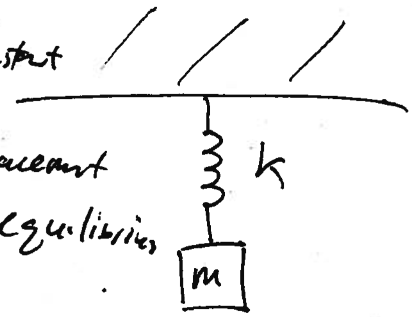
Simple Harmonic Oscillator (SHO)

A mass on a spring is a classical example of a SHO: $F = -kx$

spring constant

displacement from equilibrium



Newton's 2nd Law says

$$-kx = m\ddot{x} = m\frac{d^2x}{dt^2}$$

$$\frac{dx^2}{dt^2} + \frac{k}{m}x = \varnothing \qquad \text{Define } \omega_0 = \sqrt{k/m} = \text{natural frequency}$$

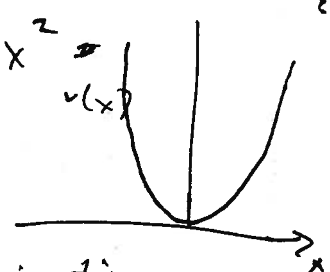
$$\frac{d^2x}{dt^2} + \omega_0^2 x = \varnothing$$

arbitrary constants (determined by initial conditions)

Classical Solution: $x(t) = A\cos(\omega_0 t + \delta)$

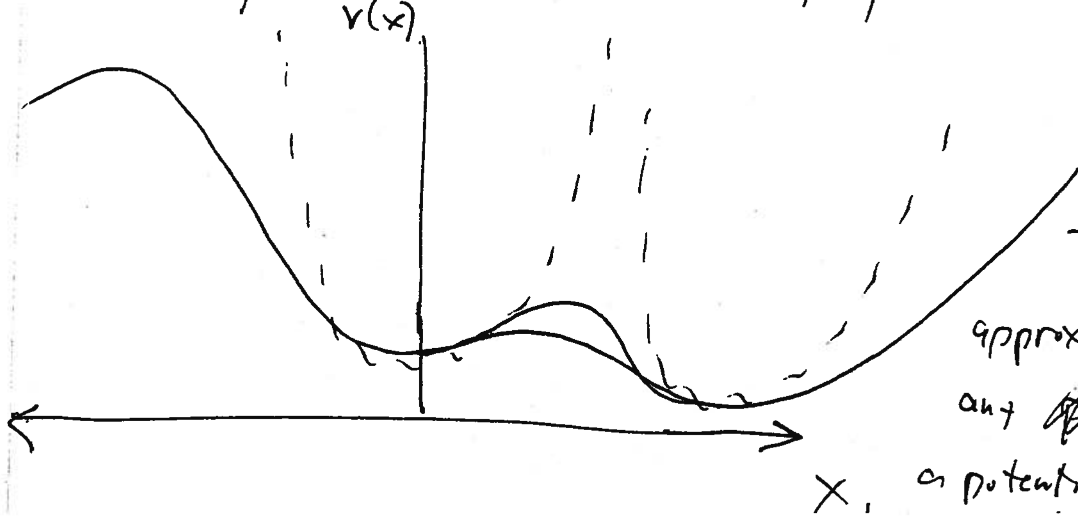
$KE = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 = \frac{1}{2}m\dot{x}^2 = \frac{p^2}{2m}$

Potential energy $V(x) = +\int_0^x kx'\,dx' = \frac{1}{2}kx^2$



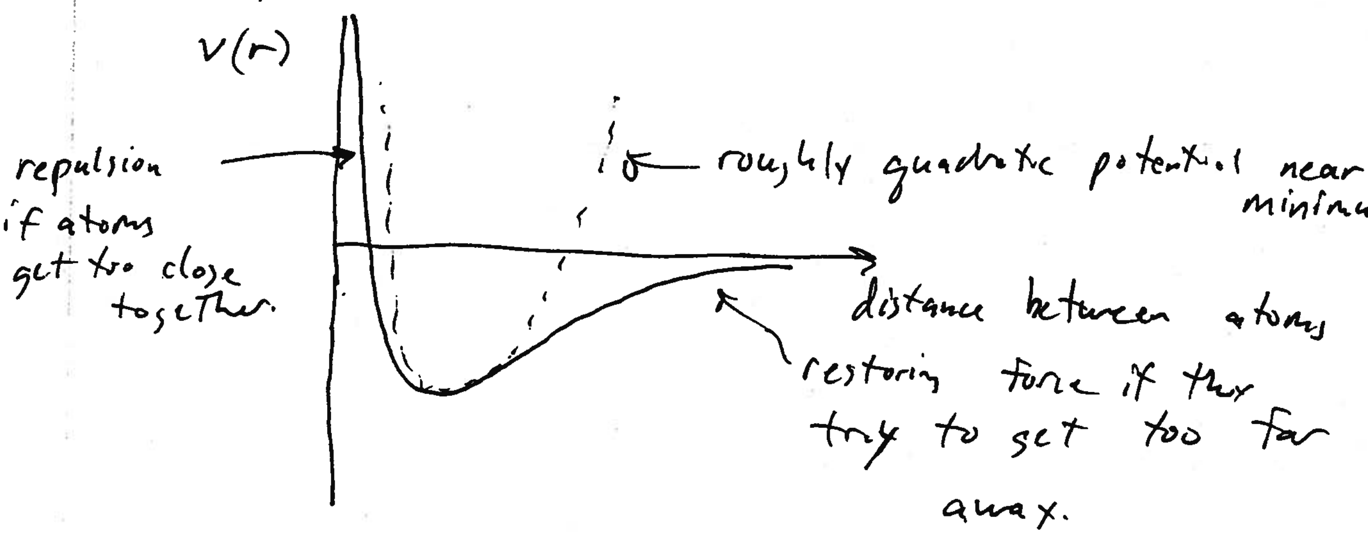
Total Energy $= \frac{p^2}{2m} + \frac{1}{2}kx^2$

~~The SHO~~, the SHO makes a good approximation for the potential near almost any potential minimum.



To a good approximation, almost any ~~pot~~ minimum in a potential function

~~SHO~~ In QM, the SHO is a good model for most molecules. Imagine 2 atoms bound together, like 2 Hydrogen atoms bond into H_2: The potential is roughly



The Hamiltonian is taken from the classical energy:

$$E_{classical} = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

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$$\therefore \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}kx^2$$

The TISE is

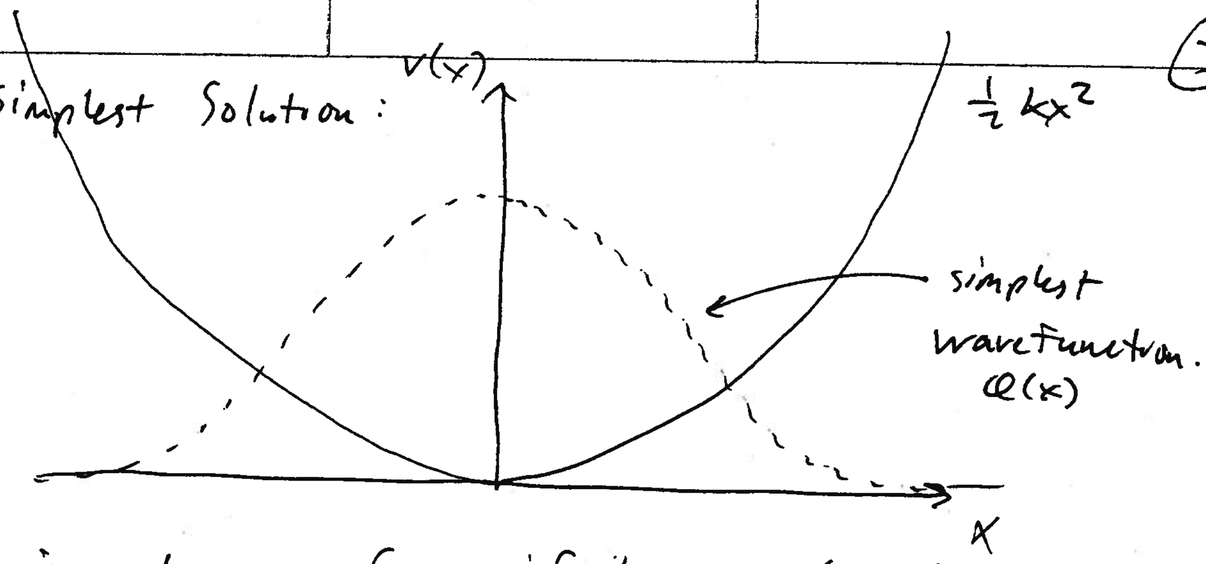
$$\hat{H}\, \varphi = E\varphi \leftarrow \text{e.v. equation for } \hat{H}.$$

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} + \frac{1}{2}kx^2\varphi(x) = E\,\varphi(x)$$

The simplest solution to this differential eq. is a Gaussian

$$\varphi(x) = A\, e^{-\beta^2x^2/2}, \text{ where } \beta^2 = \frac{m\omega_0}{\hbar} = \frac{m}{\hbar}\sqrt{\frac{k}{m}} = \frac{\sqrt{km}}{\hbar}$$

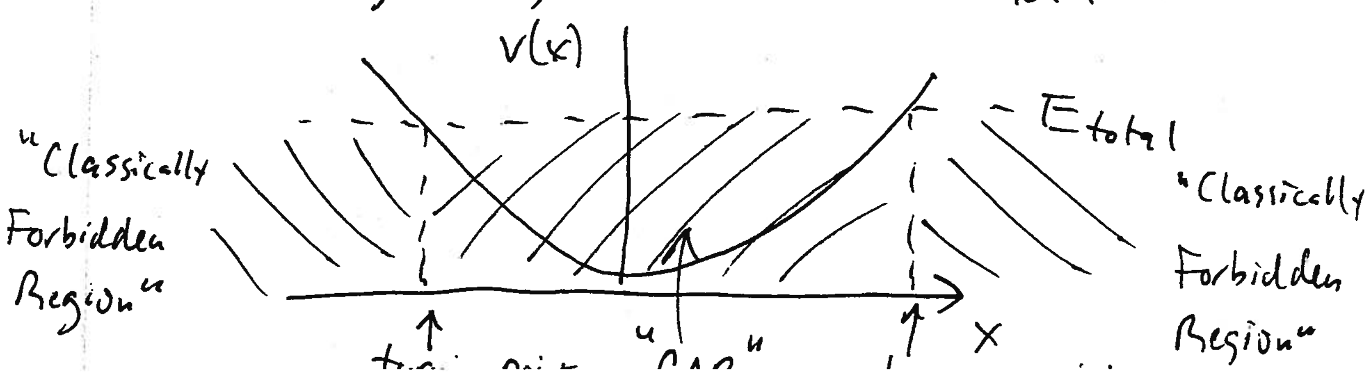
Simplest Solution:



This is only one of an infinite # of solutions. In fact, this one turns out to be the ground state, or state of lowest energy.

Also, recall from the uncertainty principle that a Gaussian Wavefunction coincidentally minimizes $\Delta x \Delta p$. For this wavefunction $\Delta x \Delta p = \hbar/2$, the absolute minimum

One interesting thing about this wavefunction is that it extends all the way to $x \to \pm\infty$. That means there is some non-zero probability to find the particle anywhere on the x-axis, although usually it will be found near $x = 0$. In fact, we might find the particle outside the "Classically Allowed Region" ("CAR"), where $V(x) \leq E_{total}$.



So a QM ~~SHO~~ particle might be observed at a location which is forbidden by energy conservation in classical mechanics. In QM, however, if we measured an "illegal" position, and then measured the energy (to try to confirm the violation of energy conservation) the position measurement would disturb the energy state. We then expect a spectrum of possible energy measurements, and we ~~could~~ ~~say~~ would learn nothing about the energy of the particle before we measured the position.

Operator Solution to the QM SHO

We could find the other, more complicated solutions to the D.E. by continuing to guess them. But a better way uses the "creation" & "annihilation" operators.

Define

$$\hat{a} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right), \quad \beta \equiv \sqrt{\frac{m\omega_0}{\hbar}}$$

What is the Hermitian Conjugate of $\hat{a}$? Well,

$$\hat{x} \rightarrow \hat{x}^{+} = \hat{x}, \quad \hat{p} \rightarrow \hat{p}^{+} = \hat{p}, \quad \& \ (i) \rightarrow (-i)$$

$$\therefore \quad \hat{a}^{+} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)$$

Using $[\hat{x},\hat{p}] = i\hbar$, we can prove that $[\hat{a},\hat{a}^{+}] = 1$

or $\hat{a}\hat{a}^{+} = 1 + \hat{a}^{+}\hat{a}$

We can also write

$$\hat{x} = \frac{\hat{a} + \hat{a}^{+}}{\sqrt{2\beta}} \quad , \quad \hat{p} = -im\omega_0 \left(\frac{\hat{a} - \hat{a}^{+}}{\sqrt{2\beta}} \right)$$

In terms of $\hat{a}$ & $\hat{a}^{+}$, the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \hbar\omega_0 \left(\hat{a}^{+}\hat{a} + \frac{1}{2} \right)$$

We also define $\hat{N} = \hat{a}^{+}\hat{a}$, so that $\hat{H} = \hbar\omega_0 (\hat{N} + \frac{1}{2})$.

$\hat{N}$ is Hermitian and has real eigenvalues (n).
We don't yet know that (n) will be an integer, but it will turn out that way. Also, since $\hat{H} = \hbar\omega_0(\hat{N} + \frac{1}{2})$, if $|n\rangle$ is an eigenstate of $\hat{N}$, it is also an eigenstate of $\hat{H}$.

So let $|n\rangle$ stand for an eigenstate of $\hat{N}$ & $\hat{H}$.
If we let (n) stand for the $\hat{N}$ eigenvalue, then

$$\hat{N}\,|n\rangle = n\,|n\rangle .$$

QM Simple Harmonic Oscillator.

We wrote

$$\hat{a} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) \quad , \quad \beta \equiv \sqrt{\frac{m\omega_0}{\hbar}}$$

& $$\hat{a}^+ \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)$$

Then $$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \hbar\omega_0\left(\underbrace{\hat{a}^+\hat{a}}_{\equiv \hat{N}} + \frac{1}{2}\right) \equiv \hbar\omega_0\left(\hat{N} + \frac{1}{2}\right),$$

We let $|n\rangle$ stand for an common eigenstate of $\hat{N}$ & $\hat{H}$, and (n) is the $\hat{N}$ eigenvalue:

$$\hat{N}|n\rangle = n|n\rangle$$, (we don't yet know that (n) is an integer).

So far we've only re-written the SHO problem in terms of a different set of operators

We can show that the state $\underline{\hat{a}|n\rangle}$ is also an eigenstate of $\hat{N}$ with eigenvalue $(n-1)$. Watch.

Let $|b\rangle \equiv \hat{a}|n\rangle$.

$$\hat{N}|b\rangle = \underbrace{(\hat{a}^+\hat{a})}_{\hat{N}}(\hat{a}|n\rangle) = \overbrace{(\hat{a}\hat{a}^+ - 1)}^{\text{commutator for } \hat{a}, \hat{a}^+}(\hat{a}|n\rangle)$$
$$= (\hat{a}\hat{a}^+\hat{a} - \hat{a})|n\rangle$$
$$= \hat{a}(\hat{a}^+\hat{a} - 1)|n\rangle$$
$$= \hat{a}(\hat{N} - 1)|n\rangle$$
$$= \hat{a}(n-1)|n\rangle$$
$$= (n-1)\hat{a}|n\rangle = (n-1)|b\rangle.$$

$\therefore$ $\hat{N}|b\rangle = (n-1)|b\rangle$, $|b\rangle$ is an eigenstate with e.v. $(n-1)$.

~~[illegible]~~ Since $|b\rangle$ has eigenvalue $(n-1)$, we might as well label it that way:

$$|b\rangle \longrightarrow |n-1\rangle$$

$$\hat{N}|n-1\rangle = (n-1)|n-1\rangle \quad , \quad \hat{a}|n\rangle \sim |n-1\rangle = A|n-1\rangle$$

some proportion constant

If we repeat the algebra again, we can prove that $\hat{a}|n-1\rangle$ is an eigenstate with eigenvalue $(n-2)$

$$\hat{N}\left(\hat{a}|n-1\rangle\right) = (n-2)\left(\hat{a}|n-1\rangle\right)$$

$$\therefore \quad \hat{a}|n-1\rangle \sim |n-2\rangle = B|n-2\rangle$$

some proportionality constant

the $\hat{a}$ operator is converting one eigenstate into the ~~next lower~~ neighboring lower eigenstate.

We call $\underline{\hat{a}}$ the "lowering operator" or "stepdown" operator" or "annihilation operator" or "demotion operator".

Note that since $\hat{a} \neq \hat{a}^{+}$, $\hat{a}$ is not Hermitian so it cannot represent an observable. But it is very useful anyway.

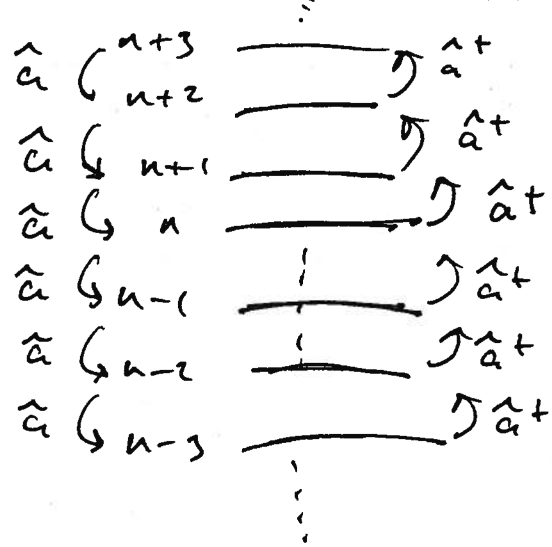
Similar Reasoning shows that

$\hat{a}^{+}|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $(n+1)$. $\therefore \quad \hat{a}^{+}|n\rangle \sim |n+1\rangle = C|n+1\rangle$

some prop. const

We call $\hat{a}^{+}$ the "promotion operator" or "creation operator" or "step-up" operator, or "raising operator.

So we have a "ladder of states"



How did we learn this without solving the Schroedinger Eq?? Two steps: we noticed that we could write $\hat{H} = \hbar\omega_0(\hat{N} + \frac{1}{2}) = \hbar\omega_0(\hat{a}^+\hat{a} + \frac{1}{2})$, plus we inferred the commutator $[\hat{a}, \hat{a}^+] = 1$ from $[\hat{x}, \hat{p}] = i\hbar$

In the Homework #6, you showed that the expectation value for any squared Hermitian operator must be ≥ 0: $\langle A \rangle \geq 0$ if $\hat{A} = \hat{A}^+$.

Since $\hat{H} \sim \hat{p}^2 + \hat{x}^2$, $\langle H \rangle \geq 0$ for any state $|\psi\rangle$.

$\therefore$ the lowest energy state can't have an eigenvalue smaller than zero:

$$\hat{H}|\text{lowest}\rangle = \hbar\omega_0(\hat{N} + \tfrac{1}{2})|\text{lowest}\rangle = \hbar\omega_0(n_{\text{lowest}} + \tfrac{1}{2})|\text{lowest}\rangle$$

$$\langle\text{lowest}|\hat{H}|\text{lowest}\rangle = \hbar\omega_0(n_{\text{lowest}} + \tfrac{1}{2})\langle\text{lowest}|\text{lowest}\rangle$$

$$= \hbar\omega_0(n_{\text{lowest}} + \tfrac{1}{2}) \geq 0.$$

$$\therefore \quad n_{\text{lowest}} \geq \frac{-1}{2}.$$

*The "ladder of states" must have a "bottom" state — it cannot

For this lowest state, applying the demotion operator must give zero: "proportionality constant"

Finish Lec 10/23 →
$$\hat{a}\,|\text{lowest}\rangle = \phi\,|\text{lowest}\rangle = \phi.$$

Also, $\hat{N}\,|\text{lowest}\rangle = \hat{a}^{+}\hat{a}\,|\text{lowest}\rangle = \hat{a}^{+}(\phi) = \phi.$
$= \phi\,|\text{lowest}\rangle.$

$\therefore$ The eigenvalue of $\hat{N}$ for $|\text{lowest}\rangle$ is zero; so call $|\text{lowest}\rangle \rightarrow |0\rangle$, (because $\hat{N}|0\rangle = \phi|0\rangle$).

Then $\hat{a}^{+}|0\rangle = A\,|1\rangle$

proportionality constant

And $\hat{N}\,|1\rangle = (1)\,|1\rangle$

eigenvalue is 1.

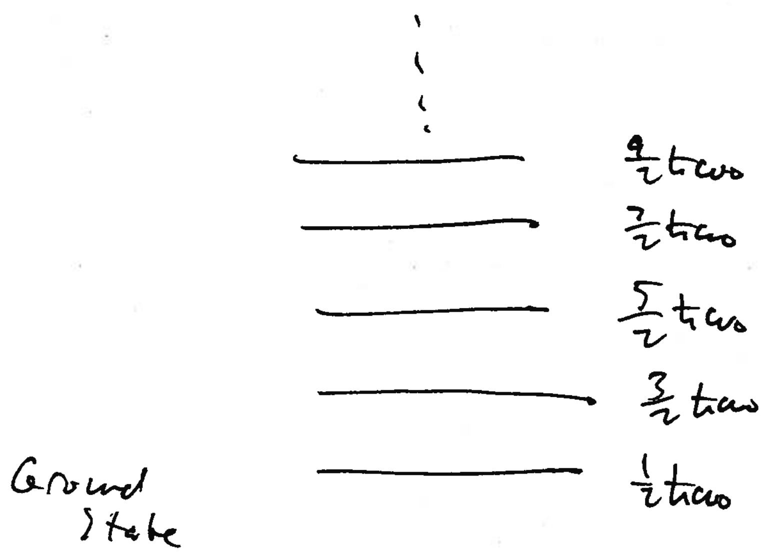
$\therefore\quad n = \text{integer} = 0, 1, 2, \ldots \rightarrow \infty.$

And $\hat{H}\,|n\rangle = \hbar\omega_0\left(n+\tfrac{1}{2}\right)|n\rangle, \quad n = 0, 1, 2, \ldots$

$E_n = \hbar\omega_0\left(n+\tfrac{1}{2}\right).$

$E_0 = \text{ground state energy} = \tfrac{1}{2}\hbar\omega_0.$

All other levels are spaced by $(\hbar\omega_0)$.



QM Simple Harmonic Oscillator

We found a "ladder-of-states" using the "step-up" & "step-down" operators.

$$\text{step down} \longrightarrow \hat{a}|n\rangle \overset{\text{proportional}}{\sim} |n-1\rangle$$

$$\text{step up} \longrightarrow \hat{a}^{+}|n\rangle \sim |n+1\rangle$$

$$\hat{H} = \hbar\omega_0\left(\hat{N} + \tfrac{1}{2}\right) = \hbar\omega_0\left(\hat{a}^{+}\hat{a} + \tfrac{1}{2}\right)$$

Then eigenvalues of energy are

$$E_n = \hbar\omega_0\left(n + \tfrac{1}{2}\right), \quad n = 0, 1, 2, \ldots\ldots$$

If we apply $\hat{a}$ to $|0\rangle$, we annihilate it

$$\hat{a}|\phi\rangle = \phi.$$

We can write this as a differential equation in position space to find the wavefunction $\varphi_0(x)$ for the ground state:

First define $\xi^2 \equiv \beta^2 x^2$, where $\beta^2 = \frac{m\omega_0}{\hbar}$, so that

$$\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) = \frac{\beta}{\sqrt{2}}\left(x + \frac{\hbar}{m\omega_0}\frac{d}{dx}\right) = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)$$

&

$$\hat{a}^{+} = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)$$

Then our ground-state-annihilation equation says

$$\frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)\varphi_0(\xi) = \phi \quad \text{In } (x\text{-space}) \text{ or } (\xi\text{-space}).$$

The solution to this Diff. Eq is

$$\varphi_0(\xi) = A e^{-\xi^2/2}$$

Normalization : $\displaystyle \underline{1} = \int_{-\infty}^{\infty} |\varphi_0|^2 \, d\xi = \sqrt{\pi} A^2$

$$\therefore \; A = \frac{1}{\sqrt[4]{\pi}} = \pi^{-1/4}$$

So $$\varphi_0(\xi) = \pi^{-1/4} e^{-\xi^2/2}$$

In x-space this is

$$\boxed{\varphi_0(x) = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} e^{-(\beta x)^2/2}}$$ Ground state wavefunction

Now that we have ~~the~~ an explicit expression for the ground state wavefunction, we can find the other states by applying the promotion operator :

$$\cancel{\varphi_1(x) \overset{\text{proportional}}{\sim} \hat{a}^+ \varphi_0(x) = A_1 \hat{a}^+ \varphi_0(x)}$$

$$\varphi_1(\xi) \overset{\text{proportional to}}{\sim} \hat{a}^+ \varphi_0(\xi) =$$

$$\varphi_1(\xi) = A_1 \left(\xi - \frac{d}{d\xi}\right) e^{-\xi^2/2}$$

$$= A_1 \, 2\xi \, e^{-\xi^2/2}$$

And $A_1 = \left(2\sqrt{\pi}\right)^{-1/2}$ by normalization

If we keep applying $\hat{a}^+$, we keep generating more & more states :

$$\varphi_n(\xi) = A_n \left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2}$$

This n^{th} order operator always gives back $e^{-\xi^2/2}$, multiplied by an n^{th} order polynomial:

$$\left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2} = H_n(\xi) e^{-\xi^2/2}$$

The eigenstates are

$$\boxed{\begin{array}{ll} \psi_n(\xi) = A_n H_n(\xi)\, e^{-\xi^2/2} & , A_n = \left(2^n n! \sqrt{\pi}\right)^{-\frac{1}{2}} \\ E_n = \hbar\omega_0 \left(n + \frac{1}{2}\right) & , n = 0, 1, 2, \ldots \end{array}}$$

The polynomials $H_n(\xi)$ are called "Hermite polynomials"

Since the eigenstates $\psi_n(\xi)$ are normalized by A_n, and since they are eigenstates of a Hermitian Operator $(\hat{H})$, they must be ortho-normal:

$\langle n | m \rangle = \delta_{nm}$ in Dirac Notation

$$\int_{-\infty}^{\infty} \psi_n^*(\xi)\, \psi_m(\xi)\, d\xi = \delta_{nm} \quad \text{in wave mechanics}$$

& They are complete:

$$\hat{I} = \sum_n |n\rangle\langle n|$$

Also, the proportionality constant for $\hat{a}$ & $\hat{a}^+$ turns out to be

$$\hat{a}|n\rangle = \sqrt{n}\, |n-1\rangle \quad , \quad \hat{a}^+|n\rangle = \sqrt{n+1}\, |n+1\rangle$$

Energy Quantization for Bound states in QM

In classical physics, most waves are described by the "wave eq" : $\frac{\partial^2 F(x,t)}{\partial t^2} = v^2 \frac{\partial^2 F(x,t)}{\partial x^2}$

For EM waves, $F \to \vec{E}$. For waves on a string, $F \to$ height of string.

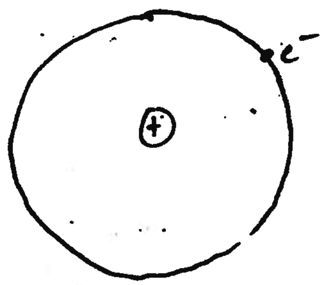
The energy carried by these classical waves is proportional to the Amplitude squared: $E \sim A^2$.

Any amplitude is possible, so any positive energy is possible.

In the 19th century, atomic spectra revealed that atoms & molecules emit & absorb EM energy at discrete, fixed values. Planck interpreted this to mean that something unusual about EM waves only allowed them to interact in "lumps". $(E = h\nu)$. Einstein suggested that the EM wave is composed entirely of "lumps" → photons.

In 1909, Rutherford found that the ~~[illegible]~~ positive charges inside an atom are lumped into a point particle, the nucleus. So ~~[illegible]~~ why is the atom stable? Shouldn't the negatively charged electrons crash into the positively charged nucleus?

For example, suppose we imagine the electron orbiting the nucleus like a planet:



The electron goes in a circle. Any charged particle moving in a circle should radiate EM energy at the frequency of its rotation. This loss of energy should cause the electron to "spiral in" very quickly, so all atoms should immediately decay.

QM solves all these problems. QM ~~shows~~ predicts that

① There is a minimal energy for any bound state. "E_0" or "E_{ground}"

② Other bound state energies are possible, but they are <u>discrete</u> rather than <u>continuous</u>.

③ For a bound state in an energy eigenstate, the expectation value for the particle does not change in time, so the particle is not "moving"

$$\frac{d}{dt}\langle x\rangle = 0 \quad \text{for a stationary state}$$

So no classical EM wave emission should be expected.

How does QM pull off this trick??

In particular, the Schroedinger Eq is a partial-differential Eq, just like the classical wave Eq. Shouldn't <u>any</u> energy be possible?

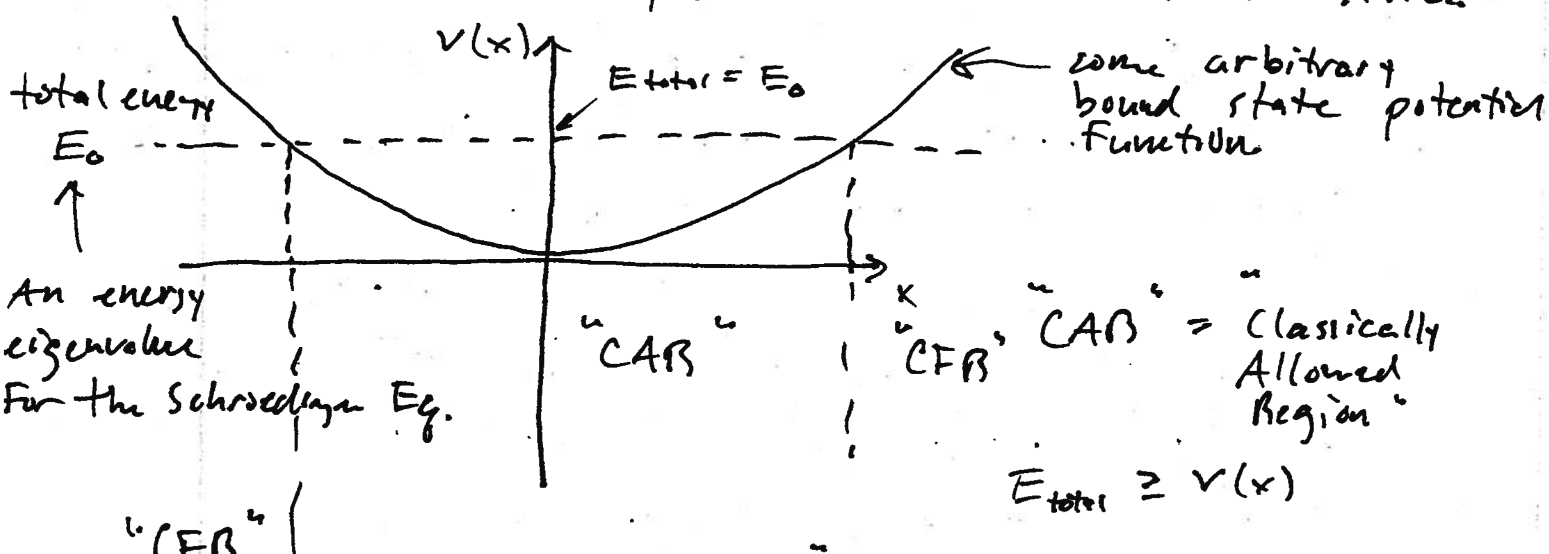
At first glance, nothing about the Schroedinger Eq appears to be discrete. It's a partial differential equation of a smooth function $\Psi(x,t)$, just like the classical wave Eq.

Here's the answer

> There <u>are</u> a continuum of energies & solutions which are <u>mathematically possible</u> for the Schroedinger Eq. However, only a <u>discrete set</u> of those solutions are <u>physically possible</u>, because most of them blow up as $x \to \infty$ or $x \to -\infty$. <u>I.E., most solutions are not normalizeable</u>

Here's why.

Suppose we have some potential function which has a minimum, so there will be bound states.



"CAB" = "Classically Allowed Region"

$E_{total} \geq V(x)$

"CFB" = "Classically Forbidden Region"

$V(x) > E_{total}$ (not possible

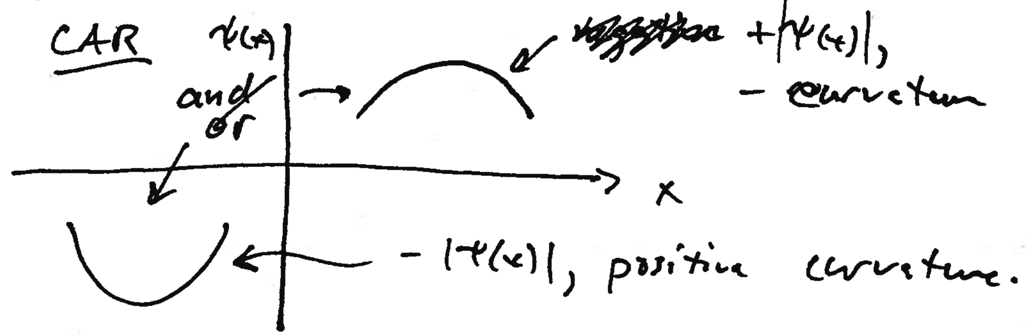
The TISE says

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

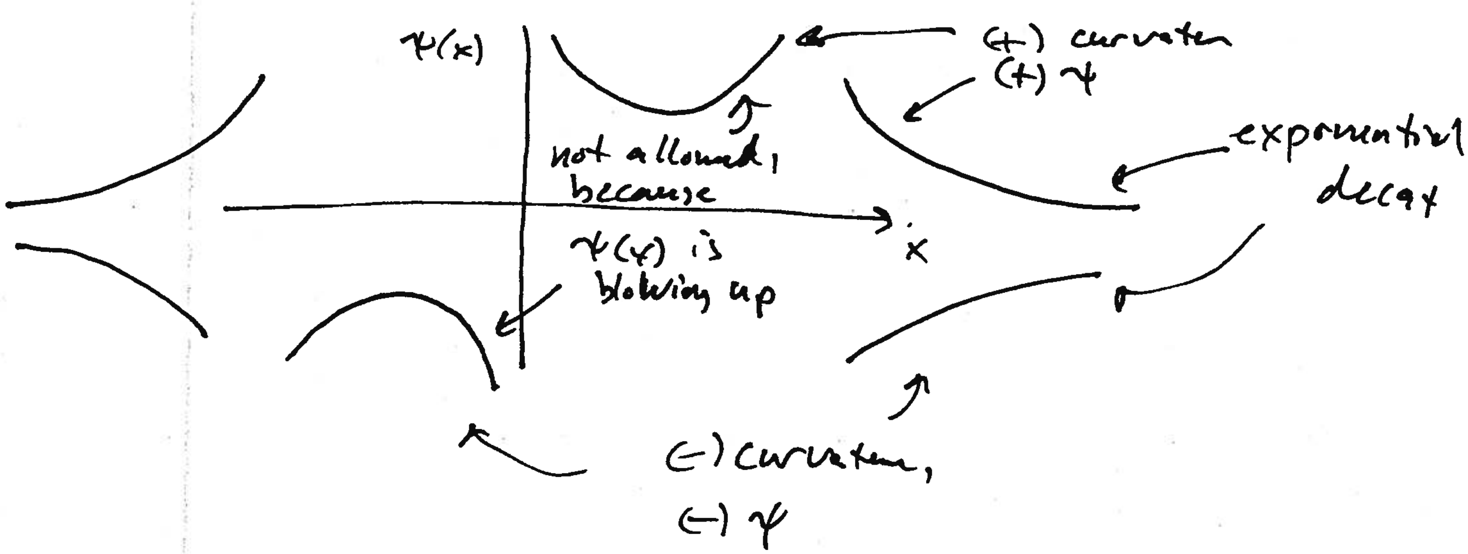
$$\psi''(x) = \frac{-2m}{\hbar^2}\left[E-V(x)\right]\psi(x)$$

For CAR, $E-V(x) > 0$, & TISE says
"The curvature of $\psi(x)$ has the opposite sign as $\psi(x)$"
For CFR, $E-V(x) < 0$, & TISE says
"The curvature of $\psi(x)$ has the same sign as $\psi(x)$"

So in a CAR, $\psi(x)$ should be like



In a CFR, $\psi(x)$ should be like

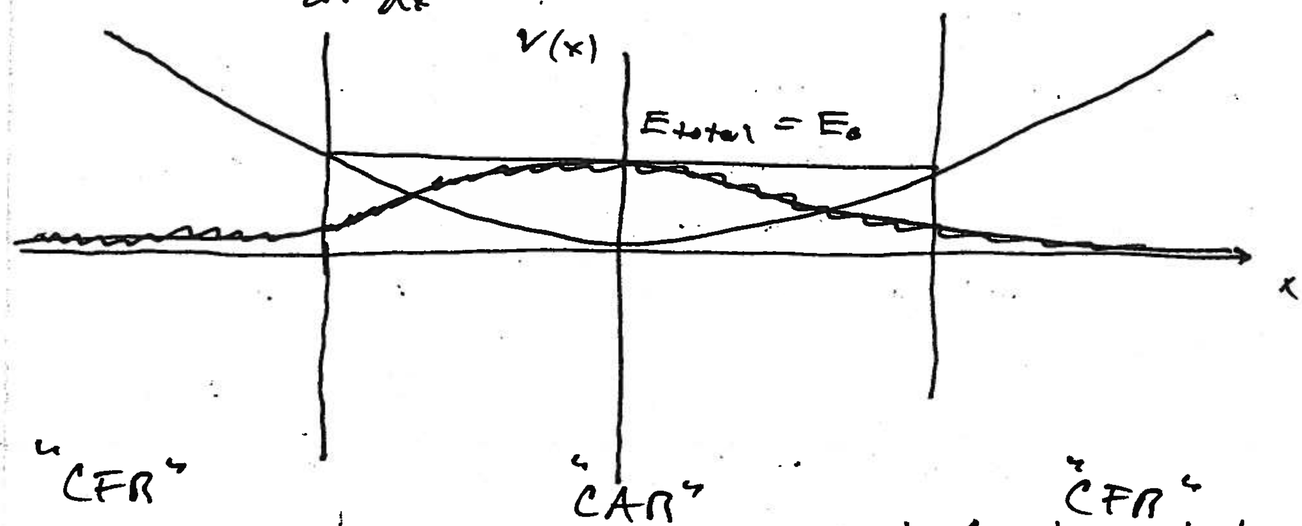


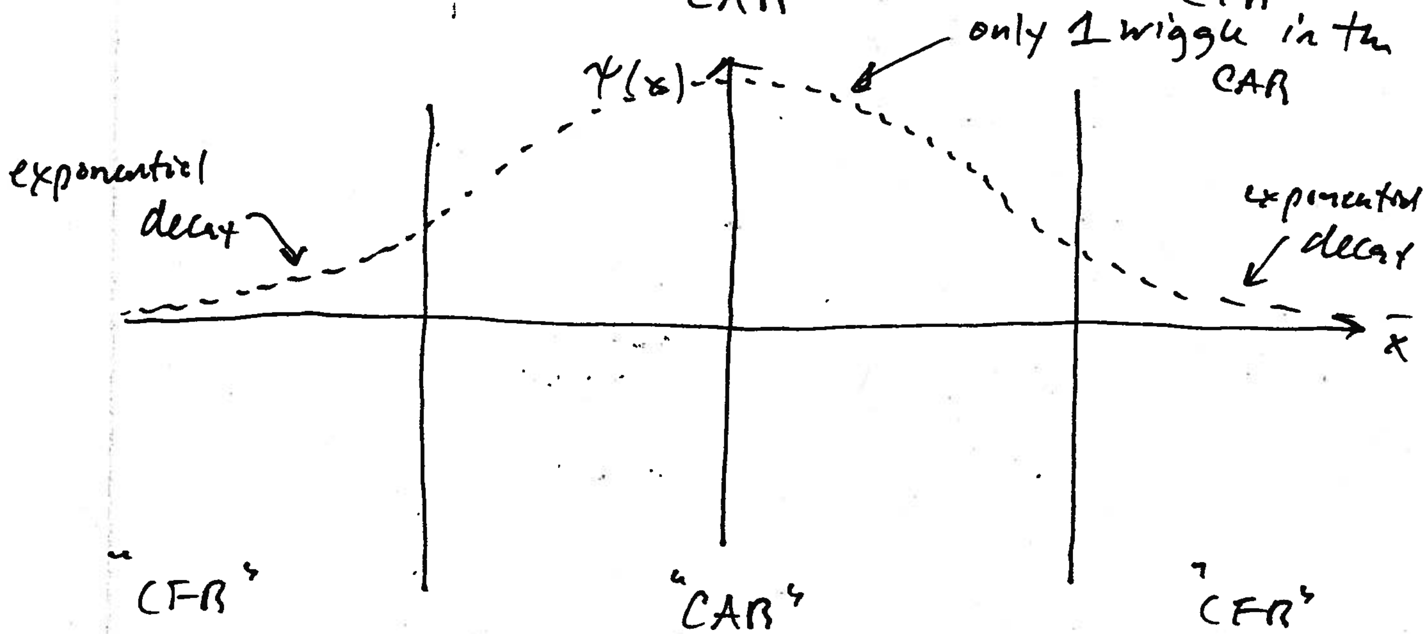
Therefore

- $\psi(x)$ oscillates in the CAR
- $\psi(x)$ decays exponentially in the CFR.

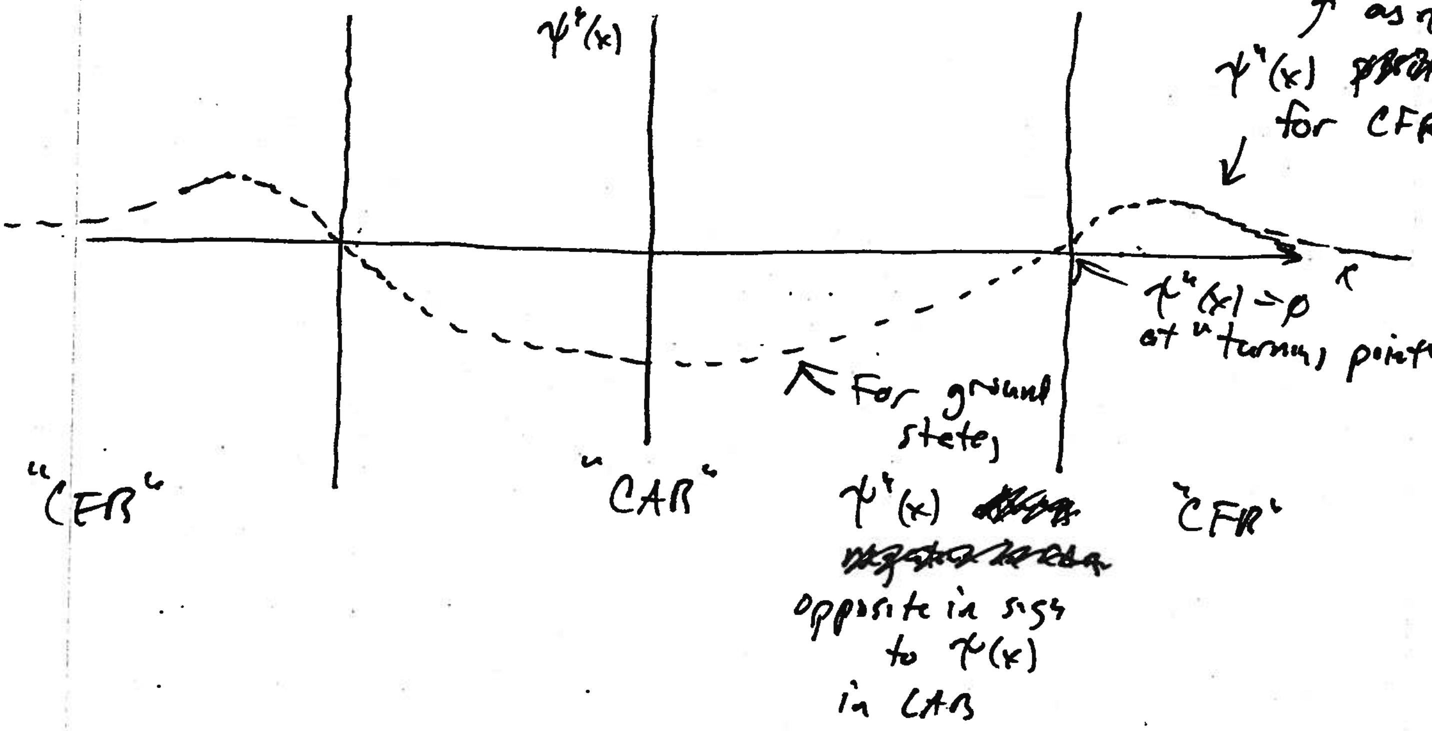
What should the ground state $\psi(x)$ look like??

$\Rightarrow$ Minimize the "number of wiggles" to minimize $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \leftarrow$ KE. in the CAR



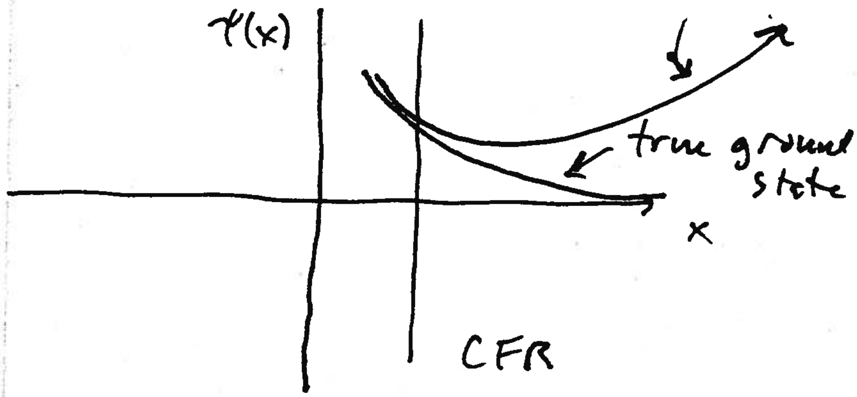


If we plot $\psi''(x)$, we see more clearly:



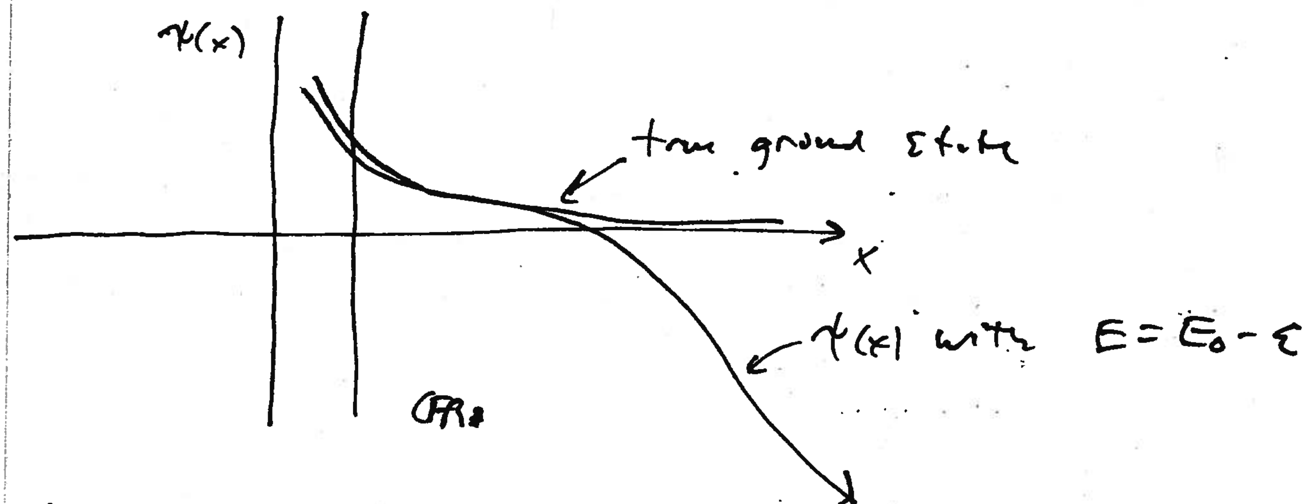
As $x \to +\infty$ or $x \to -\infty$, $\psi''(x)$ must approach ϕ so that $\psi(x) \to \phi$.

What happens to $\psi(x)$ in the CFR ~~[...]~~ if we try to increase the energy from E_0 to $E_0 + \varepsilon$?? Roughly speaking, $\psi(x)$ will have "too much" positive curvature:



This new $\psi(x)$ does not decay to zero as $x \to \infty$. It is not normalizable and un-physical.

Similarly, if we try to decrease the energy from E_0 to $E_0 - \varepsilon$, $\psi(x)$ goes away to negative infinity



Only the special value of $E = E_0$ perfectly balances the tendency of $\psi(x)$ to blow up at large x in the CFR. This is how QM "picks" the ground state, and this is why atoms & molecules have discrete & stable bound states, which they could never have in classical physics.

Exam 2 Review

Dirac Delta Function: $\frac{1}{2\pi}\int_{-\infty}^{\infty} dk \, e^{ik(x-x')} = \delta(x-x')$

& $\frac{1}{2\pi}\int_{-\infty}^{\infty} dx \, e^{i(k-k')x} = \delta(k-k')$

~~Physical Interpretation: The Fourier Transform of a plane wave is a delta function~~

$$\text{Delta Function} \xleftrightarrow{\text{Fourier Transfer}} \text{Perfect Plane Wave}$$

Physical Interpretation: A plane wave in position space is a delta function in momentum space. A plane wave in momentum space is a delta function in position space

Uncertainty Principle

$$(\Delta A)(\Delta B) \geq \frac{1}{2}\left|\langle C \rangle\right| \ , \quad \hat{C} = [\hat{A}, \hat{B}]$$

For $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$, $[\hat{x}, \hat{p}] = i\hbar$, so

$$\Delta x \, \Delta p \geq \hbar/2.$$

For a typical wavefunction, $(\Delta x)(\Delta p)$ will be larger than $\hbar/2$. Only for an gaussian wavefunction will $\Delta x \, \Delta p$ be equal to $\hbar/2$.

Meaning: The uncertainty principle does not limit the accuracy of any measurement device. It tells us how accurately we can predict the result of a single measurement, ~~of one~~ of a variable, if the ~~other~~ other variable is already known with a particular accuracy.

Dirac Notation

Common base states in QM:

$\{|n\rangle\}$: Bound state energy eigenstates. Discrete.

$\{|x\rangle\}$: Position eigenstates, continuous

$\{|k\rangle\}$: momentum eigenstates, continuous

Each of these sets of states are complete & orthonormal:

$$\langle m|n\rangle = \delta_{mn}, \qquad \hat{I} = \sum_n |n\rangle\langle n|$$

$$\langle x|x'\rangle = \delta(x-x') \qquad \hat{I} = \int |x\rangle\langle x|\, dx$$

$$\langle k|k'\rangle = \delta(k-k') \qquad \hat{I} = \int |k\rangle\langle k|\, dk$$

~~We can calculate the overlap of two arbitrary states in any basis:~~

$$\cancel{\langle a|b\rangle = \langle a|\sum_n |n\rangle\langle n|\,|b\rangle = \sum \langle a|n\rangle\langle n|b\rangle}$$

We can project any arbitrary state onto these bases:

$$\langle n|\psi\rangle = a_n \leftarrow \text{a QM amplitude} \Rightarrow |a_n|^2 = P(E_n)$$

$$\langle x|\psi\rangle = \psi(x) \qquad \Rightarrow |\psi(x)|^2 dx = P(x)dx$$

$$\langle k|\psi\rangle = \phi(k) \qquad \Rightarrow |\phi(k)|^2 dk = P(k)dk$$

We can use $\hat{I}$ to calculate the overlap of any two states

$$\langle a|b\rangle = \langle a|\sum_n |n\rangle\langle n|\,|b\rangle = \sum_n \langle a|n\rangle\langle n|b\rangle = \sum_n a_n^* b_n$$

$$\langle a|b\rangle = \langle a|\int dx\, |x\rangle\langle x|\,|b\rangle = \int \langle a|x\rangle\langle x|b\rangle\, dx = \int \psi_a^*(x)\psi_b(x)\, dx$$

$$\langle a|b\rangle = \langle a|\int dk\, |k\rangle\langle k|\,|b\rangle = \int \langle a|k\rangle\langle k|b\rangle\, dk = \int \phi_a^*(k)\phi_b(k)\, dk$$

$\langle a|b\rangle$ is a complex number, a QM amplitude. It will always be the same no matter how we calculate it.

Wave Mechanics	Dirac Notation
$\hat{A}\varphi = a\varphi$	$\hat{A}\vert\varphi\rangle = a\vert\varphi\rangle$
$\hat{H}\varphi_n = E_n\varphi_n$	$\hat{H}\vert n\rangle = E_n\vert n\rangle$
$\psi(x) = \sum_n a_n\varphi_n$	$\vert\psi\rangle = \sum_n a_n\vert n\rangle$
$a_n = \int \varphi_n^*\psi(x)\,dx$	$a_n = \langle n\vert\psi\rangle$
$\int \varphi_m^*\varphi_n\,dx = \delta_{mn}$	$\langle m\vert n\rangle = \delta_{mn}$
$\psi(x) = \frac{1}{\sqrt{2\pi}}\int\phi(k)e^{ikx}\,dk$	$\vert\psi\rangle = \int \vert k\rangle\phi(k)\,dk$
$\varphi(x) = \frac{1}{\sqrt{2\pi}}e^{ikx} \leftarrow$ m$\hat{p}$ e.f $\rightarrow$	$\langle x\vert k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx}$
$\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ particle-in-the-box	$\langle x\vert n\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$
$\varphi_n(\xi) = A_nH_n(\xi)e^{-\xi^2/2}$ SHO	$\langle x\vert n\rangle = A_nH_n(\xi)e^{-\xi^2/2}$

Hermitian Operators

$$\langle\hat{A}^+\alpha\vert\beta\rangle \equiv \langle\alpha\vert\hat{A}\beta\rangle \leftarrow \text{def. of Hermitian conjugate operator}$$

When $\hat{A}^+ = \hat{A}$, we say $\hat{A}$ is Hermitian.

Hermitian operators have

1. real eigenvalues
2. orthogonal eigenfunctions

So we require all observables to be represented by Hermitian operators.

Simple Harmonic Oscillator

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}Kx^2, \quad \omega_0 \equiv \sqrt{\frac{K}{m}}, \quad \beta \equiv \sqrt{\frac{m\omega_0}{\hbar}}$$

$$\hat{a} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) \quad \hat{a}^+ = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right), \quad \hat{N} \equiv \hat{a}^+\hat{a}$$

Then $\hat{H} = \hbar\omega_0\left(\hat{a}^+\hat{a} + \frac{1}{2}\right) = \hbar\omega_0\left(\hat{N} + \frac{1}{2}\right)$

$$E_n = \hbar\omega_0\left(n+\tfrac{1}{2}\right), \quad n = 0, 1, 2, \ldots$$

$$\hat{N}|n\rangle = n|n\rangle$$

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle, \quad \hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$\langle x|0\rangle = \varphi_0(x) = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} e^{-(\beta x)^2/2}$$

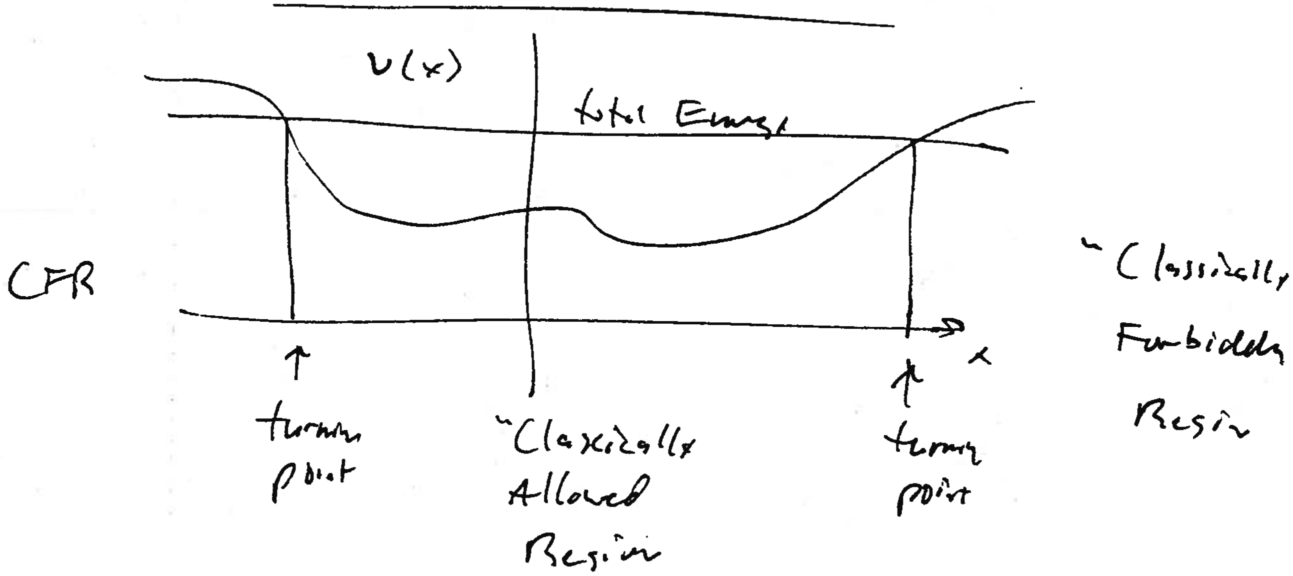
Define $\xi \equiv \beta x$

$$\langle x|n\rangle = \varphi_n(\xi) = A_n\left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2}, \quad A_n = \left(2^n n! \sqrt{\pi}\right)^{-\frac{1}{2}}$$

$$\equiv A_n H_n(\xi) e^{-\xi^2/2}$$

$H(\xi)$ = "Hermite Polynomials"

Bound State Quantization



CAR: ψ'' has opposite sign as ψ $\Rightarrow$ oscillating solutions

CFR: ψ'' has same sign as ψ $\Rightarrow$ solutions blowup or decay to zero.

In the CFR, we reject the solutions which blowup as being non-normalizable & unphysical.

The decaying solutions perfectly balance the tendency to blowup towards $(+)\infty$ & $(-)\infty$. They are discrete, so bound states have discrete eigenvalues in Q.M.