1 Basics

1.1 Bra-ket notation, delta function, position and momentum representation

Useful identities:

$$\hat{q}|x\rangle = x|x\rangle,\ \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar},$$
$$\hat{1} = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|,$$
$$f(x)\delta(x-x') = f(x')\delta(x-x').$$

a) A two-level system has a complete orthonormal basis consisting of the states $|1\rangle$ and $|2\rangle$. Consider the linear combinations $|\psi_+\rangle = 2^{-1/2}\big(|1\rangle + i|2\rangle\big)$ and $|\psi_-\rangle = 2^{-1/2}\big(|1\rangle - i|2\rangle\big)$.

• Show that these two new states still form an orthonormal basis.
• Construct the two operators $\hat{A} = |\psi_+\rangle\langle\psi_-|$ and $\hat{B} = |\psi_-\rangle\langle\psi_+|$ and show that $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ are distinct projection operators.
(Recall that $\hat{P}$ is a projection operator if $\hat{P} = \hat{P}^\dagger = \hat{P}^2$.)
• What are $\hat{A}^\dagger$ and $\hat{B}^\dagger$?
• Calculate $\mathrm{Tr}\,\hat{A}$ and $\mathrm{Tr}\,\hat{B}$; verify that $\mathrm{Tr}\,\hat{A}\hat{B} = \mathrm{Tr}\,\hat{B}\hat{A}$.
• Calculate the eigenvalues and eigenfunctions of the Hamiltonian operator

$$\hat{H} = |1\rangle\langle 1| - |2\rangle\langle 2| + i|1\rangle\langle 2| - i|2\rangle\langle 1|.$$

How can you tell without calculation that the two eigenvalues are each others opposite?
• Show that $(\hat{A}+\hat{B})^2$ is the identity operator $\hat{1}$. Use this to obtain the eigenvalues of $\hat{A}+\hat{B}$ without calculation.

b) Derive or evaluate the following integrals over delta functions:

$$\int_{-\infty}^{\infty} dy\, f(y) \frac{\partial}{\partial y}\delta(y-x) = -f'(x), \tag{1}$$
$$\int_{-\infty}^{\infty} dx\, \delta(ax) = \cdots, \tag{2}$$
$$\int_{-\infty}^{\infty} dx\, f(x)\delta(x^2-a^2) = \cdots \tag{3}$$

c) Explain or derive the following equations:

$$\langle x|x'\rangle = \delta(x-x'), \tag{4}$$
$$\langle x|\hat{q}|x'\rangle = x\delta(x-x'), \tag{5}$$
$$\langle x|\hat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x') = \langle x'|\hat{p}|x\rangle^*, \tag{6}$$
$$\langle x|\hat{q}\hat{p} - \hat{p}\hat{q}|x'\rangle = i\hbar\delta(x-x'). \tag{7}$$

1.2 Unbounded operators

KP 7.3 invokes Weyl's criterion to show that the spectrum of the position operator $\hat{q}$ includes the entire real axis $-\infty < x < \infty$. As an alternative demonstration of this fact, show that $e^{-i\hat{p}a/\hbar}|x\rangle$ is an eigenfunction of $\hat{q}$ with eigenvalue $x + a$, for any real a.

Hint: Use the commutation relation $[\hat{q}, F(\hat{p})] = i\hbar F'(\hat{p})$, which you can verify by expanding $F(\hat{p})$ in a Taylor series in $\hat{p}$.

1.3 Density matrix

The expectation value of an operator $\hat{M}$ in the state $|\Psi\rangle$ is $\langle\hat{M}\rangle = \langle\Psi|\hat{M}|\Psi\rangle$. We can write this as the trace of the product of the operator $\hat{M}$ and an operator $\hat{\rho}$,

$$\langle\hat{M}\rangle = \mathrm{Tr}\,\hat{M}\hat{\rho},\;\; \hat{\rho} = |\Psi\rangle\langle\Psi|.$$

The operator $\hat{\rho}$ is the density matrix (or state operator) corresponding to the state $|\Psi\rangle$.

a) Derive that $\mathrm{Tr}\,\hat{\rho} = 1$, $\hat{\rho} = \hat{\rho}^\dagger$, $\hat{\rho}^2 = \hat{\rho}$. What are the eigenvalues of $\hat{\rho}$?

More generally, a system can consist of a mixture of states. If the state $|\Psi_n\rangle$ occurs with probability p_n, then the density matrix is

$$\hat{\rho} = \sum_n p_n |\Psi_n\rangle\langle\Psi_n|.$$

(The states $|\Psi_n\rangle$ are normalized to unity, but they need not be orthogonal.)
b) What is now the expectation value of $\hat{M}$?

c) Derive that it still holds that $\mathrm{Tr}\,\hat{\rho} = 1$, $\hat{\rho} = \hat{\rho}^\dagger$. However, unlike for a pure (not mixed) state, it no longer holds that $\hat{\rho}^2 = \hat{\rho}$ — not even if the Ψ_n's are orthogonal.

d) Derive that $\langle\Psi|\hat{\rho}|\Psi\rangle \geqslant 0$ for each $|\Psi\rangle$. What restriction does this inequality impose on the eigenvalues of $\hat{\rho}$?

e) The evolution in time of the wave function $\Psi(t)$ is given by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = \hat{H}\Psi(t).$$

Derive the corresponding evolution in time of the density matrix,

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)].$$

f) The solution to the evolution equation is

$$\hat{\rho}(t) = e^{-i\hat{H}t/\hbar}\hat{\rho}(0)e^{i\hat{H}t/\hbar}.$$

Show that this implies that a pure state at $t = 0$ remains pure for $t > 0$.

1.4 Photon polarizations

Pauli matrices:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

a) The polarization of a photon is described by a 2×2 density matrix $\hat{\rho}$. It can be written in terms of Pauli matrices,

$$\hat{\rho} = \frac{1}{2}\left(\sigma_0 + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3\right),$$

with a vector of real coefficients $\vec{a} = (a_1, a_2, a_3)$.
Why is $|\vec{a}| \leqslant 1$? What operation on $\vec{a}$ corresponds to complex conjugation of $\hat{\rho}$? And what operation on $\vec{a}$ corresponds to a unitary transformation of $\hat{\rho}$?

The vectors $\vec{a}$ which satisfy $|\vec{a}| \leqslant 1$ form a sphere, the Bloch sphere.

b) Where on the Bloch sphere lies the density matrix $\hat{\rho} = |\Psi\rangle\langle\Psi|$ of a pure state? Derive this formula for the overlap of two pure states:

$$|\langle\Psi_1|\Psi_2\rangle|^2 = \tfrac{1}{2}(1 + \vec{a}_1 \cdot \vec{a}_2).$$

c) Derive that the expectation value of the polarization operator $n_x\sigma_1 + n_y\sigma_2 + n_z\sigma_3$ along the unit vector $\vec{n} = (n_x, n_y, n_z)$ is given by the inner product $\vec{a} \cdot \vec{n}$. Explain how you can use this property to measure the density matrix. Why is this not possible if you have only a single system at your disposal?

1.5 Heisenberg equations of motion

$$\frac{d}{dt}\hat{O} = \frac{\partial}{\partial t}\hat{O} - \frac{i}{\hbar}[\hat{O}, \hat{H}].$$

a) Solve the Heisenberg equation of motion for the position operator $\hat{q}(t)$ of a particle of mass m moving along a line in the absence of any forces acting on the particle. Show that $\hat{q}(t)$ and $\hat{q}(0)$ do not commute for $t \neq 0$.

b) Show that the expectation value $\langle \hat{q}(t) \rangle$ of the position of the free particle satisfies the classical equation of motion

$$\langle \hat{q}(t) \rangle = p_0 t / m + x_0,$$

where $x_0 = \langle \hat{q}(0) \rangle$ and $p_0 = \langle \hat{p}(0) \rangle$. This is known as Ehrenfest's theorem.

1.6 Uncertainty relation

Consider two Hermitian operators $\hat{A}$ and $\hat{B}$ with zero average. The variances in the state with density matrix $\hat{\rho}$ are given by

$$(\Delta A)^2 = \mathrm{Tr}\, \hat{\rho} \hat{A}^2, \ \ (\Delta B)^2 = \mathrm{Tr}\, \hat{\rho} \hat{B}^2.$$

The uncertainty relation provides a lower bound on the product of these two variances, in terms of the expectation value $\langle \hat{C} \rangle = \mathrm{Tr}\, \hat{\rho} \hat{C}$ of the commutator

$$[\hat{A}, \hat{B}] = i \hat{C}.$$

a) Prove that $\mathrm{Tr}\,(\hat{\rho} \hat{T}^\dagger \hat{T}) \geqslant 0$, for any operator $\hat{T}$.

b) Take any real number ω and substitute $\hat{T} = \hat{A} + i\omega \hat{B}$ to arrive at the inequality

$$(\Delta A)^2 - \omega \langle \hat{C} \rangle + \omega^2 (\Delta B)^2 \geqslant 0.$$

c) Optimize the inequality by varying ω, to obtain the uncertainty relation

$$(\Delta A)^2 (\Delta B)^2 \geqslant \frac{1}{4} \langle \hat{C} \rangle^2.$$

d) The original form of the uncertainty relation, $\Delta x \Delta p \geqslant \hbar/2$, due to Heisenberg, corresponds to $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$. Show that the lower bound $\Delta x \Delta p = \hbar/2$ is reached for a Gaussian wave packet,

$$\psi(x) = C \exp(-\alpha x^2).$$