Lecture 14

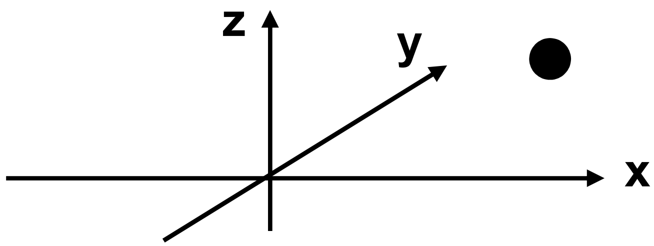
CSCOs, Energy-Time Uncertainty, and Quasi-Bound States

In this lecture you will learn:

- **Some more fundamentals of quantum physics: CSCOs**
- **The energy-time uncertainty relation in quantum physics**
- **Quasi-bound states in quantum physics**

Observables and Eigenvalue Degeneracies

Consider a particle in free-space in 3D:



The Hamiltonian is:

$$\hat{H} = \frac{\hat{\vec{p}}.\hat{\vec{p}}}{2m} = \frac{\hat{p}^2}{2m} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$$

Question: Is the <u>energy eigenvalue</u> of the particle enough to uniquely specify all that is SIMULTANEOUSLY knowable or measurable about the particle??

Answer: No!

Momentum commutes with the free-particle Hamiltonian:

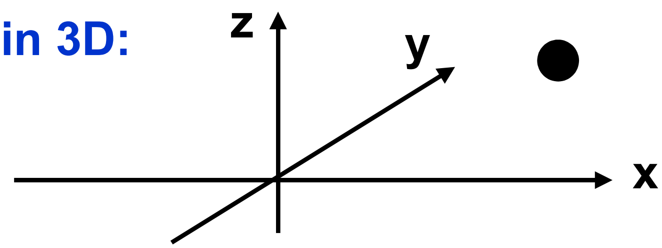
$$\left[\hat{H}, \hat{\vec{p}}\right] = 0$$

And there are many different energy eigenstates which all have the same energy eigenvalue (i.e. the same eigenvalue for the operator $\hat{p}^2/2m$) but which are also momentum eigenstates with different momentum eigenvalues:

$$\left|\vec{p} = p e_x\right\rangle \quad \left|\vec{p} = p e_y\right\rangle \quad \left|\vec{p} = (p e_x + p e_z)/\sqrt{2}\right\rangle$$

Observables and Eigenvalue Degeneracies

A particle in free-space in 3D:



$$\hat{H} = \frac{\hat{\vec{p}}.\hat{\vec{p}}}{2m} = \frac{\hat{p}^2}{2m} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m}$$

Conclusion: The Hamiltonian has degenerate eigenvalues – meaning several different energy eigenstates have the same energy eigenvalue

Therefore, specifying the eigenvalue of the Hamiltonian is not enough to uniquely specify all that is simultaneously knowable or measureable about the particle!

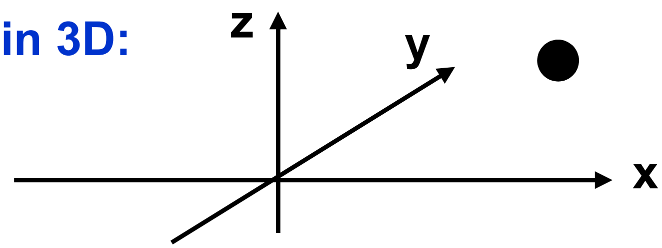
How do we fix the problem?

Suppose we take both the Hamiltonian operator $\hat{H}$ and the momentum operator $\hat{\vec{p}}$, and then ask the same question: Are the energy and the momentum eigenvalues of the particle, taken together, enough to uniquely specify all that is SIMULTANEOUSLY knowable or measurable about this particle??

Answer: Yes ……..but this is an overkill. Just specifying the momentum would do.

Observables and Eigenvalue Degeneracies

A particle in free-space in 3D:



Suppose we take just the momentum operator $\hat{\vec{p}}$, and then ask the same question again: Is the momentum eigenvalue of the particle enough to uniquely specify all that is SIMULTANEOUSLY knowable or measureable about this particle??

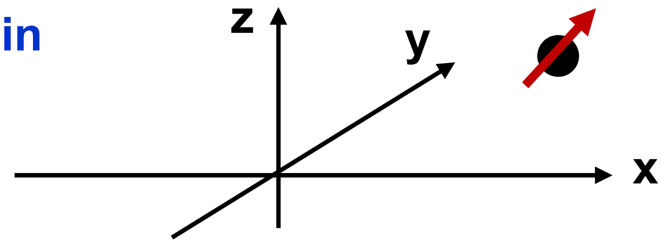
Answer: Yes!

$$\left|\vec{p} = p e_x\right\rangle \quad \left|\vec{p} = p e_y\right\rangle \quad \left|\vec{p} = \left(p e_x + p e_z\right)/\sqrt{2}\right\rangle$$

But what if the particle now has spin (e.g. an electron)????

Observables and Eigenvalue Degeneracies

A particle in free-space in 3D with spin:



Suppose we take just the momentum operator $\hat{\vec{p}}$, and then ask the same question again: Is the momentum eigenvalue of the particle enough to uniquely specify all that is SIMULTANEOUSLY knowable or measureable about this particle??

$$\left|\vec{p} = p e_x\right\rangle \qquad \left|\vec{p} = p e_y\right\rangle \qquad \left|\vec{p} = \left(p e_x + p e_z\right)/\sqrt{2}\right\rangle$$

Answer: No! we need to specify the spin too!

$$\left|\vec{p} = p e_x\right\rangle \otimes \left|\uparrow\right\rangle \qquad \left|\vec{p} = p e_y\right\rangle \otimes \left|\downarrow\right\rangle \qquad \left|\vec{p} = \left(p e_x + p e_z\right)/\sqrt{2}\right\rangle \otimes \frac{1}{\sqrt{2}}\left[\left|\uparrow\right\rangle + \left|\downarrow\right\rangle\right]$$

Note that spin operators commute with momentum and position operators:

$$\left[\hat{S}_k, \hat{p}_j\right] = 0 \qquad \left[\hat{S}_k, \hat{r}_j\right] = 0 \qquad \left\{ j, k = x, y, z \right.$$

The momentum AND spin of the particle, taken together, are enough to uniquely specify all that is SIMULTANEOUSLY knowable or measurable about this particle

Complete Set of Commuting Observables (CSCO)

Consider a Hermitian operator $\hat{O}$ corresponding to an observable *O* of a quantum system:

$$\hat{O}\left|v_j\right\rangle = \lambda_j \left|v_j\right\rangle$$

If the Hermitian operator $\hat{O}$ has all non-degenerate eigenvalues (meaning all eigenvalues λ_j are different) then we have a rather nice situation in which all possible orthogonal states of the quantum system can be uniquely distinguished by labeling it with the corresponding eigenvalue of $\hat{O}$. To put it another way, measurement of the observable *O* alone can tell us all that is simultaneously knowable about the quantum state of the system

In this case, the operator $\hat{O}$ provides a "complete set of commuting observables" or a CSCO. The set here has just one observable; the operator $\hat{O}$

But what if the following four eigenvalues $\lambda_k, \lambda_m, \lambda_n, \lambda_p$ of $\hat{O}$ are all the same?

Complete Set of Commuting Observables (CSCO)

$$\hat{O}\left|v_j\right\rangle = \lambda_j\left|v_j\right\rangle$$

But what if the following eigenvalues $\lambda_k, \lambda_m, \lambda_n, \lambda_p$ of $\hat{O}$ are all the same?

Then measurement of the observable *O* alone, can not tell us all that is simultaneously knowable about the quantum state of the system. $\hat{O}$ is then no longer a CSCO

Example: Suppose *O* is measured and the result is λ_n . That knowledge is not enough to uniquely specify the state of the system post measurement.

Question: How many observables do we need to simultaneously measure in order to gain full knowledge of all that is simultaneously knowable about the quantum state of the system?

Complete Set of Commuting Observables (CSCO)

$$\hat{O}\left|v_j\right\rangle = \lambda_j\left|v_j\right\rangle$$

The following eigenvalues $\lambda_k, \lambda_m, \lambda_n, \lambda_p$ of $\hat{O}$ are all same

Solution to the problem:

Suppose we are able to find another operator $\hat{W}$ corresponding to an observable W that is compatible with $\hat{O}$:

$$\left[\hat{O}, \hat{W}\right] = 0$$

and therefore $\left|v_j\right\rangle$ are also eigenvectors of $\hat{W}$:

$$\hat{W}\left|v_j\right\rangle = \gamma_j\left|v_j\right\rangle$$

Also suppose that $\gamma_k, \gamma_m, \gamma_n, \gamma_p$ are all different, but some other eigenvalues $\gamma_r, \gamma_s, \gamma_t$ are all the same

Therefore, using eigenvalues of both the operators $\hat{O}$ and $\hat{W}$ we can uniquely specify every common eigenstate of the system. In other words, simultaneous measurement of the two compatible observables O and W can uniquely specify the quantum state of the system post measurement

In this case, we say that the set of two operators $\hat{O}$ and $\hat{W}$ constitute a CSCO.

Complete Set of Commuting Observables (CSCO)

Formal definition of a CSCO:

Consider a set of commuting Hermitian operators $\{\hat{A}, \hat{B}, \hat{C}, \ldots\ldots\ldots\}$ corresponding to observables of a quantum system and a complete set of common eigenvectors of all these operators:

$$\hat{A}|v_j\rangle = \alpha_j |v_j\rangle$$

$$\hat{B}|v_j\rangle = \beta_j |v_j\rangle$$

$$\hat{C}|v_j\rangle = \gamma_j |v_j\rangle$$

$$\vdots$$

The set $\{\hat{A}, \hat{B}, \hat{C}, \ldots\ldots\ldots\}$ is said to constitute a CSCO if the set of corresponding eigenvalues $\{\alpha_j, \beta_j, \gamma_j, \ldots\ldots\ldots\}$, taken together, can be used to uniquely label (or identify) every common eigenvector

In other words, simultaneous measurement of all the observables *A, B, C*, …….. in a CSCO can uniquely identify the quantum state of the system

Complete Set of Commuting Observables (CSCO)

Why do we care about CSCOs?

1) It is a physically motivated assumption that for any physical quantum system there is a complete set of commuting observables. Otherwise there would be no physical or measurable way to distinguish all the various states that belong to the Hilbert space of the system.

2) So in any physical problem we are obliged to find such a complete set, and we must include all compatible operators in such a set until all the common eigenvectors of the set can be uniquely specified by the eigenvalues of these operators.

3) A CSCO need not be unique. Once we have a complete set of commuting observables, adding another commuting observable causes no harm, although it is not necessary. <u>But ideally, we want the smallest number of operators in the set.</u>

How Fast can Quantum Gates Operate? How Fast can Quantum States Evolve in Time?

The question "how fast can quantum computers operate?" is related to the question "how fast can quantum gates operate?"

↓

A quantum gate is made of up one or more quantum operations
Are there fundamental speed limits to the speed of a quantum operation?

↓

Are there fundamental limits to the speeds at which quantum states can evolve?

Quantum Time Evolution Revisited

A measure of how fast quantum states can evolve is how fast the mean value of some suitable observable changes with time

Consider the time-dependent mean value of an operator $\hat{O}$:

$$\langle \hat{O} \rangle (t) = \langle \psi(t) | \hat{O} | \psi(t) \rangle \qquad \left\{ \quad |\psi(t)\rangle = e^{-i\frac{\hat{H}}{\hbar}t} |\psi(t=0)\rangle \right.$$

Suppose $|\psi(t=0)\rangle$ is an eigenstate of the Hamiltonian with energy *E*. Then:

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

$$\Rightarrow \langle \hat{O} \rangle (t) = \langle \psi(t) | \hat{O} | \psi(t) \rangle = \langle \psi(t=0) | \hat{O} | \psi(t=0) \rangle = \langle \hat{O} \rangle (t=0)$$

Conclusion: $|\psi(t=0)\rangle$ must be a superposition of energy eigenstates for the mean value $\langle \psi(t) | \hat{O} | \psi(t) \rangle$ to change with time

No energy uncertainty → no non-trivial time development

Quantum Time Evolution Revisited

We now assume that the state $\left|\psi(t)\right\rangle$ is not an energy eigenstate but a superposition of energy eigenstates

If the state $\left|\psi(t)\right\rangle$ is a superposition of energy eigenstates then the mean and the standard deviation in the energy is:

$$\left\langle \hat{H} \right\rangle(t) = \left\langle \psi(t) \right| \hat{H} \left| \psi(t) \right\rangle$$

$$\Delta E = \sigma_H = \sqrt{\left\langle \psi(t) \right| \Delta\hat{H}^2 \left| \psi(t) \right\rangle} = \sqrt{\left\langle \psi(t) \right| \hat{H}^2 \left| \psi(t) \right\rangle - \left\langle \psi(t) \right| \hat{H} \left| \psi(t) \right\rangle^2}$$

We start from:

$$\left\langle \hat{O} \right\rangle(t) = \left\langle \psi(t) \right| \hat{O} \left| \psi(t) \right\rangle$$

Take the time derivative on both sides:

$$i\hbar \frac{\partial}{\partial t} \left\langle \hat{O} \right\rangle(t) = \left\langle \psi(t) \right| \hat{O} \left(i\hbar \frac{\partial}{\partial t} \left| \psi(t) \right\rangle \right) + \left(i\hbar \frac{\partial}{\partial t} \left\langle \psi(t) \right| \right) \hat{O} \left| \psi(t) \right\rangle$$

$$= \left\langle \psi(t) \right| \hat{O}\hat{H} \left| \psi(t) \right\rangle - \left\langle \psi(t) \right| \hat{H}\hat{O} \left| \psi(t) \right\rangle$$

$$= \left\langle \psi(t) \right| \left[\hat{O}, \hat{H} \right] \left| \psi(t) \right\rangle$$

The mean value of the observable O will NOT change with time if $\left[\hat{O}, \hat{H} \right] = 0$

Energy-Time Uncertainty Relation

$$i\hbar \frac{\partial}{\partial t}\langle \hat{O} \rangle(t) = \langle \psi(t) | [\hat{O}, \hat{H}] | \psi(t) \rangle$$

Now the standard Heisenberg uncertainty relation says:

$$\langle \psi(t) | \Delta\hat{O}^2 | \psi(t) \rangle \langle \psi(t) | \Delta\hat{H}^2 | \psi(t) \rangle \geq \left[\frac{\langle \psi(t) | [\hat{O}, \hat{H}] | \psi(t) \rangle}{2i} \right]^2$$

which gives:

$$\sqrt{\langle \psi(t) | \Delta\hat{O}^2 | \psi(t) \rangle} \sqrt{\langle \psi(t) | \Delta\hat{H}^2 | \psi(t) \rangle} \geq \frac{\hbar}{2} \frac{\partial}{\partial t} \langle \psi(t) | \hat{O} | \psi(t) \rangle$$

We define a time scale ΔT_O related to the time rate of change of the mean value of the observable O as:

$$\frac{1}{\Delta T_O} = \frac{\frac{\partial}{\partial t} \langle \psi(t) | \hat{O} | \psi(t) \rangle}{\sqrt{\langle \psi(t) | \Delta\hat{O}^2 | \psi(t) \rangle}}$$

This time scale represents a duration over which the mean value of the observable changes "significantly"

to get:

$$\Delta T_O \sqrt{\langle \psi(t) | \Delta\hat{H}^2 | \psi(t) \rangle} \geq \frac{\hbar}{2}$$

$$\Rightarrow \Delta T_O \, \Delta E \geq \frac{\hbar}{2}$$

The product of the energy standard deviation of a quantum state and the time scale over which the mean value of any observable evolves in time is greater than or equal to $\hbar/2$

Energy-Time Uncertainty Relation

$$\Delta T_O \sqrt{\langle \psi(t) | \Delta \hat{H}^2 | \psi(t) \rangle} \geq \frac{\hbar}{2}$$

$$\Rightarrow \Delta T_O \, \Delta E \geq \frac{\hbar}{2}$$

The above relation implies that the larger the energy uncertainty of a quantum state (meaning larger the superposition of different energy eigenstates a quantum state is made up of) the smaller the time scale over which the mean value of an observable can change "significantly" with time

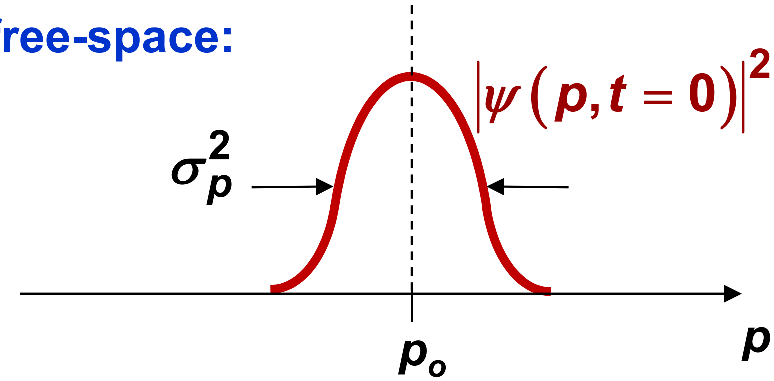
Energy-time uncertainty in quantum physics is not an uncertainty relation, strictly speaking, because time is not an operator in quantum physics

The energy-time uncertainty is a relation between the rate at which the mean value of an observable evolves in time and the uncertainty in the energy of the system

Energy-Time Uncertainty Relation: Gaussian Wavepacket

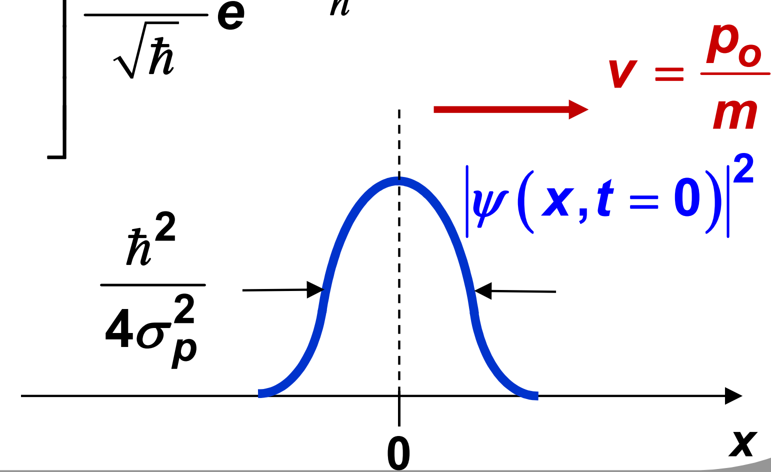
Consider a Gaussian wave-packet for a particle in free-space:

$$\left|\psi(t=0)\right\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \Bigg[\underbrace{\left(\frac{2\pi}{\sigma_p^2}\right)^{1/4} e^{-\frac{(p-p_o)^2}{4\sigma_p^2}}}_{\psi(p,t=0)} \Bigg] \left|p\right\rangle$$



$$\Rightarrow \left|\psi(t)\right\rangle = e^{-i\frac{\hat{H}}{\hbar}t}\left|\psi(t=0)\right\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \left[\left(\frac{2\pi}{\sigma_p^2}\right)^{1/4} e^{-\frac{(p-p_o)^2}{4\sigma_p^2}} \right] e^{-i\frac{E(p)}{\hbar}t} \left|p\right\rangle$$

$$\left\langle x \middle| \psi(t)\right\rangle = \psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \left[\left(\frac{2\pi}{\sigma_p^2}\right)^{1/4} e^{-\frac{(p-p_o)^2}{4\sigma_p^2}} \right] \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{\hbar}} e^{-i\frac{E(p)}{\hbar}t}$$



Energy-Time Uncertainty Relation: Gaussian Wavepacket

$$\langle x|\psi(t)\rangle = \psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \left[\left(\frac{2\pi}{\sigma_p^2} \right)^{1/4} e^{-\frac{(p-p_o)^2}{4\sigma_p^2}} \right] \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{\hbar}} e^{-i\frac{E(p)}{\hbar}t}$$

This implies the following mean values:

$$\langle\psi(t)|\hat{p}|\psi(t)\rangle = p_o$$

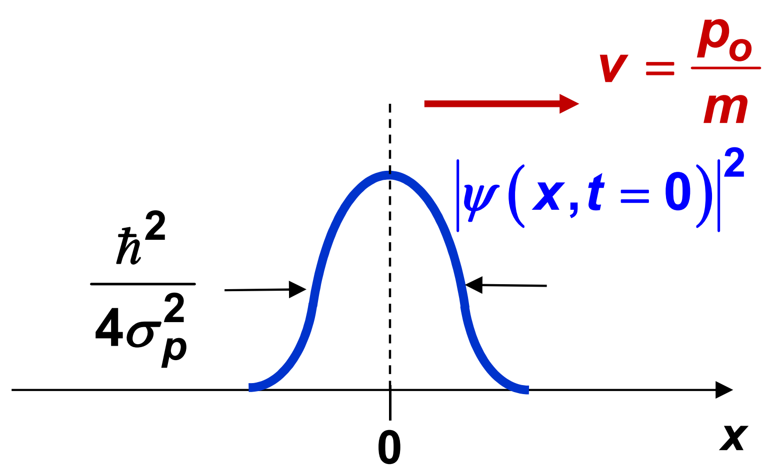
$$\Rightarrow \langle\psi(t)|\hat{x}|\psi(t)\rangle = \frac{p_o}{m}t = \frac{\langle\psi(t)|\hat{p}|\psi(t)\rangle}{m}t$$

$$\Rightarrow \langle\psi(t)|\hat{H}|\psi(t)\rangle = \frac{\langle\psi(t)|\hat{p}^2|\psi(t)\rangle}{2m} = \frac{p_o^2 + \sigma_p^2}{2m}$$

and the following mean square deviations:

$$\Rightarrow \langle\psi(t)|\Delta\hat{x}^2|\psi(t)\rangle = \frac{\hbar^2}{4\sigma_p^2} + \frac{\sigma_p^2}{m^2}t^2$$

$$\Rightarrow \langle\psi(t)|\Delta\hat{H}^2|\psi(t)\rangle = \frac{4p_o^2\sigma_p^2 + 2\sigma_p^4}{4m^2}$$

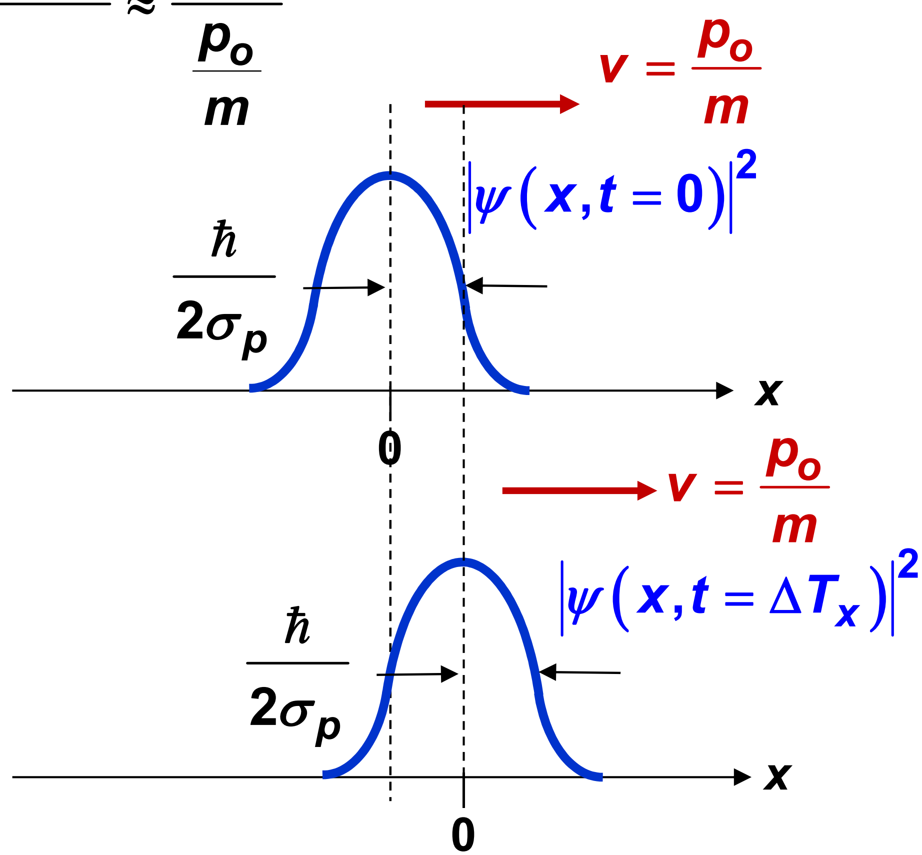


Energy-Time Uncertainty Relation: Gaussian Wavepacket

Time scale for the mean position to change significantly:

$$\Delta T_x = \frac{\sqrt{\langle \psi(t) | \Delta \hat{x}^2 | \psi(t) \rangle}}{\frac{\partial}{\partial t} \langle \psi(t) | \hat{x} | \psi(t) \rangle} = \frac{\sqrt{\frac{\hbar^2}{4\sigma_p^2} + \frac{\sigma_p^2}{m^2} t^2}}{\frac{p_o}{m}} \approx \frac{\frac{\hbar}{2\sigma_p}}{\frac{p_o}{m}}$$

ΔT_x is the time taken by the wavepacket to travel a distance equal to its width



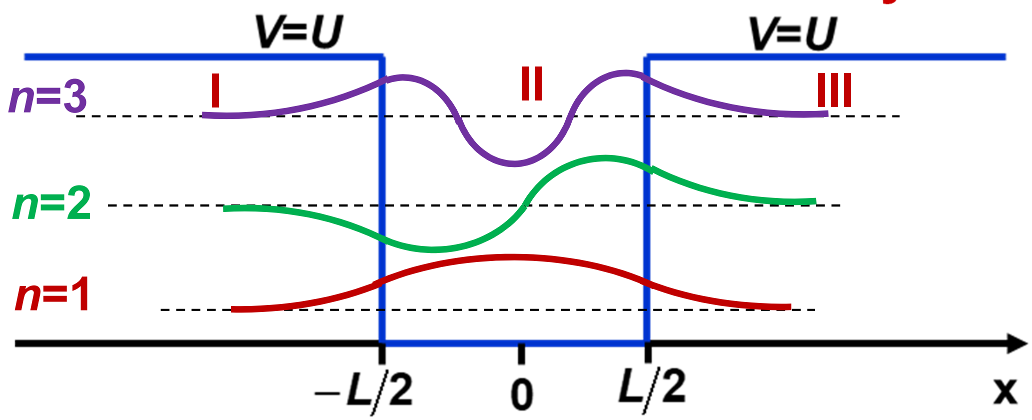
$$\Delta T_x \sqrt{\langle \psi(t) | \Delta \hat{H}^2 | \psi(t) \rangle} \geq \frac{\hbar}{2}$$

$$\Rightarrow \frac{\frac{\hbar}{2\sigma_p}}{\frac{p_o}{m}} \frac{p_o \sigma_p \sqrt{1 + \frac{\sigma_p^2}{2p_o^2}}}{m} \geq \frac{\hbar}{2}$$

$$\Rightarrow \frac{\hbar}{2} \sqrt{1 + \frac{\sigma_p^2}{2p_o^2}} \geq \frac{\hbar}{2}$$

→ Energy-time uncertainty satisfied!

Bound States in Quantum Physics



These states are all bonafide bound states!

A particle placed in any of these states will stay in that state inside the potential well forever (i.e. it has infinite lifetime for being inside the potential well)

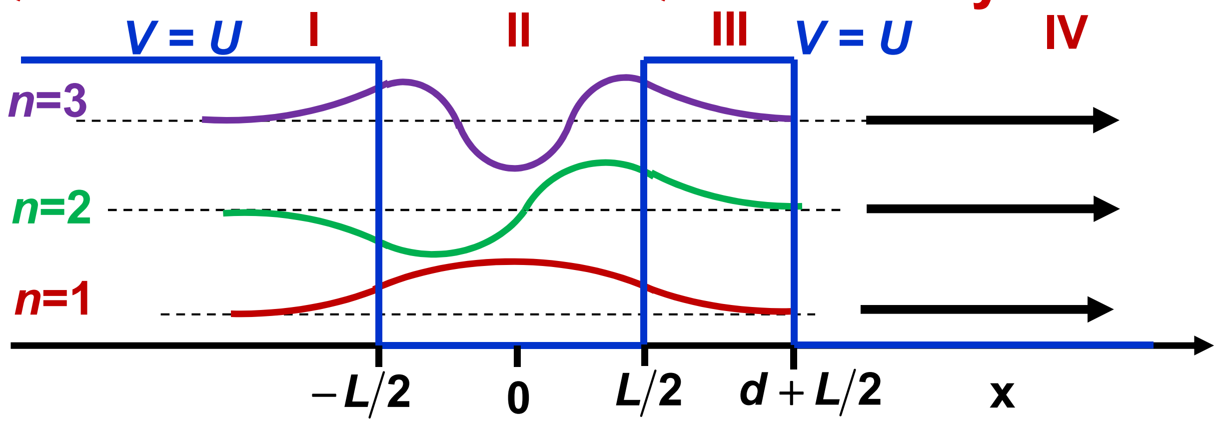
Suppose we put a particle inside the well in state n=1 at time t=0:

$$\left|\psi(t=0)\right\rangle = \left|\phi_1\right\rangle$$

$$\Rightarrow \left|\psi(t)\right\rangle = e^{-i\frac{E}{\hbar}t}\left|\phi_1\right\rangle$$

$$\Rightarrow \int_{-L/2}^{L/2} dx \left|\left\langle x|\psi(t)\right\rangle\right|^2 = \int_{-L/2}^{L/2} dx \left|\left\langle x|\psi(t=0)\right\rangle\right|^2$$

Quasi-Bound States in Quantum Physics



These states are all quasi-bound states!

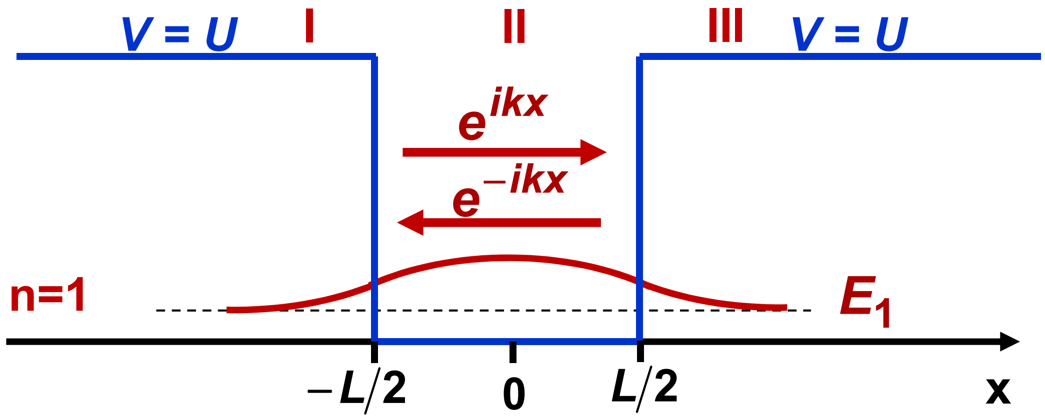
The potential barrier on the right side is not infinitely thick and there is a finite probability that a particle in the potential well tunnels through it

If the particle tunnels through the right barrier it will keep going and escape from the potential well

A particle placed in one of these states inside the potential well has a finite lifetime for being inside the well

How do we find the lifetimes of these quasi-bound states?

Lifetimes of Quasi-Bound States in Quantum Physics



STEP 1:

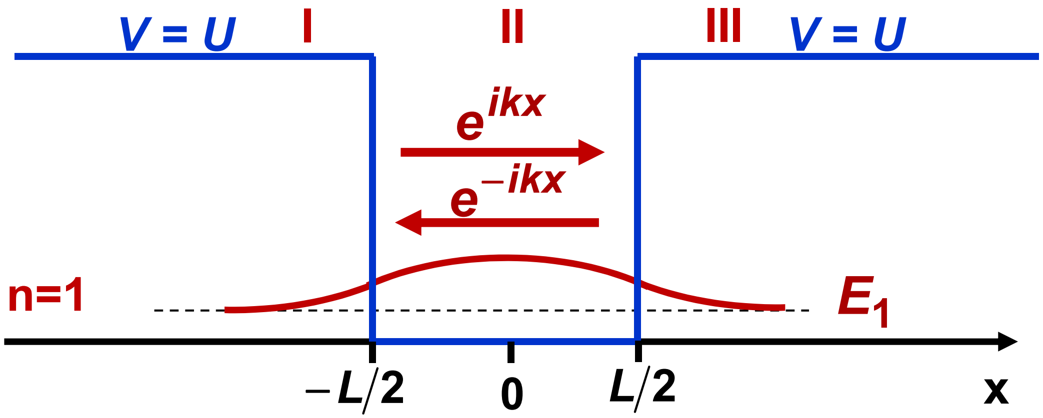
Suppose the energy of the corresponding bound state (assuming potential barriers on both sides are infinitely thick) is found to be E_1

One can think of this bound state as a plane wave of wavevector given by,

$$\frac{\hbar^2 k^2}{2m} = E_1$$

bouncing back and fourth between the two interfaces (recall that the magnitude of the reflection coefficient |r| is unity for such a bound state)

Lifetimes of Quasi-Bound States in Quantum Physics



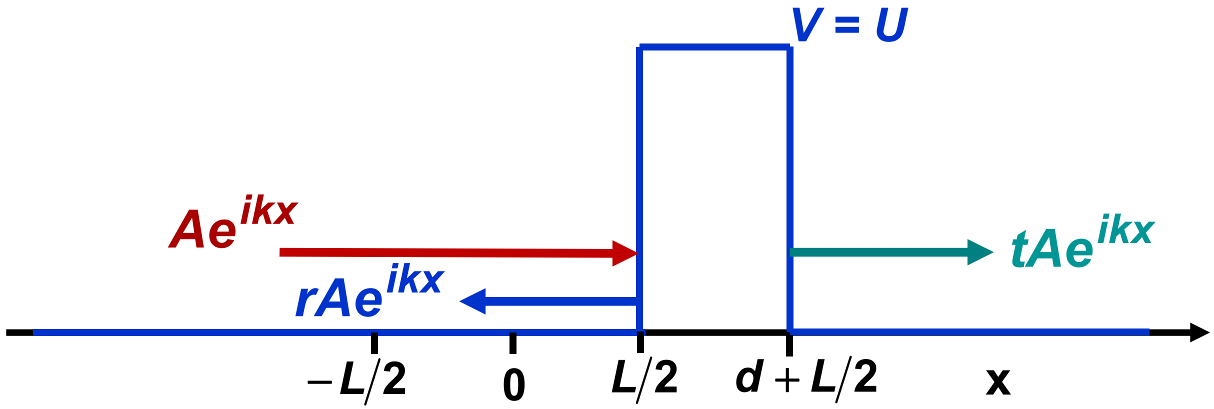
STEP 2:

Find the number of times per second this confined particle hits the right barrier:

$$f(k) \approx \frac{(\hbar k/m)}{2L}$$

This is called the attempt frequency *f(k)* !

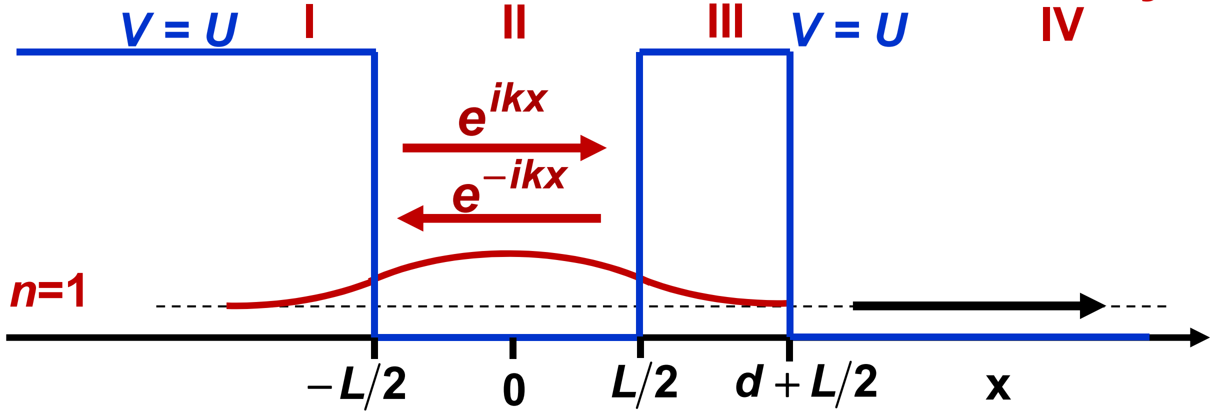
Lifetimes of Quasi-Bound States in Quantum Physics



STEP 3:

Find the transmission probability $|t(k)|^2$ by solving the above problem where the wavevector magnitude of the incident plane wave is the same as that found in STEP 1 for the bound state

Lifetimes of Quasi-Bound States in Quantum Physics



STEP 4:

The lifetime τ_1 of the quasi-bound state is then found as:

$$\frac{1}{\tau_1} = f(k)\left|t(k)\right|^2$$

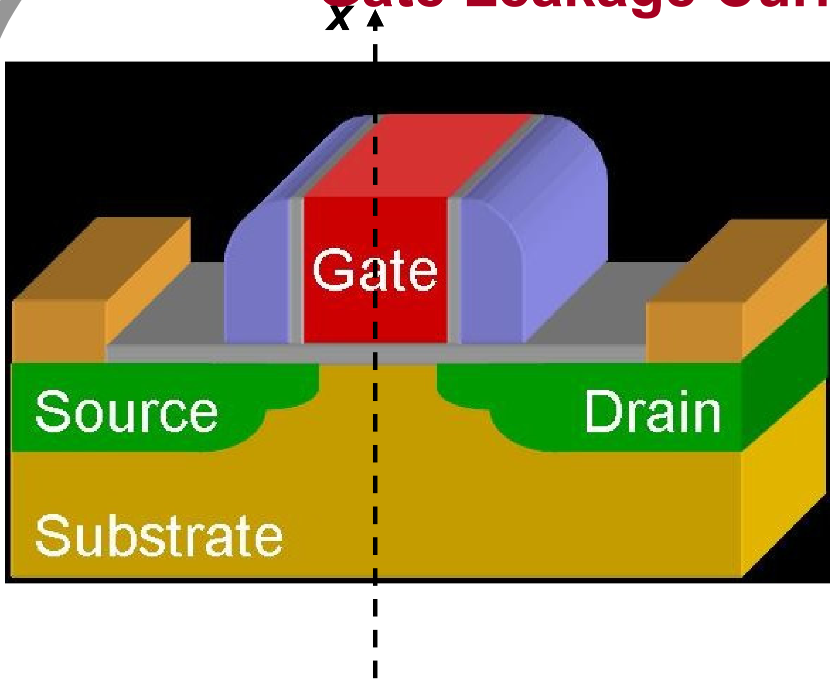
Consequence of the finite lifetime:

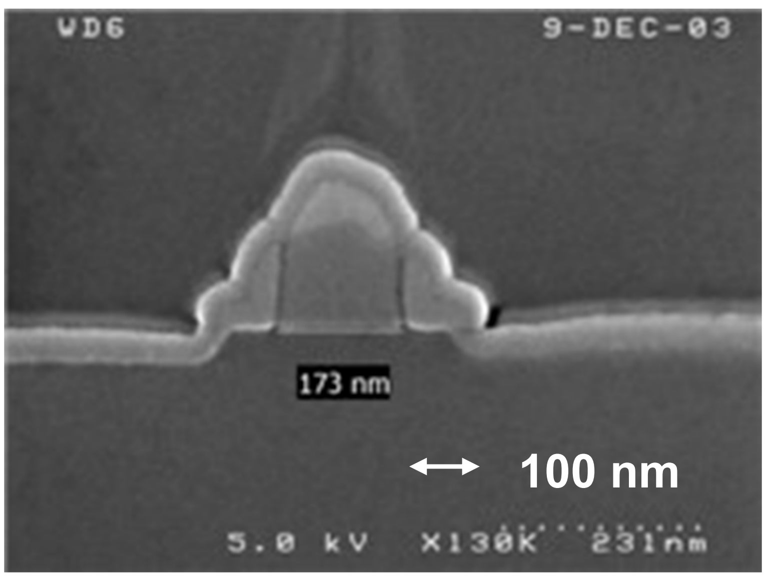
Suppose we put a particle inside the well in state n=1 at time t=0:

$$\left|\psi(t=0)\right\rangle = \left|\phi_1\right\rangle$$

$$\Rightarrow \int_{-L/2}^{L/2} dx \left|\left\langle x \middle| \psi(t)\right\rangle\right|^2 = e^{-\frac{t}{\tau_1}} \int_{-L/2}^{L/2} dx \left|\left\langle x \middle| \psi(t=0)\right\rangle\right|^2$$

Gate Leakage Current in Silicon MOS Transistors





A 50 nm gate MOS transistor (INTEL)