Lecture 21:
Simple Harmonic Oscillator: Coordinate Basis

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As you have no doubt heard before, the primary motivation for studying the simple harmonic oscillator is that, for any system subject to a potential energy \( V(x) \) and for motion around an equilibrium position \( x_0 \) (where, by definition, \( \frac{d}{dx} V(x) \bigg|_{x_0} = 0 \)), the system acts like a simple harmonic oscillator. Explicitly, the potential energy is

\[
V(x) = V(x_0) + \frac{d}{dx} V(x) \bigg|_{x_0} (x - x_0) + \frac{1}{2} \frac{d^2}{dx^2} V(x) \bigg|_{x_0} (x - x_0)^2 + \cdots
\]

The first term is an unimportant constant, the second term vanishes at \( x_0 \) because it is an equilibrium position, so the third term is the first important term. It is quadratic in the displacement from \( x_0 \), just like a simple harmonic oscillator. If the kinetic term is the usual \( \frac{p^2}{2m} \), then the Hamiltonian for the system may be approximated as

\[
\mathcal{H}(x, p) = \frac{p^2}{2m} + \frac{1}{2} k x^2
\]

where we define \( k = \frac{d^2}{dx^2} V(x) \bigg|_{x_0} \) and redefine the origin to be at \( x_0 \). That is, we have the simple harmonic oscillator.
The above argument is equally valid for multiparticle systems; in fact, the SHO approximation can be even more useful there because of the complication of dealing with so many particles.

See Shankar and any intermediate mechanics textbook (Marion and Thornton, Hand and Finch, Goldstein) for more examples.
{\langle x \rangle}-Basis Hamiltonian and Eigenvalue-Eigenvector Equation

The classical and quantum Hamiltonians are

\[ H(x, p) = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad \Rightarrow \quad H(X, P) = \frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2 \] (6.1)

As usual, we first need to find the eigenstates of the Hamiltonian, \( H \psi_E = E \psi_E \).
Also as usual, we insert completeness and take the product on the left with \( \langle x \rangle \) (repeating this completely generic step so that you are reminded of it!):

\[ \langle x | H | \psi_E \rangle = \langle x | E | \psi_E \rangle \]

\[ \int_{-\infty}^{\infty} dx' \langle x | H | x' \rangle \langle x' | \psi_E \rangle = E \langle x | \psi_E \rangle \]

\[ \int_{-\infty}^{\infty} dx' \langle x | \left( \frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2 \right) | x' \rangle \psi_{E,x}(x') = E \psi_{E,x}(x) \]
We calculated in Equations 5.27 and 5.28 the matrix elements \( \langle x | P^2 | x' \rangle \) and \( \langle x | V(X) | x' \rangle \) in a way valid for any one-dimensional problem, so we use those results:

\[
\int_{-\infty}^{\infty} dx \, \delta(x - x') \left[ -\frac{\hbar^2}{2m} \frac{d}{d(x')}^2 + \frac{1}{2} m \omega^2 (x')^2 \right] \psi_{E,x}(x') = E \psi_{E,x}(x)
\]

\[
-\frac{\hbar^2}{2m} \frac{d}{dx^2} \psi_{E,x}(x) + \frac{1}{2} m \omega^2 x^2 \psi_{E,x}(x) = E \psi_{E,x}(x) \quad (6.2)
\]

There are two natural scales, a length \( b = \sqrt{\frac{\hbar}{m \omega}} \) and an energy \( E_0 = \hbar \omega = \frac{\hbar^2}{mb^2} \). If we define \( y = \frac{x}{b} \) and \( \varepsilon = \frac{E}{E_0} \), then we may scale out the dimensions:

\[
b^2 \frac{d}{dx^2} \psi_{E,x}(x) + \frac{2mE}{\hbar^2} b^2 \psi_{E,x}(x) - \frac{m^2 \omega^2 b^4}{\hbar^2} \frac{x^2}{b^2} \psi_{E,x}(x) = 0
\]

\[
\frac{d^2}{dy^2} \psi_{\varepsilon}(y) + (2 \varepsilon - y^2) \psi_{\varepsilon}(y) = 0 \quad (6.3)
\]

The physics is now mostly done and we have a math problem. The other bit of input from the physics is the boundary condition \( \psi_{\varepsilon}(y) \to 0 \) faster than \( 1/\sqrt{|y|} \) as \( |y| \to \infty \) so that the resulting state can be normalized. We know the state should be normalizable to unity because the potential becomes infinite at large \( |x| \) and thus there can be no free states.
Solving the Differential Equation

We must now find the solutions of Equation

\[
\frac{d^2}{dy^2} \psi_\epsilon(y) + (2\epsilon - y^2) \psi_\epsilon(y) = 0
\]

subject to the boundary condition \(\psi_\epsilon(y) \to 0\) faster than \(1/\sqrt{|y|}\) as \(|y| \to \infty\). \(\epsilon\) is a parameter that gives the energy eigenvalue.

This is a second-order linear differential equation with non-constant, polynomial coefficients, so you know from your math classes that one has to construct a series solution. In principle, this is all straightforward. However, we will go through much of the calculation in detail because this is the first such case we have encountered. Also, for the sake of your mathematical physics education, it is important to become adept at doing this kind of thing: just as differentiation and integration are second nature to you by now, and hopefully you are getting to a similar point on linear algebra, you need to internalize methods of solving differential equations.
Let's first consider the asymptotic behavior of the equation: this will put the problem in a cleaner form for the series solution. At large $|y|$, $y^2 \gg \varepsilon$, so we have

$$\frac{d^2}{dy^2} \psi_\varepsilon(y) - y^2 \psi_\varepsilon(y) = 0$$

(Notice that the equation no longer depends on $\varepsilon$ and hence we can drop the $\varepsilon$ label for now.) A solution to this equation, in the same limit $|y| \to \infty$, is

$$\psi(y) = A y^m e^{\pm \frac{y^2}{2}}$$

which we can see by direct substitution:

$$\frac{d^2}{dy^2} \psi(y) = \frac{d}{dy} \left( \left[m y^{m-1} + y^m (\pm y)\right] A e^{\pm \frac{y^2}{2}} \right)$$

$$= \left[ (m (m - 1) y^{m-2} \pm (m + 1) y^m) + (m y^{m-1} \pm y^{m+1}) (\pm y) \right] A e^{\pm \frac{y^2}{2}}$$

$$= \left[y^{m+2} \pm (2 m + 1) y^m + m (m - 1) y^{m-2}\right] A e^{\pm \frac{y^2}{2}}$$
Now take the $|y| \to \infty$ limit:

$$\frac{d^2}{dy^2} \psi(y) \mid_{|y| \to \infty} y^2 A y^m e^{\pm \frac{y^2}{2}} = y^2 \psi(y)$$

The asymptotic solution works. So, our solution must asymptote to $y^m e^{\pm \frac{y^2}{2}}$ at large $|y|$. To be normalizable, and hence physically allowed, the + solution is disallowed, leaving only

$$\psi(y) \mid_{|y| \to \infty}^m y e^{-\frac{y^2}{2}}$$

(6.4)
In order to further constrain the form of the solution, let us consider the $|y| \ll \varepsilon$ limit, in which we can ignore the $y^2$ term, giving

$$\frac{d^2}{dy^2} \psi_\varepsilon(y) + 2 \varepsilon \psi_\varepsilon(y) = 0$$

This is a second-order linear differential equation with constant coefficients, so we know the solution is a sum of harmonic functions:

$$\psi_\varepsilon(y) = \alpha \cos \left( \sqrt{2\varepsilon} y \right) + \beta \sin \left( \sqrt{2\varepsilon} y \right)$$

Notice that the solution depends on $\varepsilon$ in this limit. Since we ignored the term of order $y^2$ in the differential equation in this limit, we only need to consider this solution to first order in $y$, which gives

$$\psi_\varepsilon(y) \left|_{|y| \to 0} \right. \to \alpha + \beta \sqrt{2 \varepsilon} y \quad (6.5)$$

That is, the solution behaves like a polynomial as $|y| \to 0$. 
A full solution that would satisfy the above limits is

$$\psi_\epsilon(y) = u_\epsilon(y) e^{-\frac{y^2}{2}}$$  \hspace{1cm} (6.6)

where $u(y) \xrightarrow{|y| \to 0} \alpha + \beta \sqrt{2 \epsilon}y$ and $u(y) \xrightarrow{|y| \to \infty} y^m$. (Note that $u_\epsilon(y)$ now carries the $\epsilon$ subscript because the Gaussian portion has no dependence on $\epsilon$ by construction.)

Let us plug this into the full differential equation and obtain a differential equation for $u(y)$:

$$\left[ \frac{d^2}{dy^2} + (2 \epsilon - y^2) \right] \left( u_\epsilon(y) e^{-\frac{y^2}{2}} \right) = 0$$

$$\left[ \frac{d^2}{dy^2} u_\epsilon(y) - 2y \frac{d}{dy} u_\epsilon(y) + \left( y^2 - 1 + 2 \epsilon - y^2 \right) u_\epsilon(y) \right] e^{-\frac{y^2}{2}} = 0$$

$$\frac{d^2}{dy^2} u_\epsilon(y) - 2y \frac{d}{dy} u_\epsilon(y) + (2 \epsilon - 1) u_\epsilon(y) = 0$$  \hspace{1cm} (6.7)

Our asymptotic considerations indicate that the solution to this differential equation behaves like a polynomial both as $|y| \to 0$ and as $|y| \to \infty$. This leads us to try a series solution of the form $u_\epsilon(y) = \sum_{n=0}^{\infty} C_{\epsilon,n} y^n$. 
Feeding the series solution form into the differential equation yields

\[
\sum_{n=0}^{\infty} C_{\varepsilon,n} \left[ n(n-1)y^{n-2} - 2ny^n + (2\varepsilon - 1)y^n \right] = 0
\]

\[
\sum_{m=0}^{\infty} C_{\varepsilon,m+2} (m+2)(m+1)y^m = \sum_{n=0}^{\infty} C_{\varepsilon,n} (2n+1-2\varepsilon)y^n
\]

where, for the first piece, we relabeled the sum over \( n \) to be a sum over \( m = n - 2 \); the \( m \) index starts at 0, not \(-2\), because the first two terms of that series vanish \( n(n-1) = 0 \) for \( n = 0, 1 \), and we moved the second and third pieces to the right side. Since the functions \( \{y^n\} \) are linearly independent (recall, we argued that they could be used as a basis for a function space on the interval \([a, b]\) because no one of them can be written as sum of the others), the sums must be equal term-by-term, so

\[
C_{\varepsilon,n+2} = C_{\varepsilon,n} \frac{2n+1-2\varepsilon}{(n+2)(n+1)}
\]

The coefficients \( C_{\varepsilon,0} \) and \( C_{\varepsilon,1} \) are left to be determined by initial conditions.
Now, as is usual in these circumstances, we require that the series terminate at some point so that the asymptotic behavior is obeyed: as we have it now, the series goes on forever rather than converging to $y^m$ for some $m$. This also explains why we have obtained no quantization condition on $\varepsilon$ yet: as we explained in Section 5.3, quantization of the energy arises because of the bound-state condition that the solution must decay sufficiently quickly at $\infty$; our solution does not yet satisfy this condition!

Shankar complicates this issue by following the unterminated solution to its logical conclusion. That is unnecessary: we know that $\sum_{n=0}^{\infty} C_n y^n \xrightarrow{|y|\to\infty} y^m$ is impossible unless $C_n = 0$ for $n > m$ by the same linear independence argument as made before.
So, let's just require termination:

\[
0 = C_{\varepsilon, n+2} = C_{\varepsilon, n} \frac{2n + 1 - 2\varepsilon}{(n + 2)(n + 1)}
\]

\[
0 = 2n + 1 - 2\varepsilon
\]

\[
\varepsilon = \frac{2n + 1}{2}
\]

We obtain the condition that \(\varepsilon\) must be an odd half-integer.

The above condition only terminates either the odd or even coefficients, depending on whether the \(n\) set by \(\varepsilon\) is odd or even. To ensure termination, we must require \(C_{\varepsilon, 1} = 0\) when \(n\) is even so that the odd terms all vanish and, conversely, \(C_{\varepsilon, 0} = 0\) when \(n\) is odd so all the even powers vanish.

To summarize, with \(\varepsilon\) an odd half-integer of the form \(\varepsilon = \frac{2n + 1}{2}\), \(u_{\varepsilon}(y)\) is a polynomial of order \(n = \frac{2\varepsilon - 1}{2}\) and containing only the odd or even powers of \(y\) depending on whether \(n\) is even or odd, respectively. This solution matches our asymptotic conditions.
Explicit Form for the SHO Solutions

Our solutions are of the form

\[
\psi_{E_n,x}(x) = \left( \frac{m \omega}{\pi \hbar 2^n (n!)^2} \right)^{1/4} H_n \left( x \sqrt{\frac{m \omega}{\hbar}} \right) e^{-\frac{m \omega x^2}{2 \hbar}} \quad E_n = \left( n + \frac{1}{2} \right) \hbar \omega
\]  

(6.8)

where \( H_n(y) \) are the Hermite polynomials

\[
H_0(y) = 1 \quad H_1(y) = 2y \\
H_2(y) = -2 \left( 1 - 2y^2 \right) \quad H_3(y) = -12 \left( y - \frac{2}{3} y^3 \right)
\]

where the choice of the \( C_0 \) and \( C_1 \) coefficients in each case is arbitrary but is a convention (one that allows the given simple form for the normalization). The normalization can be calculated by some tedious integrations that we will not go through. The different eigenfunctions are of course orthonormal,

\[
\langle \psi_{E_n} | \psi_{E_m} \rangle = \int_{-\infty}^{\infty} dx \, \psi_{E_n,x}^*(x) \psi_{E_m,x}(x) = \delta_{nm}.
\]

The related orthogonality and normalization of the Hermite polynomials alone is given in Shankar, as well as a recurrence relation that we will not need.