1 Fundamental concepts

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 Heisenberg equation of motion and Ehrenfest theorem

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

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 the *Ehrenfest theorem.*

1.3 Hellmann-Feynman theorem

If the Hamiltonian $\hat{H}(\lambda)$ depends on some parameter $\lambda \in \mathbb{R}$, then the eigenvalues $E_n(\lambda)$ and eigenfunctions $\psi_n(\lambda)$ will also depend on λ.

a) Prove the *Hellmann-Feynman theorem*

$$\frac{dE_n(\lambda)}{d\lambda} = \left\langle \psi_n(\lambda) \left| \frac{d\hat{H}(\lambda)}{d\lambda} \right| \psi_n(\lambda) \right\rangle.$$

This theorem can be applied to the dispersion relation in a wave guide, which is the dependence $E_n(p)$ of the n-th mode in the wave guide on the momentum p along the wave guide.

b) Explain why the expectation value v_n of the velocity in the n-th mode is given by the derivative $dE_n(p)/dp$.

1.4 Uncertainty relation

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

$$(\Delta A)^2 = \langle \psi | \hat{A}^2 | \psi \rangle, \ (\Delta B)^2 = \langle \psi | \hat{B}^2 | \psi \rangle.$$

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

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

a) Prove that $\langle\psi|\hat{T}^\dagger\hat{T}|\psi\rangle \geqslant 0$, 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,

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