The Hamiltonian

Recall the 3rd postulate which prescribes the time-development of any state $|\psi\rangle$

$$\boxed{i\hbar \frac{\partial}{\partial t} |\psi\rangle = \mathcal{H} |\psi\rangle} \quad (1)$$

$\mathcal{H}$ is the Hamiltonian, a hermitian operator.

Most generally, we obtain the Hamiltonian as follows

1) Start with the Lagrangian formulation of classical mechanics dealing with generalized coordinates q_i and their generalized velocities $\dot{q}_i$.

$$\boxed{\text{Lagrangian} = L(q_i, \dot{q}_i, t)} \quad (2)$$

The classical equations of motion are obtained by extremizing the action

$$\boxed{S = \int_{t_1}^{t_2} dt \; L(q_i, \dot{q}_i, t)} \quad (3)$$

subject to the boundary conditions

$$\boxed{q_i(t_1) = q_{i1} \qquad q_i(t_2) = q_{i2}} \quad (4)$$

This leads to the Euler-Lagrange equations

$$\boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i}} \quad (5)$$

one for each i

2) From the Lagrangian define the canonical momentum conjugate to q_i as

$$\boxed{p_i = \frac{\partial L}{\partial \dot{q}_i}} \quad (6)$$

3) Take a Legendre transform of L to make q_i, p_i the independent variables instead of $q_i, \dot{q}_i$ by defining the Hamiltonian

$$\boxed{\mathcal{H} = \sum_i p_i \dot{q}_i - L} \quad (7)$$

To verify that the independent variables are q_i, p_i consider

$$d\mathcal{H} = \sum_i \left(\cancel{p_i d\dot{q}_i} + \dot{q}_i dp_i\right) - \sum_i \left(\frac{\partial L}{\partial q_i} dq_i + \cancel{\frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i}\right)$$

and note the cancellation of the $d\dot{q}_i$ term due to the definition of p_i

$$\Rightarrow \quad \frac{\partial \mathcal{H}}{\partial p_i} = \dot{q}_i \qquad \frac{\partial \mathcal{H}}{\partial q_i} = -\frac{\partial L}{\partial q_i} = -\dot{p}_i$$

$$\boxed{\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}} \quad (8)$$

Hamilton's eq^{n}s

4) Now promote q_i and p_i to Hermitian operators $\mathbb{q}_i$ and $\mathbb{p}_i$ satisfying canonical commutation relations

$$\boxed{[\mathbb{q}_i, \mathbb{p}_j] = i\hbar\, \delta_{ij}} \quad (9)$$

$$\boxed{H(q_i, p_i) \Rightarrow \mathbb{H}(\mathbb{q}_i, \mathbb{p}_i)} \quad (10)$$

is the quantum Hamiltonian operator

Here is how this works for a particle in 1D moving in a potential $V(x)$

$$\boxed{L(x, \dot{x}) = \frac{1}{2} M \dot{x}^2 - V(x)} \quad (11)$$

$$\frac{\partial L}{\partial \dot{x}} = M\dot{x} \qquad \frac{\partial L}{\partial x} = -\frac{dV}{dx}$$

Euler-Lagrange eq^n $\quad \boxed{M\ddot{x} = -\frac{dV}{dx}} \quad (12)$

$$\boxed{p = \frac{\partial L}{\partial \dot{x}} = M\dot{x}} \quad (13) \quad \text{or} \quad \dot{x} = p/M$$

$$H = p\dot{x} - \frac{1}{2} M\dot{x}^2 + V(x)$$

$$\boxed{H = \frac{p^2}{M} - \frac{1}{2M} p^2 + V(x) = \frac{p^2}{2M} + V(x)} \quad (14)$$

So $\quad \boxed{\mathbb{H} = \frac{\mathbb{P}^2}{2M} + V(\mathbb{X})} \quad (15)$

Since $\mathcal{H}$ is a hermitian operator it has a complete set of eigenkets with real eigenvalues

$$\boxed{\mathcal{H}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \qquad \langle\alpha|\beta\rangle = \delta_{\alpha\beta} \qquad \sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{1}} \quad (16)$$

Now consider $$\boxed{i\hbar\frac{\partial}{\partial t}|\alpha(t)\rangle = \mathcal{H}|\alpha(t)\rangle = \varepsilon_\alpha|\alpha(t)\rangle} \quad (17)$$

$$\Rightarrow \boxed{|\alpha(t)\rangle = e^{-\frac{i\varepsilon_\alpha t}{\hbar}}|\alpha(0)\rangle} \quad (18)$$

It is convenient to have a time-independent basis so we will henceforth set $|\alpha(0)\rangle \equiv |\alpha\rangle$

$$\Rightarrow \boxed{|\alpha(t)\rangle = e^{-\frac{i\varepsilon_\alpha t}{\hbar}}|\alpha\rangle} \quad (19)$$

Eigenstates of $\mathcal{H}$ are stationary. The expectation value of any physical observable in such a state is time-independent

$$\boxed{\langle\alpha(t)|\mathbb{A}|\alpha(t)\rangle = \langle\alpha|\mathbb{A}|\alpha\rangle} \quad (20)$$

We will be spending quite a bit of time in the rest of the course finding the eigenstates of simple Hamiltonians.

Any ket $|\psi\rangle$ can be expanded as

$$\boxed{|\psi(t)\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|\psi(t)\rangle = \sum_\alpha |\alpha\rangle \psi_\alpha(t)} \quad (21)$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \sum_\alpha |\alpha\rangle\, i\hbar\frac{\partial\psi_\alpha}{\partial t} = \mathcal{H}|\psi(t)\rangle = \sum_\alpha |\alpha\rangle\, \varepsilon_\alpha \psi_\alpha(t)$$

(22)

$$\Rightarrow \quad i\hbar\frac{\partial\psi_\alpha}{\partial t} = \varepsilon_\alpha\psi_\alpha \quad \Rightarrow \quad \boxed{\psi_\alpha(t) = e^{\frac{-i\varepsilon_\alpha t}{\hbar}}\psi_\alpha(0)}$$

$$\boxed{|\psi(t)\rangle = \sum_\alpha |\alpha\rangle\,\psi_\alpha(0)\, e^{-i\varepsilon_\alpha t/\hbar}} \quad (23)$$

Thus, once one knows $|\alpha\rangle$ one can find the time-dependence of any state.

Now consider (24)

$$\boxed{\langle\psi(t)|A|\psi(t)\rangle = \sum_{\alpha,\beta} e^{i(\varepsilon_\alpha-\varepsilon_\beta)t/\hbar}\,\langle\alpha|A|\beta\rangle}$$

If $[A,\mathcal{H}]=0$ then we know that they share eigenstates, so eigenstates of $\mathcal{H}$ are also eigenstates of A

(25)

$$\Rightarrow \quad \boxed{\langle\alpha|A|\beta\rangle = \delta_{\alpha\beta}\,\langle\alpha|A|\alpha\rangle \quad \text{if } [A,\mathcal{H}]=0}$$

So $\boxed{\langle\psi(t)|A|\psi(t)\rangle \text{ is time-independent if } [A,\mathcal{H}]=0}$

(26)

Given a state $|\psi\rangle$ and an operator $\mathbb{A}$, one can compute expectation values of powers of $\mathbb{A}$

$$\boxed{\langle\psi|\mathbb{A}|\psi\rangle = \bar{A}} = \text{mean or expectation value of } \mathbb{A} \text{ in } |\psi\rangle \quad (27)$$

$$\boxed{(\Delta A)^2 \equiv \langle\psi|\mathbb{A}^2|\psi\rangle - \left(\langle\psi|\mathbb{A}|\psi\rangle\right)^2} \quad (28)$$ is the variance of $\mathbb{A}$ in $|\psi\rangle$

$$\boxed{\Delta A = \text{Uncertainty of } \mathbb{A} \text{ in } |\psi\rangle} \quad (29)$$

Let's consider a simple example. Consider a normalized wavefunction at $t=0$

$$\boxed{\langle x|\psi(0)\rangle = \psi(x,0) = \frac{e^{-x^2/2a^2}}{\sqrt{a\sqrt{\pi}}}} \quad (30)$$

Let the particle be free, that is, $V(x)=0$

$$\boxed{\mathbb{H} = \frac{\mathbb{P}^2}{2M}} \quad (31)$$

Clearly $[\mathbb{P},\mathbb{H}]=0$ so eigenstates of $\mathbb{P}$ are also eigenstates of $\mathbb{H}$. We should therefore expand $|\psi\rangle$ in $|p\rangle$

$$\boxed{|\psi\rangle = \int_{-\infty}^{\infty} dp \; |p\rangle \, \tilde{\psi}(p)} \quad (32)$$

$$\Rightarrow \boxed{\psi(x) = \int_{-\infty}^{\infty} dp \; \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \, \tilde{\psi}(p)} \quad (33)$$

with the inverse transform

$$\boxed{\tilde{\psi}(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \, e^{-ipx/\hbar} \, \psi(x)} \quad (34)$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{a\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2a^2} - ipx/\hbar} \, dx$$

Complete squares

$$-\frac{x^2}{2a^2} - \frac{ipx}{\hbar} = -\frac{1}{2a^2}\left[x^2 + \frac{2ia^2p}{\hbar} x\right]$$

$$= -\frac{1}{2a^2}\left[\left(x + \frac{ia^2p}{\hbar}\right)^2 + \frac{a^4p^2}{\hbar^2}\right]$$

Shift the variable of integration to $\tilde{x} = x + \frac{ia^2p}{\hbar}$ and do the integral

$$\boxed{\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{a\sqrt{\pi}}} \sqrt{2\pi a^2} \, e^{-\frac{a^2p^2}{2\hbar^2}} = \sqrt{\frac{a}{\hbar\sqrt{\pi}}} \, e^{-\frac{a^2p^2}{2\hbar^2}}} \quad (35)$$

So $\boxed{|\psi(0)\rangle = \sqrt{\frac{a}{\hbar\sqrt{\pi}}} \int_{-\infty}^{\infty} dp \, |p\rangle \, e^{-\frac{a^2p^2}{2\hbar^2}}}$ (36)

Now $\mathcal{H}|p\rangle = \frac{p^2}{2M}|p\rangle \Rightarrow |p(t)\rangle = e^{-\frac{ip^2}{2M\hbar}t}|p\rangle$

$$\Rightarrow \boxed{|\psi(t)\rangle = \sqrt{\frac{a}{\hbar\sqrt{\pi}}} \int_{-\infty}^{\infty} dp \, |p\rangle \, e^{-\frac{a^2p^2}{2\hbar^2} - i\frac{p^2t}{2M\hbar}}} \quad (37)$$

Consider the mean and variance of x in $|\psi(t)\rangle$

$$\boxed{\langle \psi(t)|\, X\, |\psi(t)\rangle = \int_{-\infty}^{\infty} dx \ \langle \psi(t)|x\rangle\, x\, \langle x|\psi(t)\rangle} \quad (38)$$

So we need $\langle x|\psi(t)\rangle$

$$= \psi(x,t) = \sqrt{\frac{a}{\hbar\sqrt{\pi}}} \int_{-\infty}^{\infty} dp \ \frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}} \ e^{-p^2\left[\frac{a^2}{2\hbar^2} + \frac{it}{2M\hbar}\right]}$$

Let $\alpha = \frac{a^2}{2\hbar^2} + \frac{it}{2M\hbar}$

$$-\alpha p^2 + \frac{ipx}{\hbar} = -\alpha\left[p^2 - \frac{ip}{\alpha\hbar}x\right]$$

$$= -\alpha\left[p - \frac{ix}{2\alpha\hbar}\right]^2 - \frac{x^2}{4\alpha\hbar^2}$$

As usual, shift the $p \to p - \frac{ix}{2\alpha\hbar}$ and do the integral

$$\psi(x,t) = \sqrt{\frac{a}{\hbar\sqrt{\pi}}} \ \frac{1}{\sqrt{2\pi\hbar}} \ \sqrt{\frac{\pi}{\frac{a^2}{2\hbar^2} + \frac{it}{2M\hbar}}} \ e^{-\frac{x^2}{2a^2 + 2i\hbar t/M}}$$

$$\boxed{\psi(x,t) = \sqrt{\frac{a/\sqrt{\pi}}{a^2 + \frac{it\hbar}{M}}} \ e^{-\frac{x^2}{2a^2 + 2it\hbar/M}}} \quad (39)$$

define $\boxed{\beta = \frac{\hbar}{Ma^2}}$ (40) which has dimensions of $1/\text{time}$

$$\boxed{\psi(x,t) = \frac{1}{\sqrt{a\sqrt{\pi}}} \ \frac{1}{\sqrt{1+i\beta t}} \ e^{-\frac{x^2}{2a^2(1+i\beta t)}}} \quad (41)$$

$$|\psi(x,t)|^2 = \frac{1}{a\sqrt{\pi}} \frac{1}{\sqrt{1+\beta^2 t^2}} e^{-\frac{x^2}{a^2}\frac{1}{1+\beta^2 t^2}}$$

$$\boxed{\langle \psi(t) | \mathbb{x} | \psi(t) \rangle = \frac{1}{a\sqrt{\pi}} \frac{1}{\sqrt{1+\beta^2 t^2}} \int_{-\infty}^{\infty} dx \; x \; e^{-\frac{x^2}{a^2(1+\beta^2 t^2)}} = 0} \quad (42)$$

$$\boxed{\langle \psi(t) | \mathbb{x}^2 | \psi(t) \rangle = \frac{1}{a\sqrt{\pi}} \frac{1}{\sqrt{1+\beta^2 t^2}} \int_{-\infty}^{\infty} dx \; x^2 \; e^{-\frac{x^2}{a^2(1+\beta^2 t^2)}} = \frac{a^2}{2}(1+\beta^2 t^2)} \quad (43)$$

so $\boxed{(\Delta x)^2 = \frac{a^2}{2}(1+\beta^2 t^2)}$ (44)