SQ14)

$$\boxed{[\hat{x}, \hat{p}] = i\hbar \quad ; \quad \hat{x} = x \quad ; \quad \hat{p} = -i\hbar\frac{d}{dx}}$$ ⇐ You should remember this!

① Demonstrate how this commutator works ; wave function = $\psi(x)$

$$\boxed{\text{* Product rule ;} \quad \frac{d}{dx}(x\psi(x)) = x\frac{d}{dx}\psi(x) + \psi(x)}$$

$$\begin{aligned}
L.H.S. &= [\hat{x}, \hat{p}]\psi(x) \\
&= (\hat{x}\hat{p} - \hat{p}\hat{x})\psi(x) \\
&= (x)(-i\hbar\frac{d}{dx})\psi(x) - (-i\hbar\frac{d}{dx})(x\psi(x)) \\
&= -i\hbar x\frac{d}{dx}\psi(x) + i\hbar x\frac{d}{dx}\psi(x) + i\hbar\psi(x) = i\hbar\psi(x) = R.H.S.
\end{aligned}$$

true for any $\psi(x)$

② Angular momentum $\hat{L}$;

$$\vec{L} = \vec{r}\times\vec{p} \Rightarrow \begin{cases} L_x = yp_z - zp_y \\ L_y = zp_x - xp_z \\ L_z = xp_y - yp_x \end{cases} \Rightarrow \begin{cases} \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{cases} \text{with} \begin{cases} \hat{x} = x \;;\; \hat{p}_x = i\hbar\frac{d}{dx} \\ \hat{y} = y \;;\; \hat{p}_y = i\hbar\frac{d}{dy} \\ \hat{z} = z \;;\; \hat{p}_z = i\hbar\frac{d}{dz} \end{cases}$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

③ Useful commutator relations ;

A. $[\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$ B. $[\hat{L}_i, \hat{L}_j] = i\hbar\underbrace{\varepsilon_{ijk}}_{\text{remark *}}\hat{L}_k$ C. $[\hat{A}\hat{B}, \hat{C}] = A[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$

To show B ;

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= (yp_z - zp_y)(zp_x - xp_z) - (zp_x - xp_z)(yp_z - zp_y) \\
&= yp_zzp_x - yxp_z^2 - z^2p_yp_x + zxp_yp_z - zyp_xp_z + z^2p_xp_y + xyp_z^2 - xp_zzp_y \\
&= y(p_zz)p_x - y(zp_z)p_x + x(zp_z)p_y - x(p_zz)p_y \\
&= y[p_z, z]p_x + x[z, p_z]p_y \\
&= -i\hbar yp_x + i\hbar xp_y = i\hbar(xp_y - yp_x) = i\hbar\hat{L}_z
\end{aligned}$$

To show C ;

This is the trick!

$$\begin{aligned}
[\hat{A}\hat{B}, \hat{C}] &= \hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B} \\
&= \hat{A}\hat{B}\hat{C}\underline{- \hat{A}\hat{C}\hat{B} + \hat{A}\hat{C}\hat{B}} - \hat{C}\hat{A}\hat{B} \\
&= \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}
\end{aligned}$$

Remark * ;

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) \text{ is } (1,2,3), (2,3,1) \text{ or } (3,1,2) \\ -1 & \text{if } (i,j,k) \text{ is } (3,2,1), (1,3,2) \text{ or } (2,1,3) \\ 0 & \text{if } i=j \text{ or } j=k \text{ or } k=i \end{cases}$$

We are now ready to calculate $[\hat{L}^2, \hat{L}_x]$!

$$
\begin{aligned}
[\hat{L}^2, \hat{L}_x] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] \\
&= [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x] \qquad \text{*using B and C} \\
&= \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y + \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z \\
&= \hat{L}_y(-i\hbar\hat{L}_z) + (-i\hbar\hat{L}_z)\hat{L}_y + \hat{L}_z(i\hbar\hat{L}_y) + (i\hbar\hat{L}_y)\hat{L}_z \\
&= i\hbar[\hat{L}_z\hat{L}_y - \hat{L}_z\hat{L}_y + \hat{L}_y\hat{L}_z - \hat{L}_y\hat{L}_z] \\
&= 0
\end{aligned}
$$

It is also true that $[\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$

$\therefore [\hat{L}^2, \hat{L}_i] = 0$

$\hat{L}^2$ commutes with every component of $\hat{L}$ $\qquad [\hat{L}^2, \hat{L}_i] = 0$

but different componet of $\hat{L}$ do not commute $\qquad [\hat{L}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}\hat{L}_k$

$\Uparrow$

In summary, for angular momentum $\hat{L}$, the components $\hat{L}_x, \hat{L}_y, \hat{L}_z$ and $\hat{L}^2$ satisfy these relations

Solution by: Leung Hing Shing

SQ.15

(P.1)

Aim: To construct the Hamiltonian from Lagrangian and to construct the Hamiltonian of 2D rigid rotar system

Before writing down a Hamiltonian, you have to know the way of constructing the required Hamiltonian.

Step ① Writ down the Lagrangian

$$\boxed{L(\{x_i\}, \{\dot{x}_i\}) = K.E. - P.E.}$$

Stop ② Finding the conjugate momentum for each coordinate.

$$\boxed{P_i = \frac{\partial L}{\partial \dot{x}_i}}$$

Step ③ Constructing the Hamiltonian of the system.

$$\boxed{H(\{x_i\}, \{p_i\}) = \sum_i p_i \dot{x}_i - L}$$

(a) For a mass in a 2D plane,

$K.E. = \frac{1}{2}mv^2 = \frac{m}{2}(\dot{r}^2 + r^2\dot{\theta}^2)$

In our case, we want $P.E. = 0$

We want to $\boxed{\text{construct } H}$

① Write down the Lagrangian

$$L = K.E. - P.E.$$
$$= \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2)$$

coordinates : r, θ

generalized velocity (time-derivative of coordinate) : $\dot{r}, \dot{\theta}$

② Finding the conjugate momentum

$$p_i = \frac{\partial L}{\partial \dot{x}_i}$$

$$p_r = \frac{\partial L}{\partial \dot{r}}$$
$$= m\dot{r} \text{ (radial momentum)}$$
$$p_\theta = \frac{\partial L}{\partial \dot{\theta}}$$
$$= mr^2\dot{\theta} \text{ (angular momentum)}.$$

③ Constructing H

$$H = \sum_i p_i \dot{x}_i - L$$
$$= p_r\dot{r} + p_\theta\dot{\theta} - L$$
$$= m\dot{r}^2 + mr^2\dot{\theta}^2 - [\tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2)]$$
$$= \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2)$$

Make sure that H is expressed in terms of coordinates and momentums only. We don't want "velocity"

$$H = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2)$$

$$= \frac{1}{2}m\left[\left(\frac{P_r}{m}\right)^2 + r^2\left(\frac{P_\theta}{mr^2}\right)^2\right]$$

$$= \frac{P_r^2}{2m} + \frac{P_\theta^2}{2mr^2}$$

Also, we want to find out the conserved momentum.

Using the Euler-Lagrange equation

$$\boxed{\frac{\partial L}{\partial x_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} = 0}$$

For r: $\frac{\partial L}{\partial r} - \frac{d}{dt}\frac{\partial L}{\partial \dot{r}} = 0$

$$(mr\dot{\theta}^2) - \frac{d}{dt}(m\dot{r}) = 0$$

$$\frac{d}{dt}(P_r) = mr\dot{\theta}^2$$

For θ: $\frac{\partial L}{\partial \theta} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}} = 0$

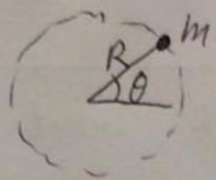
$$(0) - \frac{d}{dt}(mr^2\dot{\theta}) = 0$$

$$\frac{d}{dt}P_\theta = 0$$

$$\boxed{P_\theta = \text{constent}}$$

Therefore, the angular momentum is conserved.

(b) For 2D rigid rotator, $r=R$.
Therefore, θ and $\dot{\theta}$ are the only variables in Lagrangian.



① $L(\theta,\dot{\theta}) = \frac{1}{2} m R^2 \dot{\theta}^2$

② $p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mR^2\dot{\theta}$

Moment of inertia
$\underline{I} = mR^2$

③ $$H = p_\theta \dot{\theta} - L$$
$$= mR^2\dot{\theta}^2 - \frac{1}{2}mR^2\dot{\theta}^2$$
$$= \frac{1}{2}mR^2\dot{\theta}^2$$
$$= \frac{p_\theta^2}{2mR^2} = \frac{p_\theta^2}{2I}$$

We want to convert H, θ and p_θ into operators.

$$H \rightarrow \hat{H}$$
$$\theta \rightarrow \hat{\theta}$$
$$p_\theta \rightarrow \hat{L}_\theta$$

To find $\hat{L}_\theta$ we use the definition of angular momentum

classical: $\underbrace{p_\theta}_{\text{angular momentum}} \hat{z}_{unit} = (\underbrace{R}_{\text{radius}}\hat{r}_{unit}) \times \underbrace{(p\,\hat{\theta}_{unit})}_{\text{momentum in } \theta \text{ direction}}$

In operator form,

$$\underbrace{(\hat{z}_{unit}\hat{L}_\theta)}_{\text{angular momentum}} = \underbrace{(R\,\hat{r}_{unit})}_{\text{rad Vector}} \times \underbrace{\left(\hat{\theta}_{unit}\left(\frac{\hbar}{i}\vec{\nabla}_\theta\right)\right)}_{\text{momentum in }\theta\text{ direction}}$$

In cylindrical coordinate

$$\vec{\nabla} = \hat{r}_{unit}\frac{\partial}{\partial r} + \hat{\theta}_{unit}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{z}\frac{\partial}{\partial z}.$$

Since there is only θ dependence in the system,

$$\therefore \vec{\nabla} = \hat{\theta}_{unit}\frac{1}{R}\frac{\partial}{\partial \theta}.$$

and $\vec{\nabla}_\theta = \frac{1}{R}\frac{\partial}{\partial \theta}$.

$$\therefore \hat{z}_{unit}\hat{L}_\theta = (R\,\hat{r}_{unit}) \times \left(\hat{\theta}_{unit}\frac{\hbar}{i}\frac{1}{R}\frac{\partial}{\partial \theta}\right)$$

$$\hat{L}_\theta = \frac{\hbar}{i}\frac{\partial}{\partial \theta}.$$

$\hat{r}_{unit} \times \hat{\theta}_{unit} = \hat{z}_{unit}$.

$\therefore$

$$\boxed{\begin{aligned} &\theta \to \hat{\theta} \\ &p_\theta \to \hat{L}_\theta = \frac{\hbar}{i}\frac{\partial}{\partial \theta} \\ &H \to \hat{H} = \frac{\hat{L}_\theta^2}{2I} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial \theta^2}. \end{aligned}}$$

It looks like these operators are similar to those in x-coordinate. The similarity is listed in the table.

x - coordinate	θ - coordinate
$x \to \hat{x}$	$\theta \to \hat{\theta}$
$p \to \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$	$p_\theta \to \hat{L}_\theta = \frac{\hbar}{i}\frac{\partial}{\partial \theta}$
$H \to \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	$H \to \hat{H} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial \theta^2}$

When θ-coordinate is used, x is replaced by θ as shown in the table. m, a quantity measuring translational inertial is replaced by I, a quantity measuring rotational inertial.

The time-independent Schrödinger eq is

$$\hat{H}\,\psi(\theta) = E\,\psi(\theta)$$

$$\boxed{-\frac{\hbar^2}{2I}\frac{\partial^2\psi}{\partial\theta^2} = E\,\psi(\theta).}$$

SQ.16

Aim: Write down the TISE of an oscillator in momentum space and find the ground state solution of the TISE

Before write down the TISE, we check that whether $p \to \hat{p}$ and $x \to \hat{x} = i\hbar\frac{\partial}{\partial p}$ satisfy $[\hat{x},\hat{p}] = i\hbar$.

$$\hat{x}\hat{p}\, f(p) = i\hbar \frac{\partial}{\partial p}(p\, f(p))$$

$$= i\hbar\, f(p) + i\hbar p \frac{\partial}{\partial p} f(p).$$

$$\hat{p}\hat{x}\, f(p) = i\hbar p \frac{\partial}{\partial p} f(p).$$

$$[\hat{x},\hat{p}] f(p) = (i\hbar f(p) + i\hbar p \frac{\partial}{\partial p} f(p) - i\hbar p \frac{\partial}{\partial p} f(p))$$

$$= i\hbar\, f(p)$$

$\therefore$ $p \to \hat{p}$ and $x \to i\hbar\frac{\partial}{\partial p}$ satisfy $[\hat{x},\hat{p}] = i\hbar$.

The first aim is write down the TISE of an oscillator in momentum space.

we first write down the classical Harmitonian ①. Then, find the correspoinding Hamitonian operator in terms of momentum. ②

Finally, we write down the TISE ③

① The classical $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$,

② $\hat{H}$ Operator in terms of momentum

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

$$= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(\frac{\hbar}{i}\frac{\partial}{\partial p}\right)^2$$

$$= \frac{p^2}{2m} - \frac{\hbar^2}{2\left(\frac{1}{m\omega^2}\right)}\frac{\partial^2}{\partial p^2}$$

$$= -\frac{\hbar^2}{2\left(\frac{1}{m\omega^2}\right)}\frac{\partial^2}{\partial p^2} + \frac{1}{2}\left(\frac{1}{m\omega^2}\right)\omega^2 p^2$$

we define the hypothetic effective mass in momentum space, which is $m_{eff} = \frac{1}{m\omega^2}$.

Then $\hat{H} = -\frac{\hbar^2}{2m_{eff}}\frac{\partial^2}{\partial p^2} + \frac{1}{2}m_{eff}\,\omega^2 p^2$.

③ Write down the TISE in momentum space

$$\hat{H}\,\psi(p) = E\psi(p)$$

$$\Rightarrow -\frac{\hbar^2}{2m_{eff}}\frac{\partial^2\tilde{\psi}(p)}{\partial p^2} + \frac{1}{2}m_{eff}\,\omega^2 p^2\tilde{\psi}(p) = E\tilde{\psi}(p)$$

This TISE in momentum space looks like that in real space. The similarity is listed in the table.

x-coordinate	p-coordinate
$x \rightarrow \hat{x}$ $p \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$	$p \rightarrow \hat{p}$ $x \rightarrow -\frac{\hbar}{i}\frac{\partial}{\partial p}$
mass : m	effective mass : $m_{eff} = \frac{1}{m\omega^2} \propto \frac{1}{m}$
TISE : $-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2}m\omega^2\psi(x)$ $= E\psi(x)$	TISE : $-\frac{\hbar^2}{2m_{eff}}\frac{\partial^2 \tilde{\psi}}{\partial p^2} + \frac{1}{2}m_{eff}\omega^2\tilde{\psi}(p)$ $= E\tilde{\psi}(p)$

since $\psi(x)$ and $\tilde{\psi}(p)$ have the same form of TISE. If the eigenfunctions of $\psi(x)$ are $\phi_n(x; m, \omega)$, then the eigenfunctions of $\tilde{\psi}(p)$ are $\phi_n(p; m_{eff}, \omega)$. $E_n = \hbar\omega(n+\frac{1}{2})$.

The second aim is to find the ground state solution.

The ground state wavefunction in real space is

P.10

$$\phi_0(x; m, \omega) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{x^2}{4\left(\frac{\hbar}{2m\omega}\right)}}$$

Then the ground state wavefunction in momentum space is

$$\phi_0(p; m_{eff}, \omega) = \left(\frac{m_{eff}\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{p^2}{4\left(\frac{\hbar}{2m_{eff}\omega}\right)}}$$

Then, we test whether the solution satisfy the TISE in momentum space.

$$\frac{\partial}{\partial p}\phi_0(p; m_{eff}, \omega)$$

$$= \left(\frac{m_{eff}\omega}{\pi\hbar}\right)^{1/4}\left[(-p)/\left(\frac{\hbar}{m_{eff}\omega}\right)\right] e^{-\frac{p^2}{4\left(\frac{\hbar}{2m_{eff}\omega}\right)}}$$

$$\frac{\partial^2}{\partial p^2}\phi_0(p; m_{eff}, \omega)$$

$$= \left(\frac{m_{eff}\omega}{\pi\hbar}\right)^{1/4}\left(\left[p^2/\left(\frac{\hbar^2}{m_{eff}^2\omega^2}\right)\right] - \left[1/\left(\frac{\hbar}{m_{eff}\omega}\right)\right]\right) e^{-\frac{p^2}{4\left(\frac{\hbar}{2m_{eff}\omega}\right)}}$$

$$= \left\{\left[p^2/\left(\frac{\hbar^2}{m_{eff}^2\omega^2}\right)\right] - \left[1/\left(\frac{\hbar}{m_{eff}\omega}\right)\right]\right\}\phi_0(p; m_{eff}, \omega)$$

$$-\frac{\hbar^2}{2m_{eff}}\frac{\partial^2\phi_0}{\partial p^2} + \frac{1}{2}m_{eff}\omega^2 p^2\phi_0$$

$$= \left\{-\frac{1}{2}m_{eff}\omega^2 p^2 + \frac{1}{2}\hbar\omega\right\}\phi_0$$

$$+\frac{1}{2}m_{eff}\omega^2 p^2\phi_0$$

$= \frac{1}{2}\hbar\omega\,\phi_0.$

$$E_0 = \frac{1}{2}\hbar\omega.$$

$\therefore$ The proposed $\phi_0(p)$ is really a solution to TISE in momentum space and $E_0 = \frac{1}{2}\hbar\omega$.

Extra:

You can check that $\sigma_x{}^2 = \frac{\hbar}{2m\omega}$.

and $\sigma_p{}^2 = \frac{\hbar}{2m_{eff}\,\omega}$.

If $m\uparrow$, $\sigma_x\uparrow$.

If $m\uparrow$, $m_{eff}\downarrow$, $\sigma_p\downarrow$.

This is consistent with the uncertainty principle.

Also, $\sigma_x{}^2\sigma_p{}^2 = \frac{\hbar^2}{4m\,m_{eff}\,\omega^2} = \frac{\hbar^2}{4} \geq \frac{\hbar^2}{4}$,

which is the uncertainty principle.