Name: 陈稼霖
StudentID: 45875852

Problem 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.

Solution:

(a) According to Ehrenfest's theorem
$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{1}{m}\langle\hat{p}_x\rangle \tag{1}$$
$$\frac{d\langle\hat{p}_x\rangle}{dt} = -\langle\vec{\nabla}\hat{V}(\hat{x})\rangle \tag{2}$$
For a free particle, $V(\hat{x})$ is a constant, so
$$\frac{d\langle\hat{p}_x\rangle}{dt} = -\langle\frac{\partial}{\partial x}\hat{V}(\hat{x})\rangle = 0 \tag{3}$$
the mean value $\langle\hat{p}_x\rangle$ remains constant. In this way,
$$\frac{d\langle\hat{\vec{r}}\rangle}{dt} = \frac{1}{m}\langle\hat{p}_x\rangle \tag{4}$$
is also a constant, so
$$\langle\hat{x}\rangle = \frac{\langle\hat{p}_x\rangle}{m}t + x_0 \tag{5}$$
$\langle\hat{x}\rangle$ is a linear function of time, where x_0 is a integration constant.

(b) The equations of motion for mean value $\langle\hat{x}^2\rangle$ is
$$\frac{d\langle\hat{x}^2\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{x}^2,\hat{H}]\rangle \tag{6}$$
Since
$$\begin{aligned}
[\hat{x}^2,\hat{H}] =& [\hat{x}^2,\frac{\hat{p}_x^2}{2m}+\hat{V}(\hat{x})] = [\hat{x}^2,\frac{\hat{p}_x^2}{2m}] + [\hat{x}^2,\hat{V}(\hat{x})]\\
=&\frac{1}{2m}\left(\hat{x}[\hat{x},\hat{p}_x^2]+[\hat{x},\hat{p}_x^2]\hat{x}\right) + (\hat{x}\hat{V}(\hat{x})-\hat{V}(\hat{x})\hat{x})\\
=&\frac{1}{2m}\left(\hat{x}(\hat{p}_x[\hat{x},\hat{p}_x]+[\hat{x},\hat{p}_x]\hat{p}_x)+(\hat{p}_x[\hat{x},\hat{p}_x]+[\hat{x},\hat{p}_x]\hat{p}_x)\hat{x}\right) + (xV(x)-V(x)x)\\
=&\frac{i\hbar}{m}(\hat{x}\hat{p}_x+\hat{p}_x\hat{x})
\end{aligned} \tag{7}$$

Name: 陈稼霖
StudentID: 45875852

we have

$$\frac{d\langle\hat{x}^2\rangle}{dt}=\frac{1}{m}\langle\hat{x}\hat{p}_x+\hat{p}_x\hat{x}\rangle \tag{8}$$

The equation of motion for mean value $\langle\hat{x}\hat{p}_x+\hat{p}_x\hat{x}\rangle$ is

$$\frac{d\langle\hat{x}\hat{p}_x+\hat{p}_x\hat{x}\rangle}{dt}=\frac{1}{i\hbar}\langle[\hat{x}\hat{p}_x+\hat{p}_x\hat{x},\hat{H}]\rangle \tag{9}$$

Since

$$\begin{aligned}
[\hat{x}\hat{p}_x+\hat{p}_x\hat{x},\hat{H}]=&[\hat{x}\hat{p}_x+\hat{p}_x\hat{x},\frac{\hat{p}^2}{2m}+\hat{V}(\hat{x})]\\
=&[\hat{x}\hat{p}_x,\frac{\hat{p}_x^2}{2m}]+[\hat{p}_x\hat{x},\frac{\hat{p}_x^2}{2m}]+[\hat{x}\hat{p}_x,\hat{V}(\hat{x})]+[\hat{p}_x\hat{x},\hat{V}(\hat{x})]\\
=&\frac{1}{2m}[\hat{x}\hat{p}_x,\hat{p}_x^2]+\frac{1}{2m}[\hat{p}_x\hat{x},\hat{p}_x^2]\\
&+(\hat{x}\hat{p}_x\hat{V}(\hat{x})-\hat{V}(\hat{x})\hat{x}\hat{p}_x)+(\hat{p}_x\hat{x}\hat{V}(\hat{x})-\hat{V}(\hat{x})\hat{p}_x\hat{x})\\
=&\frac{1}{2m}\left(\hat{x}[\hat{p}_x,\hat{p}_x^2]+[\hat{x},\hat{p}_x^2]\hat{p}_x+\hat{p}_x[\hat{x},\hat{p}_x^2]+[\hat{p}_x,\hat{p}_x^2]\hat{x}\right)\\
=&\frac{1}{2m}\left(\hat{x}(\hat{p}_x[\hat{p}_x,\hat{p}_x]+[\hat{p}_x,\hat{p}_x]\hat{p}_x)+(\hat{p}_x[\hat{x},\hat{p}_x]+[\hat{x},\hat{p}_x]\hat{p}_x)\hat{p}_x\right.\\
&\left.+\hat{p}_x(\hat{p}_x[\hat{x},\hat{p}_x]+[\hat{x},\hat{p}_x]\hat{p}_x)+(\hat{p}_x[\hat{p}_x,\hat{p}_x]+[\hat{p}_x,\hat{p}_x]\hat{p}_x)\hat{x}\right)\\
=&\frac{2i\hbar}{m}\hat{p}_x^2
\end{aligned} \tag{10}$$

we have

$$\frac{d\langle\hat{x}\hat{p}_x+\hat{p}_x\hat{x}\rangle}{dt}=\frac{2}{m}\langle\hat{p}_x^2\rangle \tag{11}$$

The equation of motion of the mean value $\langle\hat{p}_x^2\rangle$ is

$$\frac{d\langle\hat{p}_x^2\rangle}{dt}=\frac{1}{i\hbar}\langle[\hat{p}_x^2,\hat{H}]\rangle \tag{12}$$

Since

$$\begin{aligned}
[\hat{p}_x^2,\hat{H}]=&[\hat{p}_x^2,\frac{\hat{p}_x^2}{2m}+\hat{V}(\hat{x})]\\
=&\frac{1}{2m}[\hat{p}_x^2,\hat{p}_x^2]+[\hat{p}_x^2,\hat{V}(\hat{x})]\\
=&0
\end{aligned} \tag{13}$$

we have

$$\frac{d\langle\hat{p}_x^2\rangle}{dt}=0 \tag{14}$$

so $\langle\hat{p}_x^2\rangle$ is a constant.
Using this fact, integrate the equation of motion for the mean value $\langle\hat{x}\hat{p}_x+\hat{p}_x\hat{x}\rangle$ to get

$$\langle\hat{x}\hat{p}_x+\hat{p}_x\hat{x}\rangle=\frac{2\langle\hat{p}_x^2\rangle}{m}t+\langle\hat{x}\hat{p}_x+\hat{p}_x\hat{x}\rangle|_{t=0} \tag{15}$$

where $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle|_{t=0}$ is a integration constant.

Using the conclusion above, we have

$$\frac{d\langle \hat{x}^2\rangle}{dt} = \frac{2\langle \hat{p}_x^2\rangle}{m^2}t + \frac{\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle|_{t=0}}{m} \tag{16}$$

Integrate the equation of motion for the mean value $\langle \hat{x}^2\rangle$ to get

$$\langle \hat{x}^2\rangle = \frac{\langle \hat{p}_x^2\rangle}{m^2}t^2 + \frac{\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle|_{t=0}}{m}t + \langle \hat{x}^2\rangle\big|_{t=0} \tag{17}$$

where $\langle \hat{x}^2\rangle|_{t=0}$ is another integration constant.

(c) The root-mean square deviation Δx can be written as

$$(\Delta x)^2 = \langle \hat{x}^2\rangle - \langle \hat{x}\rangle^2 \tag{18}$$

where, using the conclusion obtained for last question

$$\langle \hat{x}^2\rangle = \frac{\langle \hat{p}_x^2\rangle}{m^2}t^2 + \frac{\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle|_{t=0}}{m}t + \langle \hat{x}^2\rangle\big|_{t=0} \tag{19}$$

and using the conclusion for (a)

$$\langle \hat{x}\rangle = \frac{\langle \hat{p}_x\rangle}{m}t + x_0 \tag{20}$$

Suitably choosing the time origin to make $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x}\rangle|_{t=0} = 2\langle \hat{p}_x\rangle x_0$, then

$$(\Delta x)^2 = \frac{\langle \hat{p}_x^2\rangle - \langle \hat{p}_x\rangle^2}{m^2}t^2 + \langle \hat{x}^2\rangle\big|_{t=0} - x_0^2 = \frac{1}{m^2}(\Delta p_x)_0^2 t^2 + (\Delta x)_0^2, \tag{21}$$

where constant $(\Delta x)_0^2 = \langle \hat{x}^2\rangle|_{t=0} - x_0^2$.

According to the equation derived above, the width of the wave packet is a monotonically increasing function of time.

Physcial interpretation: the group velocity of the particle is different from its phase particle, making the probability density for finding the particle diffuse in the space as it spreads.

□

Problem 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 $\frac{\partial}{\partial t}|\langle p_x|\psi(t)\rangle|^2$ and $\frac{\partial}{\partial p_x}|\langle p_x|\psi(t)\rangle|^2$. Integrate the equation thus obtained; give a physical interpretation.

Solution:

(a) According to Ehrenfest's theorem, the mean value for the position satisfies

$$\frac{d\langle\hat{x}\rangle}{dt}=\frac{1}{m}\langle\hat{p}_x\rangle \tag{22}$$

The mean value for the momentum satisfies

$$\frac{d\langle\hat{p}_x\rangle}{dt}=-\langle\frac{\partial}{\partial x}\hat{V}(\hat{x})\rangle=f \tag{23}$$

Integrate the equation above to get

$$\langle\hat{p}_x\rangle=ft+\langle\hat{p}_x\rangle|_{t=0} \tag{24}$$

where $\langle\hat{p}_x\rangle|_{t=0}$ is an integration constant. Plug the equation above into the first equation in this solution to get

$$\frac{d\langle\hat{x}\rangle}{dt}=\frac{ft+\langle\hat{p}_x\rangle|_{t=0}}{m} \tag{25}$$

Intergrate the equation above to get

$$\langle\hat{x}\rangle=\frac{f}{2m}t^2+\frac{\langle\hat{p}_x\rangle|_{t=0}}{m}t+\langle\hat{x}\rangle|_{t=0} \tag{26}$$

where $\langle\hat{x}\rangle|_{t=0}$ is an integration constant.

The equations obtained from integration can depict the classical motion in an uniform potential field well, such as that momentum is a linear function about the time and the position quadratic function.

(b) According to Ehrenfest theorem, the mean value of the square of the momentum satisfies

$$\frac{d\langle\hat{p}_x\rangle}{dt}=\frac{1}{i\hbar}\langle[\hat{p}_x^2,\hat{H}]\rangle \tag{27}$$

Since

$$\begin{aligned}
[\hat{p}_x^2,\hat{H}]\psi=&\left([\hat{p}_x^2,\frac{\hat{p}_x^2}{2m}+\hat{V}(\hat{x})]\right)\psi\\
=&\left(\frac{1}{2m}[\hat{p}_x^2,\hat{p}_x^2]+[\hat{p}_x^2,\hat{V}(\hat{x})]\right)\psi\\
=&\left(\hat{p}_x^2\hat{V}(\hat{x})-\hat{V}(\hat{x})\hat{p}_x^2\right)\psi\\
=&\left(-\hbar^2\frac{d^2}{dx^2}(-fx)-(-fx)(-\hbar^2)\frac{d^2}{dx^2}\right)\psi\\
=&2\hbar^2f\frac{d}{dx}\psi
\end{aligned} \tag{28}$$

$$\Longrightarrow[\hat{p}_x^2,\hat{H}]=2\hbar^2f\frac{d}{dx}=2i\hbar f\hat{p}_x \tag{29}$$

we have

$$\frac{d\langle\hat{p}_x^2\rangle}{dt} = 2f\langle\hat{p}_x\rangle = 2f(ft + \langle\hat{p}_x\rangle|_{t=0}) \tag{30}$$

so the mean value of the momentum of is

$$\langle\hat{p}_x^2\rangle = ft^2 + 2f\ \langle\hat{p}_x\rangle|_{t=0}\, t + \langle\hat{p}_x^2\rangle\big|_{t=0} \tag{31}$$

where the integration constant $\langle\hat{p}_x^2\rangle|_{t=0} = [\langle\hat{p}_x\rangle|_{t=0}]^2$.
Therefore, the root-mean-square deviation of the momentum is

$$\Delta p_x = \sqrt{\langle\hat{p}_x^2\rangle - \langle\hat{p}_x\rangle^2} = 0 \tag{32}$$

which does not vary over time.

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

$$i\hbar\frac{\partial}{\partial t}\bar{\psi}(p_x,t) = \left[\frac{p_x^2}{2m} + \hat{V}(i\hbar\frac{d}{dx})\right]\bar{\psi}(p_x,t) \tag{33}$$

where $\bar{\psi}(p_x,t)$ is the wave function in the momentum representation.
In the potential energy $\hat{V}(\hat{x}) = -f\hat{x}$, the Schrödinger equation can be written as

$$i\hbar\frac{\partial}{\partial t}\bar{\psi}(p_x,t) = \left(\frac{p_x^2}{2m} - i\hbar f\frac{\partial}{\partial p_x}\right)\bar{\psi}(p_x,t) \tag{34}$$

Using the equation above,

$$\begin{aligned}
\frac{\partial}{\partial t}|\bar{\psi}(p_x,t)|^2 =& \bar{\psi}^*(p_x,t)\frac{\partial\psi(\bar{p_x},t)}{\partial t} + \bar{\psi}(p_x,t)\frac{\partial\bar{\psi}^*(p_x,t)}{\partial t}\\
=& -\bar{\psi}^*(p_x,t)\left(\frac{ip_x^2}{2m\hbar} + f\frac{\partial}{\partial p_x}\right)\bar{\psi}(p_x,t) + \bar{\psi}(p_x,t)\\
&+ \bar{\psi}(p_x,t)\left(\frac{ip_x^2}{2m\hbar} - f\frac{\partial}{\partial p_x}\right)\bar{\psi}^*(p_x,t)\\
=& -f\left(\bar{\psi}^*(p_x,t)\frac{\partial\bar{\psi}(p_x,t)}{\partial p_x} + \bar{\psi}(p_x,t)\frac{\partial\bar{\psi}^*(p_x,t)}{\partial p_x}\right)\\
=& -f\frac{\partial}{\partial p_x}|\bar{\psi}(p_x,t)|^2
\end{aligned} \tag{35}$$

Let

$$r = p - ft \tag{36}$$

$$s = p + ft \tag{37}$$

then

$$\frac{\partial|\bar{\psi}(p_x,t)|^2}{\partial p} = \frac{\partial|\bar{\psi}(p_x,t)|^2}{\partial r} + \frac{\partial|\bar{\psi}(p_x,t)|^2}{\partial s} \tag{38}$$

$$\frac{\partial|\bar{\psi}(p_x,t)|^2}{\partial t} = -f\frac{\partial|\bar{\psi}(p_x,t)|^2}{\partial r} + f\frac{\partial|\bar{\psi}(p_x,t)|^2}{\partial s} \tag{39}$$

Name: 陈稼霖
StudentID: 45875852

so

$$\frac{\partial|\bar{\psi}(p_x,t)|^2}{\partial s}=0 \tag{40}$$

which means that $|\bar{\psi}(p_x,t)|^2$ is a function of r along

$$|\bar{\psi}(p_x,t)|^2=P(p-ft) \tag{41}$$

where P is an arbitrary function and

$$|\bar{\psi}(p_x,t)|^2=|\bar{\psi}(p_x-ft,0)|^2 \tag{42}$$

Physical interpretation: the probability density in momentum representation moves according to the classical equation of motion, $p=p_0+ft$.

Reference: http://scipp.ucsc.edu/∼haber/ph215/QMsol18_2.pdf □

Problem 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 $\vec{B}=\vec{\nabla}\times\vec{A}(\vec{r})$. Show that

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

Solution:

(a) The probability current is

$$\begin{aligned}
\vec{J}(\vec{r}) =& \frac{\hbar}{2im}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*)\\
=& \frac{\hbar}{2im}\left(\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\vec{\nabla}\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})} - \sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}\vec{\nabla}\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\right)\\
=& \frac{\hbar}{2im}\left[\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\left(e^{i\xi(\vec{r})}\vec{\nabla}\sqrt{\rho(\vec{r})} + \sqrt{\rho(\vec{r})}\vec{\nabla}e^{i\xi(\vec{r})}\right)\right.\\
&\left.-\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}\left(e^{-i\xi(\vec{r})}\vec{\nabla}\sqrt{\rho(\vec{r})} + \sqrt{\rho(\vec{r})}\vec{\nabla}e^{-i\xi(\vec{r})}\right)\right]\\
=& \frac{\hbar}{2im}\left[\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\left(e^{i\xi(\vec{r})}\frac{\vec{\nabla}\rho(\vec{r})}{2\sqrt{\rho(\vec{r})}} + \sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}i\vec{\nabla}\xi(\vec{r})\right)\right.\\
&\left.-\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}\left(e^{-i\xi(\vec{r})}\frac{\vec{\nabla}\rho(\vec{r})}{2\sqrt{\rho(\vec{r})}} + \sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}(-i\vec{\nabla}\xi(\vec{r}))\right)\right]\\
=& \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\xi(\vec{r})
\end{aligned} \tag{43}$$

For a wave function with the same density $\rho(\vec{r}) = |\psi(\vec{r})|^2$ differing by a global phase vector

$$\varphi(\vec{r}) = \psi(\vec{r})e^{i\psi} = \sqrt{\rho(\vec{r})}e^{i[\xi(\vec{r})+\phi]} \tag{44}$$

its probability

$$\begin{aligned}
\vec{J}_1(\vec{r}) =& \frac{\hbar}{2im}(\varphi^*\vec{\nabla}\varphi - \varphi\vec{\nabla}\varphi^*)\\
=& \frac{\hbar}{2im}\left(\sqrt{\rho(\vec{r})}e^{-i[\xi(\vec{r})+\phi(\vec{r})]}\vec{\nabla}\sqrt{\rho(\vec{r})}e^{i[\xi(\vec{r})+\phi]} - \sqrt{\rho(\vec{r})}e^{i[\xi(\vec{r})+\phi]}\vec{\nabla}\sqrt{\rho(\vec{r})}e^{-i[\xi(\vec{r})+\phi]}\right)\\
=& \frac{\hbar}{2im}\left[\sqrt{\rho(\vec{r})}e^{-i[\xi(\vec{r})+\phi]}\left(e^{i[\xi(\vec{r})+\phi]}\vec{\nabla}\sqrt{\rho(\vec{r})} + \sqrt{\rho(\vec{r})}\vec{\nabla}e^{i[\xi(\vec{r})+\phi]}\right)\right.\\
&\left.-\sqrt{\rho(r)}e^{i[\xi(\vec{r})+\phi]}\left(e^{-i[\xi(\vec{r})+\phi]}\vec{\nabla}\sqrt{\rho(\vec{r})} + \sqrt{\rho(\vec{r})}\vec{\nabla}e^{-i[\xi(\vec{r})+\phi]}\right)\right]\\
=& \frac{\hbar}{2im}\left[\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\left(e^{i[\xi(\vec{r})+\phi]}\frac{\vec{\nabla}\rho(\vec{r})}{2\sqrt{\rho(\vec{r})}} + \sqrt{\rho(\vec{r})}e^{i[\xi(\vec{r})+\phi]i\vec{\nabla}\xi(\vec{r})}\right)\right.\\
&\left.-\sqrt{\rho(\vec{r})}\left(e^{-i[\xi(\vec{r})+\phi]}\frac{\vec{\nabla}\rho(\vec{r})}{2\sqrt{\rho(\vec{r})}} + \sqrt{\rho(\vec{r})}e^{-i[\xi(\vec{r})+\phi]}(-i\vec{\nabla}\xi(\vec{r}))\right)\right]\\
=& \frac{\hbar}{m}\rho(\vec{r})\vec{\nabla}\xi(\vec{r})
\end{aligned} \tag{45}$$

is the same as $\psi(\vec{r})$'s.

Therefore, two wave functions leading to the same density and current can differ only by a global phase factor

(b) For an arbitrary wave function $\psi(\vec{r})$,

$$\vec{\nabla}\times\vec{v}(\vec{r}) = \nabla\times\frac{\hbar}{m}\vec{\nabla}\xi(\vec{r}) = 0$$

Therefore, a quantum state $\psi(\vec{r})$ can be associated withe $\rho(\vec{r})$ and $\vec{J}(\vec{r})$ only if $\vec{\nabla}\times\vec{v}(\vec{r}) = 0$.

Name: 陈稼霖
StudentID: 45875852

(c) In the magnetic field $\vec{B} = \vec{\nabla} \times \vec{A}(\vec{r})$, the probability current is

$$\begin{aligned}\vec{J}(\vec{r},t) =& \frac{\hbar}{2m}\left\{\psi^*(\vec{r},t)[-i\hbar\vec{\nabla} - q\vec{A}(\vec{r})]\psi(\vec{r},t) - \psi(\vec{r},t)[-i\hbar\vec{\nabla} - q\vec{A}(\vec{r})]\psi^*(\vec{r},t)\right\}\\ =& \frac{\hbar}{2m}\left\{\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}[-i\hbar\vec{\nabla} - q\vec{A}(\vec{r})]\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}\right.\\ &\left.-\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}[-i\hbar\vec{\nabla} - q\vec{A}(\vec{r})]\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\right\}\\ =& \frac{\hbar}{2m}\left\{\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\left[-i\hbar e^{i\xi(\vec{r})}\frac{\vec{\nabla}\rho(\vec{r})}{2\sqrt{\rho(\vec{r})}} - i\hbar\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}i\vec{\nabla}\xi(\vec{r}) - q\vec{A}\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}\right]\right.\\ &\left.-\sqrt{\rho(\vec{r})}e^{i\xi(\vec{r})}\left[-i\hbar e^{-i\xi(\vec{r})}\frac{\vec{\nabla}\rho(\vec{r})}{2\sqrt{\rho(\vec{r})}} - i\hbar\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}(-i\vec{\nabla}\xi(\vec{r})) - q\vec{A}\sqrt{\rho(\vec{r})}e^{-i\xi(\vec{r})}\right]\right\}\\ =& \frac{\rho(\vec{r})}{m}[\hbar\vec{\nabla}\xi(\vec{r}) - q\vec{A}(\vec{r})]\end{aligned} \tag{46}$$

The curl of the velocity is

$$\vec{\nabla} \times \vec{v}(\vec{r}) = \nabla \times \frac{\vec{J}(\vec{r})}{\rho(\vec{r})} = \frac{1}{m}\nabla \times [\hbar\vec{\nabla}\xi(\vec{r}) - q\vec{A}(\vec{r})] = -\frac{q}{m}\vec{\nabla} \times \vec{A}(\vec{r}) = -\frac{q}{m}\vec{B}(\vec{r}) \tag{47}$$

□

Problem 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 $|\varphi_n(1)\rangle \otimes |\varphi_q(2)\rangle$.

(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 $\rho(0)$ 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?

Solution:

(a) The eigenstates of the operator $\hat{H}=\hat{H}(1)+\hat{H}(2)$ are

$$|\varphi_n\varphi_q\rangle = |\varphi_n(1)\rangle\otimes|\varphi_q(2)\rangle \tag{48}$$

The eigenequation are

$$\hat{H}|\varphi_n\varphi_q\rangle = [\hat{H}(1)1(2)+1(1)\hat{H}(2)]|\varphi_n(1)\rangle\otimes|\varphi_q(2)\rangle = \left[\frac{n^2\pi^2\hbar^2}{2ma^2}+\frac{q^2\pi^2\hbar^2}{2ma^2}\right]|\varphi_n(1)\rangle\otimes|\varphi_q(2)\rangle \tag{49}$$

so the eigenvalues are

$$\frac{n^2\pi^2\hbar^2}{2ma^2}+\frac{q^2\pi^2\hbar^2}{2ma^2}, \quad n=1,2,3,\cdots,q=1,2,3,\cdots \tag{50}$$

The eigenvalue of the lowest energy level

$$\frac{1^2\pi^2\hbar^2}{2ma^2}+\frac{1^2\pi^2\hbar^2}{2ma^2}=\frac{\pi^2\hbar^2}{ma^2} \tag{51}$$

requires

$$n=1, q=1 \tag{52}$$

so the degree of degeneracy of the lowest energy level is 1.

The eigenvalue of the second lowest energy level

$$\frac{1^2\pi^2\hbar^2}{2ma^2}+\frac{2^2\pi^2\hbar^2}{2ma^2}=\frac{5\pi^2\hbar^2}{ma^2} \tag{53}$$

requires

$$n=1,q=2 \text{ or } n=2,q=1 \tag{54}$$

so the degree of degeneracy of the second lowest energy level is 2.

(b) i. The state of the system at time $t=0$ is

$$|\psi(0)\rangle=\frac{1}{\sqrt{6}}|\varphi_1(1)\rangle\otimes|\varphi_1(2)\rangle+\frac{1}{\sqrt{3}}|\varphi_1(1)\rangle\otimes|\varphi_2(2)\rangle+\frac{1}{\sqrt{6}}|\varphi_2(1)\rangle\otimes|\varphi_1(2)\rangle+\frac{1}{\sqrt{3}}|\varphi_2(1)\rangle\otimes|\varphi_2(2)\rangle \tag{55}$$

The state of the system at time t is

$$\begin{aligned}|\psi(t)\rangle=&\frac{1}{\sqrt{6}}e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(1)\rangle\otimes e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(2)\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(1)\rangle\otimes e^{-i\frac{2\pi^2\hbar^2}{ma^2}t/\hbar}|\varphi_2(2)\rangle\\&+\frac{1}{\sqrt{6}}e^{-i\frac{2\pi^2\hbar^2}{ma^2}t/\hbar}|\varphi_2(1)\rangle\otimes e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(2)\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{2\pi^2\hbar^2}{ma^2}t/\hbar}|\varphi_2(1)\rangle\otimes e^{-i\frac{2\pi^2\hbar^2}{ma^2}t/\hbar}|\varphi_2(2)\rangle\\=&\frac{1}{\sqrt{6}}e^{-i\frac{2\pi^2\hbar}{2ma^2}t}|\varphi_1(1)\rangle\otimes|\varphi_1(2)\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_1(1)\rangle\otimes|\varphi_2(2)\rangle\\&+\frac{1}{\sqrt{6}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_2(1)\rangle\otimes|\varphi_1(2)\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{4\pi^2\hbar}{ma^2}t}|\varphi_2(1)\rangle\otimes|\varphi_2(2)\rangle\\=&\frac{1}{\sqrt{6}}e^{-i\frac{2\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_2\rangle+\frac{1}{\sqrt{6}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_2\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{4\pi^2\hbar}{ma^2}t}|\varphi_2\varphi_2\rangle\end{aligned} \tag{56}$$

ii. The possible measure results for $\hat{H}$ and their corresponding probabilities are shown in the table below

Results	Probabilities
$\frac{\pi^2\hbar^2}{ma^2}$	$\frac{1}{6}$
$\frac{5\pi^2\hbar^2}{2ma^2}$	$\frac{1}{2}$
$\frac{4\pi^2\hbar^2}{ma^2}$	$\frac{1}{3}$

iii. The possible measure results for $\hat{H}(1)$ and their corresponding probabilities are shown in the table below

Results	Probabilities
$\frac{\pi^2\hbar^2}{2ma^2}$	$\frac{1}{2}$
$\frac{2\pi^2\hbar^2}{ma^2}$	$\frac{1}{2}$

(c) i. $|\psi(0)\rangle$ is a tensor product state:

$$|\psi(0)\rangle=\left(\frac{1}{\sqrt{2}}|\psi_1(1)\rangle+\frac{1}{\sqrt{2}}|\psi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}|\psi_1(1)\rangle+\frac{\sqrt{2}}{\sqrt{3}}|\psi_2(2)\rangle\right) \tag{57}$$

When the system is in this state,

$$\begin{aligned}
\langle\hat{H}(1)\rangle =&\langle\varphi(0)|\hat{H}(1)|\varphi(0)\rangle\\
=&\left(\frac{1}{\sqrt{2}}\langle\varphi_1(1)|+\frac{1}{\sqrt{2}}\langle\varphi_2(1)|\right)\otimes\left(\frac{1}{\sqrt{3}}\langle\varphi_1(1)|+\frac{\sqrt{2}}{\sqrt{3}}\langle\varphi_2(2)|\right)\hat{H}(1)1(2)\\
&\left(\frac{1}{\sqrt{2}}|\varphi_1(1)\rangle+\frac{1}{\sqrt{2}}|\varphi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}|\varphi_1(1)\rangle+\frac{\sqrt{2}}{\sqrt{3}}|\varphi_2(2)\rangle\right)\\
=&\frac{1}{2}\frac{\pi^2\hbar^2}{2ma^2}+\frac{1}{2}\frac{2\pi^2\hbar^2}{ma^2}=\frac{5\pi^2\hbar^2}{4ma^2}
\end{aligned}$$

$$\begin{aligned}
\langle\hat{H}(2)\rangle =&\langle\psi(0)|\hat{H}(2)|\psi(0)\rangle\\
=&\left(\frac{1}{\sqrt{2}}\langle\psi_1(1)|+\frac{1}{\sqrt{2}}\langle\psi_2(1)|\right)\otimes\left(\frac{1}{\sqrt{3}}\langle\psi_1(1)|+\frac{\sqrt{2}}{\sqrt{3}}\langle\psi_2(2)|\right)1(1)\hat{H}(2)\\
&\left(\frac{1}{\sqrt{2}}|\psi_1(1)\rangle+\frac{1}{\sqrt{2}}|\psi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}|\psi_1(1)\rangle+\frac{\sqrt{2}}{\sqrt{3}}|\psi_2(2)\rangle\right)\\
=&\frac{1}{3}\frac{\pi^2\hbar^2}{2ma^2}+\frac{2}{3}\frac{2\pi^2\hbar^2}{ma^2}=\frac{3\pi^2\hbar^2}{2ma^2}
\end{aligned}$$

$$\begin{aligned}
&\langle\hat{H}(1)\hat{H}(2)\rangle=\langle\psi(0)|\hat{H}(1)\hat{H}(2)|\psi(0)\rangle\\
=&\left(\frac{1}{\sqrt{2}}\langle\psi_1(1)|+\frac{1}{\sqrt{2}}\langle\psi_2(1)|\right)\otimes\left(\frac{1}{\sqrt{3}}\langle\psi_1(1)|+\frac{\sqrt{2}}{\sqrt{3}}\langle\psi_2(2)|\right)\hat{H}(1)\hat{H}(2)\\
&\left(\frac{1}{\sqrt{2}}|\psi_1(1)\rangle+\frac{1}{\sqrt{2}}|\psi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}|\psi_1(1)\rangle+\frac{\sqrt{2}}{\sqrt{3}}|\psi_2(2)\rangle\right)\\
=&\left(\frac{1}{\sqrt{2}}\langle\psi_1(1)|+\frac{1}{\sqrt{2}}\langle\psi_2(1)|\right)\otimes\left(\frac{1}{\sqrt{3}}\langle\psi_1(1)|+\frac{\sqrt{2}}{\sqrt{3}}\langle\psi_2(2)|\right)\hat{H}(1)\\
&\left(\frac{1}{\sqrt{2}}|\psi_1(1)\rangle+\frac{1}{\sqrt{2}}|\psi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}\frac{\pi^2\hbar^2}{2ma^2}|\psi_1(1)\rangle+\frac{\sqrt{2}}{\sqrt{3}}\frac{2\pi^2\hbar^2}{ma^2}|\psi_2(2)\rangle\right)\\
=&\left(\frac{1}{\sqrt{2}}\langle\psi_1(1)|+\frac{1}{\sqrt{2}}\langle\psi_2(1)|\right)\otimes\left(\frac{1}{\sqrt{3}}\langle\psi_1(1)|+\frac{\sqrt{2}}{\sqrt{3}}\langle\psi_2(2)|\right)\\
&\left(\frac{1}{\sqrt{2}}\frac{\pi^2\hbar^2}{2ma^2}|\psi_1(1)\rangle+\frac{1}{\sqrt{2}}\frac{2\pi^2\hbar^2}{ma^2}|\psi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}\frac{\pi^2\hbar^2}{2ma^2}|\psi_1(1)\rangle+\frac{\sqrt{2}}{\sqrt{3}}\frac{2\pi^2\hbar^2}{ma^2}|\psi_2(2)\rangle\right)\\
=&\frac{15}{8}\left(\frac{\pi^2\hbar^2}{ma^2}\right)^2
\end{aligned}\tag{58}$$

$$\langle\hat{H}(1)\rangle\langle\hat{H}(2)\rangle=\langle\hat{H}(2)\hat{H}(1)\rangle\tag{59}$$

Explanation: Since the two particles (1) and (2) do not interact with each other, their Hamiltonians are independent.

ii. At time t,

$$\begin{aligned}\langle\hat{H}(1)\rangle=&\left(\frac{1}{\sqrt{6}}e^{i\frac{2\pi^2\hbar}{2ma^2}t}\langle\varphi_1\varphi_1|+\frac{1}{\sqrt{3}}e^{i\frac{5\pi^2\hbar}{2ma^2}t}\langle\varphi_1\varphi_2|+\frac{1}{\sqrt{6}}e^{i\frac{5\pi^2\hbar}{2ma^2}t}\langle\varphi_2\varphi_1|+\frac{1}{\sqrt{3}}e^{i\frac{4\pi^2\hbar}{ma^2}t}\langle\varphi_2\varphi_2|\right)\hat{H}(1)\\&\left(\frac{1}{\sqrt{6}}e^{-i\frac{2\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_2\rangle+\frac{1}{\sqrt{6}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_2\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{4\pi^2\hbar}{ma^2}t}|\varphi_2\varphi_2\rangle\right)\\=&\frac{1}{6}\frac{\pi^2\hbar^2}{2ma^2}+\frac{1}{3}\frac{\pi^2\hbar^2}{2ma^2}+\frac{1}{6}\frac{2\pi^2\hbar^2}{ma^2}+\frac{1}{3}\frac{2\pi^2\hbar^2}{ma^2}=\frac{5}{4}\frac{\pi^2\hbar^2}{ma^2}\end{aligned}\tag{60}$$

$$\begin{aligned}\langle\hat{H}(2)\rangle=&\left(\frac{1}{\sqrt{6}}e^{i\frac{2\pi^2\hbar}{2ma^2}t}\langle\varphi_1\varphi_1|+\frac{1}{\sqrt{3}}e^{i\frac{5\pi^2\hbar}{2ma^2}t}\langle\varphi_1\varphi_2|+\frac{1}{\sqrt{6}}e^{i\frac{5\pi^2\hbar}{2ma^2}t}\langle\varphi_2\varphi_1|+\frac{1}{\sqrt{3}}e^{i\frac{4\pi^2\hbar}{ma^2}t}\langle\varphi_2\varphi_2|\right)\hat{H}(2)\\&\left(\frac{1}{\sqrt{6}}e^{-i\frac{2\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_2\rangle+\frac{1}{\sqrt{6}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_2\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{4\pi^2\hbar}{ma^2}t}|\varphi_2\varphi_2\rangle\right)\\=&\frac{1}{6}\frac{\pi^2\hbar^2}{2ma^2}+\frac{1}{3}\frac{2\pi^2\hbar^2}{ma^2}+\frac{1}{6}\frac{\pi^2\hbar^2}{2ma^2}+\frac{1}{3}\frac{2\pi^2\hbar^2}{ma^2}=\frac{3\pi^2\hbar^2}{2ma^2}\end{aligned}\tag{61}$$

$$\begin{aligned}\langle\hat{H}(1)\hat{H}(2)\rangle=&\left(\frac{1}{\sqrt{6}}e^{i\frac{2\pi^2\hbar}{2ma^2}t}\langle\varphi_1\varphi_1|+\frac{1}{\sqrt{3}}e^{i\frac{5\pi^2\hbar}{2ma^2}t}\langle\varphi_1\varphi_2|+\frac{1}{\sqrt{6}}e^{i\frac{5\pi^2\hbar}{2ma^2}t}\langle\varphi_2\varphi_1|+\frac{1}{\sqrt{3}}e^{i\frac{4\pi^2\hbar}{ma^2}t}\langle\varphi_2\varphi_2|\right)\hat{H}(1)\hat{H}(2)\\&\left(\frac{1}{\sqrt{6}}e^{-i\frac{2\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_2\rangle+\frac{1}{\sqrt{6}}e^{-i\frac{5\pi^2\hbar}{2ma^2}t}|\varphi_2\varphi_1\rangle+\frac{1}{\sqrt{3}}e^{-i\frac{4\pi^2\hbar}{ma^2}t}|\varphi_2\varphi_2\rangle\right)\\=&\left(\frac{1}{6}\times\frac{1}{2}\times\frac{1}{2}+\frac{1}{3}\times\frac{1}{2}\times2+\frac{1}{6}\times2\times\frac{1}{2}+\frac{1}{3}\times2\times2\right)\left(\frac{\pi^2\hbar^2}{ma^2}\right)=\frac{15}{8}\left(\frac{\pi^2\hbar^2}{ma^2}\right)\end{aligned}\tag{62}$$

Still,

$$\langle\hat{H}(1)\rangle\langle\hat{H}(2)\rangle=\langle\hat{H}(2)\hat{H}(1)\rangle\tag{63}$$

Therefore, the preceding results remain valid when the state is the state $|\psi(t)\rangle$ calculated in (b).

(d) i. Assume that $|\psi(0)\rangle$ can be put in the form of a tensor product

$$|\psi(0)\rangle=\sum_i a_i|\varphi_i(1)\rangle\otimes\sum_j b_j|\varphi_j(2)\rangle=\sum_{i,j}a_ib_j|\varphi_i(1)\rangle\otimes|\varphi_j(2)\rangle=\sum_{i,j}a_ib_j|\varphi_i\varphi_j\rangle\tag{64}$$

where

$$\sum_i|a_i|^2=1\tag{65}$$

$$\sum_j|b_j|^2=1\tag{66}$$

If so,

$$a_1b_1=\sqrt{\frac{1}{5}}\tag{67}$$

$$a_1b_2=\sqrt{\frac{3}{5}}\tag{68}$$

$$a_2b_1=\sqrt{\frac{1}{5}}\tag{69}$$

$$a_ib_j=0\quad(\text{for } i\neq1,j\neq1)\tag{70}$$

Name: 陈稼霖
StudentID: 45875852

From equation (68) and (69), we know

$$a_2 \neq 0, \quad b_2 \neq 0 \tag{71}$$

which means

$$a_2 b_2 \neq 0 \tag{72}$$

contradicting equation (70).

Therefore, the assumption above is incorrect and $|\psi(0)\rangle$ cannot be put in the form of a tensor product.

When the system is in this state,

$$\begin{aligned}
\langle \hat{H}(1) \rangle =& \left(\frac{1}{\sqrt{5}} \langle \varphi_1 \varphi_1 | + \sqrt{\frac{3}{5}} \langle \varphi_1 \varphi_2 | + \frac{1}{\sqrt{5}} \langle \varphi_2 \varphi_1 | \right) \hat{H}(1) \\
& \left(\frac{1}{\sqrt{5}} | \varphi_1 \varphi_1 \rangle + \sqrt{\frac{3}{5}} | \varphi_1 \varphi_2 \rangle + \frac{1}{\sqrt{5}} | \varphi_2 \varphi_1 \rangle \right) \\
=& \left(\frac{1}{\sqrt{5}} \langle \varphi_1(1) | \otimes \langle \varphi_1(2) | + \sqrt{\frac{3}{5}} \langle \varphi_1(1) | \otimes \langle \varphi_2(2) | + \frac{1}{\sqrt{5}} \langle \varphi_2(1) | \otimes \langle \varphi_1(2) | \right) \hat{H}(1) 1(2) \\
& \left(\frac{1}{\sqrt{5}} | \varphi_1(1) \rangle \otimes | \varphi_1(2) \rangle + \sqrt{\frac{3}{5}} | \varphi_1(1) \rangle \otimes | \varphi_2(2) \rangle + \frac{1}{\sqrt{5}} | \varphi_2(1) \rangle \otimes | \varphi_2(2) \rangle \right) \\
=& \frac{1}{5} \frac{\pi^2 \hbar^2}{2ma^2} + \frac{3}{5} \frac{\pi^2 \hbar^2}{2ma^2} + \frac{1}{5} \frac{2\pi^2 \hbar^2}{ma^2} = \frac{4\pi^2 \hbar^2}{5ma^2}
\end{aligned} \tag{73}$$

$$\begin{aligned}
\langle \hat{H}(2) \rangle =& \left(\frac{1}{\sqrt{5}} \langle \varphi_1 \varphi_1 | + \sqrt{\frac{3}{5}} \langle \varphi_1 \varphi_2 | + \frac{1}{\sqrt{5}} \langle \varphi_2 \varphi_1 | \right) \hat{H}(2) \\
& \left(\frac{1}{\sqrt{5}} | \varphi_1 \varphi_1 \rangle + \sqrt{\frac{3}{5}} | \varphi_1 \varphi_2 \rangle + \frac{1}{\sqrt{5}} | \varphi_2 \varphi_1 \rangle \right) \\
=& \left(\frac{1}{\sqrt{5}} \langle \varphi_1(1) | \otimes \langle \varphi_1(2) | + \sqrt{\frac{3}{5}} \langle \varphi_1(1) | \otimes \langle \varphi_2(2) | + \frac{1}{\sqrt{5}} \langle \varphi_2(1) | \otimes \langle \varphi_1(2) | \right) 1(1) \hat{H}(2) \\
& \left(\frac{1}{\sqrt{5}} | \varphi_1(1) \rangle \otimes | \varphi_1(2) \rangle + \sqrt{\frac{3}{5}} | \varphi_1(1) \rangle \otimes | \varphi_2(2) \rangle + \frac{1}{\sqrt{5}} | \varphi_2(1) \rangle \otimes | \varphi_2(2) \rangle \right) \\
=& \frac{1}{5} \frac{\pi^2 \hbar^2}{2ma^2} + \frac{3}{5} \frac{2\pi^2 \hbar^2}{ma^2} + \frac{1}{5} \frac{2\pi^2 \hbar^2}{ma^2} = \frac{17\pi^2 \hbar^2}{10ma^2}
\end{aligned} \tag{74}$$

$$\langle \hat{H}(1)\hat{H}(2)\rangle = \left(\frac{1}{\sqrt{5}}\langle\varphi_1\varphi_1| + \sqrt{\frac{3}{5}}\langle\varphi_1\varphi_2| + \frac{1}{\sqrt{5}}\langle\varphi_2\varphi_1|\right)\hat{H}(1)\hat{H}(2)$$
$$\left(\frac{1}{\sqrt{5}}|\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}}|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}}|\varphi_2\varphi_1\rangle\right)$$
$$= \left(\frac{1}{\sqrt{5}}\langle\varphi_1\varphi_1| + \sqrt{\frac{3}{5}}\langle\varphi_1\varphi_2| + \frac{1}{\sqrt{5}}\langle\varphi_2\varphi_1|\right)\hat{H}(1)$$
$$\left(\frac{1}{\sqrt{5}}\frac{\pi^2\hbar^2}{2ma^2}|\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}}\frac{2\pi^2\hbar^2}{ma^2}|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}}\frac{2\pi^2\hbar^2}{ma^2}|\varphi_2\varphi_1\rangle\right)$$
$$= \left(\frac{1}{5}\times\frac{1}{2}\times\frac{1}{2} + \frac{3}{5}\times\frac{1}{2}\times 2 + \frac{1}{5}\times 2\times\frac{1}{2}\right)\left(\frac{\pi^2\hbar^2}{ma^2}\right)^2 = \frac{17}{20}\left(\frac{\pi^2\hbar^2}{ma^2}\right) \tag{75}$$

$$\langle\hat{H}(1)\rangle\langle\hat{H}(2)\rangle \neq \langle\hat{H}(1)\hat{H}(2)\rangle \tag{76}$$

Explanation: The state $|\psi(0)\rangle$ cannot be put in the form of a tensor product, and thus, is not an existent state that satisfies that the Hamiltonians of the two particles are independent.

ii. The state at time t derived from the above-given $|\psi(0)\rangle$ is

$$|\psi(t)\rangle = \frac{1}{\sqrt{5}}e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(1)\rangle\otimes e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(2)\rangle + \frac{\sqrt{3}}{\sqrt{5}}e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(1)\rangle\otimes e^{-i\frac{2\pi^2\hbar^2}{ma^2}t/\hbar}|\varphi_2(2)\rangle$$
$$+ \frac{1}{\sqrt{5}}e^{-i\frac{2\pi^2\hbar^2}{ma^2}t/\hbar}|\varphi_2(1)\rangle\otimes e^{-i\frac{\pi^2\hbar^2}{2ma^2}t/\hbar}|\varphi_1(2)\rangle$$
$$= \frac{1}{\sqrt{5}}e^{-i\frac{\pi^2\hbar}{ma^2}t}|\varphi_1(1)\rangle\otimes|\varphi_1(2)\rangle + \frac{\sqrt{3}}{\sqrt{5}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t}|\varphi_1(1)\rangle\otimes|\varphi_2(2)\rangle + \frac{1}{\sqrt{5}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t}|\varphi_2(1)\rangle\otimes|\varphi_1(2)\rangle$$
$$= \frac{1}{\sqrt{5}}e^{-i\frac{\pi^2\hbar}{ma^2}t}|\varphi_1\varphi_1\rangle + \frac{\sqrt{3}}{\sqrt{5}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t}|\varphi_2\varphi_1\rangle \tag{77}$$

When the state is in the state $|\psi(t)\rangle$,

$$\langle\hat{H}(1)\rangle = \left(\frac{1}{\sqrt{5}}e^{i\frac{\pi^2\hbar}{ma^2}t}\langle\varphi_1\varphi_1| + \sqrt{\frac{3}{5}}e^{i\frac{3\pi^2\hbar}{2ma^2}t}\langle\varphi_1\varphi_2| + \frac{1}{\sqrt{5}}e^{i\frac{3\pi^2\hbar}{2ma^2}t}\langle\varphi_2\varphi_1|\right)\hat{H}(1)$$
$$\left(\frac{1}{\sqrt{5}}e^{-i\frac{\pi^2\hbar}{ma^2}t}|\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t}|\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t}|\varphi_2\varphi_1\rangle\right)$$
$$= \left(\frac{1}{\sqrt{5}}\langle\varphi_1(1)|\otimes\langle\varphi_1(2)| + \sqrt{\frac{3}{5}}\langle\varphi_1(1)|\otimes\langle\varphi_2(2)| + \frac{1}{\sqrt{5}}\langle\varphi_2(1)|\otimes\langle\varphi_1(2)|\right)\hat{H}(1)1(2)$$
$$\left(\frac{1}{\sqrt{5}}|\varphi_1(1)\rangle\otimes|\varphi_1(2)\rangle + \sqrt{\frac{3}{5}}|\varphi_1(1)\rangle\otimes|\varphi_2(2)\rangle + \frac{1}{\sqrt{5}}|\varphi_2(1)\rangle\otimes|\varphi_2(2)\rangle\right)$$
$$= \frac{1}{5}\frac{\pi^2\hbar^2}{2ma^2} + \frac{3}{5}\frac{\pi^2\hbar^2}{2ma^2} + \frac{1}{5}\frac{2\pi^2\hbar^2}{ma^2} = \frac{4\pi^2\hbar^2}{5ma^2} \tag{78}$$

Name: 陈稼霖
StudentID: 45875852

$$
\begin{aligned}
\langle \hat{H}(2) \rangle =& \left(\frac{1}{\sqrt{5}} e^{i\frac{\pi^2\hbar}{ma^2}t} \langle \varphi_1\varphi_1| + \sqrt{\frac{3}{5}} e^{i\frac{3\pi^2\hbar}{2ma^2}t} \langle \varphi_1\varphi_2| + \frac{1}{\sqrt{5}} e^{i\frac{3\pi^2\hbar}{2ma^2}t} \langle \varphi_2\varphi_1| \right) \hat{H}(2) \\
& \left(\frac{1}{\sqrt{5}} e^{-i\frac{\pi^2\hbar}{ma^2}t} |\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}} e^{-i\frac{3\pi^2\hbar}{2ma^2}t} |\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}} e^{-i\frac{3\pi^2\hbar}{2ma^2}t} |\varphi_2\varphi_1\rangle \right) \\
=& \left(\frac{1}{\sqrt{5}} \langle \varphi_1(1)| \otimes \langle \varphi_1(2)| + \sqrt{\frac{3}{5}} \langle \varphi_1(1)| \otimes \langle \varphi_2(2)| + \frac{1}{\sqrt{5}} \langle \varphi_2(1)| \otimes \langle \varphi_1(2)| \right) 1(1)\hat{H}(2) \\
& \left(\frac{1}{\sqrt{5}} |\varphi_1(1)\rangle \otimes |\varphi_1(2)\rangle + \sqrt{\frac{3}{5}} |\varphi_1(1)\rangle \otimes |\varphi_2(2)\rangle + \frac{1}{\sqrt{5}} |\varphi_2(1)\rangle \otimes |\varphi_2(2)\rangle \right) \\
=& \frac{1}{5} \frac{\pi^2\hbar^2}{2ma^2} + \frac{3}{5} \frac{2\pi^2\hbar^2}{ma^2} + \frac{1}{5} \frac{2\pi^2\hbar^2}{ma^2} = \frac{17\pi^2\hbar^2}{10ma^2}
\end{aligned} \tag{79}
$$

$$
\begin{aligned}
\langle \hat{H}(1)\hat{H}(2) \rangle =& \left(\frac{1}{\sqrt{5}} e^{i\frac{\pi^2\hbar}{ma^2}t} \langle \varphi_1\varphi_1| + \sqrt{\frac{3}{5}} e^{i\frac{3\pi^2\hbar}{2ma^2}t} \langle \varphi_1\varphi_2| + \frac{1}{\sqrt{5}} e^{i\frac{3\pi^2\hbar}{2ma^2}t} \langle \varphi_2\varphi_1| \right) \hat{H}(1)\hat{H}(2) \\
& \left(\frac{1}{\sqrt{5}} e^{-i\frac{\pi^2\hbar}{ma^2}t} |\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}} e^{-i\frac{3\pi^2\hbar}{2ma^2}t} |\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}} e^{-i\frac{3\pi^2\hbar}{2ma^2}t} |\varphi_2\varphi_1\rangle \right) \\
=& \left(\frac{1}{\sqrt{5}} e^{i\frac{\pi^2\hbar}{ma^2}t} \langle \varphi_1\varphi_1| + \sqrt{\frac{3}{5}} e^{i\frac{3\pi^2\hbar}{2ma^2}t} \langle \varphi_1\varphi_2| + \frac{1}{\sqrt{5}} e^{i\frac{3\pi^2\hbar}{2ma^2}t} \langle \varphi_2\varphi_1| \right) \hat{H}(1) \\
& \left(\frac{1}{\sqrt{5}} e^{-i\frac{\pi^2\hbar}{ma^2}t} \frac{\pi^2\hbar^2}{2ma^2} |\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}} e^{-i\frac{3\pi^2\hbar}{2ma^2}t} \frac{2\pi^2\hbar^2}{ma^2} |\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}} e^{-i\frac{3\pi^2\hbar}{2ma^2}t} \frac{\pi^2\hbar^2}{2ma^2} |\varphi_2\varphi_1\rangle \right) \\
=& \left(\frac{1}{5} \times \frac{1}{2} \times \frac{1}{2} + \frac{3}{5} \times \frac{1}{2} \times 2 + \frac{1}{5} \times 2 \times \frac{1}{2} \right) \left(\frac{\pi^2\hbar^2}{ma^2} \right) = \frac{17\pi^2\hbar^2}{20ma^2}
\end{aligned} \tag{80}
$$

Still,

$$
\langle \hat{H}(1) \rangle \langle \hat{H}(2) \rangle \neq \langle \hat{H}(1)\hat{H}(2) \rangle \tag{81}
$$

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 tensor product of the state $|\psi(0)\rangle = \left(\frac{1}{\sqrt{2}} |\varphi_1(1)\rangle + \frac{1}{\sqrt{2}} |\varphi_2(1)\rangle \right) \left(\frac{1}{\sqrt{3}} |\varphi_1(2)\rangle + \frac{\sqrt{2}}{\sqrt{3}} |\varphi_2(2)\rangle \right)$ given in (b) can be written as

$$
|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \vdots \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0 & \cdots \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 & 0 & \cdots \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{82}
$$

Name: 陈稼霖
StudentID: 45875852

The density matrix corresponding to the ket $|\psi(0)\rangle$ is

$$\rho(0)=|\psi(0)\rangle\langle\psi(0)|=\begin{pmatrix}\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 & 0 & \cdots\\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & 0 & 0 & \cdots\\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}=\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots\\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix} \tag{83}$$

At time t, the tensor product of the state is

$$\begin{aligned}|\psi(t)\rangle=&\left(\frac{1}{\sqrt{2}}e^{-i\frac{\pi^2\hbar}{2ma^2}t}|\varphi_1(1)\rangle+\frac{1}{\sqrt{2}}e^{-i\frac{2\pi^2\hbar}{ma^2}}t|\varphi_2(1)\rangle\right)\left(\frac{1}{\sqrt{3}}e^{-i\frac{\pi^2\hbar}{2ma^2}t}|\varphi_1(2)\rangle+\frac{\sqrt{2}}{\sqrt{3}}|\varphi_2(2)\rangle\right)\\ =&\begin{pmatrix}\frac{1}{\sqrt{2}}e^{-i\frac{\pi^2\hbar}{2ma^2}t}\\ \frac{1}{\sqrt{2}}e^{-i\frac{2\pi^2\hbar}{ma^2}t}\\ 0\\ 0\\ \vdots\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{3}}e^{-i\frac{\pi^2\hbar}{2ma^2}t} & \frac{\sqrt{2}}{\sqrt{3}}e^{-i\frac{2\pi^2\hbar}{ma^2}} & 0 & 0 & \cdots\end{pmatrix}\\ =&\begin{pmatrix}\frac{1}{\sqrt{6}}e^{-i\frac{\pi^2\hbar}{ma^2}t} & \frac{1}{\sqrt{3}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t} & 0 & 0 & \cdots\\ \frac{1}{\sqrt{6}}e^{-i\frac{3\pi^2\hbar}{2ma^2}t} & \frac{1}{\sqrt{3}}e^{-i\frac{4\pi^2\hbar}{ma^2}t} & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}\end{aligned}$$

The matrix element of the partial trace $\rho(1)$ is

$$\begin{aligned}\langle\varphi_n(1)|\rho(1)|\varphi_{n'}(1)\rangle=&\sum_p(\langle\varphi_n(1)|\otimes\langle\varphi_p(2)|)\left(\frac{1}{\sqrt{2}}|\varphi_1(1)\rangle+\frac{1}{\sqrt{2}}|\varphi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}|\varphi_1(2)\rangle+\frac{\sqrt{2}}{\sqrt{3}}|\varphi_2(2)\rangle\right)\\ &\left(\frac{1}{\sqrt{2}}\langle\varphi_1(1)|+\frac{1}{\sqrt{2}}\langle\varphi_2(1)|\right)\otimes\left(\frac{1}{\sqrt{3}}\langle\varphi_1(2)|+\frac{\sqrt{2}}{\sqrt{3}}\langle\varphi_2(2)|\right)(|\varphi_{n'}(1)\rangle\otimes|\varphi_p(2)\rangle)\\ =&\frac{1}{2}\left(\delta_{1n}+\delta_{2n}\right)\left(\delta_{1n'}+\delta_{2n'}\right)\end{aligned} \tag{84}$$

$$\Longrightarrow\rho(1)=\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots\\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ 0 & 0 & 0 & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix} \tag{85}$$

Name: 陈稼霖
StudentID: 45875852

Similarly,

$$\begin{aligned}\langle\varphi_p(1)|\rho(1)|\varphi_{p'}(1)\rangle =& \sum_n (\langle\varphi_n(1)|\otimes\langle\varphi_p(2)|)\left(\frac{1}{\sqrt{2}}|\varphi_1(1)\rangle+\frac{1}{\sqrt{2}}|\varphi_2(1)\rangle\right)\otimes\left(\frac{1}{\sqrt{3}}|\varphi_1(2)\rangle+\frac{\sqrt{2}}{\sqrt{3}}|\varphi_2(2)\rangle\right)\\ &\left(\frac{1}{\sqrt{2}}\langle\varphi_1(1)|+\frac{1}{\sqrt{2}}\langle\varphi_2(1)|\right)\otimes\left(\frac{1}{\sqrt{3}}\langle\varphi_1(2)|+\frac{\sqrt{2}}{\sqrt{3}}\langle\varphi_2(2)|\right)(|\varphi_n(1)\rangle\otimes|\varphi_{p'}(2)\rangle)\\ =&\left(\frac{1}{\sqrt{3}}\delta_{1p}+\frac{\sqrt{2}}{\sqrt{3}}\delta_{2p}\right)\left(\frac{1}{\sqrt{3}}\delta_{1p'}+\frac{\sqrt{2}}{\sqrt{3}}\delta_{2p'}\right) \qquad (86)\end{aligned}$$

$$\Longrightarrow \rho(2)=\begin{pmatrix}\frac{1}{3}&\frac{\sqrt{2}}{3}&0&0&\cdots\\ \frac{\sqrt{2}}{3}&\frac{2}{3}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix} \qquad (87)$$

Since

$$\rho^2=\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix}\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix}=\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix} \qquad (88)$$

$$\mathrm{Tr}(\rho^2)=\mathrm{Tr}\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix}=1 \qquad (89)$$

$$\rho^2(1)=\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix}\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix}=\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix} \qquad (90)$$

$$\mathrm{Tr}\rho^2(1)=\mathrm{Tr}\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ \frac{1}{2}&\frac{1}{2}&0&0&\cdots\\ 0&0&0&0&\cdots\\ 0&0&0&0&\cdots\\ \vdots&\vdots&\vdots&\vdots&\ddots\end{pmatrix}=1 \qquad (91)$$

$$\rho^2(2) = \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & 0 & 0 & \cdots \\ \frac{\sqrt{2}}{3} & \frac{2}{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & 0 & 0 & \cdots \\ \frac{\sqrt{2}}{3} & \frac{2}{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & 0 & 0 & \cdots \\ \frac{\sqrt{2}}{3} & \frac{2}{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{92}$$

$$\mathrm{Tr}\rho^2(2) = \mathrm{Tr} \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & 0 & 0 & \cdots \\ \frac{\sqrt{2}}{3} & \frac{2}{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} = 1 \tag{93}$$

the density operators ρ, $\rho(1)$ and $\rho(2)$ all describe pure states.

$$\rho(1) \otimes \rho(2) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} & 0 & 0 & \cdots \\ \frac{\sqrt{2}}{3} & \frac{2}{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \rho \tag{94}$$

Interpretation: Since the density operators ρ, $\rho(1)$ and $\rho(2)$ all describe pure states, ρ can be factored into $\rho(1)$ and $\rho(2)$.

□

Problem 5. [C-T Exercise 3-17] Let $\hat{\rho}$ be the density operator of an arbitrary system, where $|\chi_l\rangle$ and π_l are the eigenvectors and eigenvalues of $\hat{\rho}$. Write $\hat{\rho}$ and $\hat{\rho}^2$ in terms of the $|\chi_l\rangle$ and π_l. What do the matrices representing these two operators in the $\{\chi_l\}$ 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, $\hat{\rho}$ 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.

Solution:

$$\hat{\rho} = \sum_l \pi_l |\xi_l\rangle\langle\xi_l| \tag{95}$$

$$\hat{\rho}^2 = \sum_l \pi_l^2 |\xi_l\rangle\langle\xi_l| \tag{96}$$

Name: 陈稼霖
StudentID: 45875852

The matrix representation of these operators in the $\{\xi_l\}$ are

$$\hat{\rho} = \begin{pmatrix} \pi_1 & 0 & 0 & \cdots \\ 0 & \pi_2 & 0 & \cdots \\ 0 & 0 & \pi_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{97}$$

$$\hat{\rho}^2 = \begin{pmatrix} \pi_1^2 & 0 & 0 & \cdots \\ 0 & \pi_2^2 & 0 & \cdots \\ 0 & 0 & \pi_3^2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{98}$$

where

$$0 \leq \pi_l \leq 1 \tag{99}$$

$$\sum_l \pi_l = 1 \tag{100}$$

In the case where $\hat{\rho}$ describes a pure state,

$$\hat{\rho^2} = \begin{pmatrix} \pi_1^2 & 0 & 0 & \cdots \\ 0 & \pi_2^2 & 0 & \cdots \\ 0 & 0 & \pi_3^2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \hat{\rho} = \begin{pmatrix} \pi_1 & 0 & 0 & \cdots \\ 0 & \pi_2 & 0 & \cdots \\ 0 & 0 & \pi_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{101}$$

$$\mathrm{Tr}\hat{\rho}^2 = \pi_1^2 + \pi_2^2 + \pi_3^2 + \cdots = 1 \tag{102}$$

$$\Longrightarrow \pi_l = \begin{cases} 1, & \text{for one certain } l \\ 0, & \text{otherwise} \end{cases} \tag{103}$$

the matrices representing of these operators in the $\{\xi_l\}$ are diagonal matrix whose diagonal elements are all zeros except one is 1.
In the case of a statistical mixture of states,

$$0 \leq \mathrm{Tr}\hat{\rho}^2 = \sum_l \pi_l^2 =< 1 \tag{104}$$

the matrices representing of these operators in the $\{\xi_l\}$ are diagonal matrix whose diagonal elements are all all at the range of $[0, 1)$ and satisfies $0 \leq \sum_l \pi^2 \leq 1$.
The necessacity has been proven above.

Sufficiency: If the trace of $\hat{\rho}^2$ is equal to 1,

$$0 \leq \pi_l \leq 1 \tag{105}$$

$$0 \leq \sum_l \pi_l = 1 \tag{106}$$

$$\mathrm{Tr}\hat{\rho}^2 = \sum_l \pi_l^2 = 1 \tag{107}$$

$$\Longrightarrow \pi_l = \begin{cases} 1, & \text{for one certain } l \\ 0, & \text{otherwise} \end{cases} \tag{108}$$

In this way, $\hat{\rho}$ corresponds to a pure case.

Therefore, if only if the trace of $\hat{\rho}^2$ is equal to 1, $\hat{\rho}$ corresponds to a pure case. $\square$