The Classical limit and Heisenberg's Uncertainty relations

Let us restrict ourselves to the simplest type of Hamiltonian

$$\boxed{\mathcal{H} = \frac{\vec{P}^2}{2M} + V(\vec{x})} \quad (1)$$

Say at time t the system is in the state

$$\boxed{|\psi(t)\rangle} \quad (2)$$

which has to satisfy the Schrödinger Eq^n

$$\boxed{i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle} \quad (3)$$

Thus

$$\boxed{\frac{\partial}{\partial t}|\psi(t)\rangle = -\frac{i}{\hbar}\mathcal{H}|\psi(t)\rangle \quad \text{and} \quad \frac{\partial}{\partial t}\langle\psi(t)| = \frac{i}{\hbar}\langle\psi(t)|\mathcal{H}} \quad (4)$$

Now consider the time-dependence of some operator $\mathbb{O}$ made of $\vec{x}$ & $\vec{P}$, with no explicit time-dependence. We want

$$\frac{d}{dt}\langle\psi(t)|\mathbb{O}|\psi(t)\rangle = \left(\frac{\partial}{\partial t}\langle\psi(t)|\right)\mathbb{O}|\psi(t)\rangle + \langle\psi(t)|\mathbb{O}\frac{\partial}{\partial t}|\psi(t)\rangle$$

$$= \frac{i}{\hbar}\langle\psi(t)|\mathcal{H}\,\mathbb{O}|\psi(t)\rangle - \frac{i}{\hbar}\langle\psi(t)|\mathbb{O}\mathcal{H}|\psi(t)\rangle \quad (5)$$

$$\boxed{\frac{d}{dt}\langle\psi(t)|\mathbb{O}|\psi(t)\rangle = \frac{i}{\hbar}\langle\psi(t)|[\mathcal{H},\mathbb{O}]|\psi(t)\rangle}$$

Let's take a few simple operators to see how this goes.

Say $\boxed{\mathbb{O} = x_i}$ (6) $i = 1, 2, 3$ components

Let's define $\bar{x}_i(t) = \langle \psi(t) | x_i | \psi(t) \rangle$

$$\boxed{\frac{d}{dt} \bar{x}_i(t) = \frac{i}{\hbar} \langle \psi(t) | [\mathcal{H}, x_i] | \psi(t) \rangle} \quad (7)$$

The only part of $\mathcal{H}$ that does not commute with x_i is $\vec{\mathbb{P}}^2/2M$

$$\boxed{\left[\frac{\mathbb{P}_j \mathbb{P}_j}{2M}, x_i \right] = \frac{1}{2M} \left\{ \mathbb{P}_j [\mathbb{P}_j, x_i] + [\mathbb{P}_j, x_i] \mathbb{P}_j \right\}} \quad (8)$$

Note how the commutator acts like a derivative.

$$[\mathbb{P}_i, x_j] = -i\hbar \, \delta_{ij}$$

So $$\boxed{[\mathcal{H}, x_i] = -i\hbar \frac{\mathbb{P}_i}{M} = -i\hbar \frac{\partial \mathcal{H}}{\partial \mathbb{P}_i}} \quad (9)$$

So
$$\boxed{\frac{d}{dt} \bar{x}_i(t) = \langle \psi(t) | \frac{\mathbb{P}_i}{M} | \psi(t) \rangle \equiv \frac{\bar{P}_i(t)}{M}} \quad (10)$$

Now consider the time-dependence of $\mathbb{P}_i$

$$\boxed{\frac{d}{dt} \bar{P}_i(t) = \frac{i}{\hbar} \langle \psi(t) | [\mathcal{H}, \mathbb{P}_i] | \psi(t) \rangle = \frac{i}{\hbar} \langle \psi(t) | [V(\vec{x}), \mathbb{P}_i] | \psi(t) \rangle} \quad (11)$$

Now $$\boxed{V(\vec{\mathbb{x}}) = \int d^3x' \, |\vec{x}'\rangle V(\vec{x}') \langle \vec{x}'|} \quad (12)$$

We already know

$$\boxed{\begin{aligned} \mathbb{P}_i |\vec{x}'\rangle &= +i\hbar \frac{\partial}{\partial x_i'} |\vec{x}'\rangle \\ \Rightarrow \langle \vec{x}' | \mathbb{P}_i &= -i\hbar \frac{\partial}{\partial x_i'} \langle \vec{x}'| \end{aligned}} \quad (13)$$

$$\boxed{\begin{aligned} [V(\vec{\mathbb{x}}), \mathbb{P}_i] &= \int d^3x' \, V(\vec{x}') \left\{ |\vec{x}'\rangle\langle \vec{x}'| \mathbb{P}_i - \mathbb{P}_i |\vec{x}'\rangle\langle\vec{x}'| \right\} \\ &= \int d^3x' \, V(\vec{x}') \left(-i\hbar \frac{\partial}{\partial x_i'} \left\{ |\vec{x}'\rangle\langle\vec{x}'| \right\} \right) \end{aligned}} \quad (14)$$

Integrate by parts. As long as we assume that $\langle \vec{x}' | \psi\rangle$ vanishes as $|\vec{x}'| \to \infty$ we can ignore boundary terms.

$$\boxed{\begin{aligned} \Rightarrow [V(\vec{\mathbb{x}}), \mathbb{P}_i] &= \int d^3x' \, i\hbar \frac{\partial V(\vec{x}')}{\partial x_i'} |\vec{x}'\rangle\langle\vec{x}'| \\ &\equiv i\hbar \frac{\partial V(\vec{\mathbb{x}})}{\partial x_i} \equiv i\hbar \frac{\partial \mathcal{H}}{\partial x_i} \end{aligned}} \quad (15)$$

$$\Rightarrow \quad \boxed{\frac{d\bar{p}_i}{dt} = -\langle \psi(t) | \frac{\partial \mathcal{H}}{\partial x_i}(\vec{\mathbb{x}}) | \psi(t)\rangle} \quad (16)$$

(10), (16) are called Ehrenfest's Theorem. They look very similar to the classical Hamilton's eq^{n}s

$$\boxed{\dot{x}_i = \frac{\partial \mathcal{H}}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial x_i}} \qquad (17)$$

If we could replace the operator $\vec{x}$ inside (16) by its average $\langle \vec{x}(t) \rangle$ then we would have the correspondence principle.

However, before one can make this classical correspondence we need to insist on some properties of $|\psi(t)\rangle$, which we have ignored so far.

The problem is the second Hamilton eq^n. Let's write out (16) explicitly

$$\boxed{\dot{p}_i = -\int d^3x' \, \langle \psi(t) | \vec{x}' \rangle \frac{\partial V}{\partial x_i'}(\vec{x}') \langle \vec{x}' | \psi(t) \rangle} \qquad (18)$$

In general $\frac{\partial V}{\partial x_i'}$ can be expanded in a Taylor series around $\bar{x}_i(t)$

$$\boxed{\begin{aligned} \frac{\partial V}{\partial x_i'}(\vec{x}') = {} & \frac{\partial V}{\partial x_i'}(\bar{x}_i) + (x_j' - \bar{x}_j) \frac{\partial}{\partial x_j'} \frac{\partial V}{\partial x_i'}(\bar{x}) \\ & + (x_j' - \bar{x}_j)(x_k' - \bar{x}_k) \frac{1}{2!} \frac{\partial}{\partial x_j'} \frac{\partial}{\partial x_k'} \frac{\partial V}{\partial x_i'} \end{aligned}} \qquad (19)$$

Now $|\psi(t)\rangle$ is normalized, so

$$\int d^3x' \, \langle \psi(t) | \vec{x}' \rangle \langle \vec{x}' | \psi(t) \rangle = \int d^3x' \, |\psi(\vec{x}', t)|^2 = 1$$

Since $\bar{x}_i$ is the average of x_i

$$\boxed{\int d^3x' \langle \psi(t)|\vec{x}'\rangle (x'_j - \bar{x}_j(t)) \langle \vec{x}'|\psi(t)\rangle = 0} \quad (20)$$

However,

$$\int d^3x' \langle \psi(t)|\vec{x}'\rangle \left(x'_j - \bar{x}_j(t)\right)\left(x'_k - \bar{x}_k(t)\right) \langle \vec{x}'|\psi(t)\rangle \neq 0$$

So Eq (16) becomes

$$\boxed{\dot{\bar{p}}_i = -\frac{\partial V(\bar{\vec{x}})}{\partial x_i} - \frac{1}{2}\frac{\partial^3 V(\bar{\vec{x}})}{\partial x_i \partial x_j \partial x_k} \langle (x_j - \bar{x}_j(t))(x_k - \bar{x}_k(t)) \rangle + \cdots} \quad (21)$$

In order to have the classical correspondance we need the higher order terms to be negligible compared to the leading term.

This can be made to happen if $\langle \vec{x}'|\psi(t)\rangle$ is sharply peaked around the classical value $\bar{\vec{x}}(t)$.

How sharply peaked can both $\vec{x}$ and $\vec{p}$ be?

The answer is given by Heisenberg's Uncertainty principle.

Heisenberg Uncertainty Principle

Consider two arbitrary Hermitian operators $\mathbb{A}$ and $\mathbb{B}$ corresponding to observables.

As we know, in any state we can compute the means and variances of $\mathbb{A}$ & $\mathbb{B}$

$$\boxed{\begin{aligned} \bar{A} &= \langle \psi | \mathbb{A} | \psi \rangle & \bar{B} &= \langle \psi | \mathbb{B} | \psi \rangle \\ (\Delta A)^2 &= \langle \psi | (\mathbb{A} - \bar{A})^2 | \psi \rangle & (\Delta B)^2 &= \langle \psi | (\mathbb{B} - \bar{B})^2 | \psi \rangle \end{aligned}} \quad (22)$$

For convenience let's define the shifted operators

$$\boxed{\tilde{\mathbb{A}} = \mathbb{A} - \bar{A} \qquad \tilde{\mathbb{B}} = \mathbb{B} - \bar{B}} \quad (23)$$

Now $(\Delta A)^2 = \langle \psi | \tilde{\mathbb{A}}^2 | \psi \rangle = \langle \tilde{\mathbb{A}}^\dagger \psi | \tilde{\mathbb{A}} \psi \rangle = \langle \tilde{\mathbb{A}} \psi | \tilde{\mathbb{A}} \psi \rangle$

and $(\Delta B)^2 = \langle \tilde{\mathbb{B}} \psi | \tilde{\mathbb{B}} \psi \rangle$ (24)

Now we use the Schwarz inequality

$$\boxed{\langle \Psi | \Psi \rangle \langle \Phi | \Phi \rangle \geq |\langle \Psi | \Phi \rangle|^2} \quad (25)$$

$$\Rightarrow \boxed{(\Delta A)^2 (\Delta B)^2 \geq \langle \tilde{\mathbb{A}} \psi | \tilde{\mathbb{B}} \psi \rangle \langle \tilde{\mathbb{B}} \psi | \tilde{\mathbb{A}} \psi \rangle} \quad (26)$$

$$\text{RHS} = \langle \psi | \tilde{\mathbb{A}} \tilde{\mathbb{B}} | \psi \rangle \langle \psi | \tilde{\mathbb{B}} \tilde{\mathbb{A}} | \psi \rangle$$

$$\boxed{\begin{aligned}\tilde{A}\tilde{B} &= \frac{1}{2}(\tilde{A}\tilde{B}+\tilde{B}\tilde{A}) + \frac{1}{2}[\tilde{A},\tilde{B}] \\ \tilde{B}\tilde{A} &= \frac{1}{2}(\tilde{A}\tilde{B}+\tilde{B}\tilde{A}) - \frac{1}{2}[\tilde{A},\tilde{B}]\end{aligned}} \quad (27)$$

So

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq \left(\frac{1}{4}\langle\psi|(\tilde{A}\tilde{B}+\tilde{B}\tilde{A})|\psi\rangle\right)^2 - \frac{1}{4}\left(\langle\psi|[\tilde{A},\tilde{B}]|\psi\rangle\right)^2} \quad (28)$$

Now recall that since $\tilde{A}, \tilde{B}$ are hermitian,

$$[\tilde{A},\tilde{B}] = \text{antihermitian} = i\,\Gamma$$

Γ hermitian

On the other hand

$$\tilde{A}\tilde{B}+\tilde{B}\tilde{A} = \text{hermitian} \quad (29)$$

$$\Rightarrow \boxed{\langle\psi|\tilde{A}\tilde{B}+\tilde{B}\tilde{A}|\psi\rangle = \text{real} \qquad \langle\psi|[\tilde{A},\tilde{B}]|\psi\rangle = \text{imaginary}}$$

So both terms on the RHS are positive.

We can drop the 1st term while preserving the inequality.

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\left|\langle\psi|[\tilde{A},\tilde{B}]|\psi\rangle\right|^2} \quad (30)$$

This is the general form of the Uncertainty principle.

Let's apply it in some simple cases.

If $A = X$, $B = P$ in 1 dimension

$[\mathbb{x}, \mathbb{p}] = i\hbar \mathbb{1}$

$$\boxed{(\Delta x)^2 (\Delta p)^2 \geq \frac{\hbar^2}{4} \quad \Rightarrow \quad \Delta x \; \Delta p \geq \frac{\hbar}{2}} \quad (31)$$

The nice thing about this is that it is universal. The inequality holds for any $|\psi\rangle$.

Can the inequality be saturated? This would require us to first saturate the Schwartz inequality, which implies

$$\boxed{\tilde{\mathbb{x}} |\psi\rangle = z \, \tilde{\mathbb{p}} |\psi\rangle} \quad (32) \qquad z = \text{complex number}$$

and demanding

$$\boxed{\langle \psi | \tilde{\mathbb{x}} \tilde{\mathbb{p}} + \tilde{\mathbb{p}} \tilde{\mathbb{x}} |\psi\rangle = 0} \quad (33)$$

Focus on (32) first. In real space

$$\boxed{(x - \bar{x}) \psi(x) = z \left(-i\hbar \frac{d\psi}{dx} - \bar{p}\, \psi\right)} \quad (34)$$

or $\psi'(x) = \frac{i}{\hbar z} \left(x - \bar{x} + z\bar{p} \right) \psi$

$$\Rightarrow \boxed{\begin{aligned} \psi(x) &= \psi(0)\, e^{\frac{i}{2\hbar z}(x - \bar{x} + z\bar{p})^2} \\ &= \psi(0)\, e^{i\bar{p}(x-\bar{x}) + \frac{iz\bar{p}^2}{2\hbar} + \frac{i(x-\bar{x})^2}{2\hbar z}} \end{aligned}} \quad (35)$$

Now let's apply the condition (33)

We write it in the form

$$\boxed{\langle \tilde{x}\psi | \tilde{p}\psi\rangle + \langle \tilde{p}\psi | \tilde{x}\psi\rangle = 0} \quad (36)$$

We already know

$$\boxed{\begin{aligned} &|\tilde{x}\psi\rangle = z\,|\tilde{p}\psi\rangle \\ \Rightarrow\ &\langle \tilde{x}\psi| = z^*\langle \tilde{p}\psi| \end{aligned}} \quad (37)$$

So $\boxed{(z+z^*)\,\langle \tilde{p}\psi|\tilde{p}\psi\rangle = 0}$ (38)

which means z is purely imaginary

Looking at (35) we see that if $\psi(x)$ is normalizable $\boxed{z = -i\,\frac{2\ell^2}{\hbar}}$ (39) where ℓ = real

$$\Rightarrow \boxed{\psi(x) = \text{Const}\ e^{\frac{i\bar{p}(x-\bar{x})}{\hbar}}\ e^{-\frac{(x-\bar{x})^2}{2\ell^2}}} \quad (40)$$

This is the minimum uncertainty wavepacket

Let us consider a more complicated example. You probably know that the commutation relations satisfied by the angular momentum operators

$$\boxed{\begin{aligned} &\vec{\mathbb{L}} = \mathbb{L}_x\hat{i} + \mathbb{L}_y\hat{j} + \mathbb{L}_z\hat{k} \\ &[\mathbb{L}_i, \mathbb{L}_j] = i\hbar\,\epsilon_{ijk}\,\mathbb{L}_k \end{aligned}} \quad (41)$$

are

As we will learn later, the orbital angular momentum operators are quantized with eigenstates $|\ell, m\rangle$ $\ell, m =$ integers $m \in [-\ell, \ell]$

$$\boxed{\begin{aligned} \vec{\mathbb{L}}^2 |\ell,m\rangle &= \hbar^2 \ell(\ell+1) |\ell,m\rangle \\ \mathbb{L}_z |\ell,m\rangle &= \hbar m |\ell,m\rangle \end{aligned}} \quad (42)$$

If the system is in a state of maximal $\mathbb{L}_z$, which is $|\ell,\ell\rangle$ then in this state

$$\boxed{\begin{aligned} (\Delta L_x)^2 (\Delta L_y)^2 &\geq \frac{\hbar^2 \ell^2}{4} \\ \Delta L_x \, \Delta L_y &\geq \frac{\hbar}{2} \ell \end{aligned}} \quad (43)$$

The Energy-time Uncertainty Relation

This has a very different status than those of dynamical variables like x, p. Remember, t is a parameter in QM. There are a couple of different ways to interpret the Et uncertainty relation.

The simplest way to think about the energy-time uncertainty relation is simply via Fourier transforms.

Say we have a plane wave of light of nominal frequency ω. We open a shutter for a finite time T to let the wave go through and then we close the shutter.

$$\Rightarrow \boxed{f(x,t) = \cos(kx - \omega t)\ \Theta\left(x - ct + \frac{cT}{2}\right)\ \Theta\left(\frac{cT}{2} - x + ct\right)} \quad (44)$$

The step functions make sure $|x - ct| < \frac{T}{2}$

Let's Fourier transform this

$$\boxed{\begin{aligned} f(x,t) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\, f(x,\omega')\, e^{-i\omega' t} \\ \Rightarrow f(x,\omega') &= \int_{-\infty}^{\infty} dt\, e^{i\omega' t}\, f(x,t) \end{aligned}} \quad (45)$$

$$\boxed{= \int_{-T/2+x/c}^{T/2+x/c} \cos(kx-\omega t)\, e^{i\omega' t}\, dt = \frac{1}{2}\int_{-\frac{T}{2}+\frac{x}{c}}^{\frac{T}{2}+\frac{x}{c}} dt\, e^{-i\omega' t}\left[e^{i(kx-\omega t)} + e^{-ikx+\omega t}\right]} \quad (46)$$

$$= \frac{1}{2} e^{ikx} \frac{e^{-i(\omega+\omega')(T/2+x/c)} - e^{-i(\omega+\omega')(-T/2+x/c)}}{-i(\omega+\omega')}$$

$$+ \frac{1}{2} e^{-ikx} \frac{e^{-i(\omega'-\omega)(\frac{T}{2}+\frac{x}{c})} - e^{-i(\omega'-\omega)(-\frac{T}{2}+\frac{x}{c})}}{-i(\omega'-\omega)}$$

Recall, for light in vacuum $k = \omega/c$, $k' = \omega'/c'$

$$\boxed{f(x,\omega') = e^{-ik'x}\left\{\frac{\sin\left[(\omega+\omega')T/2\right]}{\omega+\omega'} + \frac{\sin\left[(\omega'-\omega)T/2\right]}{\omega'-\omega}\right\}} \quad (47)$$

This contains all frequencies, not just ω.

However, it is sharply peaked around $\omega' = \pm\omega$, with a "width" $\boxed{\Delta\omega' \simeq \frac{1}{T}}$ (48)

So opening the shutter for a time Δt leads to an uncertainty of frequency of

$$\boxed{\Delta\omega' \simeq \frac{1}{\Delta t}} \quad (49)$$

$$\boxed{\Delta\varepsilon = \hbar\Delta\omega' \simeq \frac{\hbar}{\Delta t}} \quad (50)$$

Here is a more physical interpretation of the $\Delta E \, \Delta t$ uncertainty relation.

Consider an initial state that is a superposition of energy eigenstates.

$$\boxed{\begin{gathered} \mathcal{H}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \qquad \langle\alpha|\beta\rangle = \delta_{\alpha\beta} \\ |\psi(0)\rangle = \sum_\alpha \psi_\alpha |\alpha\rangle \end{gathered}} \quad \text{S1}$$

This state has some energy uncertainty ΔE

$$\boxed{\begin{gathered} \bar{E} = \langle\psi|\mathcal{H}|\psi\rangle = \sum_\alpha |\psi_\alpha|^2 \varepsilon_\alpha \\ (\Delta E)^2 = \langle\psi|(\mathcal{H}-\bar{E})^2|\psi\rangle = \sum_\alpha |\psi_\alpha|^2 \varepsilon_\alpha^2 - \left(\sum_\alpha |\psi_\alpha|^2 \varepsilon_\alpha\right)^2 \end{gathered}} \quad \text{S2}$$

We can time evolve it

$$\boxed{|\psi(t)\rangle = \sum_\alpha |\alpha\rangle e^{-i\varepsilon_\alpha t/\hbar} \psi_\alpha} \quad \text{S3}$$

Clearly $\bar{E}$ and ΔE are time-independent.

Consider some operator $\mathbb{A}$. If it commutes with $\mathcal{H}$ its mean $\bar{A}$ and $(\Delta A)^2$ will be time-independent, which is not interesting. So let's focus on the case where $[\mathcal{H}, \mathbb{A}] \neq 0$.

Now we know from the most general uncertainty relation Eq (30)

$$\boxed{(\Delta E)^2 (\Delta A)^2 \geq \frac{1}{4} \left| \langle \psi | [\mathcal{H}, A] | \psi \rangle \right|^2} \quad (54)$$

Also, from Eq (5) $\boxed{\langle \psi | [\mathcal{H}, A] | \psi \rangle = -i\hbar \langle \psi | \dot{A} | \psi \rangle}$ (55)

Thus $\boxed{\Delta E \; \Delta A \geq \frac{\hbar}{2} \langle \dot{A} \rangle}$ (56)

How long does it take to decide that $\langle A \rangle$ is changing? If this is Δt, then we demand

$$\boxed{\langle \dot{A} \rangle \Delta t \simeq \Delta A} \quad (57)$$

This means that unless $\langle \dot{A} \rangle \Delta t$ is of order ΔA we don't know that there is any time-dependence in $\langle A \rangle$ at all. We must wait for at least

$$\boxed{\Delta t \geq \hbar / 2 \Delta E} \quad (58)$$

to measure it. The nice thing is A drops out! However, how can a state in a superposition of energies arise? Typically it is because some interaction has been turned on or off.