Very Important potential: The Quantum Harmonic oscillator (QHO).

Consider an arbitrary binding potential: 

\[ V(x) = V_0 \quad \text{at} \quad x = x_0 \] 

For low enough energy bound states, 

we are near the minimum of \( V(x) \), so we expand about that minimum: 

\[ V(x) = V_0 + V''(x_0)(x-x_0)^2 \]

neglecting higher terms if \( |x-x_0| \) is small, we see that we have a parabolic potential — a harmonic oscillator potential.

Now set the zero of energy so that \( V=0 \), 
and choose a new word system so that \( x_0 = 0 \); then 

\[ V(x) = \frac{1}{2} N'' x^2 = \frac{1}{2} m \omega^2 x^2 \quad \text{with} \quad \omega^2 = \frac{V}{m} \]

\( N'' \) is the "spring constant," \( k \).

Examples: diatomic molecules, atoms in a crystal (phonons), also photons (oscillating mode of EM field) can be described using this formalism!

So we solve \( H \psi = E \psi \Rightarrow -\frac{1}{2m} \psi'' + \frac{1}{2} m \omega^2 \psi = E \psi \)

with \( \psi \rightarrow 0 \) as \( x \rightarrow \pm \infty \), since \( V(x) \sim \infty \) there.

There are only discrete bound state solutions, no continuum. 

Since \( V(x) = V(-x) \), solutions will have alternating signs: \( \psi(x) = \pm \psi(-x) \).

\( \psi \) will be oscillating between the turning points \( \pm x_0 = \pm \sqrt{2E/m \omega^2} \)

and decay for \( |x| > x_0 \). Higher \( E \) solutions will have larger \( x_0 \); more wigglies. Expect: 

\[ E_n = n \hbar \omega \]

\[ \psi_n(x) = \frac{1}{\sqrt{2^n n!}} e^{-\frac{1}{2} \frac{m \omega^2 x^2}{\hbar^2}} \sin \left( \frac{n \pi x}{x_0} \right) \]
To solve this Sch. Eqn, it is useful to shift to dimensionless variables. The dimensionless variables (our disposal are $t$, $x$, $\omega$).

We can form a time - $\frac{t}{\omega}$; an energy - $\frac{E}{\hbar \omega}$, and a length - $b = \frac{\sqrt{\hbar / \omega}}{m}$. ($b$ = "oscillator length").

So we convert: $E = E + \omega$, $x = b z$, $t = t / \omega$

where $E$, $z$, and $t$ are dimensionless.

\[
\left(\frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2\right) \psi = E \psi
\]

\[
\Rightarrow \left(\frac{d^2}{dz^2} + \frac{1}{2} b^2 \psi\right) = E \psi
\]

\[
\Rightarrow \left(\frac{d^2}{dz^2} + \frac{1}{2} z^2\right) \psi = E \psi \Rightarrow \psi'' = (z^2 - 2E) \psi
\]

(when ' denotes $\frac{d}{dz}$).

**Step 2:** Obtain asymptotic solutions $\psi_{z \to \infty}, 0$:

As $z \to \infty$,

\[
\Rightarrow \psi'' = (z^2 - 2E) \psi \to z^2 \psi
\]

Try $\psi = e^{-z^2} \Rightarrow \psi' = -2z \psi \Rightarrow \psi'' = -4z^2 \psi + z^4 \psi \to 0$

Thus, the dominant behavior at large $z$ will be Gaussian (decaying), so $\psi \to 0$.

So assume $\psi = H(0) e^{-z^2}$

\[
\psi' = -2z \psi + H' e^{-z^2}
\]

\[
\psi'' = -4z^2 \psi + H'' e^{-z^2} - z H' e^{-z^2}
\]

\[
= \left[ (z^2 - 2E) \psi \right] H'' e^{-z^2}
\]

Plug in to $\psi'' = (z^2 - 2E) \psi$

\[
\Rightarrow H'' - 2z H' + (2E - 1) H = 0
\]

**Step 3:** Now form a "transcendental" form $e^{\pm \sqrt{E}}$ of $\psi$, assume that the remainder, $H$, is a simple polynomial: $H = \sum_{n=0}^{\infty} a_n z^n$

with $a_0$ to be determined. Then

\[
H' = \sum_{n=0}^{\infty} n a_n z^{n-1}, \quad H'' = \sum_{n=0}^{\infty} (n-1) a_n z^{n-2}
\]

\[
\Rightarrow \sum_{n=0}^{\infty} \left[ n(n-1) a_n z^{n-2} - 2n a_n z^n + (2E - 1) a_n z^n \right] = 0
\]
Note that the 2nd and 3rd terms are \( O(z^n) \), while the 1st is of order \( O(z^{n-2}) \).

Since \( n \) is a (non-negative integer) summation variable, we are free to relabel, e.g., the 1st term: 
\[
(n(n-1)z^{n-2}) \rightarrow (n+2)(n+1) a_{n+2} z^n
\]

\[
\sum_{n=0}^{\infty} \left[ (n+2)(n+1) a_{n+2} - 2 n a_n + (2z-1) a_n \right] z^n = 0
\]

In order for this to be true for all \( z \), the coefficients of each power of \( z \) must separately equal zero.

\[
(n+2)(n+1) a_{n+2} = (2n - 2z + 1) a_n \quad \text{for all } n.
\]

This is a recursion relation for the coefficients, the \( a_n \)’s.

Note it relates every other coefficient, \( a_{2n+2} \) with \( a_n \).

From part 1, we know there will be an even solution, with \( a_0 = 1 \), \( a_1 = 0 \), and \( a_{2k} = 0 \) by recursion, and an odd solution, with \( a_0 = 0 \), \( a_1 = 1 \), and \( a_{2k+1} = 0 \) by recursion.

\[
a_{2n+2} = -\frac{(2z - 1 - 2n)}{(n+2)(n+1)} a_n
\]

We are free to choose \( a_0 = 1 \) or \( a_1 = 1 \), since the equation is linear in \( H \), so there will be an overall normalization constant.

So now we can determine the \( H \)'s from the recursion relation.

\textbf{Step 5:} All, but does the series converge to a finite result?

Look again at asymptotic behavior as \( |z| \rightarrow \infty \):

- Since \( H = \sum a_n z^n \), the large \( n \) terms will dominate.
- As \( n \rightarrow \infty \), \( a_{2n+2} \rightarrow +\frac{2}{n} a_n \).

What will this give? Consider \( e^{z^2} = \sum b_n z^n \), \( b_0 = \frac{1}{(2!)^2} \), \( b_{2n} = \frac{b_n}{(n+1)!} \rightarrow +\frac{2^2}{n^2} b_n \).

So, ultimately, at large \( z \), \( H \rightarrow e^{z^2} \), \( \Psi = H e^{-z^2} \rightarrow e^{+z^2} \rightarrow \infty \).

No good! To prevent this, we require the series to terminate.
or $\lim_{r \to 0} = 0$ for some $n = \rho$;
then $2\epsilon - 1 - 2\rho = 0$, or $\epsilon = \rho + \frac{1}{2}$.
(The same argument works for $\rho$ even or odd).
So requiring finite solutions at $|z| = \infty$ leads to energy quantization:

$\Rightarrow E^2 = E_{\rho} = \rho + \frac{1}{2}$ (\(\rho = \text{non-negative integer}\)), and

the polynomial solutions are:

- $\rho = 0, \quad E = \frac{1}{2}, \quad a_0 = 1, \quad a_1 = 0, \quad H_0 = 1$
- $\rho = 1, \quad E = \frac{3}{2}, \quad a_0 = 0, \quad a_1 = 1, \quad H_1 = z$
- $\rho = 2, \quad E = 3, \quad a_0 = 1, \quad a_1 = 0, \quad a_2 = -2, \quad H_2 = 1 - 2z^2$
- $\rho = 3, \quad E = \frac{7}{2}, \quad a_0 = 0, \quad a_1 = 1, \quad a_2 = 0, \quad a_3 = -3, \quad H_3 = 2 - \frac{3}{2}z^3$
- $\rho = 4, \quad E = 5, \quad a_0 = 1, \quad a_1 = 0, \quad a_2 = 0, \quad a_3 = 1, \quad a_4 = \frac{1}{3}, \quad H_4 = 1 - 4z^2 + \frac{2}{3}z^3$

With $E = \rho + \frac{1}{2}$, $H_{\rho}'' - 2zH_{\rho}' + 2\rho H_{\rho} = 0$ - Hermite's differential equation when $H_{\rho}(z) = \text{Hermite polynomial of order } \rho$.

Step 6:
$S$ now wherever $\Psi_n = C_n H_n (z) e^{-\frac{z^2}{2}}, \quad z = x/\hbar, \quad \hbar = \sqrt{\hbar/mc}$
with phase $\hat{P} \Psi_n = (-i)^n \Psi_n$.

Fix normalization: $\int \frac{1}{\Psi_n^* \Psi_m} = \delta_{nm} = \int_{-\infty}^{\infty} \Psi_n^* (x) \Psi_m (x) dx$

$\Rightarrow C_n = \sqrt{\frac{1}{2^n n! 4\pi}}$

and, indeed, the solutions are orthogonal.
Stationary States in the Harmonic Oscillator Potential

$\varphi(x)$
Stationary States in the Harmonic Oscillator Potential

$|\psi(x)|^2$
QHO wavepacket motion:

Suppose we construct a wave packet at $t=0$, corresponding to a localized particle in a $l=0$, linear superposition of the $\Psi_m$'s (the oscillator eigenfunctions): $|\Psi_0\rangle = \frac{1}{\sqrt{\Omega}} \sum_m a_m |\Psi_m(x)\rangle = \sum_m a_m |l_m\rangle$

where $|l_m\rangle$ denote the QHO TISE eigenfunctions: $C_n H_n(x) e^{-x^2/2}$.

And we want to know $|\Psi(x,t)\rangle$ at a later time $t$.

Well, $\langle \Psi_n | \psi \rangle = \sum_m a_m \langle \Psi_n | \Psi_m \rangle = \sum_m a_m \delta_{mn} = a_n$, so

$|\psi(x,t)\rangle = \sum_m a_m |m\rangle |l_m\rangle = \sum_m |l_m\rangle \langle m|\psi\rangle$.

Now, each eigenstate evolves in time as

$e^{-i E_n t / \hbar} = e^{-i \epsilon_n t} = e^{-i (E_m t / \hbar)}$, with $t = \omega t$, $E_n = E_m + \omega$.

So $|\psi(x,t)\rangle = \sum_m |l_m\rangle e^{-i \epsilon_n m t / \hbar} \langle m|\psi\rangle$

$= e^{-i \epsilon \omega t} \sum_m |l_m\rangle e^{-i \epsilon m t} \langle m|\psi\rangle$.

The overall phase in front is unimportant; $P(x,t) = \langle \psi(x,t) | \psi(x,t) \rangle$ since it's $t$.

When $t = n \pi$, $\epsilon$ even, then $\langle \psi(x, n\pi) | \psi(x, 0) \rangle = |\psi_0\rangle$ unchanged.

But when $t = p\pi$, $\epsilon$ odd, then all the odd $m$ contribute

pick up a minus sign, these correspond to eigenfunctions $-\Psi_m(x) \leftrightarrow \Psi_m(x)$

so, overall $\langle \psi(x, p\pi) | \psi(-x, 0) \rangle = 0$ odd.

Thus:

- $t = 0, 2\pi, 4\pi, \ldots$
- $t = n\pi, 2n\pi, 3n\pi$

The motion of the wavepacket is thus periodic with period $2\pi$, as in the harmonic case, and which is expected from Ehrenfest's Theorem.

\[ \frac{\partial}{\partial t} \langle p \rangle = -\frac{\partial}{\partial x} \langle x \rangle, \quad \frac{\partial}{\partial t} \langle x \rangle = \langle p \rangle \Rightarrow \frac{\partial}{\partial t} \langle x \rangle = \langle x \rangle \]
Motion of Wave Packet in Harmonic Oscillator Potential

\[ |\psi(x,t)|^2 \]

\[ a = 0.500 a_0/\sqrt{2} \]
Note that a Gaussian wavepacket in a QTO does not disperse away over time (as it does in any other potential).

It remains coherent, i.e., the particles remain with fixed phases with respect to each other, no dispersion.

These are important in quantum optics!
We have solved the (1D) H.O. 
\[ \hat{H} = \frac{1}{2m} \hat{p}^2 + \frac{1}{2} \alpha^2 x^2 = \frac{1}{2m} \left( -\frac{\hbar^2}{i} \frac{d^2}{dx^2} + m^2 \beta^2 x^2 \right) , \quad \hat{H} \Psi_n(x) = E_n \Psi_n(x) \]
and found eigenfunctions and eigenvalues 
\[ \Psi_n = C_n H_n(x) e^{-i b x^2} , \quad E_n = (n + \frac{1}{2}) \hbar \omega , \quad b = \sqrt{\frac{\hbar}{2m \omega}} \]
Once again, let's change to dimensionless variables to explore with true physics. 
\[ \hat{H} = \hat{H}_x \hat{p}_x , \quad Q = \sqrt{\frac{\hbar}{\mu}} x \quad P = \frac{\hbar}{\sqrt{2 \mu \omega}} \]
(we've been calling \( \alpha = \omega \)).
\[ \Rightarrow \hat{H} = \frac{\hbar}{\sqrt{2 \mu \omega}} \left( P^2 + Q^2 \right) \quad (\text{drop the } \hat{\alpha} \text{ over everything}) \]
\( P, Q, \hat{H} \) are Hermitian operators, and \[ [Q, P] = i \Rightarrow \hat{P} = -i \frac{\hbar}{\sqrt{2 \mu \omega}} \]
Now define annihilation and creation operators:
\[ a = \frac{\sqrt{2 \mu \omega}}{\hbar} \left( Q + i P \right) , \quad a^+ = \frac{\sqrt{2 \mu \omega}}{\hbar} \left( Q - i P \right) \]
These are not Hermitian: \( \hat{a}^+ \neq a \).
The commutator \[ [a, a^+] = -\frac{i \hbar}{\sqrt{2 \mu \omega}} [Q, P] + \frac{\hbar}{2 \mu \omega} [P, Q] = 1 \]
Thus, \[ \hat{H} = \frac{\hbar}{\sqrt{2 \mu \omega}} (aa^+ + a^+a) \]
(Using \( Q = \frac{\sqrt{2 \mu \omega}}{\hbar} (a + a^+) \), \( P = \frac{\hbar}{\sqrt{2 \mu \omega}} (a - a^+) \))
\[ H = \frac{\hbar}{\sqrt{2 \mu \omega}} (aa^+ + a^+a + \frac{\hbar}{\sqrt{2 \mu \omega}}) \]
Also, \[ \langle A \rangle = \langle a^+ a + a a^+ \rangle = \langle a \rangle \langle a^+ \rangle \Rightarrow 0 \text{ since } \hat{a}, \hat{a}^+ \text{ are Hermitian (real)} \]
Thus, \[ \langle \hat{N} \rangle = -\frac{\hbar}{2 \mu \omega} \]
In fact, \[ \langle \psi | \hat{N} | \psi \rangle = \langle \psi | a^+ a | \psi \rangle = \langle a | a \psi \rangle = \| a \psi \|_2^2 \geq 0 \]
What are the eigenfunctions of \( \hat{N} \)? Under \( \hat{N} | n \rangle = n | n \rangle \)
What about \( a | n \rangle \)? \[ Na | n \rangle = a^+ a | n \rangle = (a^+ a - 1) | n \rangle = a^+ a | n - 1 \rangle \]
\[ = a (\hat{N} - 1) | n \rangle = a (n - 1) | n - 1 \rangle = (n - 1) a | n - 1 \rangle \]
So, if \( | n \rangle \) is an eigenfunction of \( \hat{N} \) with eigenvalue \( n \),
\( a | n \rangle \) is an eigenfunction \( \hat{a} \)\langle \) eigenvalue \( n - 1 \); \( a | n \rangle \propto | n - 1 \rangle \)
Similarly, can show \( a^+ | n \rangle \propto | n + 1 \rangle \).
Therefore, the operators a and \( a^+ \) lower and raise the eigenvalue of \( \hat{N} \) by 1 unit - and repeated operation of a or \( a^+ \) makes us go "down the ladder" or "up the ladder" - they are "ladder" operators. So far, we have not specified the values \( n \) can take. Now we will see that they must be non-negative integers. To see this, remember 
\[
\langle \hat{N} \rangle \geq 0.
\]
Then, eigenvalues \( \langle n \rangle \), \( \langle a|n\rangle \), \( \langle a^+|n\rangle \), ... \( \langle a^m|n\rangle \) 

 eigenvalues \( n, n-1, n-2, ... n-m 

down to, not including, \( n-m < 0 \), since all eigenvalues must be \( \geq 0 \). We will call the lowest eigenvalue \( n_0 \). Operators again, with \( a^+ \) must give \( a|n_0\rangle = \phi \).
\[
\text{Then } a^+ a|n_0\rangle = \hat{N}|n_0\rangle = n_0|n_0\rangle = a^+|n_0\rangle = \phi = \phi = 1 \Rightarrow n_0 = 0.
\]
So the lowest eigenvalue is \( n_0 = 0 \), and \( \hat{N} (a^+|n_0\rangle) = \hat{N} (1|1\rangle) = (n_0+1) (a^+|n_0\rangle) = 1 (a^+|n_0\rangle) = (n_0+1) (a^+|n_0\rangle) = 1 \cdot (a^+|n_0\rangle) 
So the next eigenvalue is \( n = 1 \), etc - all non-negative integers!

Th state \( |n\rangle \) possesses n "quanta". \( a \) "annihilates" \( |0\rangle = a|0\rangle = \phi \).
\( a^+ \) "creates" one new quantum: \( a^+|n\rangle = |n+1\rangle \).

What is the proportionality constant? Let \( a^+|n\rangle = c|n-1\rangle \).
\[
\langle n|\hat{N}|n\rangle = n \langle n|n\rangle = n \text{ (normalized)}
\]
\[
= \langle n|a^+a|n\rangle = \langle a^+a|n\rangle = \|a|n\rangle^2 = n = \|a|n\rangle^2 \Rightarrow n = \|a|n\rangle^2 = n \Rightarrow \|a|n\rangle^2 = \sqrt{n} \Rightarrow |a|n\rangle = \sqrt{n} |n-1\rangle
\]
Similarly: \( \langle n|\hat{N}|n\rangle = n = \langle n|a^+a|n\rangle = \langle n|a^+a-1|n\rangle = \langle a^n|a^n\rangle - 1
\]
\[
\Rightarrow \|a^n\rangle\| = n+1 \Rightarrow \|a^n\rangle = n+1 \Rightarrow \|a^+|n\rangle = \sqrt{n+1} |n+1\rangle
\]

Check: \( \hat{N}|n\rangle = a^+a|n\rangle = a^+ a \sqrt{n} |n-1\rangle = \sqrt{n} \sqrt{n} |n\rangle = n|n\rangle \).
To summarize the algebraic solution of the AHO problem:

1. \[ A = \frac{\hbar^2}{2m} + \frac{1}{2} m \omega^2 x^2 \]
   \[ \hat{\Psi} = \hat{\Psi}_0 \]

2. Define
   \[ a = \frac{\hbar}{\sqrt{2m \omega}} \left( \sqrt{\frac{\omega}{2m}} \hat{x} + i \frac{\sqrt{2m \omega}}{\hbar} \hat{p} \right) \]
   \[ a^\dagger = \frac{\hbar}{\sqrt{2m \omega}} \left( \sqrt{\frac{\omega}{2m}} \hat{x} - i \frac{\sqrt{2m \omega}}{\hbar} \hat{p} \right) \]
   \[ [a, a^\dagger] = 1 \]

3. \[ \hat{N} = a^\dagger a \]
   \[ \hat{N} \langle n \rangle = n \langle n \rangle \]
   \[ \hat{a} \langle n \rangle = \hbar \omega (a + \frac{1}{2}) \langle n \rangle \]

4. \[ a^\dagger \langle n \rangle = \sqrt{n+1} \langle n+1 \rangle \] "raising", "creation" (adder operator)
   \[ a \langle n \rangle = \sqrt{n} \langle n-1 \rangle \] "lowering", "annihilation" (adder operator)

These are direct consequences of \[ [a, a^\dagger] = 1 \] - nothing else!

5. Since \( \langle \hat{N} \rangle \geq 0 \), must have a ground state.

   \[ a \langle \text{ground state} \rangle = 0 \] - annihilates the ground state
   \[ \Rightarrow \langle \text{ground state} \rangle = \langle 0 \rangle \]
   \[ \Rightarrow \text{all excited states correspond to positive integers} \]
   \[ E_n = \hbar \omega (n + \frac{1}{2}), \quad n = \text{non-negative integer} \]

6. \[ \langle n \rangle = \text{AHO state in } \text{"number" representation}; \]
   the state composed of \( n \) "particles"
So now we have the energy spectrum, and eigenstates in the "number representation" (more on representations, later) for the 1D QHO.

We can use the creation operators to generate the states in the "position rep":
\[ a^+ = \frac{1}{\sqrt{2}} (Q - i P) = \frac{i}{\sqrt{2}} (Q - \frac{\hbar}{i} \frac{\partial}{\partial Q}) \]
\[ a = \frac{1}{\sqrt{2}} (Q + i P) = \frac{i}{\sqrt{2}} (\frac{\partial}{\partial Q} + i \frac{\hbar}{\partial P}) \]

Grand state: \[ |0\rangle = 0 \Rightarrow \frac{i}{\sqrt{2}} (Q + i P) \varphi_0(Q) = 0 \]

Solution: \[ \varphi_0(Q) = A_0 \ e^{-\frac{Q^2}{2\hbar}} \quad (Q = \sqrt{\frac{\hbar}{2\mu}} X) \]

Normalize: \[ \int_{-\infty}^{\infty} |\varphi_0(Q)|^2 dQ = 1 \Rightarrow A_0 = \frac{1}{\sqrt{\pi \hbar}} \]

or,
\[ \varphi_0(Q) = \left( \frac{\mu \hbar}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\frac{\mu Q^2}{2\hbar}} \]

Then, \[ |1\rangle = \frac{i}{\sqrt{2}} a^+ |0\rangle \]

\[ |1\rangle = \frac{i}{\sqrt{2}} a^+ |0\rangle = \frac{i}{\sqrt{2}} (a^+ |1\rangle) = \frac{i}{\sqrt{2}} \left( \frac{\partial}{\partial Q} \right) |0\rangle \]

and in general, \[ |n\rangle = \frac{i}{\sqrt{n+1}} (a^+)^{n+1} |0\rangle \]

So \[ \varphi_n(Q) = A_n (Q - \frac{1}{\sqrt{n+1}}) e^{-\frac{Q^2}{2\hbar}} \]

\[ = A_n Q e^{-\frac{Q^2}{2\hbar}} \quad \text{and} \quad A_n = \left( \frac{\pi}{(n+1)!} \right)^{\frac{1}{2}} \]

And \[ \varphi_n(Q) = A_n (Q - \frac{1}{\sqrt{n+1}}) e^{-\frac{Q^2}{2\hbar}} = A_n H_n(Q) e^{-\frac{Q^2}{2\hbar}} \]

is a Hermite polynomial.

We can generate the Hermite polynomials, one at a time, this way:

\[ A_n = \left( \frac{1}{n!} \right)^{\frac{1}{2}} \quad n! \quad (2n)! \quad (2\pi)^{-\frac{1}{2}} \quad H_n(Q) = (-1)^n \left( e^{\frac{Q^2}{2\hbar}} \frac{\partial^n}{\partial Q^n} e^{-\frac{Q^2}{2\hbar}} \right) \]

It can also be shown that \[ \langle n\mid m \rangle = \delta_{nm}, \quad \text{or} \]

\[ A_n A_m \int_{-\infty}^{\infty} H_n(Q) H_m(Q) e^{-\frac{Q^2}{2\hbar}} dQ = \delta_{nm} \]

Matrix elements - Suppose that at some time, \[ |\psi\rangle = \sum_n A_n |n\rangle \]

Then we can write the expectation value for \[ Q, \]

\[ \langle Q \rangle = \sum_n \langle n \mid Q \mid n \rangle = \sum_n A_n^* A_n \langle n \mid Q \mid n \rangle \]

So it is useful to consider the matrix elements \[ \langle n \mid Q \mid m \rangle \]

\[ Q_{nm} = \langle n \mid Q \mid m \rangle = \int_{-\infty}^{\infty} dQ \; \psi_n^*(Q) \psi_m(Q) Q \]

\[ = A_m^* A_m \int_{-\infty}^{\infty} dQ \; H_n(Q) H_m(Q) Q e^{-\frac{Q^2}{2\hbar}} \]
Van packets, matrix elements, transitions

- We can construct localized van packets $\phi_n$ from energy eigenstates, in the usual way: $|\psi\rangle = \sum_n c_n |\phi_n\rangle$

- The wave function dependence: $|\psi\rangle = \sum_n c_n |\phi_n\rangle \propto e^{-E_n \sum_\tau \frac{\hbar}{\epsilon}}$

- As we have seen before, these localized van packets behave like classical particles in a H.O potential, undergoing simple harmonic oscillatory motion.

- If the particle is charged, it will radiate, with EM waves of angular frequency $\omega$.

- The amount of radiation depends on the electric dipole moment of the charge distribution: $\langle \psi | \hat{\mathbf{E}} \cdot \mathbf{x} | \psi \rangle = \langle \mathbf{x} \rangle$ (electric dipole moment operator $\hat{\mathbf{E}} = \mathbf{E}$)

- If $\psi = \psi(x)$, then $\langle \psi | \hat{\mathbf{E}} \cdot \mathbf{x} | \psi \rangle = \int dx \, |\psi|^2 \mathbf{E} \cdot \mathbf{x}$

- If the charge distribution is symmetric, no net dipole.

- If $\psi$ is not symmetric, $\langle \mathbf{x} \rangle \neq 0 \Rightarrow$ dipole radiation, with rate $R \propto e^{-|\langle \psi | \hat{\mathbf{E}} \cdot \mathbf{x} | \psi \rangle|^2}$ (classical EM)

- So let's calculate $\langle \psi | \hat{\mathbf{E}} \cdot \mathbf{x} | \psi \rangle = \sum_{nm} c_n c^*_m \langle m | \hat{\mathbf{E}} \cdot \mathbf{x} | n \rangle = \sum_n |c_n|^2 \langle m | \hat{\mathbf{E}} \cdot \mathbf{x} | n \rangle$ (diagonal terms)

- $+ \sum_n \sum_{m \neq n} |c_n|^2 \langle m | \hat{\mathbf{E}} \cdot \mathbf{x} | n \rangle \langle n | \hat{\mathbf{E}} \cdot \mathbf{x}^* | m \rangle$

- The oscillation of the dipole moment corresponds to transitions between states that are "linked" by non-diagonal matrix elements $\langle m | \hat{\mathbf{E}} \cdot \mathbf{x} | n \rangle$. These transitions occur by absorption or emission of a "quantum" of energy: photon (EM field) or phonon (lattice vibration).

- So we must evaluate the matrix elements $\langle m | \hat{\mathbf{E}} \cdot \mathbf{x} | n \rangle = \int \, d\mathbf{Q} \, \langle m | \phi(\mathbf{Q}) \rangle \cdot \mathbf{E} \cdot \mathbf{Q} \cdot \langle \phi(\mathbf{Q}) | n \rangle$ = $\sum_{Qm} \langle m | \phi_0 | n \rangle \int \, d\mathbf{Q} \, \psi_m^*(\mathbf{Q}) \cdot \mathbf{Q} \cdot \psi_n(\mathbf{Q}) \, e^{-\frac{\hbar}{\epsilon} \sum_\tau \frac{Q^2}{2m}}$
This is easy, using creation-annihilation operators, \( Q = \frac{i\hbar}{\alpha_v} (\hat{a} + \hat{a}^\dagger) \)
\[ Q_{nm} = \frac{i\hbar}{\alpha_v} <n\mid (\hat{a} + \hat{a}^\dagger) \mid m> = \frac{i\hbar}{\alpha_v} \left[ \sum_m <n\mid \hat{a} \mid m> + \sum_m <n\mid \hat{a}^\dagger \mid m> \right] \]
\[ = \frac{\hbar}{\alpha_v} \sqrt{n} \sum_m \sqrt{m} <n\mid \hat{a} \mid m-1> + \frac{\hbar}{\alpha_v} \sqrt{n} \sum_m \sqrt{m+1} <n\mid \hat{a}^\dagger \mid m+1> \]

Or, as a real symmetric (Hermitian) matrix:
\[
Q_{nm} = \begin{pmatrix}
0 & \frac{\hbar}{\alpha_v} & 0 & \cdots \\
\frac{\hbar}{\alpha_v} & 0 & \frac{\hbar}{\alpha_v} & \cdots \\
0 & \frac{\hbar}{\alpha_v} & 0 & \cdots \\
\vdots & \vdots & \vdots & \ddots 
\end{pmatrix}
\]

Diagonal \( = 0 \) : \( Q_{nn} = 0 \), only one off-diagonal term \( n \neq n+1 \)

\[ \text{Parity selection rule:} \quad n \neq n+1 \]

Note that \( <n\mid \hat{a} \mid m> = (n-\frac{1}{2})\sqrt{m} = <n\mid \hat{a} \mid m> + <n\mid \hat{a}^\dagger \mid m> \).

But from VBS, with \( V \propto \sqrt{x^2} \), \( \langle V=\langle T \rangle = \frac{3}{2} \langle H \rangle \)

thus, \( \langle x^2 \rangle, \langle p^2 \rangle \propto (n+\frac{1}{2}) \), so that higher states are more dispersed and have greater kinetic energies.

This formulation is the essence of the QM description of the interaction of matter + energy.

The matter system moves up or down one quantum of energy, and the energy system (EM, phonons) simultaneously moves down or up, one quantum.

The rate for these exchanges of energy is proportional to the squares of matrix elements:
\[ \text{Rate} \propto <\text{matter: } n, \, \text{reduction: } n+1>^2 \text{ and } <\text{matter: } n, \, \text{reduction: } n-1>^2 \]
So far, we have taken a semi-classical approach:

quantize the matter, but not the EM field (no monopoles and/or instantons!)

In relativistic QM, you will also quantize the EM field:

"second quantization"

The EM field is described as a collection of H.O.'s, of different w's:

- a continuous, infinite spectrum of w's.
- Each of these w number of "modes" can have an energy
  \[ E = \hbar \omega (n_\omega + \frac{1}{2}) \]
  with different \( n_\omega \) for each \( \omega \).

This means that even in the absence of excitations, there are an \( \infty \) number of modes with \( E = \hbar \omega \), leading to a total energy
  \[ E = \sum_\omega \left( \hbar \omega \right) = \infty ! \]

We can always "subtract" out this \( \infty \) energy of the vacuum by redefining the zero of energy; but the "zero-point energy" of the vacuum leads to observable effects! \( \Rightarrow \)

the vacuum is not empty!

In Quantum Field Theory, the vacuum is thought of as seething with virtual excitations, even in the absence of real excitations.

Thus vacuum can even be manipulated:

- of Jeff Kimble's "squeezed light" - blacker than darkness!
Zero-point energy

the QHD spectrum $E = (n + \frac{1}{2}) \hbar \omega$ is like a ladder:

but the 1st rung (ground state) is not at zero, it's at $\frac{\hbar \omega}{2}$.

This is completely non-classical; it's non-classical.

Nearly, that's not a problem, we need only realize

the zero of energy. But it shows up in physical systems!

the ground state (absence of an excitation of the H O)

is the vacuum. Eqt. an empty metal cavity at temperature $T = 0$.

There are still "zero-point" excitations $\Rightarrow$ the vacuum is not empty!

There is a quantum "noise" associated with the vacuum.

- It is a consequence of Heisenberg uncertainty.

- A QHD "mass on a spring" cannot be localized in space

  perfectly, so it cannot be perfectly at rest. It is always

  "jiggly" a little bit - quantum noise!

- One consequence:

  - emission of photons by atoms, under the influence of an applied EM field,

    stimulated emission

    (caser = light amplification by stimulated emission of radiation)

  - Atoms emit photons even when an EM field is not applied

    spontaneous emission. Actually, this is emission

    stimulated by the zero-point energy of the vacuum:

    there is always some EM field in the vicinity of an atom,

    even if a field is not applied!

- Similarly, the ground state of the hydrogen atom, $E = -R_y \frac{e^2}{2\hbar^2}$

  is a "zero-point" energy for the central potential, a consequence

  of Heisenberg uncertainty - it ensures ground state stability!

- Similarly, in an $\infty$ square well, ground state $\frac{\hbar^2}{8m a^2}$, not $\phi$. 
But there are contracances! The proof is in the observation of redshifts and redshifting of light, (simplified emission).

According to atomic theory, in the 20's, a process called the 'electric transition' of Helium was discovered. In this process, an atom of helium, with a photon of energy, $E = 0$, in a dark room, schematically:

$\text{He} \rightarrow \text{He}^+$

But if you ask it really seriously, you can dream about atoms and the government supports high research.

A special atom, E.P. energy is a loyal friend, in the theory. The energy is high, but the atom is free.

If you ask about the day when it was once or actually if it was ever a sea of zero-point energy, for fun, profit —

...
Zero-point energy

- The QHO spectrum $E_n = (n+1/2)\hbar \omega$ is like a ladder, but the lowest rung is at $\hbar \omega$, not $\hbar \nu$. In ground state, $\langle x \rangle = 0 = \langle p^2 \rangle$, but $\langle x^2 \rangle \neq 0$, $\langle p^2 \rangle \neq 0$,

\[ \Delta x \Delta p > \hbar / 2 \]

Natural minimum $\langle x \rangle = \langle x^2 \rangle = \langle p^2 \rangle$ in a vibrational state, and this is what gives the QHO its natural state.

- Seen they, for a square well $E_{\text{bound}} = \frac{\hbar^2 n^2}{2m a^2}$ and Coulomb potential of hydrogen $E_{\text{bound}} = -\frac{e^2}{n^2}$, $n=1$

- Not an intrinsic problem, need only redefine the zero of energy. The zero-point energy represents the ground state cannot take it out. It is quantum uncertainty, or quantum "noise".

A QHO mass on spring cannot be localized in space perfectly $\langle x^2 \rangle = 0$ so it cannot be perfectly at rest $\langle p^2 \rangle = 0 \implies 0$

- Thus, perfectly quantized.

- The ground state is achieved with all external energy sources are removed, e.g., thermal $T \to 0$ (and the oscillator is allowed to vibrate away all its energy as radiation).

- All oscillatory phenomenon can be quantized like QHO:

  - Include the EM field (made possible by $\hbar \in$ a canary, at time $T$).
  - Second quantization
  - Each mode coupled with $\omega = \sqrt{\epsilon} = \frac{2\pi n}{2L} \implies$ continuum
  - So a zero point energy $\omega = \sqrt{\epsilon}$ even at $T=0$, after away all the energy ("vacuum"), $E_0 = \int \sqrt{\epsilon} d\omega \to \infty$

  $\implies$ Infinite vacuum energy!