathbf{O}] \neq \mathbf{0}$. When you expand into $\left[O_x \hat{\mathbf{x}} + O_y \hat{\mathbf{y}} + \cdots, O_x^2 + O_y^2 + \cdots\right]$, you get terms like $\hat{\mathbf{x}} \left[O_x, O_y^2\right]$ which may not commute. Therefore, we cannot assume that $\left\langle \left[\mathbf{v}, \frac{1}{2} m \mathbf{v} \cdot \mathbf{v}\right] \right\rangle = 0$.

We will start by rewriting the Hamiltonian in terms of the velocity operator.

$$H = \frac{1}{2} m \mathbf{v} \cdot \mathbf{v} + qU (\mathbf{r}, t) \tag{19}$$

Computing $[v_i, v_j]$

It is useful to compute the commutators of the different components of $\mathbf{v}$.

$$[v_i, v_j] = \frac{1}{m^2}\left[p_i - qA_i\left(\mathbf{r},t\right), p_j - qA_j\left(\mathbf{r},t\right)\right] \tag{20}$$

$$= \frac{1}{m^2}\left\{[p_i, p_j] + q^2\left[A_i\left(\mathbf{r},t\right), A_j\left(\mathbf{r},t\right)\right] - q\left[p_i, A_j\left(\mathbf{r},t\right)\right] - q\left[A_i\left(\mathbf{r},t\right), p_j\right]\right\} \tag{21}$$

$$= -\frac{q}{m^2}\left\{\left[p_i, A_j\left(\mathbf{r},t\right)\right] + \left[A_i\left(\mathbf{r},t\right), p_j\right]\right\} \tag{22}$$

We can use the identity $[p_i, f(x)] = -i\hbar\partial_x f(x)$ [see Appendix] to obtain $[p_i, A_j\left(\mathbf{r},t\right)] = -i\hbar\partial_i A_j\left(\mathbf{r},t\right)$ and $\left[A_i\left(\mathbf{r},t\right), p_j\right] = -\left[p_j, A_i\left(\mathbf{r},t\right)\right] = i\hbar\partial_j A_i\left(\mathbf{r},t\right)$ where i, j are x, y, z.

$$[v_i, v_j] = -\frac{q}{m^2}\left\{-i\hbar\partial_i A_j\left(\mathbf{r},t\right) + i\hbar\partial_j A_i\left(\mathbf{r},t\right)\right\} \tag{23}$$

$$= \frac{i\hbar q}{m^2}\left\{\partial_i A_j\left(\mathbf{r},t\right) - \partial_j A_i\left(\mathbf{r},t\right)\right\} \tag{24}$$

We can simplify this by recognizing it is in the form of a cross product.

$$\left(\nabla \times \mathbf{A}\right)_x = \partial_y A_z - \partial_z A_y \tag{25}$$

$$\left(\nabla \times \mathbf{A}\right)_y = \partial_z A_x - \partial_x A_z \tag{26}$$

$$\left(\nabla \times \mathbf{A}\right)_z = \partial_x A_y - \partial_y A_x \tag{27}$$

Note: This can be written very compactly with the Levi-Civita tensor ϵ_{ijk}. The rule is that $\epsilon_{ijk} = +1$ if ijk are "in order," that is, $ijk = xyz$, or yzx, or zxy. If ijk are "out of order," that is, $ijk = xzy$ or yxz or zyx, then $\epsilon_{ijk} = -1$. If any indices are repeated, such as $ijk = xxy$, then $\epsilon_{ijk} = 0$. In this notation, any cross product can be written as

$$\left(\mathbf{A} \times \mathbf{B}\right)_i = \sum_{jk} \epsilon_{ijk} A_j B_k. \tag{28}$$

Computing $[\mathbf{v}, \mathbf{v}\cdot\mathbf{v}]$

Let's begin with one component $[v_x, \mathbf{v}\cdot\mathbf{v}]$.

$$[v_x, \mathbf{v}\cdot\mathbf{v}] = \left[v_x, v_x^2 + v_y^2 + v_z^2\right] \tag{29}$$

$$= \left\{v_y\left[v_x, v_y\right] + \left[v_x, v_y\right]v_y + v_z\left[v_x, v_z\right] + \left[v_x, v_z\right]v_z\right\} \tag{30}$$

$$= \frac{i\hbar q}{m^2}\left\{v_y\left[\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right]_z + \left[\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right]_z v_y - v_z\left[\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right]_y - \left[\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right]_y v_z\right\} \tag{31}$$

$$= \frac{i\hbar q}{m^2}\left\{\left(\mathbf{v} \times \left(\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right)\right)_x - \left(\left(\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right) \times \mathbf{v}\right)_x\right\} \tag{32}$$

$$= \frac{2i\hbar q}{m^2}\left\{\mathbf{v} \times \left[\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right]\right\}_x \tag{33}$$

Because there is nothing particularly special about x as opposed to y and z, this rule should hold for all v_x, v_y, v_z.

$$[v_i, \mathbf{v}\cdot\mathbf{v}] = \frac{2i\hbar q}{m^2}\left\{\mathbf{v} \times \left[\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right]\right\}_I \tag{34}$$

The total commutator $[\mathbf{v}, \mathbf{v}\cdot\mathbf{v}]$ is simply

$$[\mathbf{v}, \mathbf{v}\cdot\mathbf{v}] = \frac{2i\hbar q}{m^2}\left\{\mathbf{v} \times \left[\nabla \times \mathbf{A}\left(\mathbf{r},t\right)\right]\right\} \tag{35}$$

Computing $[\mathbf{v}, U(\mathbf{r}, t]$

Recall that functions of $\mathbf{r}$ commute with other functions of $\mathbf{r}$ because all of r_x, r_y, r_z commute with each other. Recall also that $[p_x, f(x)] = -i\hbar\partial_x f(x)$ and that the gradient is defined as $\nabla f(\mathbf{r}) = \sum_i \hat{\mathbf{e}}_i \partial_i f(\mathbf{r})$. Here, $\hat{\mathbf{e}}_i$ is the unit vector in the ith direction.

$$
\begin{aligned}
[\mathbf{v}, U(\mathbf{r}, t)] &= \frac{1}{m}\left[\mathbf{p} - q\mathbf{A}(\mathbf{r}, t), U(\mathbf{r}, t)\right] && (36)\\
&= \frac{1}{m}\left[\mathbf{p}, U(\mathbf{r}, t)\right] - \frac{q}{m}\left[\mathbf{A}(\mathbf{r}, t), U(\mathbf{r}, t)\right] && (37)\\
&= \frac{1}{m}\sum_i \hat{\mathbf{e}}_i \left[p_i, U(\mathbf{r}, t)\right] && (38)\\
&= -\frac{i\hbar}{m}\sum_i \hat{\mathbf{e}}_i \partial_i U(\mathbf{r}, t) && (39)\\
&= -\frac{i\hbar}{m}\nabla U(\mathbf{r}, t) && (40)
\end{aligned}
$$

Computing $[\mathbf{v}, H]$

We can finally assemble everything.

$$
\begin{aligned}
[\mathbf{v}, H] &= \left[\mathbf{v}, \frac{1}{2}m\mathbf{v}\cdot\mathbf{v} + qU(\mathbf{r}, t)\right] && (41)\\
&= q\left[\mathbf{v}, U(\mathbf{r}, t\right] + \sum_i \hat{\mathbf{e}}_i \left[v_i, \frac{1}{2}m\mathbf{v}\cdot\mathbf{v}\right] && (42)\\
&= -\frac{i\hbar q}{m}\nabla U(\mathbf{r}, t) + \frac{i\hbar q}{m}\left\{\mathbf{v}\times\left[\nabla\times\mathbf{A}(\mathbf{r}, t)\right]\right\} && (43)
\end{aligned}
$$

The explicit time dependence of $\mathbf{v}$ is all in $\mathbf{A}(\mathbf{r}, t)$.

$$
\begin{aligned}
\frac{\partial\mathbf{v}}{\partial t} &= \frac{\partial}{\partial t}\left[\frac{\mathbf{p} - q\mathbf{A}(\mathbf{r}, t)}{m}\right] && (44)\\
&= -\frac{q}{m}\frac{\partial\mathbf{A}(\mathbf{r}, t)}{\partial t} && (45)
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}\langle\mathbf{v}\rangle &= \frac{1}{i\hbar}\langle[\mathbf{v}, H]\rangle + \left\langle\frac{\partial\mathbf{v}}{\partial t}\right\rangle && (46)\\
&= -\frac{q}{m}\langle\nabla U(\mathbf{r}, t)\rangle + \frac{q}{m}\langle\mathbf{v}\times[\nabla\times\mathbf{A}(\mathbf{r}, t)]\rangle - \frac{q}{m}\left\langle\frac{\partial\mathbf{A}(\mathbf{r}, t)}{\partial t}\right\rangle && (47)
\end{aligned}
$$

And that's the answer! In order to make sense of this, we need to employ the relationship between the *classical* electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ with the vector potential.

$$
\begin{aligned}
\mathbf{B} &= \nabla\times\mathbf{A}(\mathbf{r}, t) && (48)\\
\mathbf{E} &= -\nabla U(\mathbf{r}, t) - \frac{\partial\mathbf{A}(\mathbf{r}, t)}{\partial t} && (49)
\end{aligned}
$$

If we substitute these relations, we obtain

$$
\langle\mathbf{F}\rangle = m\frac{d}{dt}\langle\mathbf{v}\rangle = q\left[\langle\mathbf{E}\rangle + \langle\mathbf{v}\times\mathbf{B}\rangle\right] \tag{50}
$$

which is exactly the form of the classical Lorentz force $\mathbf{F} = q(\mathbf{E} + \mathbf{v}\times\mathbf{B})$.

3 Density matrices

(a) Pure ensemble

$$|\psi\rangle = \begin{pmatrix} \sqrt{3/4} \\ -i/2 \end{pmatrix} \tag{51}$$

$$\langle\psi| = \begin{pmatrix} \sqrt{3/4} & i/2 \end{pmatrix} \tag{52}$$

$$\rho_{\text{pure}} = |\psi\rangle\langle\psi| = \begin{pmatrix} 3/4 & i\sqrt{3}/4 \\ -i\sqrt{3}/4 & 1/4 \end{pmatrix} \tag{53}$$

(b) Impure ensemble

$$\rho_1 = \frac{3}{4}|g\rangle\langle g| = \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{54}$$

$$\rho_2 = \frac{1}{4}|e\rangle\langle e| = \frac{1}{4}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{55}$$

$$\rho_{\text{impure}} = \rho_1 + \rho_2 = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix} \tag{56}$$

(c) Experimental determination

In the pure ensemble, all atoms are in a definite state $|\psi\rangle$. In the impure ensemble, a proportion of atoms are in each state. Therefore, if we could devise an experiment to determine the likelihood of an atom being in $|\psi\rangle$, we would get different answers for the two ensembles. For (a), we would get unity. For (b), we would get an answer based on the projection of the component states onto $|\psi\rangle$. Let $A = |\psi\rangle\langle\psi|$ be the observable that we can measure.

$$\langle A\rangle_{(\text{pure})} = \text{Tr}\left[\rho_{\text{pure}}A\right] = \text{Tr}\left[\rho_{\text{pure}}^2\right] = 1 \tag{57}$$

$$\langle A\rangle_{(\text{impure})} = \text{Tr}\left[\rho_{\text{impure}}A\right] = \text{Tr}\left[\begin{pmatrix} (3/4)^2 & i3^{3/2}/16 \\ -i\sqrt{3}/16 & 1/16 \end{pmatrix}\right] = 10/16 \tag{58}$$

(d) Entropy

If we use a basis in which ρ is diagonal, the entropy is simply

$$S = -k_B \text{Tr}\left[\rho\ln\rho\right] = -k_B\sum_k \rho_k^{(\text{diag})}\ln\rho_k^{(\text{diag})}. \tag{59}$$

For the pure state, the eigenvalues of 1 and 0.

$$S_{\text{pure}} = -k_B\left[1\cdot\ln 1 + \lim_{x\to 0^+} x\ln x\right]. \tag{60}$$

We can evaluate the limit using L'hopital's rule. Note that we have to write it as a fraction.

$$\lim_{x\to 0^+} x\ln x = \lim_{x\to 0^+}\frac{\ln x}{1/x} = \lim_{x\to 0^+} -\frac{1/x}{1/x^2} = \lim_{x\to 0^+} -x = 0 \tag{61}$$

So the entropy of a pure state is zero!

$$S_{\text{pure}} = 0 \tag{62}$$

For the mixed state,

$$S_{\text{impure}} = -k_B\left[3/4\cdot\ln 3/4 + 1/4\cdot\ln 1/4\right] \approx 0.562 k_B \tag{63}$$

(e) Thermal state

In this case, we only consider two state $|g\rangle$ and $|e\rangle$, with energy 0 and 1.

$$\rho = \frac{1}{Z}\left(|g\rangle\langle g| + e^{-1/k_B T}|e\rangle\langle e|\right) \tag{64}$$

At $T = 0$, $e^{-1/k_B T} \to 0$ and the population is purely in the ground state. As $T \to \infty$, $e^{-1/k_B T} \to 1$ and the density matrix is a statistical mixture of ground and excited.

$$\rho_{T\to\infty} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \tag{65}$$

Appendices

Commutator of momentum and a position-dependent function

$$\begin{aligned} \langle x|[\hat{p}, f(\hat{x})]|\psi\rangle &= \langle x|(\hat{p}f(\hat{x}) - f(\hat{x})\hat{p})|\psi\rangle && (66)\\ &= -i\hbar\partial_x\left(f(x)\psi(x)\right) - i\hbar f(x)\partial_x\psi(x) && (67)\\ &= -i\hbar\left(\partial_x f(x)\right)\psi(x) && (68) \end{aligned}$$

$$\to [p, f(x)] = -i\hbar\partial_x f(x) \tag{69}$$