i.e. Let $\varphi = \int d\alpha\, \varphi_\alpha\, \underline{u}_\alpha = \int d\alpha \langle u_\alpha | \varphi \rangle\, \underline{u}_\alpha$

and $\psi = \int d\beta\, \psi_\beta\, \underline{u}_\beta = \int d\beta \langle u_\beta | \psi \rangle\, \underline{u}_\beta$.

Then
$$\begin{aligned}
\langle \varphi | \psi \rangle = \langle \varphi, \psi \rangle &= \left\langle \int d\alpha \langle u_\alpha | \varphi \rangle \underline{u}_\alpha , \int d\beta \langle u_\beta | \psi \rangle \underline{u}_\beta \right\rangle \\
&= \overline{\int d\alpha \langle u_\alpha | \varphi \rangle} \int d\beta \langle u_\beta | \psi \rangle \langle u_\alpha | u_\beta \rangle \\
&= \int d\alpha \langle \varphi | u_\alpha \rangle \int d\beta \langle u_\beta | \psi \rangle \langle u_\alpha | u_\beta \rangle \\
&= \int d\alpha \langle \varphi | u_\alpha \rangle \langle u_\alpha | \psi \rangle . \quad //
\end{aligned}$$

Probabilistic Interpretation.

The probability of a system in a state $|\psi\rangle$ to be between the eigenstates $|u_\alpha\rangle$ and $|u_{\alpha + d\alpha}\rangle$ is:

$$P(\alpha)\, d\alpha \equiv \frac{|\langle u_\alpha | \psi \rangle|^2}{\langle \psi | \psi \rangle}\, d\alpha = \frac{|\psi_\alpha|^2}{\langle \psi | \psi \rangle}\, d\alpha .$$

i.e. if $|\psi\rangle$ is normalised such that $\langle \psi | \psi \rangle = 1$ then the coefficients $\psi_\alpha \equiv \langle u_\alpha | \psi \rangle$ of the continuous basis vectors square to give the probability of being in state $|u_\alpha\rangle$.

Transformations Between Different Bases.

Given a state $|\psi\rangle \in \mathcal{H}$ it can be expressed in different bases of $\mathcal{H}$ using the completeness relation.

For example let $\{\underline{u}_n\}$ be a countable basis and $\{v_\alpha\}$ be a continuous basis, then:

$$\langle v_\alpha | \psi \rangle = \psi_\alpha \quad , \quad \langle u_n | \psi \rangle = \psi_n .$$

Then,

$$\psi_\alpha = \langle v_\alpha | \psi \rangle$$
$$= \sum_n \langle v_\alpha | u_n \rangle \langle u_n | \psi \rangle$$
$$= \sum_n u_n(\alpha)\, \psi_n.$$

Where $u_n(\alpha) \equiv \langle v_\alpha | u_n \rangle$.

While,

$$\psi_n = \langle u_n | \psi \rangle$$
$$= \int d\alpha \langle u_n | v_\alpha \rangle \langle v_\alpha | \psi \rangle$$
$$= \int d\alpha \; u_n^*(\alpha)\, \psi_\alpha.$$

The Schrödinger Equation.

Just as the (dynamical) time-evolution of a system represented in phase space is given by Hamilton's equations, the time evolution of a quantum system is described by Schrödinger's equation:

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

A typical Hamiltonian in the positions basis is

$$\hat{H} = -\frac{\hbar^2}{2} \sum_i \frac{1}{m_i} \frac{\partial^2}{\partial q_i^2} + \sum_i V(q_i)$$

Theorem: The inner product is time-independent.

Proof: (For typical $\hat{H}$).

$$\langle \psi, \varphi \rangle = \int_{\mathbb{R}^k} d^k q \; \psi_q^* \varphi_q.$$

So,

$$\frac{d}{dt} \langle \psi, \varphi \rangle = \int_{\mathbb{R}^k} d^k q \left(\frac{\partial}{\partial t}(\psi_q^*) \phi_q + \psi_q^* \frac{\partial}{\partial t}(\phi_q) \right)$$
$$= \int_{\mathbb{R}^k} d^k q \left(+\frac{i}{\hbar} (\hat{H}^* \psi_q^*) \phi_q + \psi_q^* \left(-\frac{i}{\hbar} \hat{H} \phi_q \right) \right)$$

Using Schrödinger's equation we have $-i\hbar \frac{\partial}{\partial t} \psi^* = \hat{H}^* \psi^*$.

For the typical Hamiltonian $\hat{H}^* = \hat{H}$ and we have:

$$\frac{d}{dt}\langle\psi|\psi\rangle = \int_{\mathbb{R}^k} d^k q \left(+\frac{i}{\hbar}\left(-\frac{\hbar^2}{2}\sum_i \frac{1}{m_i}\frac{\partial^2 \psi^*}{\partial q^2} + \sum_i V(q_i)\psi^* \right)\right)\psi.$$

$$+ \psi^* \left(\frac{-i}{\hbar}\left(-\frac{\hbar^2}{2}\sum_i \frac{1}{m_i}\frac{\partial^2}{\partial q^2}\psi + \sum_i V(q_i)\psi \right)\right).$$

$$= \int_{\mathbb{R}^k} d^k q \left(\frac{-i\hbar}{2}\sum_i \frac{1}{m_i}\left[\frac{\partial^2 \psi^*}{\partial q^2}\psi - \psi^* \frac{\partial^2 \psi}{\partial q^2} \right]\right).$$

$$= \int_{\mathbb{R}^k} d^k q \left(\frac{-i\hbar}{2}\sum_i \frac{1}{m_i}\left(-\frac{\partial \psi^*}{\partial q}\frac{\partial \psi}{\partial q} + \frac{\partial \psi^*}{\partial q}\frac{\partial \psi}{\partial q} \right)\right) + \dots$$

$$= 0 \qquad \text{if the surface term vanishes.}$$

N.B. The surface term is $\left[\frac{\partial \psi^*}{\partial q}\psi - \psi^* \frac{\partial \psi}{\partial q} \right]_{-\infty}^{\infty} \left(\frac{-i\hbar}{2}\sum_i \frac{1}{m_i} \right)$

and well-behaved ψ and ψ (which have compact support on $\mathcal{H}$) will vanish at infinity.

The probability density $\rho(q,t) = \psi^*(q,t)\psi(q,t)$ is conserved: $\frac{\partial}{\partial t}\int d^k q\, \rho(q,t) = 0.$

Equivalently, $\frac{\partial}{\partial t}(\rho(q,t)) = \sum_i \frac{\partial}{\partial q_i}\left(\frac{-i\hbar}{2m_i}\left[\frac{\partial \psi^*}{\partial q_i}\psi - \psi^* \frac{\partial \psi}{\partial q_i} \right]\right)$

$$\equiv -\sum_i \frac{\partial}{\partial q_i} J^i$$

The surface term. (once $\int d^k q$ is removed.)

J^i is called the probability current and is:

$$J^i \equiv +\frac{i\hbar}{2m}\left(\frac{\partial \psi^*}{\partial q_i}\psi - \psi^* \frac{\partial \psi}{\partial q_i} \right)$$

$$\therefore \quad \frac{\partial}{\partial t}(\rho) + \sum_i \frac{\partial}{\partial q_i} J^i = 0.$$

The Heisenberg and Schrödinger Pictures.

1. The Schrödinger Picture.

In the Schrödinger picture the states are time-dependent $\Psi = \Psi(q,t)$ but the operators do not: $\frac{d}{dt}A = 0$.

For the states we solve the Schrödinger equation:

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

Giving a formal solution:

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

In the energy / Hamiltonian eigenvector basis:

$$|\psi(t)\rangle = \sum_n |E_n\rangle\langle E_n|\psi(0)\rangle e^{-iEt/\hbar}.$$

i.e. $\hat{H}|\psi(0)\rangle = E|\psi(0)\rangle$. (also $|\psi(t)\rangle = e^{-\frac{iEt}{\hbar}}|\psi(0)\rangle$).

2. The Heisenberg Picture.

In the Heisenberg picture the states are time-independent but the operators are time-dependent:

$$|\psi\rangle_H = e^{+i\hat{H}t/\hbar}|\psi(t)\rangle_S = |\psi(0)\rangle_S.$$

While,
$$A_H(t) = e^{i\hat{H}t/\hbar} A_S e^{-i\hat{H}t/\hbar}.$$

Theorem: The picture changing transformations leave the inner product invariant.

Proof: $_H\langle\varphi|\psi\rangle_H = {}_S\langle\varphi|e^{-i\hat{H}t/\hbar}e^{+i\hat{H}t/\hbar}|\psi\rangle_S = {}_S\langle\varphi|\psi\rangle_S.$

Theorem: The operator matrix elements are also invariant under the picture-changing transformations.

Proof: $$_H\langle\varphi|A(t)|\psi\rangle_H = {}_S\langle\varphi|e^{-i\hat{H}t/\hbar}A(t)e^{i\hat{H}t/\hbar}|\psi\rangle_S.$$
$$= {}_S\langle\varphi|e^{-i\hat{H}t/\hbar}e^{i\hat{H}t/\hbar}A_S e^{-i\hat{H}t/\hbar}e^{i\hat{H}t/\hbar}|\psi\rangle_S.$$
$$= {}_S\langle\varphi|A_S|\psi\rangle_S.$$

The dynamics is now described by:

$$\frac{d}{dt}(A_H(t)) = \frac{i\hat{H}}{\hbar}A_H(t) - A_H(t)\frac{i\hat{H}}{\hbar} = \frac{i}{\hbar}[\hat{H}, A_H]$$
$$\therefore \quad i\hbar\frac{d}{dt}(A_H(t)) = [A_H(t), \hat{H}].$$

N.B. the canonical commutation relations are unchanged by picture changing:

$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}.$$

i.e. $$\hat{q}_i(t) = e^{i\hat{H}t/\hbar}\hat{q}_i e^{-i\hat{H}t/\hbar}.$$
$$\hat{p}_j(t) = e^{i\hat{H}t/\hbar}\hat{p}_j e^{-i\hat{H}t/\hbar}.$$

then, $$[\hat{q}_i(t), \hat{p}_j(t)] = e^{i\hat{H}t/\hbar}[\hat{q}_i, \hat{p}_j]e^{-i\hat{H}t/\hbar}$$
$$= i\hbar\delta_{ij}.$$

Examples.

1. The Harmonic Oscillator.

$$\mathcal{L} = \tfrac{1}{2}m\dot{q}^2 - \tfrac{1}{2}kq^2$$

e.o.m.: $\quad \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\right) - \frac{\partial \mathcal{L}}{\partial q} = m\ddot{q} + kq = 0.$

$$\therefore \quad \ddot{q} = -\,{}^{k}\!/_{m}\, q$$

$$\left(\Rightarrow \quad q = A\cos(\omega t) + B\sin(\omega t)\right)$$

with $\omega = \sqrt{k/m}$.

$p = m\dot{q}$

Hamiltonian: $\quad H = \dot{q}p - \mathcal{L}$

$$= {}^{p^2}\!/_{2m} + {}^{k}\!/_{2}\, q^2.$$

$$= \tfrac{1}{2}m\omega^2 q^2 + \left(\tfrac{1}{2m}\right)p^2.$$

Quantisation: $\quad (q,p) \longrightarrow (\hat{q},\hat{p})$.

Now introduce the variables:

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right), \quad \alpha^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right)$$

Then observe that:

$$[\alpha, \alpha^{+}] = \frac{m\omega}{2\hbar}\left[\hat{q} + \frac{i}{m\omega}\hat{p}, \hat{q} - \frac{i}{m\omega}\hat{p}\right]$$

$$= \frac{m\omega}{2\hbar}\left(\left[\hat{q}, \frac{-i}{m\omega}\hat{p}\right] + \left[\frac{i}{m\omega}\hat{p}, \hat{q}\right]\right)$$

$$= \frac{m\omega}{2\hbar}\left(\frac{\hbar}{m\omega} + \frac{\hbar}{m\omega}\right)$$

$$= 1.$$

Now $\quad \hat{q} = \sqrt{\frac{\hbar}{2m\omega}}\left(\alpha + \alpha^{+}\right), \quad \hat{p} = -i\sqrt{\frac{\hbar m\omega}{2}}\left(\alpha - \alpha^{+}\right)$

$$\therefore \quad \hat{H} = \tfrac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}\right)(\alpha+\alpha^{+})(\alpha+\alpha^{+}) + \frac{1}{2m}(-1)\left(\frac{\hbar m\omega}{2}\right)(\alpha-\alpha^{+})(\alpha-\alpha^{+})$$

$$= \frac{\hbar\omega}{4}\left[(\alpha+\alpha^{+})(\alpha+\alpha^{+}) - (\alpha-\alpha^{+})(\alpha-\alpha^{+})\right]$$

$$= \frac{\hbar\omega}{2}\left(\alpha\alpha^{+} + \alpha^{+}\alpha\right). \;//$$

Using $[\alpha, \alpha^+] = \alpha\alpha^+ - \alpha^+\alpha = 1$ we find:

$$\hat{H} = \tfrac{1}{2}\omega\hbar\,(1 + 2\alpha^+\alpha)$$

$$= \omega\hbar\,(\tfrac{1}{2} + \alpha^+\alpha).$$

The Hilbert space can then be constructed as follows:

Let $|n\rangle$ be a basis such that $\hat{H}$ is diagonalised:

$$\hat{H}\,|n\rangle \equiv E_n\,|n\rangle.$$

Now, $$[\hat{H}, \alpha^+] = \tfrac{1}{2}\omega\hbar\,\alpha^+ + \omega\hbar\,\alpha^+\alpha\alpha^+ - \tfrac{1}{2}\omega\hbar\,\alpha^+ - \omega\hbar\,\alpha^+\alpha^+\alpha.$$

$$= \omega\hbar\,\alpha^+[\alpha, \alpha^+]$$

$$= \omega\hbar\,\alpha^+.$$

Similarly, $[\hat{H}, \alpha] = -\omega\hbar\,\alpha.$

$$\therefore\ \hat{H}\,\alpha^+\,|n\rangle = (\alpha^+\hat{H} + \omega\hbar\,\alpha^+)\,|n\rangle$$

$$= (E_n + \omega\hbar)\,\alpha^+\,|n\rangle.$$

And, $\hat{H}\,\alpha\,|n\rangle = (E_n - \omega\hbar)\,\alpha\,|n\rangle.$

i.e. α^+ is the creation operator and α is the annihilation operator.

Recall that $\langle\ |\ \rangle \geq 0$ on a Hilbert space.

In particular, $\langle n|\,\alpha^+\alpha\,|n\rangle \geq 0$

$$\langle n|\,\frac{\hat{H}}{\omega\hbar} - \frac{1}{2}\,|n\rangle = \left(\frac{E_n}{\omega\hbar} - \frac{1}{2}\right) \geq 0.$$

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

$\therefore$ The ladder operators cannot create an infinite series of eigenstates in the negative energy direction. The eigenstates must terminate:

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

$$\hat{H}\alpha^2|n\rangle = (\hat{H}\alpha.\alpha)|n\rangle$$

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

$$= (\alpha(\alpha\hat{H} - \omega\hbar\alpha) - \omega\hbar\alpha^2)|n\rangle$$

$$= (E_n - 2\omega\hbar)\alpha^2|n\rangle.$$

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

As $E_n \geq \frac{1}{2}\omega\hbar$ there must be a ground state eigenfunction $|0\rangle$ such that $\alpha|0\rangle = 0$. In fact if $\alpha|0\rangle = 0$ then $\langle 0|\alpha^+\alpha|0\rangle = 0$ $\Rightarrow E_0 = \frac{1}{2}\omega\hbar$. and the Hilbert space can be constructed by acting on $|0\rangle$ with α^+.

More concretely we can find an n-particle eigenstate:

$|n\rangle$ with energy $E_n = \frac{1}{2}\omega\hbar + n\omega\hbar$.

The operator $N = \alpha^+\alpha$ is the number operator and counts the number of particles/excitations as:

$$\langle n|\alpha^+\alpha|n\rangle = \langle n|\frac{\hat{H}}{\omega\hbar} - \frac{1}{2}|n\rangle = (\tfrac{1}{2} + n - \tfrac{1}{2})\langle n|n\rangle = n.$$

We would like to find $|n-1\rangle$ from n. Let us denote

$$|n-1\rangle = k\,\alpha|n\rangle \qquad k \in \mathbb{C}.$$

Then,

$$\langle n-1|\alpha^+\alpha|n-1\rangle = \langle n|\alpha^+ k^* \alpha^+\alpha\, k\alpha|n\rangle$$

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

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

$$= |k|^2\left(\langle n|\alpha^+\alpha\left(\frac{1}{2}+n\right) - \alpha^+\alpha|n\rangle - \frac{1}{2}n\right)$$

$$= |k|^2\left(\left(\frac{1}{2}+n\right)n - n - \frac{1}{2}n\right)$$

$$= |k|^2\left(n(n-1)\right).$$

$$= (n-1).$$

$$\Rightarrow \quad k = 1/\sqrt{n}.$$

$$\therefore \quad \alpha|n\rangle = \sqrt{n}\,|n-1\rangle$$

and similarly,

$$\alpha^+|n\rangle = \sqrt{n+1}\,|n+1\rangle.$$

With $\alpha|0\rangle = 0.$