PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 17, March 30, 2021 (Tuesday)

- Reading:
  Harmonic Oscillator: My Notes and Griffiths 2.3
  Angular Momentum: Griffiths 4.1 and 4.3
- Assignments: Problem Set 8 due April 07 (Wednesday).
  Submit your homework assignments to Canvas.

Topics for Today: Harmonic Oscillator [Griffiths 2.3]

4.3 The Harmonic Oscillator in the Coordinate Basis [Griffiths 2.3.2]

Topics for Next Lecture: Angular Momentum

4.4 Oscillator in Higher Dimensions

5.1 Rotations in Three Dimensions

4.3 The Harmonic Oscillator in the Coordinate Basis

In the x basis, the Hamiltonian for the Harmonic Oscillator is give by

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2.$$

Since the Hamiltonian has no time dependence, we have stationary solutions. We know that the wave function for stationary solutions are

$$\Psi(x,t) = \psi_E(x)e^{-iEt/\hbar}$$

and the time independent Schrödinger Equation

$$\begin{aligned} H\psi_E(x) &= E\psi_E(x) \quad \text{becomes} \\ \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi_E(x) &= E\psi_E(x) \end{aligned}$$

where $\psi_E(x)$ is the eigenfunction of the Hamiltonian with energy E.

The energy associated with the oscillator must be positive. It can be seen by writing

$$\langle H \rangle = \int \psi_E^*(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) \psi_E(x) \, dx \geq 0 \, ,$$

since it is the sum of two squares. Thus $E \geq 0$ for this system.

The Schrödinger equation can be rewritten as

$$\frac{d^2 \psi_E}{dx^2} + \frac{2m}{\hbar} \left(E - \frac{1}{2} m \omega^2 x^2 \right) \psi_E = 0 \, .$$

It is always useful to rewrite it in terms of dimensionless arguments so that we can write down logarithmic or exponential solutions.

There are three dimensionful parameters in our theory

$$[\hbar] = M L^2 T^{-1} \, , \quad [m] = M \, , \quad \text{and} \quad [\omega] = T^{-1} \, .$$

Thus

$$\left[\frac{m\omega}{\hbar}\right] = \frac{MT^{-1}}{ML^2T^{-1}} = L^{-2}.$$

If we define

$$\xi \equiv \left(\frac{m\omega}{\hbar}\right)^{1/2} x$$

then ξ will be dimensionless.

Applying the the chain rule of derivative, we obtain

$$\frac{d}{dx} = \frac{d\xi}{dx}\frac{d}{d\xi} = \left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{d}{d\xi}\,.$$

Putting this back in the equation of ψ_E, we have

$$\frac{m\omega}{\hbar}\frac{d^2\psi_E(\xi)}{d\xi^2} + \frac{2m}{\hbar}\left(E - \frac{1}{2}m\omega^2 \cdot \frac{\hbar}{m\omega}\xi^2\right)\psi_E(\xi) = 0$$

or

$$\frac{d^2\psi_E(\xi)}{d\xi^2} + \left(\frac{2E}{\hbar\omega} - \xi^2\right)\psi_E(\xi) = 0\,.$$

In addition, let us define

$$\epsilon \equiv \frac{2E}{\hbar\omega}.$$

Clearly, ϵ is dimensionless. Then the equation becomes

$$\frac{d^2\psi_E(\xi)}{d\xi^2} + (\epsilon - \xi^2)\psi_E(\xi) = 0\,.$$

Solutions in the limits $\xi \to \infty$ and $\xi \to 0$

Before deriving the solution, it is useful to find out the asymptotic forms for the solutions both in the limits $\xi \to \infty$ and $\xi \to 0$. For a finite ϵ in the limit $\xi \to \infty$, the equation of motion (EOM) becomes

$$\frac{d^2\psi_E(\xi)}{d\xi^2} - \xi^2\psi_E(\xi) = 0.$$

The solution of this equation is

$$\lim_{\xi \to \infty} \psi_E(\xi) = \xi^m e^{\pm \frac{1}{2}\xi^2}$$

for any finite m. This can be easily checked by noticing that

$$\begin{aligned}
\lim_{\xi \to \infty} \frac{d^2\psi_E(\xi)}{d\xi^2} &= \lim_{\xi \to \infty} e^{\pm \frac{1}{2}\xi^2}[m(m-1)\xi^{m-2} \pm (2m+1)\xi^m + \xi^{m+2}] \\
&= e^{\pm \frac{1}{2}\xi^2}\xi^{m+2} \\
&= \xi^2 \psi_E(\xi) \,.
\end{aligned}$$

Although both $\xi^m e^{\pm \frac{1}{2}\xi^2}$ represent an asymptotic solution, there is only one physical solution

$$\psi_E(\xi) \sim \xi^m e^{-\frac{1}{2}\xi^2}.$$

N.B. $\psi_E(x) \to 0$ as $x \to \infty$.

In the limit, $\xi \to 0$, the EOM reduces to

$$\frac{d^2\psi_E(\xi)}{d\xi^2} + \epsilon\psi_E(\xi) = 0\,, \quad \text{and} \quad \lim_{\xi\to 0}\psi_E(\xi) \to f(\xi)$$

where $f(\xi)$ is a polynomial of ξ in terms of a power series.

General solutions

Recall that the equation of motion is

$$\frac{d^2\psi_E(\xi)}{d\xi^2} + (\epsilon - \xi^2)\psi_E(\xi) = 0 \quad \text{with} \quad \psi_E(\xi) = f(\xi)e^{-\frac{1}{2}\xi^2}\,.$$

Putting this back into the EOM for the oscillator we have

$$f''(\xi) - 2\xi f'(\xi) + (\xi^2 - 1)f(\xi) + (\epsilon - \xi^2)f(\xi) = 0$$

or

$$f''(\xi) - 2\xi f'(\xi) + (\epsilon - 1)f(\xi) = 0\,.$$

We have found the equation of motion

$$f''(\xi) - 2\xi f'(\xi) + (\epsilon - 1) f(\xi) = 0\,.$$

Let us try a power series solution,

$$\begin{aligned}
f(\xi) &= \sum_{n=0}^{\infty} c_n \xi^n\,, \quad \frac{df(\xi)}{d\xi} = f'(\xi) = \sum_{n=1}^{\infty} n c_n \xi^{n-1}\,, \\
\frac{d^2 f(\xi)}{d\xi^2} &= f''(\xi) = \sum_{n=2}^{\infty} n(n-1) c_n \xi^{n-2} = \sum_{m=0}^{\infty} (m+2)(m+1) c_{m+2} \xi^m\,.
\end{aligned}$$

Putting these back into the EOM, we have

$$\sum_{m=0}^{\infty} (m+2)(m+1) c_{m+2} \xi^m - \sum_{m=0}^{\infty} 2m c_m \xi^m + (\epsilon - 1) \sum_{m=0}^{\infty} c_m \xi^m = 0$$

or

$$\sum_{m=0}^{\infty} \left[(m+2)(m+1) c_{m+2} + (\epsilon - 1 - 2m) c_m \right] \xi^m = 0\,.$$

If this equation were to be true for all m, then we must have

$$(m+2)(m+1)c_{m+2} + (\epsilon - 1 - 2m)c_m = 0,$$

that is

$$c_{m+2} = -\frac{(\epsilon - 1 - 2m)}{(m+2)(m+1)} c_m.$$

This defines a recursion relation for the coefficients. It is clear that all coefficients can be expressed in terms of c_0 and c_1.

For example,

$$\begin{aligned} c_2 &= -\frac{(\epsilon - 1)}{2} c_0, \\ c_3 &= -\frac{(\epsilon - 3)}{6} c_1, \\ c_4 &= -\frac{(\epsilon - 5)}{2 \cdot 6} c_2 = \frac{(\epsilon - 5)(\epsilon - 1)}{24} c_0. \end{aligned}$$

This system has a symmetry $x \to -x$.

Thus, we expect the solutions to be of two types, odd and even.

- If $c_0 = 0$, then all even powers in the expansion of $f(\xi)$ would vanish and hence it would be antisymmetric.
- On the other hand, if $c_1 = 0$, then $f(\xi)$ would contain only even powers in the expansion and, therefore, would be symmetric.
- In general, unless the series terminates at some point, its dominant asymptotic form can be inferred from the ratio

$$\lim_{n\to\infty} \frac{c_{n+2}}{c_n} \to \frac{2}{n}\,.$$

This is an unphysical solution if $n \to \infty$.

- Thus for a physical solution to exist the series must terminate, such that the numerator of the recursion relation vanishes,

$$c_{n+2} = -\frac{(\epsilon - 1 - 2n)}{(n+2)(n+1)} c_n\,.$$

Thus if for some n,

$$\epsilon - 1 - 2n = 0$$

then all higher coefficients would vanish and the series would terminate.

This implies

$$\begin{aligned} \frac{2E_n}{\hbar\omega} &= \epsilon_n = 2n+1 \\ E_n &= \left(n + \frac{1}{2}\right)\hbar\omega\,. \end{aligned}$$

Therefore, only if the oscillator has the above energy values would physical solutions be allowed.

When a solution is allowed for each value of n, the solution becomes

$$\psi_n(\xi) = f_n(\xi)e^{-\frac{1}{2}\xi^2} \quad \text{where} \quad f_n(\xi) = \sum_{m=0}^{n} c_m \xi^m$$

with the coefficients satisfying the above recursion formula.

The Hermite equation

The function $f_n(\xi)$ satisfies the following differential equation

$$f_n''(\xi) - 2\xi f_n'(\xi) + 2n f_n(\xi) = 0 \quad \text{with} \quad \epsilon_n = 2n + 1\,.$$

- This is called the Hermite equation and the solution $f_n(\xi)$ are the nth Hermite polynomial represented as $H_n(\xi)$.
- Every Hermite polynomial is completely determined in terms of one arbitrary constant: c_0 or c_1 depending on whether n is even or odd.

The first few of the Hermite polynomials are

$$\begin{aligned} H_0(\xi) &= 1 \\ H_1(\xi) &= 2\xi \\ H_2(\xi) &= 4\xi^2 - 2 \\ H_3(\xi) &= 8\xi^3 - 12\xi \end{aligned}$$

and so on.

The Hermite polynomials have the following orthogonality relations

$$\int_{-\infty}^{\infty} H_m(\xi)H_n(\xi)e^{-\xi^2}\,d\xi = \begin{cases} 0\,, & \text{for } n \neq m, \text{ and} \\ \sqrt{\pi}2^n \cdot n!\,, & \text{for } n = m. \end{cases}$$

The harmonic oscillator wave function is written as

$$\psi_n(\xi) = A_n f_n(\xi)e^{-\frac{1}{2}\xi^2} = A_n H_n(\xi)e^{-\frac{1}{2}\xi^2}.$$

Thus the constant A_n can be determined from normalization.
Putting back

$$\xi = \left(\frac{m\omega}{\hbar}\right)^{1/2} x$$

we obtain

$$\psi_n(x) = A_n H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right] e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}\,.$$

Furthermore, we want

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = 1.$$

In terms of the ξ variables, this equation becomes

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{1}{\left(\frac{m\omega}{\hbar}\right)^{1/2}} |\psi_n(\xi)|^2 \, d\xi &= |A_n|^2 \left(\frac{\hbar}{m\omega}\right)^{1/2} \int_{-\infty}^{\infty} H_n(\xi)^2 e^{-\xi^2} \, d\xi \\
&= |A_n|^2 \left(\frac{\hbar}{m\omega}\right)^{1/2} \sqrt{\pi} 2^n \cdot n! \\
&= 1\,.
\end{aligned}$$

Choosing A_n to be real, we have

$$A_n = A_n^* = \left[\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \frac{1}{2^n \cdot n!}\right]^{1/2} .$$

Thus the normalized eigenfunctions for the oscillator are

$$\begin{aligned}\psi_n(x) &= A_n H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right] e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{(2^n \cdot n!)^{1/2}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}\,.\end{aligned}$$

And the wave function becomes

$$\Psi_n(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{(2^n \cdot n!)^{1/2}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} e^{-iE_n t/\hbar}$$

with

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega\,.$$

That is the same energy derived from the matrix operator formalism.

There are two most frequently used pictures in quantum mechanics.

A. The Schrödinger picture

(a) In the Schrödinger picture, the state vector $|\psi(t)\rangle$ is time dependent and operators are chosen to be time independent.

(b) The equation of motion for the state vector is

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle \,.$$

B. The Heisenberg picture

(a) In the Heisenberg picture, the operators (Ω) are time dependent and the state vector $|\Psi\rangle = |\Psi(0)\rangle$ is chosen to be time independent.

(b) The equation of motion for the operators are

$$i\hbar \frac{d}{dt}\Omega(t) = [\Omega, H] \quad \text{or} \quad \frac{d}{dt}\Omega(t) = -\frac{i}{\hbar}[\Omega, H] \,.$$

In both pictures H is the Hamiltonian operator.

In the energy basis of the Harmonic Oscillator, the state vectors are time independent. Hence it is the Heisenberg picture of motion where the operators have time dependence. For example,

$$i\hbar \frac{da}{dt} = [a, H] \quad \text{or} \quad \frac{da}{dt} = -\frac{i}{\hbar}[a, H] = -\frac{i}{\hbar}\hbar\omega a = -i\omega a\,.$$

Thus

$$a(t) = a(0)e^{-i\omega t}\,.$$

Furthermore,

$$i\hbar \frac{da^\dagger}{dt} = [a^\dagger, H] \quad \text{or} \quad \frac{da^\dagger}{dt} = -\frac{i}{\hbar}[a^\dagger, H] = -\frac{i}{\hbar}(-\hbar\omega a^\dagger) = i\omega a^\dagger\,.$$

Thus

$$a^\dagger(t) = a^\dagger(0)e^{i\omega t}\,.$$

We often express the annihilation and creation operators in terms of X and P operators and vice versa

$$
\begin{aligned}
a &= \sqrt{\frac{m\omega}{2\hbar}}\left(X + \frac{i}{m\omega}P\right) \quad \text{and} \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(X - \frac{i}{m\omega}P\right) ; \\
X &= \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \quad \text{and} \quad P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger) .
\end{aligned}
$$

Thus

$$
\begin{aligned}
X(t) &= \sqrt{\frac{\hbar}{2m\omega}}\left(a(0)e^{-i\omega t} + a^\dagger(0)e^{i\omega t}\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left[\left(a(0) + a^\dagger(0)\right)\cos(\omega t) - i\left(a(0) - a^\dagger(0)\right)\sin(\omega t)\right] \\
&= X_0\cos(\omega t) + \frac{1}{m\omega}P_0\sin(\omega t)
\end{aligned}
$$

and

$$
P(t) = P_0\cos(\omega t) - (m\omega)X_0\sin(\omega t) .
$$

In general therefore, in any picture we can write

$$\langle X \rangle_t = \langle X \rangle_0 \cos(\omega t) + \frac{1}{m\omega} \langle P \rangle_0 \sin(\omega t)$$

and

$$\langle P \rangle_t = \langle P \rangle_0 \cos(\omega t) - (m\omega) \langle X \rangle_0 \sin(\omega t) \,.$$

The energy of a quantum oscillator for the n-th eigenstate is

$$E_n = (n + \frac{1}{2}) \hbar \omega \,.$$

- The minimum of the energy is not zero.
- This arises basically because of the inability to simultaneously specify both the position as well as the momentum.

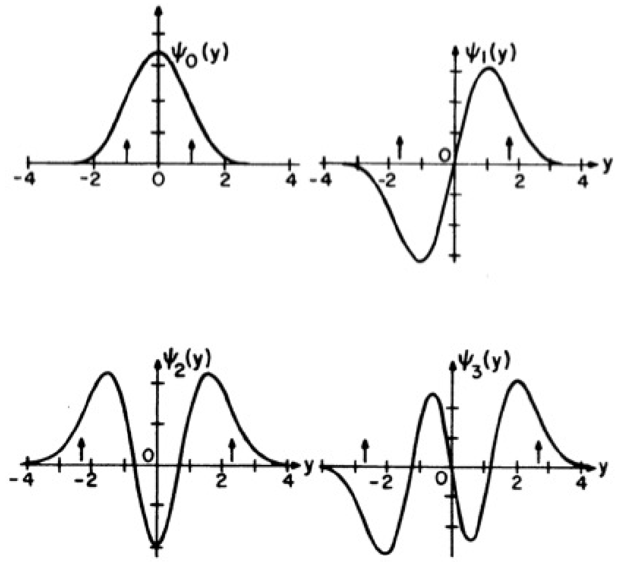

Figure 1: Normalized eigenfunctions versus $y = \xi = (m\omega/\hbar)^{1/2}x$.

If we plot the probability density for the oscillator in the ground state its maximum probability is around the point of equilibrium $(x = 0)$ and tails off at large distances. This is the opposite of classical prediction.

However, if we plot the probability for large values of the quantum number (n) the behavior is as follows:

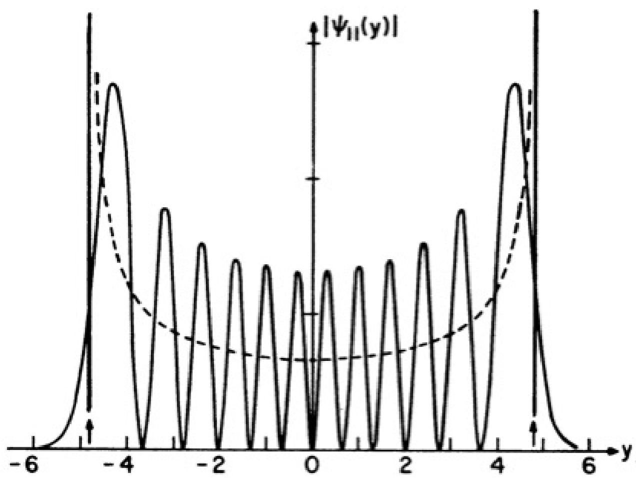

Figure 2: Probability density for $n = 11$ versus $y = \xi = (m\omega/\hbar)^{1/2}x$.

Thus as $n \to \infty$ the average of these plots behave like the classical oscillator. This is what the correspondence principle says, namely, when the energy becomes large the system must behave like a macroscopic system.