Quantum Mechanics

Solutions to the Problems in Homework Assignment 09

Fall, 2019

1. **[C-T Exercise 3-4]** Consider a free particle in one dimension.
   (a) Show, applying Ehrenfest's theorem, that $\langle \hat{x} \rangle$ is a linear function of time, the mean value $\langle \hat{p}_x \rangle$ remaining constant.
   (b) Write the equations of motion for the mean values $\langle \hat{x}^2 \rangle$ and $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x} \rangle$. Integrate these equations.
   (c) Show that, with a suitable choice of the time origin, the root-mean square deviation Δx is given by

$$(\Delta x)^2 = \frac{1}{m^2}(\Delta p_x)_0^2 t^2 + (\Delta x)_0^2,$$

where $(\Delta x)_0$ and $(\Delta p_x)_0$ are the root-mean-square deviations at the initial time.
How does the width of the wave packet vary as a function of time? Give a physical interpretation.

(a) Ehrenfest's theorem states that

$$\frac{d\langle \hat{x} \rangle}{dt} = \frac{1}{m}\langle \hat{p}_x \rangle,$$
$$\frac{d\langle \hat{p}_x \rangle}{dt} = -\langle \hat{V}'(\hat{x}) \rangle .$$

For a free particle, $\hat{V}(\hat{x}) = 0$. The second equation in Ehrenfest's theorem becomes

$$\frac{d\langle \hat{p}_x \rangle}{dt} = 0.$$

Integrating, we have

$$\langle \hat{p}_x \rangle(t) = \langle \hat{p}_x \rangle_0,$$

where $\langle \hat{p}_x \rangle_0$ is the value of $\langle \hat{p}_x \rangle$ at the initial time. Inserting $\langle \hat{p}_x \rangle(t) = \langle \hat{p}_x \rangle_0$ into the first equation in Ehrenfest's theorem, we have

$$\frac{d\langle \hat{x} \rangle}{dt} = \frac{1}{m}\langle \hat{p}_x \rangle_0 .$$

Integrating, we have

$$\langle \hat{x} \rangle(t) = \frac{\langle \hat{p}_x \rangle_0}{m} t + \langle \hat{x} \rangle_0,$$

where $\langle \hat{x} \rangle_0$ is the value of $\langle \hat{x} \rangle$ at the initial time. From the above results, we see that $\langle \hat{x} \rangle$ is a linear function of time, the mean value $\langle \hat{p}_x \rangle$ remaining constant.

(b) The mean value $\langle \hat{x}^2 \rangle$ is given by

$$\langle \hat{x}^2 \rangle = \langle \psi(t)|\hat{x}^2|\psi(t) \rangle,$$

where $|\psi(t)\rangle$ is the state vector of the particle. Note that $\hat{x}^2$ does not depend on time explicitly. Differentiating the above equation with respect to t, we obtain

$$\frac{d\langle \hat{x}^2 \rangle}{dt} = \left[\frac{d}{dt}\langle \psi(t)|\right]\hat{x}^2|\psi(t)\rangle + \langle \psi(t)|\hat{x}^2\left[\frac{d}{dt}|\psi(t)\rangle\right].$$

Making use of

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle,\ -i\hbar\frac{d}{dt}\langle \psi(t)| = \langle \psi(t)|\hat{H},$$

we have

$$\begin{aligned}
\frac{d\left\langle \hat{x}^2 \right\rangle}{dt} &= -\frac{1}{i\hbar}\left\langle \psi(t)|\hat{H}\hat{x}^2|\psi(t)\right\rangle + \frac{1}{i\hbar}\left\langle \psi(t)|\hat{x}^2\hat{H}|\psi(t)\right\rangle \\
&= \frac{1}{i\hbar}\left\langle \psi(t)|\left[\,\hat{x}^2, \hat{H}\,\right]|\psi(t)\right\rangle = \frac{1}{i\hbar}\left\langle \left[\,\hat{x}^2, \hat{H}\,\right]\right\rangle .
\end{aligned}$$

For a free particle

$$\hat{H} = \frac{\hat{p}_x^2}{2m}.$$

The commutator $\left[\,\hat{x}^2, \hat{H}\,\right]$ is given by

$$\begin{aligned}
\left[\,\hat{x}^2, \hat{H}\,\right] &= \frac{1}{2m}\left[\,\hat{x}^2, \hat{p}_x^2\,\right] = \frac{1}{2m}\hat{x}\left[\,\hat{x}, \hat{p}_x^2\,\right] + \frac{1}{2m}\left[\,\hat{x}, \hat{p}_x^2\,\right]\hat{x} \\
&= \frac{1}{2m}\hat{x}\hat{p}_x\left[\,\hat{x}, \hat{p}_x\,\right] + \frac{1}{2m}\hat{x}\left[\,\hat{x}, \hat{p}_x\,\right]\hat{p}_x + \frac{1}{2m}\hat{p}_x\left[\,\hat{x}, \hat{p}_x\,\right]\hat{x} + \frac{1}{2m}\left[\,\hat{x}, \hat{p}_x\,\right]\hat{p}_x\hat{x} \\
&= \frac{i\hbar}{m}\big(\hat{x}\hat{p}_x + \hat{p}_x\hat{x}\big).
\end{aligned}$$

We thus have

$$\frac{d\left\langle \hat{x}^2 \right\rangle}{dt} = \frac{1}{m}\left\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\right\rangle .$$

For $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle$, we have

$$\frac{d}{dt}\left\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\right\rangle = \frac{1}{i\hbar}\left\langle \left[\,\hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{H}\,\right]\right\rangle .$$

The commutator $\left[\,\hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{H}\,\right]$ is given by

$$\begin{aligned}
\left[\,\hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{H}\,\right] &= \frac{1}{2m}\left[\,\hat{x}\hat{p}_x + \hat{p}_x\hat{x}, \hat{p}_x^2\,\right] \\
&= \frac{1}{2m}\left[\,\hat{x}, \hat{p}_x^2\,\right]\hat{p}_x + \frac{1}{2m}\hat{p}_x\left[\,\hat{x}, \hat{p}_x^2\,\right] \\
&= \frac{2i\hbar}{m}\hat{p}_x^2.
\end{aligned}$$

We thus have

$$\frac{d}{dt}\left\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\right\rangle = \frac{2}{m}\left\langle \hat{p}_x^2\right\rangle .$$

For $\langle \hat{p}_x^2\rangle$, we have

$$\frac{d\left\langle \hat{p}_x^2\right\rangle}{dt} = \frac{1}{i\hbar}\left\langle \left[\,\hat{p}_x^2, \hat{H}\,\right]\right\rangle .$$

For a free particle, $\hat{H} = \hat{p}_x^2/2m$. We then have $\left[\,\hat{p}_x^2, \hat{H}\,\right] = 0$ and

$$\frac{d\left\langle \hat{p}_x^2\right\rangle}{dt} = 0.$$

Integrating the above equation yields

$$\langle \hat{p}_x^2\rangle = \langle \hat{p}_x^2\rangle_0,$$

where $\langle \hat{p}_x^2\rangle_0$ is the value of $\langle \hat{p}_x^2\rangle$ at the initial time.
Inserting $\langle \hat{p}_x^2\rangle = \langle \hat{p}_x^2\rangle_0$ into the equation of motion for $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle$, we have

$$\frac{d}{dt}\left\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\right\rangle = \frac{2}{m}\left\langle \hat{p}_x^2\right\rangle_0 .$$

Integrating the above equation yields

$$\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle(t) = \frac{2}{m}\langle \hat{p}_x^2\rangle_0\, t + \langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0,$$

where $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0$ is the value of $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle$ at the initial time. Inserting the above expression of $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle$ into the equation of motion for $\langle \hat{x}^2\rangle$, we have

$$\frac{d\langle \hat{x}^2\rangle}{dt} = \frac{2}{m^2}\langle \hat{p}_x^2\rangle_0\, t + \frac{1}{m}\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0\,.$$

Integrating the above equation yields

$$\langle \hat{x}^2\rangle = \frac{1}{m^2}\langle \hat{p}_x^2\rangle_0\, t^2 + \frac{1}{m}\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0\, t + \langle \hat{x}^2\rangle_0,$$

where $\langle \hat{x}^2\rangle_0$ is the value of $\langle \hat{x}^2\rangle$ at the initial time.

(c) From the above results for $\langle \hat{x}\rangle$ and $\langle \hat{x}^2\rangle$, we have

$$\begin{aligned}
(\Delta x)^2 &= \langle \hat{x}^2\rangle - \big(\langle \hat{x}\rangle\big)^2 \\
&= \frac{1}{m^2}\langle \hat{p}_x^2\rangle_0\, t^2 + \frac{1}{m}\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0\, t + \langle \hat{x}^2\rangle_0 - \left(\frac{\langle \hat{p}_x\rangle_0}{m} t + \langle \hat{x}\rangle_0\right)^2 \\
&= \frac{1}{m^2}\Big[\langle \hat{p}_x^2\rangle_0 - \big(\langle \hat{p}_x\rangle_0\big)^2\Big] t^2 + \frac{1}{m}\big[\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0 - 2\langle \hat{p}_x\rangle_0\langle \hat{x}\rangle_0\big] t + \langle \hat{x}^2\rangle_0 - \big(\langle \hat{x}\rangle_0\big)^2 \\
&= \frac{1}{m^2}(\Delta p_x)_0^2 t^2 + (\Delta x)_0^2 + \frac{1}{m}\big[\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0 - 2\langle \hat{p}_x\rangle_0\langle \hat{x}\rangle_0\big] t,
\end{aligned}$$

where

$$\begin{aligned}
(\Delta p_x)_0^2 &= \langle \hat{p}_x^2\rangle_0 - \big(\langle \hat{p}_x\rangle_0\big)^2, \\
(\Delta x)_0^2 &= \langle \hat{x}^2\rangle_0 - \big(\langle \hat{x}\rangle_0\big)^2.
\end{aligned}$$

If we choose the initial time so that

$$\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle_0 - 2\langle \hat{p}_x\rangle_0\langle \hat{x}\rangle_0 = 0,$$

we then have

$$(\Delta x)^2 = \frac{1}{m^2}(\Delta p_x)_0^2 t^2 + (\Delta x)_0^2.$$

$\langle \hat{x}\rangle$ gives us the center of the wave packet while Δx gives us the width of the wave packet. The width of the wave packet varies with time in the following manner

$$\Delta x = \sqrt{(\Delta p_x)_0^2 t^2/m^2 + (\Delta x)_0^2}.$$

From the above expression of Δx, we see that the time dependence of Δx arises from the uncertainty $(\Delta p_x)_0$ in the momentum at the initial time. Because of the spread in momentum, the different components of the wave packet travel with different velocities, which leads to the spread of the wave packet with time. Obviously, a wave packet with $(\Delta p_x)_0 = 0$ (a wave packet with only a single component) will not spread with time.

2. **[C-T Exercise 3-5]** In a one-dimensional problem, consider a particle of potential energy $\hat{V}(\hat{x}) = -f\hat{x}$, where f is a positive constant [$\hat{V}(\hat{x})$ arises, for example, from a gravity field or a uniform electric field].

(a) Write Ehrenfest's theorem for the mean values of the position $\hat{x}$ and the momentum $\hat{p}_x$ of the particle. Integrate these equations; compare with the classical motion.

(b) Show that the root-mean-square deviation Δp_x does not vary over time.

(c) Write the Schrödinger equation in the $\{|p_x\rangle\}$ representation. Deduce from it a relation between $\frac{\partial}{\partial t}\big|\langle p_x|\psi(t)\rangle\big|^2$ and $\frac{\partial}{\partial p_x}\big|\langle p_x|\psi(t)\rangle\big|^2$. Integrate the equation thus obtained; give a physical interpretation.

(a) For $V(x) = -fx$, we have

$$\frac{dV(x)}{dx} = -f.$$

Ehrenfest's theorem reads in this case

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{1}{m}\langle\hat{p}_x\rangle,$$
$$\frac{d\langle\hat{p}_x\rangle}{dt} = f.$$

Integrating the second equation yields

$$\langle\hat{p}_x\rangle(t) = ft + \langle\hat{p}_x\rangle_0 .$$

Inserting $\langle\hat{p}_x\rangle(t) = ft + \langle\hat{p}_x\rangle_0$ into the first equation in Ehrenfest's theorem yields

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{f}{m}t + \frac{\langle\hat{p}_x\rangle_0}{m}.$$

Integrating the above equation yields

$$\langle\hat{x}\rangle(t) = \frac{f}{2m}t^2 + \frac{\langle\hat{p}_x\rangle_0}{m}t + \langle\hat{x}\rangle_0 .$$

The above equations are the same as those for the classical motion with the averages corresponding to the classical quantities.

(b) The equation of motion for $\langle\hat{p}_x^2\rangle$ is given by

$$\frac{d\langle\hat{p}_x^2\rangle}{dt} = \frac{1}{i\hbar}\left\langle\left[\,\hat{p}_x^2, \hat{H}\,\right]\right\rangle .$$

With

$$\hat{H} = \frac{\hat{p}_x^2}{2m} - f\hat{x},$$

we have

$$\left[\,\hat{p}_x^2, \hat{H}\,\right] = -f\left[\,\hat{p}_x^2, \hat{x}\,\right] = -f\hat{p}_x\left[\,\hat{p}_x, \hat{x}\,\right] - f\left[\,\hat{p}_x, \hat{x}\,\right]\hat{p}_x = 2i\hbar f\hat{p}_x.$$

We thus have

$$\frac{d\langle\hat{p}_x^2\rangle}{dt} = 2f\langle\hat{p}_x\rangle .$$

Inserting $\langle\hat{p}_x\rangle(t) = ft + \langle\hat{p}_x\rangle_0$ into the above equation yields

$$\frac{d\langle\hat{p}_x^2\rangle}{dt} = 2f^2t + 2f\langle\hat{p}_x\rangle_0 .$$

Integrating the above equation, we have

$$\langle\hat{p}_x^2\rangle(t) = f^2t^2 + 2f\langle\hat{p}_x\rangle_0 t + \langle\hat{p}_x^2\rangle_0 .$$

The square of the root-mean-square deviation Δp_x is then given by

$$\begin{aligned}\left(\Delta p_x\right)^2 &= \langle\hat{p}_x^2\rangle(t) - \left[\langle\hat{p}_x\rangle(t)\right]^2 \\ &= f^2t^2 + 2f\langle\hat{p}_x\rangle_0 t + \langle\hat{p}_x^2\rangle_0 - \left[ft + \langle\hat{p}_x\rangle_0\right]^2 \\ &= \langle\hat{p}_x^2\rangle_0 - \langle\hat{p}_x\rangle_0^2 = \left(\Delta p_x\right)_0^2.\end{aligned}$$

Therefore, the root-mean-square deviation Δp_x does not vary over time.

(c) The Schrödinger equation in the $\{|p_x\rangle\}$ representation reads

$$i\hbar\frac{\partial\langle p_x|\psi(t)\rangle}{\partial t} = -i\hbar f\frac{\partial\langle p_x|\psi(t)\rangle}{\partial p_x} + \frac{p_x^2}{2m}\langle p_x|\psi(t)\rangle\,.$$

The complex conjugate of the above equation is given by

$$-i\hbar\frac{\partial\langle\psi(t)|p_x\rangle}{\partial t} = i\hbar f\frac{\partial\langle\psi(t)|p_x\rangle}{\partial p_x} + \frac{p_x^2}{2m}\langle\psi(t)|p_x\rangle\,.$$

Multiplying the first equation with $\langle\psi(t)|p_x\rangle$ and the second equation with $\langle p_x|\psi(t)\rangle$ and then subtracting the two resultant equations, we obtain

$$i\hbar\left[\langle\psi(t)|p_x\rangle\,\frac{\partial\langle p_x|\psi(t)\rangle}{\partial t} + \langle p_x|\psi(t)\rangle\,\frac{\partial\langle\psi(t)|p_x\rangle}{\partial t}\right] = -i\hbar f\left[\langle\psi(t)|p_x\rangle\,\frac{\partial\langle p_x|\psi(t)\rangle}{\partial p_x} + \langle p_x|\psi(t)\rangle\,\frac{\partial\langle\psi(t)|p_x\rangle}{\partial p_x}\right].$$

Combining the two terms on each side and cancelling $i\hbar$ on both sides, we have

$$\frac{\partial}{\partial t}\big|\langle p_x|\psi(t)\rangle\big|^2 = -f\frac{\partial}{\partial p_x}\big|\langle p_x|\psi(t)\rangle\big|^2.$$

For the convenience of integrating the above equation, we set $u(p_x,t) = \big|\langle p_x|\psi(t)\rangle\big|^2$. Then the above equation is written as

$$\frac{\partial u(p_x,t)}{\partial t} + f\frac{\partial u(p_x,t)}{\partial p_x} = 0.$$

Together with the initial condition $u(p_x,t=0) = \big|\langle p_x|\psi(0)\rangle\big|^2$, we have the following initial-value problem with a first-order partial differential equation

$$\begin{cases} \dfrac{\partial u}{\partial t} + f\dfrac{\partial u}{\partial p_x} = 0 & (-\infty < p_x < \infty,\ t \geq 0), \\ u\big|_{t=0} = \big|\langle p_x|\psi(0)\rangle\big|^2 & (-\infty < p_x < \infty). \end{cases}$$

The above problem can be solved by using the method of characteristic curves. Let $p_x = p_x(t)$. We introduce the function $U(t)$ with $U(t) \equiv u[x(t),t]$. We can then cast the original initial-value problem with a first-order partial differential equation into two initial-value problems with first-order ordinary differential equations: The initial-value problem for $p_x(t)$ and the initial-value problem for $U(t)$. The statements for these two initial-value problems read

$$\begin{cases} \dfrac{dp_x}{dt} = f, \\ p_x\big|_{t=0} = c, \end{cases} \qquad \begin{cases} \dfrac{dU}{dt} = 0, \\ U\big|_{t=0} = \big|\langle c|\psi(0)\rangle\big|^2, \end{cases}$$

where c is a parameter that is to be eliminated. The solutions of the above two initial-value problems are given by

$$\begin{aligned} &p_x = ft + c, \\ &U(t) = \big|\langle c|\psi(0)\rangle\big|^2. \end{aligned}$$

From $p_x = ft + c$, we have $c = p_x - ft$. Inserting $c = p_x - ft$ into the expression of $U(t)$, we have

$$u(p_x,t) = \big|\langle p_x - ft|\psi(0)\rangle\big|^2.$$

We have thus obtained

$$\big|\langle p_x|\psi(t)\rangle\big|^2 = \big|\langle p_x - ft|\psi(0)\rangle\big|^2.$$

The above result indicates that the probability density at the point p_x of momentum space at time t is equal to that at the point $p_x - ft$ of momentum space at the initial time $t = 0$. This reflects the prediction of classical physics that the increase of the momentum of the particle at time t in the force field $-fx$ is equal to ft. The quantum mechanical probability distribution in momentum space is shifted over time. Using the above-obtained probability density in momentum space, we can verify the result derived for $\langle \hat{p}_x \rangle(t)$ in Part (a) and the results derived for $\langle \hat{p}_x^2 \rangle(t)$ and $\left(\Delta p_x\right)^2$ in Part (b). For $\langle \hat{p}_x \rangle(t)$, we have

$$\begin{aligned}\langle \hat{p}_x \rangle(t) &= \int_{-\infty}^{\infty} dp_x \; p_x \big|\langle p_x|\psi(t)\rangle\big|^2 = \int_{-\infty}^{\infty} dp_x \; p_x \big|\langle p_x - ft|\psi(0)\rangle\big|^2 \\ &= \int_{-\infty}^{\infty} dp'_x \; (p'_x + ft)\big|\langle p'_x|\psi(0)\rangle\big|^2 = \langle \hat{p}_x \rangle_0 + ft\end{aligned}$$

which is identical with that derived in Part (a).
For $\langle \hat{p}_x^2 \rangle(t)$, we have

$$\begin{aligned}\langle \hat{p}_x^2 \rangle(t) &= \int_{-\infty}^{\infty} dp_x \; p_x^2 \big|\langle p_x|\psi(t)\rangle\big|^2 = \int_{-\infty}^{\infty} dp_x \; p_x^2 \big|\langle p_x - ft|\psi(0)\rangle\big|^2 \\ &= \int_{-\infty}^{\infty} dp'_x \; (p'_x + ft)^2\big|\langle p'_x|\psi(0)\rangle\big|^2 = \langle \hat{p}_x^2 \rangle_0 + 2ft\,\langle \hat{p}_x \rangle_0 + (ft)^2\end{aligned}$$

which is identical with that derived in Part (b).

From the just-obtained results for $\langle \hat{p}_x \rangle(t)$ and $\langle \hat{p}_x^2 \rangle(t)$, we can obtain the same result for $\left(\Delta p_x\right)^2$ as in Part (b).

3. **[C-T Exercise 3-9]** One wants to show that the physical state of a (spinless) particle is completely defined by specifying the probability density $\rho(\vec{r}) = |\psi(\vec{r})|^2$ and the probability current $\vec{J}(\vec{r})$.

   (a) Assume the function $\psi(\vec{r})$ known and let $\xi(\vec{r})$ be its argument, $\psi(\vec{r}) = \sqrt{\rho(\vec{r})}\, e^{i\xi(\vec{r})}$. Show that

   $$\vec{J}(\vec{r}) = \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\xi(\vec{r}).$$

   Deduce that two wave functions leading to the same density $\rho(\vec{r})$ and current $\vec{J}(\vec{r})$ can differ only by a global phase factor.

   (b) Given arbitrary functions $\rho(\vec{r})$ and $\vec{J}(\vec{r})$, show that a quantum state $\psi(\vec{r})$ can be associated with them only if $\vec{\nabla} \times \vec{v}(\vec{r}) = 0$, where $\vec{v}(\vec{r}) = \vec{J}(\vec{r})/\rho(\vec{r})$ is the velocity associated with the probability fluid.

   (c) Now assume that the particle is submitted to a magnetic field $\vec{B}(\vec{r}) = \vec{\nabla} \times \vec{A}(\vec{r})$. Show that

   $$\begin{aligned}\vec{J}(\vec{r}) &= \frac{\rho(\vec{r})}{m}\big[\,\hbar\vec{\nabla}\xi(\vec{r}) - q\vec{A}(\vec{r})\,\big], \\ \vec{\nabla} \times \vec{v}(\vec{r}) &= -\frac{q}{m}\vec{B}(\vec{r}).\end{aligned}$$

(a) With $\psi(\vec{r}) = \sqrt{\rho(\vec{r})}\, e^{i\xi(\vec{r})}$, the probability current $\vec{J}(\vec{r})$ is given by

$$\begin{aligned}\vec{J}(\vec{r}) &= \frac{\hbar}{2im}\big[\,\psi^*(\vec{r})\vec{\nabla}\psi(\vec{r}) - \psi(\vec{r})\vec{\nabla}\psi^*(\vec{r})\,\big] \\ &= \frac{\hbar}{2im}\bigg\{\sqrt{\rho(\vec{r})}\, e^{-i\xi(\vec{r})}\bigg[\,\frac{e^{i\xi(\vec{r})}}{2\sqrt{\rho(\vec{r})}}\vec{\nabla}\rho(\vec{r}) + i\sqrt{\rho(\vec{r})}\, e^{i\xi(\vec{r})}\vec{\nabla}\xi(\vec{r})\,\bigg] \\ &\quad - \sqrt{\rho(\vec{r})}\, e^{i\xi(\vec{r})}\bigg[\,\frac{e^{-i\xi(\vec{r})}}{2\sqrt{\rho(\vec{r})}}\vec{\nabla}\rho(\vec{r}) - i\sqrt{\rho(\vec{r})}\, e^{-i\xi(\vec{r})}\vec{\nabla}\xi(\vec{r})\,\bigg]\bigg\} \\ &= \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\xi(\vec{r}).\end{aligned}$$

Assume that

$$\begin{aligned}\rho_1(\vec{r}) &= |\psi_1(\vec{r})|^2, \\ \rho_2(\vec{r}) &= |\psi_2(\vec{r})|^2.\end{aligned}$$

From $\rho_1(\vec{r}) = \rho_2(\vec{r})$, we have $|\psi_1(\vec{r})|^2 = |\psi_2(\vec{r})|^2$ from which we have

$$\xi_2(\vec{r}) = \xi_1(\vec{r}) + \chi(\vec{r}).$$

Let $|\psi_1(\vec{r})|^2 = |\psi_2(\vec{r})|^2 = \rho(\vec{r})$. The probability currents corresponding to the two wave functions are respectively given by

$$\begin{aligned} \vec{J}_1(\vec{r}) &= \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\xi_1(\vec{r}), \\ \vec{J}_2(\vec{r}) &= \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\xi_2(\vec{r}) = \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\xi_1(\vec{r}) + \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\chi(\vec{r}). \end{aligned}$$

For $\vec{J}_1(\vec{r}) = \vec{J}_2(\vec{r})$ to hold for any $\rho(\vec{r})$, we must have

$$\vec{\nabla}\chi(\vec{r}) = 0.$$

That is, $\chi(\vec{r})$ is independent of $\vec{r}$. Thus, two wave functions leading to the same density $\rho(\vec{r})$ and current $\vec{J}(\vec{r})$ can differ only by a global phase factor.

(b) From the expressions of the probability density and current

$$\begin{aligned} \rho(\vec{r}) &= |\psi(\vec{r})|^2, \\ \vec{J}(\vec{r}) &= \frac{\hbar}{2im}\big[\,\psi^*(\vec{r})\vec{\nabla}\psi(\vec{r}) - \psi(\vec{r})\vec{\nabla}\psi^*(\vec{r})\,\big], \end{aligned}$$

we have

$$\frac{\vec{J}(\vec{r})}{\rho(\vec{r})} = \frac{\hbar}{2im}\left[\frac{\vec{\nabla}\psi(\vec{r})}{\psi(\vec{r})} - \frac{\vec{\nabla}\psi^*(\vec{r})}{\psi^*(\vec{r})}\right] = \frac{\hbar}{2im}\left[\vec{\nabla}\ln\psi(\vec{r}) - \vec{\nabla}\ln\psi^*(\vec{r})\right] = \frac{\hbar}{2im}\vec{\nabla}\ln\frac{\psi(\vec{r})}{\psi^*(\vec{r})}.$$

Since the right hand side is proportional to the gradient of a scalar function, its curl is zero. Thus, the curl of $\vec{J}(\vec{r})/\rho(\vec{r})$ must be zero. That is,

$$\vec{\nabla}\times\frac{\vec{J}(\vec{r})}{\rho(\vec{r})} = 0.$$

Therefore, the condition that $\vec{\nabla}\times\big[\,\vec{J}(\vec{r})/\rho(\vec{r})\,\big] = 0$ is necessary.

To prove that the condition that $\vec{\nabla}\times\big[\,\vec{J}(\vec{r})/\rho(\vec{r})\,\big] = 0$ is sufficient, we assume that $\vec{\nabla}\times\big[\,\vec{J}(\vec{r})/\rho(\vec{r})\,\big] = 0$ holds. From $\psi(\vec{r}) = \sqrt{\rho(\vec{r})}\,e^{i\xi(\vec{r})}$, we have

$$\frac{\vec{J}(\vec{r})}{\rho(\vec{r})} = \frac{\hbar}{2im}\vec{\nabla}\ln\frac{\psi(\vec{r})}{\psi^*(\vec{r})} = \frac{\hbar}{2im}\vec{\nabla}\ln e^{2i\xi(\vec{r})} = \frac{\hbar}{m}\vec{\nabla}\xi(\vec{r}).$$

Since $\vec{\nabla}\times\big[\,\vec{J}(\vec{r})/\rho(\vec{r})\,\big] = 0$, we can always find $\xi(\vec{r})$ from the above equation. Therefore, the condition that $\vec{\nabla}\times\big[\,\vec{J}(\vec{r})/\rho(\vec{r})\,\big] = 0$ is sufficient.

(c) The probability current for the particle in a magnetic field $\vec{B}(\vec{r}) = \vec{\nabla}\times\vec{A}(\vec{r})$ is giben by

$$\vec{J}(\vec{r}) = \frac{1}{m}\,\mathrm{Re}\Big\{\psi^*(\vec{r})\big[-i\hbar\vec{\nabla} - q\vec{A}(\vec{r})\big]\psi(\vec{r})\Big\}.$$

Making use of $\psi(\vec{r}) = \sqrt{\rho(\vec{r})}\,e^{i\xi(\vec{r})}$, we have

$$\begin{aligned} -\,i\hbar\vec{\nabla}\psi(\vec{r}) &= -i\hbar\frac{e^{i\xi(\vec{r})}}{2\sqrt{\rho(\vec{r})}}\vec{\nabla}\rho(\vec{r}) + \hbar\sqrt{\rho(\vec{r})}\,e^{i\xi(\vec{r})}\vec{\nabla}\xi(\vec{r}), \\ \psi^*(\vec{r})\big[-i\hbar\vec{\nabla} - q\vec{A}(\vec{r})\big]\psi(\vec{r}) &= -i\hbar\frac{1}{2}\vec{\nabla}\rho(\vec{r}) + \hbar\rho(\vec{r})\vec{\nabla}\xi(\vec{r}) - q\vec{A}(\vec{r})\rho(\vec{r}). \end{aligned}$$

Thus,

$$\begin{aligned}\vec{J}(\vec{r}) &= \frac{1}{m}\,\mathrm{Re}\big[-i\hbar\frac{1}{2}\vec{\nabla}\rho(\vec{r}) + \hbar\rho(\vec{r})\vec{\nabla}\xi(\vec{r}) - q\vec{A}(\vec{r})\rho(\vec{r})\big] \\ &= \frac{\rho(\vec{r})}{m}\big[\hbar\vec{\nabla}\xi(\vec{r}) - q\vec{A}(\vec{r})\big].\end{aligned}$$

For $\vec{\nabla}\times\vec{v}(\vec{r})$, we have

$$\begin{aligned}\vec{\nabla}\times\vec{v}(\vec{r}) &= \frac{1}{m}\vec{\nabla}\times\big[\hbar\vec{\nabla}\xi(\vec{r}) - q\vec{A}(\vec{r})\big] \\ &= -\frac{q}{m}\vec{\nabla}\times\vec{A}(\vec{r}) \\ &= -\frac{q}{m}\vec{B}(\vec{r}),\end{aligned}$$

where we have used $\vec{\nabla}\times\big[\vec{\nabla}\xi(\vec{r})\big] = 0$ and $\vec{\nabla}\times\vec{A}(\vec{r}) = \vec{B}(\vec{r})$.

4. **[C-T Exercise 3-16]** Consider a physical system formed by two particles (1) and (2), of the same mass m, which do not interact with each other and which are both placed in an infinite potential well of width a. Denote by $\hat{H}(1)$ and $\hat{H}(2)$ the Hamiltonians of each of the two particles and by $|\varphi_n(1)\rangle$ and $|\varphi_q(2)\rangle$ the corresponding eigenstates of the first and second particle, of energies $n^2\pi^2\hbar^2/2ma^2$ and $q^2\pi^2\hbar^2/2ma^2$. In the state space of the global system, the basis chosen is composed of the states $|\varphi_n\varphi_q\rangle$ defined by $|\varphi_n\varphi_q\rangle = |\varphi_n(1)\rangle\otimes|\varphi_q(2)\rangle$.

   (a) What are the eigenstates and the eigenvalues of the operator $\hat{H} = \hat{H}(1) + \hat{H}(2)$, the total Hamiltonian of the system? Give the degree of degeneracy of the two lowest energy levels.

   (b) Assume that the system, at time $t = 0$, is in the state

   $$|\psi(0)\rangle = \frac{1}{\sqrt{6}}\,|\varphi_1\varphi_1\rangle + \frac{1}{\sqrt{3}}\,|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{6}}\,|\varphi_2\varphi_1\rangle + \frac{1}{\sqrt{3}}\,|\varphi_2\varphi_2\rangle\,.$$

      i. What is the state of the system at time t?
      ii. The total energy $\hat{H}$ is measured. What results can be found, and with what probabilities?
      iii. Same questions if, instead of measuring $\hat{H}$, one measures $\hat{H}(1)$.

   (c) i. Show that $|\psi(0)\rangle$ is a tensor product state. When the system is in this state, calculate the following mean values: $\langle\hat{H}(1)\rangle$, $\langle\hat{H}(2)\rangle$ and $\langle\hat{H}(1)\hat{H}(2)\rangle$. Compare $\langle\hat{H}(1)\rangle\langle\hat{H}(2)\rangle$ with $\langle\hat{H}(1)\hat{H}(2)\rangle$; how can this result be explained?
      ii. Show that the preceding results remain valid when the state of the system is the state $|\psi(t)\rangle$ calculated in (b).

   (d) Now assume that the state $|\psi(0)\rangle$ is given by

   $$|\psi(0)\rangle = \frac{1}{\sqrt{5}}\,|\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}}\,|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}}\,|\varphi_2\varphi_1\rangle\,.$$

      i. Show that $|\psi(0)\rangle$ cannot be put in the form of a tensor product. When the system is in this state, calculate the following mean values: $\langle\hat{H}(1)\rangle$, $\langle\hat{H}(2)\rangle$ and $\langle\hat{H}(1)\hat{H}(2)\rangle$. Compare $\langle\hat{H}(1)\rangle\langle\hat{H}(2)\rangle$ with $\langle\hat{H}(1)\hat{H}(2)\rangle$; how can this result be explained?
      ii. Show that the preceding results remain valid when the state of the system is the state $|\psi(t)\rangle$ derived from the above-given $|\psi(0)\rangle$.

   (e) Write the matrix, in the basis of the vectors $|\varphi_n\varphi_q\rangle$, which represents the density matrix ρ corresponding to the ket $|\psi(0)\rangle$ given in (b). What is the density matrix $\rho(t)$ at time t? Calculate, at the instant $t = 0$, the partial traces $\rho(1) = \mathrm{Tr}_2\,\rho$ and $\rho(2) = \mathrm{Tr}_1\,\rho$. Do the density operators ρ, $\rho(1)$ and $\rho(2)$ describe pure states? Compare ρ with $\rho(1)\otimes\rho(2)$; what is your interpretation?

(a) Since $[\hat{H}(1), \hat{H}(2)] = 0$, we have $[\hat{H}, \hat{H}(1)] = [\hat{H}, \hat{H}(2)] = 0$. Thus, $\hat{H}$, $\hat{H}(1)$, and $\hat{H}(2)$ have common eigenvectors. Their common eigenvectors are $\{|\varphi_n\varphi_q\rangle\}$,

$$\begin{aligned}
\hat{H}\,|\varphi_n\varphi_q\rangle &= \frac{(n^2+q^2)\pi^2\hbar^2}{2ma^2}\,|\varphi_n\varphi_q\rangle, \\
\hat{H}(1)\,|\varphi_n\varphi_q\rangle &= \frac{n^2\pi^2\hbar^2}{2ma^2}\,|\varphi_n\varphi_q\rangle, \\
\hat{H}(2)\,|\varphi_n\varphi_q\rangle &= \frac{q^2\pi^2\hbar^2}{2ma^2}\,|\varphi_n\varphi_q\rangle, \\
n, q &= 1, 2, 3, \cdots .
\end{aligned}$$

Thus, the eigenvalues of $\hat{H}$ are

$$E_{nq} = \frac{(n^2+q^2)\pi^2\hbar^2}{2ma^2},\ n, q = 1, 2, 3, \cdots .$$

The corresponding eigenvectors of $\hat{H}$ are

$$|\varphi_n\varphi_q\rangle = |\varphi_n(1)\rangle \otimes |\varphi_q(2)\rangle,\ n, q = 1, 2, 3, \cdots .$$

The two lowest energy levels are

$$\begin{aligned}
E_1 \equiv E_{11} &= \frac{\pi^2\hbar^2}{ma^2}, \\
E_2 \equiv E_{12} = E_{21} &= \frac{5\pi^2\hbar^2}{2ma^2}.
\end{aligned}$$

The energy level $E_1 = \dfrac{\pi^2\hbar^2}{ma^2}$ is non-degenerate. The energy level $E_2 = \dfrac{5\pi^2\hbar^2}{2ma^2}$ is two-fold degenerate.

(b) i. The state of the system at time t is gibven by

$$|\psi(t)\rangle = \frac{1}{\sqrt{6}}e^{-iE_{11}t/\hbar}\,|\varphi_1\varphi_1\rangle + \frac{1}{\sqrt{3}}e^{-iE_{12}t/\hbar}\,|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{6}}e^{-iE_{21}t/\hbar}\,|\varphi_2\varphi_1\rangle + \frac{1}{\sqrt{3}}e^{-iE_{22}t/\hbar}\,|\varphi_2\varphi_2\rangle$$

with

$$E_{nq} = \frac{(n^2+q^2)\pi^2\hbar^2}{2ma^2},\ n, q = 1, 2, 3, \cdots .$$

ii. If the total energy $\hat{H}$ is measured, the possible results and the probabilities of obtaining these results are given in the following.

Result	**Probability**
$\dfrac{\pi^2\hbar^2}{ma^2}$	$\dfrac{1}{6}$
$\dfrac{5\pi^2\hbar^2}{2ma^2}$	$\dfrac{1}{3} + \dfrac{1}{6} = \dfrac{1}{2}$
$\dfrac{4\pi^2\hbar^2}{ma^2}$	$\dfrac{1}{3}$

iii. If $\hat{H}(1)$ is measured, the possible results and the probabilities of obtaining these results are given in the following.

Result	**Probability**
$\dfrac{\pi^2\hbar^2}{2ma^2}$	$\dfrac{1}{6} + \dfrac{1}{3} = \dfrac{1}{2}$
$\dfrac{2\pi^2\hbar^2}{ma^2}$	$\dfrac{1}{6} + \dfrac{1}{3} = \dfrac{1}{2}$

(c) i. We can rewrite $|\psi(0)\rangle$ as follows

$$\begin{aligned}
|\psi(0)\rangle &= \frac{1}{\sqrt{6}}\,|\varphi_1\varphi_1\rangle + \frac{1}{\sqrt{3}}\,|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{6}}\,|\varphi_2\varphi_1\rangle + \frac{1}{\sqrt{3}}\,|\varphi_2\varphi_2\rangle \\
&= \frac{1}{\sqrt{3}}\,|\varphi_1(1)\rangle \otimes \left[\frac{1}{\sqrt{2}}\,|\varphi_1(2)\rangle + |\varphi_2(2)\rangle\right] + \frac{1}{\sqrt{3}}\,|\varphi_2(1)\rangle \otimes \left[\frac{1}{\sqrt{2}}\,|\varphi_1(2)\rangle + |\varphi_2(2)\rangle\right] \\
&= \frac{1}{\sqrt{3}}\big[\,|\varphi_1(1)\rangle + |\varphi_2(1)\rangle\,\big] \otimes \left[\frac{1}{\sqrt{2}}\,|\varphi_1(2)\rangle + |\varphi_2(2)\rangle\right].
\end{aligned}$$

Thus, $|\psi(0)\rangle$ is a tensor product state.

The mean value of $\hat{H}(1)$ in $|\psi(0)\rangle$ is given by

$$\langle \hat{H}(1)\rangle = \frac{\pi^2\hbar^2}{2ma^2} \times \frac{1}{2} + \frac{2\pi^2\hbar^2}{ma^2} \times \frac{1}{2} = \frac{5\pi^2\hbar^2}{4ma^2}.$$

The mean value of $\hat{H}(2)$ in $|\psi(0)\rangle$ is given by

$$\langle \hat{H}(2)\rangle = \frac{\pi^2\hbar^2}{2ma^2} \times \frac{1}{3} + \frac{2\pi^2\hbar^2}{ma^2} \times \frac{2}{3} = \frac{3\pi^2\hbar^2}{2ma^2}.$$

The mean value of $\hat{H}(1)\hat{H}(2)$ in $|\psi(0)\rangle$ is given by

$$\begin{aligned}
\langle \hat{H}(1)\hat{H}(2)\rangle &= \left(\frac{\pi^2\hbar^2}{2ma^2}\right)^2 \times \frac{1}{6} + \frac{\pi^2\hbar^2}{2ma^2}\frac{2\pi^2\hbar^2}{ma^2} \times \left(\frac{1}{3} + \frac{1}{6}\right) + \left(\frac{2\pi^2\hbar^2}{ma^2}\right)^2 \times \frac{1}{3} \\
&= \frac{15}{8}\left(\frac{\pi^2\hbar^2}{ma^2}\right)^2 = \frac{15}{2}\left(\frac{\pi^2\hbar^2}{2ma^2}\right)^2.
\end{aligned}$$

From the above results, we see that

$$\langle \hat{H}(1)\rangle\langle \hat{H}(2)\rangle = \langle \hat{H}(1)\hat{H}(2)\rangle\,.$$

This is due to the fact that $|\psi(0)\rangle$ is a tensor-product state. Writing $|\psi(0)\rangle$ as

$$|\psi(0)\rangle = |\phi(1)\rangle \otimes |\chi(2)\rangle$$

with

$$\begin{aligned}
|\phi(1)\rangle &= \frac{1}{\sqrt{2}}\big[\,|\varphi_1(1)\rangle + |\varphi_2(1)\rangle\,\big], \\
|\chi(2)\rangle &= \frac{1}{\sqrt{3}}\,|\varphi_1(2)\rangle + \sqrt{\frac{2}{3}}\,|\varphi_2(2)\rangle,
\end{aligned}$$

we have

$$\langle \hat{H}(1)\hat{H}(2)\rangle_{\psi(0)} = \langle \hat{H}(1)\rangle_{\phi(1)}\langle \hat{H}(2)\rangle_{\chi(2)},$$

where

$$\begin{aligned}
\langle \hat{H}(1)\rangle_{\phi(1)} &= \langle \phi(1)|\hat{H}(1)|\phi(1)\rangle = \frac{5\pi^2\hbar^2}{4ma^2}, \\
\langle \hat{H}(2)\rangle_{\chi(2)} &= \langle \chi(2)|\hat{H}(2)|\chi(2)\rangle = \frac{3\pi^2\hbar^2}{2ma^2}.
\end{aligned}$$

Note that $|\phi(1)\rangle$ and $|\chi(2)\rangle$ are normalized.

ii. Because $|c_{p,q}|^2 = |c_{p,q}e^{-iE_{pq}t/\hbar}|^2$, the probabilities of finding the particle in the eigenstates $|\varphi_n\varphi_q\rangle = |\varphi_n(1)\rangle \otimes |\varphi_q(2)\rangle$ are the same for $|\psi(0)\rangle$ and $|\psi(t)\rangle$. Therefore, the preceding results remain valid when the state of the system is the state $|\psi(t)\rangle$ derived from the above-given $|\psi(0)\rangle$.

(d) i. If we attempt to factorize

$$|\psi(0)\rangle = \frac{1}{\sqrt{5}}\,|\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}}\,|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}}\,|\varphi_2\varphi_1\rangle,$$

we can only get this far

$$|\psi(0)\rangle = \frac{1}{\sqrt{5}}\,|\varphi_1(1)\rangle \otimes \big[\,|\varphi_1(2)\rangle + \sqrt{3}\,|\varphi_2(2)\rangle\,\big] + \frac{1}{\sqrt{5}}\,|\varphi_2(1)\rangle \otimes |\varphi_1(2)\rangle\,.$$

Therefore, $|\psi(0)\rangle$ cannot be put in the form of a tensor product.
The mean value of $\hat{H}(1)$ in $|\psi(0)\rangle$ is given by

$$\langle \hat{H}(1)\rangle = \frac{\pi^2\hbar^2}{2ma^2} \times \left(\frac{1}{5} + \frac{3}{5}\right) + \frac{2\pi^2\hbar^2}{ma^2} \times \frac{1}{5} = \frac{4\pi^2\hbar^2}{5ma^2}.$$

The mean value of $\hat{H}(2)$ in $|\psi(0)\rangle$ is given by

$$\langle \hat{H}(2)\rangle = \frac{\pi^2\hbar^2}{2ma^2} \times \left(\frac{1}{5} + \frac{1}{5}\right) + \frac{2\pi^2\hbar^2}{ma^2} \times \frac{3}{5} = \frac{7\pi^2\hbar^2}{5ma^2}.$$

The mean value of $\hat{H}(1)\hat{H}(2)$ in $|\psi(0)\rangle$ is given by

$$\begin{aligned}\langle \hat{H}(1)\hat{H}(2)\rangle &= \left(\frac{\pi^2\hbar^2}{2ma^2}\right)^2 \times \frac{1}{5} + \frac{\pi^2\hbar^2}{2ma^2}\,\frac{2\pi^2\hbar^2}{ma^2} \times \left(\frac{3}{5} + \frac{1}{5}\right) \\ &= \frac{17}{20}\left(\frac{\pi^2\hbar^2}{ma^2}\right)^2 = \frac{17}{5}\left(\frac{\pi^2\hbar^2}{2ma^2}\right)^2.\end{aligned}$$

From the above results, we see that

$$\langle \hat{H}(1)\rangle\langle \hat{H}(2)\rangle \neq \langle \hat{H}(1)\hat{H}(2)\rangle\,.$$

This is due to the fact that $|\psi(0)\rangle$ is not a tensor-product state.

ii. Because $|c_{p,q}|^2 = |c_{p,q}e^{-iE_{pq}t/\hbar}|^2$, the probabilities of finding the particle in the eigenstates $|\varphi_n\varphi_q\rangle = |\varphi_n(1)\rangle \otimes |\varphi_q(2)\rangle$ are the same for $|\psi(0)\rangle$ and $|\psi(t)\rangle$. Therefore, the preceding results remain valid when the state of the system is the state $|\psi(t)\rangle$ derived from the above-given $|\psi(0)\rangle$.

(e) The density operator $\hat{\rho}$ corresponding to the ket $|\psi(0)\rangle$ given in (b) is given by

$$\begin{aligned}\hat{\rho} &= |\psi(0)\rangle\langle\psi(0)| \\ &= \frac{1}{6}\,|\varphi_1\varphi_1\rangle\langle\varphi_1\varphi_1| + \frac{1}{3\sqrt{2}}\,|\varphi_1\varphi_2\rangle\langle\varphi_1\varphi_1| + \frac{1}{6}\,|\varphi_2\varphi_1\rangle\langle\varphi_1\varphi_1| + \frac{1}{3\sqrt{2}}\,|\varphi_2\varphi_2\rangle\langle\varphi_1\varphi_1| \\ &\quad + \frac{1}{3\sqrt{2}}\,|\varphi_1\varphi_1\rangle\langle\varphi_1\varphi_2| + \frac{1}{3}\,|\varphi_1\varphi_2\rangle\langle\varphi_1\varphi_2| + \frac{1}{3\sqrt{2}}\,|\varphi_2\varphi_1\rangle\langle\varphi_1\varphi_2| + \frac{1}{3}\,|\varphi_2\varphi_2\rangle\langle\varphi_1\varphi_2| \\ &\quad + \frac{1}{6}\,|\varphi_1\varphi_1\rangle\langle\varphi_2\varphi_1| + \frac{1}{3\sqrt{2}}\,|\varphi_1\varphi_2\rangle\langle\varphi_2\varphi_1| + \frac{1}{6}\,|\varphi_2\varphi_1\rangle\langle\varphi_2\varphi_1| + \frac{1}{3\sqrt{2}}\,|\varphi_2\varphi_2\rangle\langle\varphi_2\varphi_1| \\ &\quad + \frac{1}{3\sqrt{2}}\,|\varphi_1\varphi_1\rangle\langle\varphi_2\varphi_2| + \frac{1}{3}\,|\varphi_1\varphi_2\rangle\langle\varphi_2\varphi_2| + \frac{1}{3\sqrt{2}}\,|\varphi_2\varphi_1\rangle\langle\varphi_2\varphi_2| + \frac{1}{3}\,|\varphi_2\varphi_2\rangle\langle\varphi_2\varphi_2|\,.\end{aligned}$$

Since $\hat{\rho}$ has non-zero matrix elements only in the subspace spanned by $|\varphi_1\varphi_1\rangle$, $|\varphi_1\varphi_2\rangle$, $|\varphi_2\varphi_1\rangle$, and $|\varphi_2\varphi_2\rangle$, we write the representation matrix of $\hat{\rho}$ only in this subspace with the four basis vectors given in the stated order. We have

$$\rho = \frac{1}{6}\begin{pmatrix} 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \\ 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \end{pmatrix}.$$

$\hat{\rho}(t)$ is given by

$$\rho(t) = \frac{1}{6}\begin{pmatrix} 1 & \sqrt{2}\,e^{i(E_{11}-E_{12})t/\hbar} & e^{i(E_{11}-E_{21})t/\hbar} & \sqrt{2}\,e^{i(E_{11}-E_{22})t/\hbar} \\ \sqrt{2}\,e^{i(E_{12}-E_{11})t/\hbar} & 2 & \sqrt{2}\,e^{i(E_{12}-E_{21})t/\hbar} & 2e^{i(E_{12}-E_{22})t/\hbar} \\ e^{i(E_{21}-E_{11})t/\hbar} & \sqrt{2}\,e^{i(E_{21}-E_{12})t/\hbar} & 1 & \sqrt{2}\,e^{i(E_{21}-E_{22})t/\hbar} \\ \sqrt{2}\,e^{i(E_{22}-E_{11})t/\hbar} & 2e^{i(E_{22}-E_{12})t/\hbar} & \sqrt{2}\,e^{i(E_{22}-E_{21})t/\hbar} & 2 \end{pmatrix}.$$

The partial trace $\hat{\rho}(1)$ is given by

$$\begin{aligned} \hat{\rho}(1) &= \mathrm{Tr}_2\,\hat{\rho} \\ &= \frac{1}{6}\,|\varphi_1(1)\rangle\langle\varphi_1(1)| + \frac{1}{6}\,|\varphi_2(1)\rangle\langle\varphi_1(1)| + \frac{1}{3}\,|\varphi_1(1)\rangle\langle\varphi_1(1)| + \frac{1}{3}\,|\varphi_2(1)\rangle\langle\varphi_1(1)| \\ &\quad + \frac{1}{6}\,|\varphi_1(1)\rangle\langle\varphi_2(1)| + \frac{1}{6}\,|\varphi_2(1)\rangle\langle\varphi_2(1)| + \frac{1}{3}\,|\varphi_1(1)\rangle\langle\varphi_2(1)| + \frac{1}{3}\,|\varphi_2(1)\rangle\langle\varphi_2(1)| \\ &= \frac{1}{2}\,|\varphi_1(1)\rangle\langle\varphi_1(1)| + \frac{1}{2}\,|\varphi_1(1)\rangle\langle\varphi_2(1)| + \frac{1}{2}\,|\varphi_2(1)\rangle\langle\varphi_1(1)| + \frac{1}{2}\,|\varphi_2(1)\rangle\langle\varphi_2(1)|\,. \end{aligned}$$

The matrix representing $\hat{\rho}(1)$ in the subspace spanned by $|\varphi_1(1)\rangle$ and $|\varphi_2(1)\rangle$ is given by

$$\rho(1) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

The partial trace $\hat{\rho}(2)$ is given by

$$\begin{aligned} \hat{\rho}(2) &= \mathrm{Tr}_1\,\hat{\rho} \\ &= \frac{1}{6}\,|\varphi_1(2)\rangle\langle\varphi_1(2)| + \frac{1}{3\sqrt{2}}\,|\varphi_2(2)\rangle\langle\varphi_1(2)| + \frac{1}{3\sqrt{2}}\,|\varphi_1(2)\rangle\langle\varphi_2(2)| + \frac{1}{3}\,|\varphi_2(2)\rangle\langle\varphi_2(2)| \\ &\quad + \frac{1}{6}\,|\varphi_1(2)\rangle\langle\varphi_1(2)| + \frac{1}{3\sqrt{2}}\,|\varphi_2(2)\rangle\langle\varphi_1(2)| + \frac{1}{3\sqrt{2}}\,|\varphi_1(2)\rangle\langle\varphi_2(2)| + \frac{1}{3}\,|\varphi_2(2)\rangle\langle\varphi_2(2)| \\ &= \frac{1}{3}\,|\varphi_1(2)\rangle\langle\varphi_1(2)| + \frac{\sqrt{2}}{3}\,|\varphi_1(2)\rangle\langle\varphi_2(2)| + \frac{\sqrt{2}}{3}\,|\varphi_2(2)\rangle\langle\varphi_1(2)| + \frac{2}{3}\,|\varphi_2(2)\rangle\langle\varphi_2(2)|\,. \end{aligned}$$

The matrix representing $\hat{\rho}(2)$ in the subspace spanned by $|\varphi_1(2)\rangle$ and $|\varphi_2(2)\rangle$ is given by

$$\rho(2) = \frac{1}{3}\begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 2 \end{pmatrix}.$$

To see if $\hat{\rho}$ describes a pure state, we evaluate the square of its representation matrix. We have

$$\rho^2 = \frac{1}{36}\begin{pmatrix} 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \\ 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \end{pmatrix}\begin{pmatrix} 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \\ 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \\ 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \end{pmatrix} = \rho.$$

Thus, $\hat{\rho}$ describes a pure state.
To see if $\hat{\rho}(1)$ describes a pure state, we evaluate the square of its representation matrix. We have

$$\big[\rho(1)\big]^2 = \frac{1}{4}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \rho(1).$$

Thus, $\hat{\rho}(1)$ describes a pure state.
To see if $\hat{\rho}(2)$ describes a pure state, we evaluate the square of its representation matrix. We have

$$\big[\rho(2)\big]^2 = \frac{1}{9}\begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 2 \end{pmatrix}\begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 2 \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 2 \end{pmatrix} = \rho(2).$$

Thus, $\hat{\rho}(2)$ describes a pure state.

The tensor product of $\rho(1)$ with $\rho(2)$ is given by

$$\rho(1) \otimes \rho(2) = \frac{1}{6}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 2 \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \\ 1 & \sqrt{2} & 1 & \sqrt{2} \\ \sqrt{2} & 2 & \sqrt{2} & 2 \end{pmatrix}.$$

We see that $\rho = \rho(1) \otimes \rho(2)$. This is because $|\psi(0)\rangle$ is a tensor-product state.

5. **[C-T Exercise 3-17]** Let $\hat{\rho}$ be the density operator of an arbitrary system, where $|\chi_\ell\rangle$ and π_ℓ are the eigenvectors and eigenvalues of $\hat{\rho}$. Write $\hat{\rho}$ and $\hat{\rho}^2$ in terms of the $|\chi_\ell\rangle$ and π_ℓ. What do the matrices representing these two operators in the $\{|\chi_\ell\rangle\}$ basis look like — first, in the case where $\hat{\rho}$ describes a pure state and then, in the case of a statistical mixture of states? (Begin by showing that, in a pure case, $\hat{\rho}$ has only one non-zero diagonal element, equal to 1, while for a statistical mixture, $\hat{\rho}$ has several diagonal elements included between 0 and 1.) Show that $\hat{\rho}$ corresponds to a pure case if and only if the trace of $\hat{\rho}^2$ is equal to 1.

We assume that all the eigenvectors of $\hat{\rho}$ are normalized. In terms of $|\chi_\ell\rangle$ and π_ℓ, the density operator $\hat{\rho}$ is given by

$$\hat{\rho} = \sum_\ell \pi_\ell \, |\chi_\ell\rangle\langle\chi_\ell| \, .$$

$\hat{\rho}^2$ is given by

$$\begin{aligned} \hat{\rho}^2 &= \Big(\sum_\ell \pi_\ell \, |\chi_\ell\rangle\langle\chi_\ell|\Big)\Big(\sum_{\ell'} \pi_{\ell'} \, |\chi_{\ell'}\rangle\langle\chi_{\ell'}|\Big) \\ &= \sum_{\ell\ell'} \pi_\ell \pi_{\ell'} \, |\chi_\ell\rangle\langle\chi_\ell|\chi_{\ell'}\rangle\langle\chi_{\ell'}| \\ &= \sum_{\ell\ell'} \pi_\ell \pi_{\ell'} \, |\chi_\ell\rangle\delta_{\ell\ell'}\langle\chi_{\ell'}| \\ &= \sum_\ell \pi_\ell^2 \, |\chi_\ell\rangle\langle\chi_\ell| \, . \end{aligned}$$

From the expressions of $\hat{\rho}$ and $\hat{\rho}^2$, we see that the matrices representing these two operators in the $\{|\chi_\ell\rangle\}$ basis are diagonal matrices.

In the case where $\hat{\rho}$ describes a pure state, we have $\hat{\rho}^2 = \hat{\rho}$ and $\operatorname{Tr}\hat{\rho}^2 = \operatorname{Tr}\hat{\rho} = 1$. We then have

$$\sum_\ell \pi_\ell^2 = \sum_\ell \pi_\ell = 1.$$

For the above two equations to hold, one of π_ℓ's is equal to 1 and all others are equal to zero. Thus, $\hat{\rho}$ has only one non-zero diagonal element that is equal to 1.

For a statistical mixture, from $\operatorname{Tr}\hat{\rho} = 1$, we have

$$\operatorname{Tr}\hat{\rho} = \sum_\ell \pi_\ell = 1.$$

Since $\hat{\rho}$ is positive semi-definite, all its eigenvalues are nonnegative. Thus, for a statistical mixture, $\hat{\rho}$ has several diagonal elements included between 0 and 1.

We first show that $\operatorname{Tr}\hat{\rho}^2 = 1$ is the necessary condition for $\hat{\rho}$ to correspond to a pure case. For a pure case, we must have $\hat{\rho}^2 = \hat{\rho}$. Taking the trace of $\hat{\rho}^2 = \hat{\rho}$ and making use of $\operatorname{Tr}\hat{\rho} = 1$, we have

$$\operatorname{Tr}\hat{\rho}^2 = \operatorname{Tr}\hat{\rho} = 1.$$

Therefore, $\operatorname{Tr}\hat{\rho}^2 = 1$ is the necessary condition for $\hat{\rho}$ to correspond to a pure case.

We now show that $\mathrm{Tr}\,\hat{\rho}^2 = 1$ is also the sufficient condition for $\hat{\rho}$ to correspond to a pure case. If $\mathrm{Tr}\,\hat{\rho}^2 = 1$, we have

$$\langle\hat{\rho}\rangle = \mathrm{Tr}\,\hat{\rho}^2 = 1.$$

Assume that $\hat{\rho}$ is the density operator of a statistical mixture of the orthogonal states $|\psi_1\rangle$, $|\psi_2\rangle$, $\cdots$ with the weights p_1, p_2, $\cdots$. From the above-obtained result that $\langle\hat{\rho}\rangle = 1$, we have

$$\sum_k p_k \langle\psi_k|\hat{\rho}|\psi_k\rangle = 1.$$

Inserting $\hat{\rho} = \sum_{k'} p_{k'} |\psi_{k'}\rangle\langle\psi_{k'}|$ into the left hand side of the above equation yields

$$\sum_{kk'} p_k p_{k'} \langle\psi_k|\psi_{k'}\rangle\langle\psi_{k'}|\psi_k\rangle = 1.$$

Making use of $\langle\psi_k|\psi_{k'}\rangle = \delta_{kk'}$, we have

$$\sum_{kk'} p_k p_{k'} \delta_{kk'}^2 = 1$$

from which it follows that

$$\sum_k p_k^2 = 1.$$

We also have

$$\sum_k p_k = 1.$$

With $0 \le p_k \le 1$ taken into consideration, the above two equations can be simultaneously satisfied only if one of p_k's is equal to 1 and all others are equal to 0. This corresponds to a pure case. Therefore, $\mathrm{Tr}\,\hat{\rho}^2 = 1$ is the sufficient condition for $\hat{\rho}$ to correspond to a pure case.