Solution to Problem Set 3

P1)

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

eqs. of motion are

$$\begin{cases} \frac{dx}{dt} = \frac{p}{m} \\ \frac{dp}{dt} = -m\omega^2 x + F \end{cases}$$

The state in the Heisenberg picture is $|0\rangle$, the ground state of the SHO at $t=0$ in Schrödinger picture.

Now

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}+\hat{a}^\dagger) \quad \& \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a}^\dagger - \hat{a})$$

$$\hat{a} = \sqrt{\frac{m\hbar\omega}{2}}\left[\hat{x} + i\frac{\hat{p}}{m\omega}\right] \quad \& \quad \hat{a}^\dagger = \sqrt{\frac{m\hbar\omega}{2}}\left[\hat{x} - i\frac{\hat{p}}{m\omega}\right]$$

where $[\hat{x},\hat{p}] = i\hbar$

equation of motion for $\hat{a}$ by direct substitution is:

$$\frac{d}{dt}\hat{a} = -i\omega\hat{a} + iF\sqrt{\frac{1}{2m\hbar\omega}} \quad \Rightarrow$$

$$\hat{a}(t) = \hat{a}(0)\,e^{-i\omega t} + i\sqrt{\frac{1}{2m\hbar\omega^3}}\,F(1-e^{-i\omega t})$$

$$\hat{a}^\dagger(t) = \hat{a}^\dagger(0)\,e^{+i\omega t} - i\sqrt{\frac{1}{2m\hbar\omega^3}}\,(1-e^{i\omega t})$$

Note that

$$\langle 0|\, \hat{a}(0)\, |0\rangle = \langle 0|\, \hat{a}^{\dagger}(0)\, |0\rangle = 0$$

a)

therefore $\langle 0|\, \hat{x}\, |0\rangle = \langle 0|\, (\hat{a} + \hat{a}^{\dagger})\, |0\rangle = 0$

b) $$\langle 0|\, \hat{p}\, |0\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\, \langle 0|\, -2iF\sqrt{\frac{1}{2m\hbar\omega^3}}\,(1-e^{i\omega t})\, |0\rangle$$

$$= \frac{F}{\omega}(1-\cos\omega t)$$

$$\langle 0|\, \hat{p}\, |0\rangle = \frac{2F}{\omega}\sin^2\frac{\omega t}{2}$$

Problem 2)

$\hat{G}(t) = m\omega \cos\omega t \, \hat{x}(t) - \sin\omega t \, \hat{p}(t)$

a)

$[\hat{G}, \hat{H}] = m\omega \cos\omega t \, [\hat{x}, \hat{H}] - \sin\omega t \, [\hat{p}(t), \hat{H}]$

where $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}$ & $[\hat{x}, \hat{p}] = i\hbar$

$[\hat{x}, \hat{H}] = [\hat{x}, \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2] = \frac{i\hbar}{m} \hat{p}$

$[\hat{p}, \hat{H}] = [\hat{p}, \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2] = -i\hbar m\omega^2 \hat{x}$

$\Rightarrow [\hat{G}, \hat{H}] = i\hbar \omega \cos\omega t \, \hat{p} + i\hbar m\omega^2 \sin\omega t \, \hat{x}$

$\hat{G}, \hat{H}$ do not commute & do not simultaneously diagonalized

b)

$$\frac{d\hat{G}}{dt} = \frac{1}{i\hbar} [\hat{G}, \hat{H}] + \frac{\partial \hat{G}}{\partial t}$$

$$= \omega \cos\omega t \, \hat{p} + m\omega^2 \sin\omega t \, \hat{x} - m\omega^2 \sin\omega t \, \hat{x} - \omega \cos\omega t \, \hat{p}$$

$$\Rightarrow \boxed{\frac{d\hat{G}}{dt} = 0}$$

$\hat{G}$ is constant of a motion.

c) Since $\frac{dx}{dt} = p$ & $\frac{dp}{dt} = -\omega^2 x$ $\Rightarrow$

$$\begin{cases} x = x_0 \cos\omega t + \frac{p_0}{m\omega} \sin\omega t \\ p = p_0 \cos\omega t - m\omega x_0 \sin\omega t \end{cases}$$

where $x_0 = x(t=0)$ & $p_0 = p(t=0)$ $\Rightarrow$

$$G = m\omega\left[x_0 \cos\omega t + \frac{p_0}{m\omega}\sin\omega t\right]\cos\omega t$$

$$- \left[p_0 \cos\omega t - m\omega x_0 \sin\omega t\right]\sin\omega t = m\omega x_0$$

$$\boxed{\hat{G} = m\omega x_0}$$

Problem 3)

a) $H = \frac{p^2}{2m} + \frac{1}{2}k(x-x_0)^2 = \frac{p^2}{2m} + \frac{1}{2}kx^2 + \frac{1}{2}kx_0^2 - kxx_0$

Since $\frac{1}{2}kx_0^2$ is constant, the total Hamiltonian can be written now as

$$\boxed{H = \frac{p^2}{2m} + \frac{1}{2}kx^2 - kx_0\, x = H_0 + \alpha x}$$

b) $\begin{cases} H_0 = \hbar\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2}) \\ \alpha x = \alpha\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}) \end{cases} \Rightarrow$

In Schrödinger picture

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}) + \alpha\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a})$$

$$= \hbar\omega\left[\hat{a}^\dagger\hat{a} + c(\hat{a}^\dagger + \hat{a}) + \tfrac{1}{2}\right]$$

where $c = \alpha\sqrt{\frac{\hbar}{2m\omega}}$

if $\hat{b} = \hat{a} + c$ & $\hat{b} = \hat{a}^\dagger + c \Rightarrow$

$$\hat{H} = \hbar\omega(\hat{b}^\dagger\hat{b} + \tfrac{1}{2} - c^2)$$

The ground state has an energy

$E_0 = \hbar\omega(\frac{1}{2} - c^2)$ & $b|0\rangle = 0$

Schrödinger ground state is

$$|\psi_s(t)\rangle = e^{-i\omega t(\frac{1}{2} - c^2)}|0\rangle$$

The equation for the state in the Dirac picture is:

$$i\hbar \frac{\partial}{\partial t} \Psi_D(t) = \alpha\, x_D(t)\, \Psi_D(t)$$

where $\Psi_D(0) = \Psi_S(0)$ $\Longrightarrow$

$$\boxed{\Psi_D(t) = \Psi_S(t) - \frac{i\alpha}{\hbar}\int_0^t \Psi_D(\tau)\, x_D(\tau)\, d\tau}$$

ground
state wave function

This equation is a Volterra-type equation that can be solved by iterating, (Dyson Series).

For $x_D(t)$, we need $U_0(t) = \exp\left[-i \frac{H_0}{\hbar} t\right]$

$$U_0(t) = \exp\left[-i\omega t \left(\hat{a}^\dagger \hat{a} + \tfrac{1}{2}\right)\right]$$

$$x_D(t) = U_0^\dagger(t)\, x\, U_0(t)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\, e^{i\omega t(\hat{a}^\dagger \hat{a} + \frac{1}{2})} (\hat{a}^\dagger + \hat{a})\, e^{-i\omega t(\hat{a}^\dagger \hat{a} + \frac{1}{2})}$$

Since $[\hat{a}, \hat{H}] = \hbar\omega \hat{a}$ & $[\hat{a}^\dagger, \hat{H}] = \hbar\omega \hat{a}^\dagger$

$$\left\{ \begin{array}{l} \hat{a}\, e^{-i\omega t \hat{a}^\dagger \hat{a}} = e^{-i\omega t}\, e^{-i\omega t \hat{a}^\dagger \hat{a}}\, \hat{a} \\ \hat{a}^\dagger\, e^{-i\omega t \hat{a}^\dagger \hat{a}} = e^{i\omega t}\, e^{-i\omega t \hat{a}^\dagger \hat{a}}\, \hat{a}^\dagger \end{array} \right. \Longrightarrow$$

$$x_D(t) = \sqrt{\frac{\hbar}{2m\omega}} \left[e^{-i\omega t}\, \hat{a} + e^{i\omega t}\, \hat{a}^\dagger \right]$$

$$\boxed{x_D(t) = x_s \cos\omega t + \frac{P_s}{m\omega} \sin\omega t}$$

Problem 4)

a)

The canonical conjugate variables are (ψ, ψ°) as $\{\psi, \psi^{\circ}\} = 0$. Note that $\psi(\vec{r})$ & $\psi^{*}(r)$ are complex field quantities and because Lagrangian is real so it has to have the right dependency on ψ^{*} & ψ so, canonical variables are $\psi, \psi^{\circ}, \psi^{*}, \psi^{*\circ}$.

Once the field is considered, the Lagrangian formalism extends to the following equations:

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \psi^{\circ}} = \frac{\partial \mathcal{L}}{\partial \psi} - \sum_i \partial_i \frac{\partial \mathcal{L}}{\partial(\partial_i \psi)} \qquad (1)$$

and

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \psi^{*\circ}} = \frac{\partial \mathcal{L}}{\partial \psi^{*}} - \sum_i \partial_i \frac{\partial \mathcal{L}}{\partial(\partial_i \psi^{*})} \qquad (2)$$

where $\underline{i}$ referes to coordinate system, e.g. (x, y, z). Note that $\sum_i \hat{i}\,\partial_i \triangleq \vec{\nabla}$, where $\hat{i}$ is unit vector.

Now $\mathcal{L} = \frac{i\hbar}{2}(\psi^{*}\psi^{\circ} - \psi^{*\circ}\psi) - \frac{\hbar^2}{2m}\nabla\psi^{*}\cdot\nabla\psi - V(r)\psi^{*}\psi$

$$\frac{\partial \mathcal{L}}{\partial \psi^{*\circ}} = -i\frac{\hbar}{2}\psi \qquad (3)$$

$$\frac{\partial \mathcal{L}}{\partial \psi^*} = \frac{i\hbar}{2}\psi^{\circ} - V(r)\psi \qquad (4)$$

$$\frac{\partial \mathcal{L}}{\partial(\partial_i \psi^*)} = \frac{-\hbar^2}{2m}\partial_i \psi \quad \text{or} \quad \frac{\partial \mathcal{L}}{\partial \nabla\psi^*} = \frac{-\hbar^2}{2m}\nabla\psi \qquad (5)$$

Inserting (3), (4) & (5) in (2), we yield:

$$\boxed{i\hbar\psi^{\circ} - V(r)\psi + \frac{\hbar^2}{2m}\nabla^2\psi = 0} \quad \text{Schrödinger Equation} \quad (6)$$

b) $\psi = \psi_r + i\psi_i \implies \nabla\psi = \nabla\psi_r + i\nabla\psi_i$

then straightforwardly we get

$$\mathcal{L} = \hbar(\psi_i\psi_r^{\circ} - \psi_r\psi_i^{\circ}) - \frac{\hbar^2}{2m}\left[(\nabla\psi_r)^2 + (\nabla\psi_i)^2\right] - V(r)\left[\psi_i^2 + \psi_r^2\right] \qquad (7)$$

Note that $\mathcal{L}(\psi_r, \psi_i, \psi_r^{\circ}, \psi_i^{\circ})$.

c) $$\mathcal{L}' = 2\hbar\psi_i\psi_r^{\circ} - \frac{\hbar^2}{2m}\left[(\nabla\psi_r)^2 + (\nabla\psi_i)^2\right] - V(r)\left[\psi_i^2 + \psi_r^2\right]$$

$$L' = \int d^3r\, \mathcal{L}' = L + \frac{d}{dt}\int d^3r\, \hbar\,\psi_r\psi_i \quad \text{is now} \qquad (8)$$

independent of $\psi_i^{\circ} \implies L'(\psi_r, \psi_i, \psi_r^{\circ})$.

d) The Lagrange equation relative to ψ_i reads

$$\frac{\partial L'}{\partial \psi_i(r)} = 0 \;\; (8a) \implies 2\hbar\psi_r^{\circ} - 2V\psi_i - \frac{\hbar^2}{m}\nabla^2\psi_i = 0 \implies$$

$$\boxed{\hbar\psi_r^{\circ} - V\psi_i - \frac{\hbar^2}{2m}\nabla^2\psi_i = 0} \qquad (9)$$

Note that eq. (9) allows one to express ψ_i as a function of ψ_r°, therefore

$\mathcal{L}'(\psi_r, \psi_r^\circ, \psi_i(\psi_r^\circ))$.

Technically $\mathcal{L}'$ is now a function of ψ_r & ψ_r°.

Note one does not need to reexpress $\mathcal{L}'$ as just a function of ψ_r & ψ_r°, as it is not necessary for the following parts,

e) Using $\frac{\partial \hat{\mathcal{L}}'}{\partial \psi_r^\circ}$ as a function of the functional derivatives of $\mathcal{L}'$ ⇒

$$\frac{\partial \hat{\mathcal{L}}'}{\partial \psi_r^\circ} = \frac{\partial \mathcal{L}'}{\partial \psi_r^\circ} + \frac{\partial \mathcal{L}'}{\partial \psi_i}\frac{\partial \psi_i}{\partial \psi_r^\circ}$$

Since (8a) implies $\frac{\partial L'}{\partial \psi_i} = 0 \Rightarrow \boxed{\frac{\partial \hat{L}'}{\partial \psi_r^\circ} = \frac{\partial L'}{\partial \psi_r^\circ}}$ (10)

f) Now conjugate momentum $\Pi_r(r) = \frac{\partial \hat{L}'}{\partial \psi_r^\circ} = \frac{\partial L'}{\partial \psi_r^\circ}$

$\Rightarrow \boxed{\Pi_r(r) = 2\hbar\, \psi_i(r)}$ (11)

$\Rightarrow \boxed{\psi = \psi_r + i\psi_i = \psi_r + \frac{i}{2\hbar}\Pi_r(r)}$ (12)

g) The Hamiltonian density reads

$$\mathcal{H} = \Pi\psi^{*\circ} + \Pi^*\psi^\circ - \mathcal{L} = \Pi_r\psi_r^\circ - \mathcal{L}'$$

$$= \frac{\hbar^2}{2m}\left[(\nabla\psi_r)^2 + (\nabla\psi_i)^2\right] + V(r)\left[\psi_r^2 + \psi_i^2\right]$$

Now $\int d^3r\, \mathcal{H} = H$

then using $\int d^3r (\nabla\psi_r)^2 = -\int d^3r\, \psi_r \nabla^2 \psi_r$

$$\Big[\ \nabla\cdot(\psi_r \nabla\psi_r) = \nabla^2\psi_r + \psi_r\nabla^2\psi_r \Rightarrow$$

$$\int \nabla\cdot(\psi_r\nabla\psi_r)\, d^3r = \int \nabla^2\psi_r\, d^3r + \int \psi_r \nabla^2\psi_r\, d^3r$$

$$\oint \cancelto{0}{\psi_r\nabla\psi_r\, ds} = \int \nabla^2\psi_r\, d^3r + \int \psi_r\nabla^2\psi_r\, d^3r$$

$$\psi(r\to\infty) = 0$$

$$\Rightarrow \int d^3r\,(\nabla\psi_r)^2 = -\int d^3r\, \psi_r \nabla^2\psi_r \ \Big]$$

$$H = \int d^3r \left[\frac{-\hbar^2}{2m}(\psi_r\nabla^2\psi_r + \psi_i\nabla^2\psi_i) + V(r)(\psi_r^2+\psi_i^2) \right]$$

Now $\psi = \psi_r + i\,\psi_i$ & $\int d^3r\,(\psi_r\nabla^2\psi_i - \psi_i\nabla^2\psi_r) = 0$

$\psi^* = \psi_r - i\,\psi_i$ $\quad\Downarrow$

integration by part 2 times

$$\Rightarrow \boxed{H = \int d^3r\ \psi^* \left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\psi}$$

the same result for total energy operator from QM.

h) $[\hat{\psi}_r(\vec{r}), \hat{\Pi}_r(\vec{r}')] = i\hbar\, \delta(\vec{r}-\vec{r}')$

Since $\psi = \psi_r + \frac{i}{2\hbar}\Pi_r$ from eq. (12) $\Rightarrow$

$$[\hat{\psi}(r), \hat{\psi}^\dagger(r')] = \cancelto{0}{[\hat{\psi}_r(r), \hat{\psi}_r(r')]} + \frac{1}{4\hbar^2}\cancelto{0}{[\Pi_r(r), \Pi_r(r')]}$$

$$- \frac{i}{2\hbar}[\psi_r(r), \Pi_r(r')] + \frac{i}{2\hbar}[\Pi_r(r), \psi_r(r')]$$

$$\Rightarrow \boxed{[\hat{\psi}(r), \hat{\psi}^\dagger(r')] = \delta(r-r')} \rightarrow \text{bosons}$$

Same trend $\Rightarrow$ $\boxed{[\hat{\psi}(r), \hat{\psi}(r')] = 0} \rightarrow$ bosons

If you replace commutators by anti-commutators then we have fermions.

Problem 5)

Using $x = r\cos\phi \sin\theta$
$y = r\sin\phi \sin\theta$ for spherical coordinate,
$z = r\cos\theta$

$$\psi = Ar(\cos\phi\sin\theta + \sin\phi\sin\theta + 2\cos\theta)e^{-\alpha r}$$

the angular part is $\psi_a = A'(\cos\phi\sin\theta + \sin\phi\sin\theta + 2\cos\theta)$

$$\Rightarrow \int_0^{2\pi}\int_0^{\pi} |\psi_a|^2 d\theta\, d\phi = 1 \Rightarrow$$

$$\psi_a(\theta,\phi) = A'\left[\frac{1}{2}(e^{i\phi}+e^{-i\phi})\sin\theta + \frac{1}{2i}(e^{i\phi}-e^{-i\phi})\sin\theta + 2\cos\theta\right]$$

$$\rightarrow \psi_a(\theta,\phi) = A'\left[\frac{-1}{2}(1-i)\sqrt{\frac{8\pi}{3}}\,Y_1^1 + \frac{1}{2}(1+i)\sqrt{\frac{8\pi}{3}}\,Y_1^{-1} + 2\sqrt{\frac{4\pi}{3}}\,Y_1^0\right]$$

by orthonormality of $Y_\ell^m \Rightarrow$

$$A'^2\left[\frac{1}{2}\cdot\frac{8\pi}{3} + \frac{1}{2}\cdot\frac{8\pi}{3} + 4\cdot\frac{4\pi}{3}\right] = 1 \Rightarrow$$

$$\boxed{A' = \sqrt{\frac{1}{8\pi}}}$$

a) Since $\ell = 1 \rightarrow \boxed{\sqrt{\langle \hat{L}^2\rangle} = \sqrt{\ell(\ell+1)}\,\hbar = \sqrt{2}\,\hbar}$

b) $\langle\psi|\hat{L}_z|\psi\rangle = A'^2\left[\frac{1}{2}\cdot\frac{8\pi}{3}\hbar\,(Y_1^1)^2 + \frac{1}{2}\cdot\frac{8\pi}{3}(-\hbar)(Y_1^{-1})^2 + 4\cdot\frac{4\pi}{3}(0)(Y_1^0)^2\right] = 0 \rightarrow \boxed{\langle\hat{L}_z\rangle = 0}$

c)

$$P = |\langle L_z | \psi_a \rangle|^2 = \frac{1}{8\pi}\left(\frac{1}{2} \cdot \frac{8\pi}{3}\right) = \frac{1}{6}$$

$$\boxed{P = \frac{1}{6}}$$

A.H. Majedi