

Relativity, Mechanics and Quantum Theory

Solutions to Problem Sheet 7.

(7.1.) We have:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi.$$

$$\langle \psi | \hat{Q} \rangle = \int_{\mathbb{R}^3} d^3q \cdot \psi^* \hat{Q} \psi.$$

and

$$\frac{d}{dt} \langle \psi | \hat{Q} \rangle = \frac{d}{dt} \int_{\mathbb{R}^3} d^3q \cdot \psi^* \hat{Q} \psi = \frac{d}{dt} \int_{\mathbb{R}^3} d^3q \cdot \hat{Q} \psi^* \psi.$$

i.e. $\hat{Q} = \psi^* \hat{Q} \psi.$

(i.) $\therefore \int d^3q \frac{d}{dt} (\hat{Q}) = \int d^3q \left(\frac{\partial \psi^*}{\partial t} \hat{Q} \psi + \psi^* \frac{\partial \hat{Q}}{\partial t} \psi \right).$

n.b. $i\hbar \frac{\partial \psi^*}{\partial t} = \hat{H}^* \psi^* = \hat{H} \psi^*.$

$$\therefore \int d^3q \left(\psi^* \hat{H} \psi + \psi^* \left(\frac{\partial \hat{Q}}{\partial t} \right) \psi \right).$$

Here $\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \sum_i V(q_i).$

$$\begin{aligned} \therefore \int d^3q \frac{d}{dt} (\hat{Q}) &= \int d^3q \left(-\frac{i\hbar}{2m} \nabla^2 \psi^* \psi + \psi^* \left(\frac{\partial \hat{Q}}{\partial t} \right) \psi \right) \\ &= \int d^3q \left(\cancel{\frac{i\hbar}{2m} \nabla^2 \psi^* \psi} - \cancel{\frac{i\hbar}{2m} \nabla^2 \psi^* \psi} \right) \\ &\quad + \left[\frac{i\hbar}{2m} \nabla^2 \psi^* \psi \right]_{\mathbb{R}^3} \\ &\quad + \left[\frac{i\hbar}{2m} \nabla^2 \psi^* \psi \right]_{\mathbb{R}^3}. \end{aligned}$$

$$\int d^3q \frac{d}{dt} (\hat{Q}) = \int d^3q \left(\frac{i\hbar}{2m} \nabla^2 \psi^* \psi - \psi^* \left(\frac{\partial \hat{Q}}{\partial t} \right) \psi \right).$$

$$\therefore \frac{d}{dt} (\hat{Q}) + \sum_i \frac{d}{dt} \left(\frac{i\hbar}{2m} \nabla^2 \psi^* \psi \right) = 0. //$$

(ii) $\langle \Psi | \Phi \rangle = \int_{\mathbb{R}^k} d^k q \Psi^* \Phi.$

$\therefore \frac{d}{dt} (\langle \Psi | \Phi \rangle) = \int_{\mathbb{R}^k} d^k q \left(\frac{\partial \Psi^*}{\partial t} \Phi + \Psi^* \frac{\partial \Phi}{\partial t} \right).$

$= \int_{\mathbb{R}^k} d^k q \left(\frac{i}{\hbar} (\hat{H} \Psi^*) \Phi + \Psi^* \left(\frac{-i}{\hbar} \hat{H} \Phi \right) \right).$

$= \int_{\mathbb{R}^k} d^k q \left(\frac{i}{\hbar} \left[-\frac{\hbar^2}{2} \sum_i \frac{\partial^2 \Psi^*}{\partial q_i^2} \Phi + \frac{\hbar^2}{2} \sum_i \frac{\partial^2 \Phi}{\partial q_i^2} \Psi^* \right] \right).$

$= \int_{\mathbb{R}^k} d^k q \sum_i \frac{i\hbar}{2m_i} \left(-\frac{\partial^2 \Psi^*}{\partial q_i^2} \Phi + \Psi^* \frac{\partial^2 \Phi}{\partial q_i^2} \right).$

$= \int_{\mathbb{R}^k} d^k q \sum_i \frac{i\hbar}{2m_i} \left(\frac{\partial^2 \Psi^*}{\partial q_i^2} \Phi - \frac{\partial \Psi^*}{\partial q_i} \frac{\partial \Phi}{\partial q_i} - \frac{\partial \Phi}{\partial q_i} \frac{\partial \Psi^*}{\partial q_i} + \frac{\partial^2 \Phi}{\partial q_i^2} \Psi^* \right)$

$+ \left[\sum_i \frac{i\hbar}{2m_i} \left(-\frac{\partial \Psi^*}{\partial q_i} \Phi + \Psi^* \frac{\partial \Phi}{\partial q_i} \right) \right]_{\mathbb{R}^k}.$

The boundary term vanishes if sufficiently strong conditions are placed on Φ and Ψ . For example if $\Phi(\pm\infty) = 0$ and $\Psi^*(\pm\infty) = 0$ while $\frac{\partial \Psi^*}{\partial q_i}(\pm\infty) \neq \pm\infty$ and $\frac{\partial \Phi}{\partial q_i}(\pm\infty) \neq \pm\infty$.

Then the inner product $\langle \Psi | \Phi \rangle$ is conserved. //

(7.2.) In the Schrödinger picture the states are time-dependent

$\Psi_S \equiv \Psi(q, t)$ while the operators \hat{A}_S are time-independent:

$\frac{d\hat{A}_S}{dt} = 0$

In the Heisenberg picture the states are time-independent

$\Psi_H \equiv \Psi(q)$ while the operators \hat{A}_H are time-dependent

$\hat{A}_H \equiv A_H(q, t).$

The states $|\psi\rangle_S, |\psi\rangle_H$ and operators \hat{A}_S, \hat{A}_H are related by: 3.

$$|\psi\rangle_H = e^{+i\hat{H}t/\hbar} |\psi(t)\rangle_S //$$

(which ~~is~~ comes from a formal solution to the Schrödinger equation:

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

$$\Rightarrow |\psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}} |\psi(t)\rangle_{t=0}$$

$$\therefore |\psi(t)\rangle_{t=0} = e^{+i\hat{H}t/\hbar} |\psi(t)\rangle //$$

$\begin{matrix} \text{III} & & \text{III} \\ |\psi\rangle_H & & |\psi(t)\rangle_S \end{matrix}$

The operators in the two pictures are related by:

$$\hat{A}_H(t) = e^{+i\hat{H}t/\hbar} \hat{A}_S e^{-i\hat{H}t/\hbar} //$$

The operator matrix elements are unchanged by the picture change.

$$\begin{aligned} \langle u_n | \hat{A}_H(t) | u_m \rangle_H &= \langle u_n(t) | e^{-i\hat{H}t/\hbar} \hat{A}_H(t) e^{+i\hat{H}t/\hbar} | u_m(t) \rangle_S \\ &= \langle u_n(t) | \hat{A}_S | u_m(t) \rangle_S \\ &\equiv (\hat{A}_S)_{nm} // \end{aligned}$$

$\begin{matrix} \text{III} \\ (\hat{A}_H(t))_{nm} \end{matrix}$

For some basis $\{u_n\}$.

The Heisenberg operators evolve in time as:

$$\begin{aligned} \frac{d}{dt} \hat{A}_H(t) &= \frac{i}{\hbar} e^{+i\hat{H}t/\hbar} \hat{A}_S e^{-i\hat{H}t/\hbar} + e^{+i\hat{H}t/\hbar} \hat{A}_S e^{-i\hat{H}t/\hbar} \left(\frac{-i\hat{H}}{\hbar} \right) \\ &= \frac{i}{\hbar} [\hat{H}, \hat{A}_H(t)] // \end{aligned}$$

Where we have used $\frac{d\hat{A}_S}{dt} = 0$.

(7.3.)
$$\mathcal{L} = \frac{1}{2}(\dot{\theta}^2 + \dot{x}^2).$$

To quantise we treat θ and x as operators.

To find the Hamiltonian we make use of:

$$p_{\theta} \equiv \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = \dot{\theta} \quad \text{and} \quad p_x \equiv \frac{\partial \mathcal{L}}{\partial \dot{x}} = \dot{x}.$$

$$\begin{aligned} \therefore H &= p_i \dot{q}_i - \mathcal{L} \\ &= \dot{\theta}^2 + \dot{x}^2 - \mathcal{L} \\ &= \frac{1}{2}(\dot{\theta}^2 + \dot{x}^2) \end{aligned}$$

$$\therefore \hat{H} = \frac{1}{2}(\hat{p}_{\theta}^2 + \hat{p}_x^2).$$

In the position representation $\hat{p}_i \equiv -i\hbar \frac{\partial}{\partial q_i}$

$$\therefore \hat{p}_{\theta} = (-i\hbar) \frac{\partial}{\partial \theta} \quad \hat{p}_x = (-i\hbar) \frac{\partial}{\partial x}.$$

$$\begin{aligned} \therefore \hat{H} &= \frac{1}{2} \left(-\hbar^2 \frac{\partial^2}{\partial \theta^2} - \hbar^2 \frac{\partial^2}{\partial x^2} \right) \\ &= -\frac{\hbar^2}{2} \left(\frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial x^2} \right). \end{aligned}$$

Let $\psi(\theta, x) = \psi(\theta + 2\pi, x)$ be an eigenfunction of \hat{H} :

$$\hat{H}\psi = \lambda\psi.$$

As \hat{H} is self-adjoint $\lambda \in \mathbb{R}$.

Since $\psi(\theta, x) = \psi(\theta + 2\pi, x)$ then:

$$\psi(\theta, x) = \sum_{k \in \mathbb{Z}} e^{ik\theta} \phi(x).$$

and,

$$\hat{H}\psi = -\frac{\hbar^2}{2} \left(\sum_{k \in \mathbb{Z}} -k^2 e^{ik\theta} \phi(x) + \sum_{k \in \mathbb{Z}} e^{ik\theta} \frac{\partial^2 \phi}{\partial x^2} \right) = \lambda\psi.$$

$$\therefore -\frac{\hbar^2}{2} \left(\sum_{k \in \mathbb{Z}} e^{ik\theta} \left(-k^2 \phi(x) + \frac{\partial^2 \phi}{\partial x^2} \right) \right) = \lambda\psi = \lambda \sum_{k \in \mathbb{Z}} e^{ik\theta} \phi(x).$$

$$\Rightarrow -\frac{\hbar^2}{2} (-k^2 \phi(x)) - \lambda \phi(x) = \frac{\hbar^2}{2} \frac{\partial^2 \phi}{\partial x^2}$$

$$\Rightarrow \phi(x) = A_k e^{\sqrt{k^2 - 2\lambda/\hbar^2} x} + B_k e^{-\sqrt{k^2 - 2\lambda/\hbar^2} x}$$

$$\therefore \Psi(x, \theta) = \sum_{k \in \mathbb{Z}} (A_k e^{\mu x} + B_k e^{-\mu x}) e^{ik\theta}$$

$$\text{where } \mu = \sqrt{k^2 - 2\lambda/\hbar^2}$$

$$\therefore \mu^2 = k^2 - 2\lambda/\hbar^2$$

$$\therefore \lambda = \frac{\hbar^2 (k^2 - \mu^2)}{2} //$$

Where k and μ are determined by the eigenfunction.

(7.4.) We have:

$$\alpha \equiv \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{q} + \frac{i}{m\omega} \hat{p} \right)$$

$$\text{and } \alpha^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{q} - \frac{i}{m\omega} \hat{p} \right)$$

(i.) Using $[\hat{q}, \hat{p}] = i\hbar$, we have:

$$\begin{aligned} [\alpha, \alpha^\dagger] &= \frac{m\omega}{2\hbar} \left[\hat{q} + \frac{i}{m\omega} \hat{p}, \hat{q} - \frac{i}{m\omega} \hat{p} \right] \\ &= \frac{m\omega}{2\hbar} \left([\hat{q}, -\frac{i}{m\omega} \hat{p}] + [\frac{i}{m\omega} \hat{p}, \hat{q}] \right) \\ &= \frac{m\omega}{2\hbar} \left(\frac{\hbar}{m\omega} + \frac{\hbar}{m\omega} \right) \\ &= 1 // \end{aligned}$$

$$(ii.) \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{q}^2$$

$$\text{noting that, } \sqrt{\frac{2\hbar}{m\omega}} (\alpha + \alpha^\dagger) = 2\hat{q} \Rightarrow \hat{q} = \sqrt{\frac{\hbar}{2m\omega}} (\alpha + \alpha^\dagger)$$

$$\sqrt{\frac{2\hbar}{m\omega}} (\alpha - \alpha^\dagger) = \frac{2i}{m\omega} \hat{p} \quad \text{and} \quad \hat{p} = \frac{i}{2} \sqrt{\frac{\hbar m\omega}{2}} (\alpha - \alpha^\dagger)$$

$$\begin{aligned}
\therefore \hat{I} &= \frac{\hbar^2}{2m} \left(-\frac{\hbar m \omega}{2} (\alpha - \alpha^\dagger)(\alpha - \alpha^\dagger) \right) + \frac{m \omega^2}{2} \left(\frac{\hbar}{2m\omega} (\alpha + \alpha^\dagger)(\alpha + \alpha^\dagger) \right)^2 \\
&= -\frac{\hbar^2}{4} \left(\cancel{\alpha^2} - \alpha \alpha^\dagger - \alpha^\dagger \alpha + \cancel{(\alpha^\dagger)^2} \right) + \frac{\hbar \omega}{4} \left(\cancel{\alpha^2} + \alpha \alpha^\dagger + \alpha^\dagger \alpha + \cancel{(\alpha^\dagger)^2} \right) \\
&= \frac{\hbar \omega}{2} (\alpha \alpha^\dagger + \alpha^\dagger \alpha) \\
&= \frac{\hbar \omega}{2} ([\alpha, \alpha^\dagger] + 2\alpha^\dagger \alpha) \\
&= \hbar \omega \left(\frac{1}{2} + \alpha^\dagger \alpha \right). //
\end{aligned}$$

$$\begin{aligned}
\text{(iii.) } [\hat{H}, \alpha] &= \hbar \omega [\alpha^\dagger \alpha, \alpha] \\
&= \hbar \omega [\alpha^\dagger, \alpha] \alpha \\
&= -\hbar \omega \alpha. //
\end{aligned}$$

$$\begin{aligned}
[\hat{H}, \alpha^\dagger] &= \hbar \omega [\alpha^\dagger \alpha, \alpha^\dagger] \\
&= \hbar \omega \alpha^\dagger [\alpha, \alpha^\dagger]. \\
&= \hbar \omega \alpha^\dagger. //
\end{aligned}$$

$$\text{(iv.) We have, } \hat{H} |n\rangle = E_n |n\rangle.$$

$$\begin{aligned}
\hat{H} (\alpha^\dagger)^k |n\rangle &= (\alpha^\dagger \hat{H} (\alpha^\dagger)^{k-1} + [\hat{H}, \alpha^\dagger] (\alpha^\dagger)^{k-1}) |n\rangle. \\
&= (\alpha^\dagger \hat{H} (\alpha^\dagger)^{k-1} + \hbar \omega (\alpha^\dagger)^k) |n\rangle. \\
&= ((\alpha^\dagger)^k \hat{H} + k \hbar \omega (\alpha^\dagger)^k) |n\rangle. \\
&= (E_n + k \hbar \omega) (\alpha^\dagger)^k |n\rangle. //
\end{aligned}$$

Similarly,

$$\hat{H} (\alpha)^k |n\rangle = (E_n - k \hbar \omega) (\alpha)^k |n\rangle. //$$

(v.) We note that:

$$\langle n | \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} | n \rangle = \langle n | n \rangle \left(\frac{E_n}{\hbar\omega} - \frac{1}{2} \right)$$

||

$$\langle n | \alpha^\dagger \alpha | n \rangle = |\alpha | n \rangle|^2 \geq 0.$$

$$\therefore E_n \geq \frac{1}{2} \hbar\omega.$$

As $\alpha | n \rangle$ is an eigenstate with a lower eigenvalue

$$\text{i.e. } E_n - \hbar\omega < E_n.$$

and as we have shown there is a lower bound to the set of energy eigenstates then we conclude that not all states $(\alpha)^k | n \rangle$ exist and for some \hat{k} we find

$$\alpha^{\hat{k}} | n \rangle = 0.$$

The state $\alpha^{\hat{k}-1} | n \rangle \equiv | 0 \rangle$ is the ground state and has energy eigenvalue:

$$\hat{H} | 0 \rangle = \hbar\omega \left(\frac{1}{2} - \alpha^\dagger \alpha \right) | 0 \rangle$$

$$= \frac{1}{2} \hbar\omega | 0 \rangle \quad \text{as } \alpha | 0 \rangle \equiv 0.$$

Hence the minimum energy is the ground state energy

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

$$\begin{aligned} \text{(vi.) } \langle n | \alpha^\dagger \alpha | n \rangle &= \langle n | \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} | n \rangle \\ &= \langle n | n \rangle \left(\frac{E_n}{\hbar\omega} - \frac{1}{2} \right). \end{aligned}$$

Now as $| n \rangle \propto (\alpha^\dagger)^n | 0 \rangle$ and $E_0 = \frac{1}{2} \hbar\omega$

$$\text{the } E_n = E_0 + n \hbar\omega = \left(n + \frac{1}{2} \right) \hbar\omega.$$

$$\therefore \alpha^\dagger \alpha | n \rangle = \left(\left(n + \frac{1}{2} \right) - \frac{1}{2} \right) | n \rangle = n | n \rangle. //$$

(vii) Let us write $|n-1\rangle = \lambda \alpha |n\rangle$ For some $\lambda \in \mathbb{C}$.

then

$$\begin{aligned} \langle n-1 | n-1 \rangle &= 1 \\ &= |\lambda|^2 \langle n | \alpha^\dagger \alpha | n \rangle. \\ &= |\lambda|^2 n \langle n | n \rangle. \\ &= |\lambda|^2 n \end{aligned}$$

$$\Rightarrow |\lambda|^2 = \frac{1}{n}$$

$$\therefore |\lambda| = \frac{1}{\sqrt{n}}$$

$$\therefore \alpha |n\rangle = \frac{1}{\sqrt{n}} |n-1\rangle //$$

Similarly we have:

(Let $|n+1\rangle = \mu \alpha^\dagger |n\rangle$)

$$\begin{aligned} 1 &= \langle n+1 | n+1 \rangle \\ &= |\mu|^2 \langle n | \alpha \alpha^\dagger | n \rangle. \\ &= |\mu|^2 \langle n | [\alpha, \alpha^\dagger] + \alpha^\dagger \alpha | n \rangle \\ &= |\mu|^2 (1+n) \langle n | n \rangle \\ &= |\mu|^2 (1+n) \end{aligned}$$

$$\Rightarrow |\mu| = \frac{1}{\sqrt{1+n}}$$

$$\therefore \alpha^\dagger |n\rangle = \frac{1}{\sqrt{1+n}} |n+1\rangle //$$