Lecture 7

Quantum Harmonic Oscillator

Study Goal of This Lecture

- Harmonic oscillator model

- Hamiltonian and its properties

- Operator method

7.1 Review of Harmonic Oscillator Model

We will continue our discussions on solving T.I.S.E. for simple quantum systems. The next is the quantum harmonic oscillator model. Physics of harmonic oscillator is taught even in high schools. There, the system is defined as a particle under the influence of a "linear" restoring force:

$$F = -k(x - x_0), \tag{7.1}$$

where k and x is force constant and equilibrium position respectively. Note potential is

$$V(x) = -\int F dx + C = \frac{1}{2}kx^2, \tag{7.2}$$

where C is the absolute potential but it is not important so we let it equals to zero. We are not going to discuss about classical harmonic oscillator in class because you should have been quite familiar with the classical problem, for a short review, see Silbey p.99. Instead, we will use the spare time that we have by avoiding going over the classical problem to discuss:

7.1.1   Why Harmonic Oscillator?

Why harmonic oscillator, before we jump into the calculation and derivation, we should ask ourself this question first. We mention two points here. (You should ask yourself and figure out too!)

First Point: A particle's motions around a stable point in arbitrary potential behave like a harmonic oscillator. (use 1-D H.O. for example)
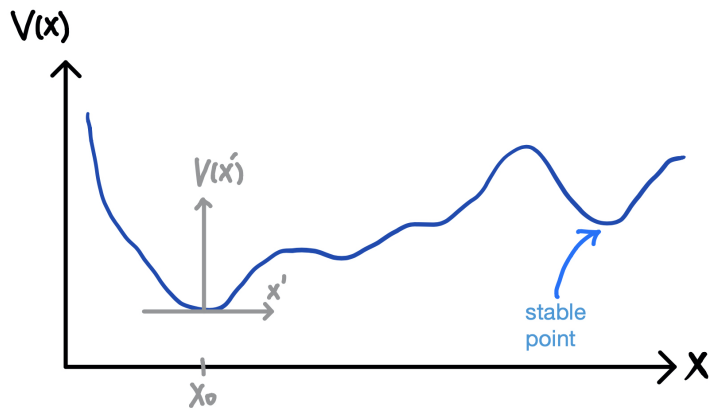

Figure 7.1: Arbitrary potential.

around these potential minima, $F = 0$, so

$$\frac{d}{dx}V(x)\bigg|_{x=x_0} = 0. \tag{7.3}$$

For motions around x_0, we perform Taylor's expansion around x_0

$$
\begin{aligned}
V(x - x_0) = V(x_0) &+ \frac{d}{dx}V(x)\bigg|_{x=x_0} \cdot (x - x_0) \\
&+ \frac{1}{2}\frac{d^2}{dx^2}V(x)\bigg|_{x=x_0}(x - x_0)^2 \\
&+ O((x - x_0)^3).
\end{aligned} \tag{7.4}
$$

Since we expand $V(x)$ around the stable point, the first derivative is zero, that is

$$V(x - x_0) \simeq V(x_0) + \frac{1}{2}\frac{d^2}{dx^2}V(x)\bigg|_{x=x_0}(x - x_0)^2. \tag{7.5}$$

The potential is equivalent to a harmonic form. The $V(x_0)$ term is a constant, absolute potential is irrelevant, we can chop it. Also, if we set $x = x - x_0$, this is the same to

$$V(x) = \frac{1}{2}kx^2, \ \text{with} \ k = \frac{d^2}{dx^2}V(x)\Big|_{x=x_0}. \tag{7.6}$$

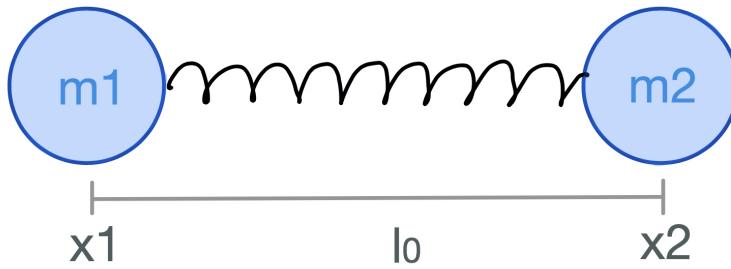**Second Point:** Diatomic molecules connected by a spring exhibit harmonic motion.

Figure 7.2: Diatomic molecule

The force:

$$F = -k(x_2 - x_1 - l_0) \equiv -k \cdot \Delta x, \tag{7.7}$$

m_1, m_2 subjected to opposing force with the same amplitude.

$$f_2 = m_2 a_2 = \begin{cases} m_2 \cdot \frac{d^2 x_2}{dt^2} & = -k(x_2 - x_1 - l_0), \\ m_1 \cdot \frac{d^2 x_1}{dt^2} & = k(x_2 - x_1 - l_0). \end{cases} \tag{7.8}$$

Substract one of the above two equations by the others.

$$\frac{d^2(x_2 - x_1)}{dt^2} = -\frac{k}{m_2}(x_2 - x_1 - l_0) - \frac{k}{m_1}(x_2 - x_1 - l_0), \tag{7.9}$$

$$\therefore \frac{d^2(x_2 - x_1 - l_0)}{dt^2} = -k(\frac{1}{m_2} + \frac{1}{m_1}) \cdot (x_2 - x_1 - l_0). \tag{7.10}$$

Define reduced mass $\mu = \frac{m_1 m_2}{m_1 + m_2}$ and $x = x_2 - x_1 - l_0$. x here is the deviation to the equilibrium position.

$$\frac{d^2 x}{dt^2} - k \cdot \frac{1}{\mu} \cdot x, \tag{7.11}$$

$$\mu a = F = -kx. \tag{7.12}$$

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This is harmonic form!

Note that the change of variable reduces the two-body problem to two one body problems.

- relative motion: vibration

- center of mass motion: translation

In fact, for a polyatomic, non-linear molecule with N atoms, there will be 3 transla- For a molecule with N tional, 3 rotational and $3N - 6$ vibrations degree of freedom. atom, there is $3N$ degree of freedom.

7.2   Quantum harmonic oscillator

7.2.1   Hamiltonian of quantum harmonic oscillator

Given the classical Hamiltonian(total energy) of a particle in a harmonic potentail:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(x). \tag{7.13}$$

Note that

$$\hat{V}(x) = \frac{1}{2}kx^2 = \frac{1}{2}\mu\omega^2 x^2 = 2\pi^2\nu^2\mu x^2, \tag{7.14}$$

$$\omega = \sqrt{\frac{k}{\mu}} : \text{angular frequency},$$

$$\nu = \frac{\omega}{2\pi} : \text{ frequency}.$$

We will use the more convenient "ω" version, so

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}\mu\omega^2\hat{x}^2. \tag{7.15}$$

According to the quantum-classical correspondance principle,

$$x \to x\cdot, \quad p \to -i\hbar\frac{d}{dx},$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2. \tag{7.16}$$

The T.I.S.E. $\hat{H}\psi(x) = E\psi(x)$:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 \right]\psi(x) = E\psi(x). \tag{7.17}$$

This is a second-order differential equation and it can be solved by using the power-series method. The process is detailed in Levine Sec.4.2 . In Silbey's textbook, the solution are given. It will be an interesting practice to solve the differential equation once in your lifetime, but we will not go that here.

We will, instead, solve this using "physics" in section 3 of this lecture. We will show that by inspecting the properties of the Hamiltonina operator, the eigenvalue problem can be solved. (logic is new, so be patient.) Below, we firstly show the solution of this T.I.S.E. directly and focus on its properties.

7.2.2   Solution of Quantum Harmonic Oscillator

With the boundary condition $\psi(x) = 0$ when $x \rightarrow \pm\infty$, it turns out that the harmonic oscillator has energy levels given by

$$E_n = (n + \frac{1}{2})h\nu = (n + \frac{1}{2})\hbar\omega \quad \text{with } n = 0, 1, 2, \cdots, \tag{7.18}$$

where n is the vibrational quantum number and $\omega = \sqrt{\frac{k}{\nu}}$. Note that the energy level are equally spaced and the zero-point energy $E_0 = \frac{1}{2}\hbar\omega$.
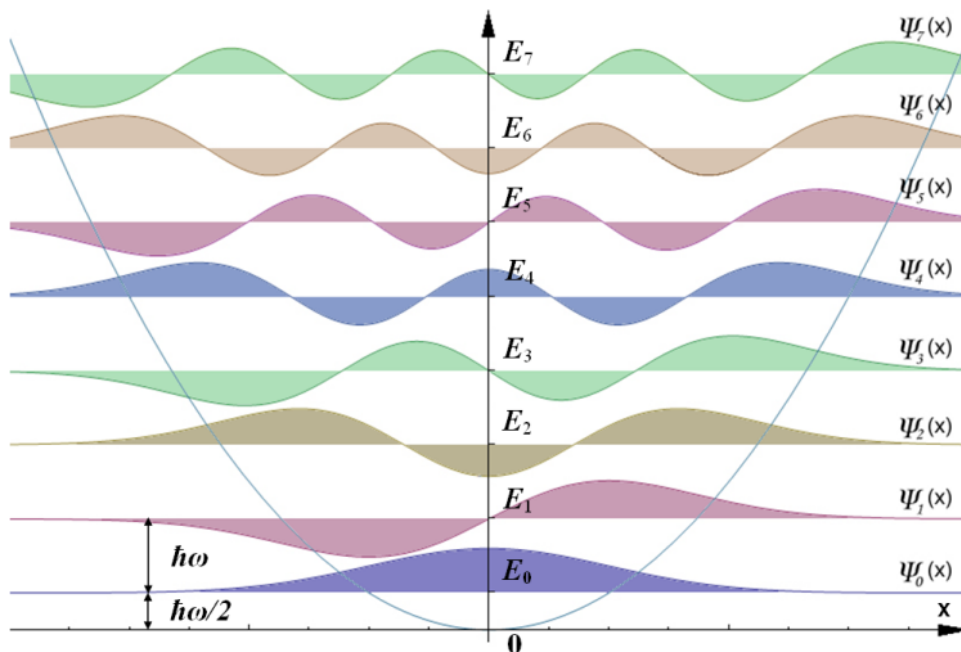

Figure 7.3: Wavefunctions of a quantum harmonic oscillator. Figure's author: AllenMcC.

The eigenfunctions are:

$$\psi_n(x) = N_n H_n(\alpha^{\frac{1}{2}} x) e^{-\alpha \frac{x^2}{2}}, \tag{7.19}$$

where

$$\alpha = \sqrt{\frac{h\mu}{\hbar^2}} = \frac{\mu\omega}{\hbar},$$

and the normalization constant

$$N_n = \frac{1}{(2^n \cdot n!)^{\frac{1}{2}}} \cdot (\frac{\alpha}{\pi})^{\frac{1}{4}}. \tag{7.20}$$

H_n are the Hermite polynomials:

$$H_n(x) = (-1)^{-n} e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}), \ n \geq 0. \tag{7.21}$$

The first few terms are:

$$H_0(x) = 1,$$
$$H_1(x) = 2x,$$
$$H_2(x) = 4x^2 - 2,$$
$$H_3(x) = 8x^3 - 12x.$$

The ground state is a "Gaussian" function

$$\psi_0(x) = (\frac{\alpha}{\pi})^{\frac{1}{4}} e^{-\frac{\alpha x^2}{2}}, \tag{7.22}$$

and the first excited state:

$$\psi_1(x) = (\frac{4\alpha^3}{\pi})^{\frac{1}{4}} x e^{\frac{-\alpha x^2}{2}}. \tag{7.23}$$

Note that similar to the particle in a finite depth well, these wavefunction also extended to the classical forbidden region. For example, the ground state:

$$E_0 = \frac{1}{2}\hbar\omega \geq \frac{1}{2}\mu\omega^2 x^2, \tag{7.24}$$

$$\therefore -\sqrt{\frac{\hbar}{\mu\omega}} \geq x \geq \sqrt{\frac{\hbar}{\mu\omega}}.$$

The probability of finding the particle at the groundstate within this classical limits is

$$P = \int_{-\sqrt{\frac{1}{\alpha}}}^{\sqrt{\frac{1}{\alpha}}} (\frac{\alpha}{\hbar})^{\frac{1}{4}} e^{-\frac{\alpha x^2}{2}} (\frac{\alpha}{\hbar})^{\frac{1}{4}} e^{-\frac{\alpha x^2}{2}} dx = (\frac{\alpha}{\hbar})^{\frac{1}{2}} \int_{-\sqrt{\frac{1}{\alpha}}}^{\sqrt{\frac{1}{\alpha}}} e^{-\alpha x^2} dx. \tag{7.25}$$

Using numerical integration we find $P \simeq 0.84$ which means that a significant fraction of the particle probability density is outside the classical region $\Rightarrow$ tunneling!!

Also note that the eigenfunctions have well defined "parity": we define for function

$$f(x) = f(-x) \Leftarrow \text{even functions,}$$
$$f(x) = -f(-x) \Leftarrow \text{odd functions.}$$
(7.26)

Note that $\cos(x)$ and e^{-x^2} are even and $\sin(x)$ and x are odd. If $f(x)$ is even and $g(x)$ is odd, then

$$f(x) \cdot f(x) : \text{even,}$$
$$g(x) \cdot g(x) : \text{even,}$$
$$f(x) \cdot g(x) : \text{odd,}$$
$$f'(x) : \text{odd,}$$
$$g'(x) : \text{even.}$$
(7.27)

This is useful for integration because by symmetry, the integration of the odd function is zero.

Now we go back to the eigenfunction of quantum harmonic oscillator:

$$\psi_n(x) \text{ is even for } n = 0, 2, 4, 6, \cdots,$$
$$\psi_n(x) \text{ is odd for } n = 1, 3, 5, 7, \cdots.$$
(7.28)

This is useful when evaluating integrals.(Which will be discussed in the next lecture.)

7.2.3 Properties of Hermite polynomials

Let's go back to discuss more about Hermite polynomials. The Hermite polynomials have some useful relations:

1. Orthonormality relation:

$$\frac{1}{(2^n n!)^{\frac{1}{2}}} \left(\frac{1}{\pi}\right)^{\frac{1}{4}} \frac{1}{(2^{n'} n'!)^{\frac{1}{2}}} \left(\frac{1}{\pi}\right)^{\frac{1}{4}} \int_\infty^\infty e^{-\frac{x^2}{2}} H_n e^{-\frac{x^2}{2}} H_{n'} dx = \delta_{n,n'}.$$
(7.29)

2. Recurrence relation:

$$xH_n = nH_{n-1} + \frac{1}{2}H_{n+1}, \ H_n = 0 \text{ for } n < 0.$$
(7.30)

3. Differential relation:
$$\frac{dH_n}{dx} = 2nH_{n-1}, \quad \frac{dH_0}{dx} = 0. \tag{7.31}$$

Note that these three rules are all we need for the evaluation of expectation value. The orthonormality relation can be used to easily proof that eigenfunctions of harmonic oscillator are orthonormal to each other.

Proof.
$$\psi_n(x) = \frac{1}{(2^n n!)^{\frac{1}{2}}} (\frac{\alpha}{\pi})^{\frac{1}{4}} H_n(\alpha^{\frac{1}{2}} x) e^{\frac{-\alpha x^2}{2}}.$$

the inner product of arbitrary two wavefunctions:
$$\int_{-\infty}^{\infty} \psi_n^*(x) \psi_m(x) dx,$$

define $y = \alpha^{\frac{1}{2}} x$, $dy = \alpha^{\frac{1}{2}} dx$ and then plug in the integral, yield the same equation as Equ(7.29) $\Rightarrow$ orthonormal! $\qquad\square$

The recurrence relation can be used to evaluate anything related to x.
e.g. $\langle x^2 \rangle$ of ground state:
$$\langle x^2 \rangle = (\frac{\alpha}{\pi})^{\frac{1}{2}} \int_{-\infty}^{\infty} H_0(\alpha^{\frac{1}{2}} x) e^{\frac{-\alpha x^2}{2}} x^2 H_0(\alpha^{\frac{1}{2}} x) e^{\frac{-\alpha x^2}{2}} dx. \tag{7.32}$$

Let $y = \alpha^{\frac{1}{2}} x$, $dy = \alpha^{\frac{1}{2}} dx$, we rewrite the above formula as:
$$\begin{aligned}
\langle x^2 \rangle &= (\frac{\alpha}{\pi})^{\frac{1}{2}} (\frac{1}{\alpha^{\frac{1}{2}}}) \int_{-\infty}^{\infty} e^{-y^2} H_0(y) \frac{y^2}{\alpha} H_0(y) dy \\
&= \frac{1}{\alpha} (\frac{1}{\pi})^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-y^2} H_0(y) [y^2 H_0(y)] dy \\
&= \frac{1}{\alpha} (\frac{1}{\pi})^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-y^2} H_0(y) [\frac{1}{2} H_0(y) + \frac{1}{4} H_2(y)] dy \qquad (7.33)\\
&= \frac{1}{2} \frac{1}{\alpha} (\frac{1}{\pi})^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-y^2} H_0(y) H_0(y) dy \\
&= \frac{1}{2} \frac{1}{\alpha} = \frac{\hbar}{2\mu\omega}.
\end{aligned}$$

Generally, we obtain:
$$\langle x^2 \rangle_n = \frac{1}{\alpha} (n + \frac{1}{2}). \tag{7.34}$$

Similarily, one can use differential relation to evaluate
$$\langle p^2 \rangle = \frac{\hbar^2 \alpha}{2} = \frac{\hbar^2}{2} \frac{\mu\omega}{\hbar} = \frac{\hbar\mu\omega}{2}. \tag{7.35}$$

By symmetry, $\langle x \rangle = 0$, $\langle p \rangle = 0$,

$$\therefore \Delta x = \sqrt{\frac{\hbar}{2\mu\omega}}, \ \Delta p = \sqrt{\frac{\hbar\mu\omega}{2}}, \ \Delta x \Delta p = \frac{\hbar}{2}.$$

We found that the ground state of harmonic oscillator has minimal uncertainty allowed by Heisenberg uncertainty principle!!

7.3 Operator Approach for Solving Quantum Harmonic Oscillator

7.3.1 Operator Adjoints

Before we start, we review the mathematics of operator adjoint:

Given an operator $\hat{A}$, we define the Hermitian adjoint, denotes as $\hat{A}^\dagger$, as the operator satisfy the following equation:

$$\int_{-\infty}^{\infty} (\hat{A}^\dagger \phi(x))^* \psi(x) dx = \int_{-\infty}^{\infty} \phi(x)^* \hat{A}\psi(x) dx \tag{7.36}$$

Actually, we have seen this before, Hermitian operator are operator that are their own adjoints: If $\hat{A}^\dagger = \hat{A}$, the $\hat{A}$ is Hermitian. Quantum observables are Hermitian operators $\Rightarrow$ eigenvalues are real.

$$\Rightarrow \hat{x}^\dagger = \hat{x}, \ \hat{p}^\dagger = \hat{p}, \ \hat{H}^\dagger = \hat{H}$$

For non-Hermitian operators, $\hat{A}^\dagger \neq \hat{A}$. There are a few useful properties of operator ajoints:

1. $(A + B)^\dagger = A^\dagger + B^\dagger$

2. $(\lambda A)^\dagger = \lambda^* A^\dagger$, where λ is a complex number

   Proof.

   $$\because \lambda \int (\hat{A}^\dagger \phi)^* \psi dx = \lambda \int \phi^* \hat{A}\psi dx \Rightarrow \int (\lambda^* \hat{A}^\dagger \phi)^* \psi dx = \int \phi^* \lambda \hat{A}\psi dx \tag{7.37}$$

   $\square$

3. $(\hat{A}^\dagger)^\dagger = \hat{A}$

4. $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$

5. $[\int \phi^* \hat{A}\psi dx]^* = \int \psi^* \hat{A}^\dagger \phi dx$

Now we are ready to solve the quantum harmonic oscillator model. The following is the operator method in Quantum Mechanics, Cohen-Tanoudji, Chapter 5. Let's consider the quantum harmonic oscillator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2. \tag{7.38}$$

The Hamiltonian has a quadratic form, and the expecatation value of $\hat{p}^2$ and $\hat{x}^2$ must be greater than zero. We notice that the total energy must be positive or zero:

$$\hat{H}\psi = E\psi, \ E \geq 0. \tag{7.39}$$

Let's rewrite the Hamiltonian for convenience:

$$\hat{H} = \hbar\omega[\ \frac{\hat{p}^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar}\hat{x}^2\ ]$$
$$= \frac{1}{2}\hbar\omega[\hat{P}^2 + \hat{X}^2], \tag{7.40}$$
$$\text{where } \hat{X} = \sqrt{\frac{m\omega}{\hbar}} \cdot \hat{x} \text{ and } \hat{P} = \sqrt{\frac{1}{m\hbar\omega}} \cdot \hat{p}.$$

Now in algebra one clearly will try to rewrite $a^2 + b^2 = (a - ib)(a + ib)$. For operators, this is not quite the same, but we will do similar thing. So, let's define:

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}) = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega}{\hbar}}\hat{x} + i\sqrt{\frac{1}{m\hbar\omega}}\hat{p}), \tag{7.41}$$

$\hat{X}$ and $\hat{P}$ are unitless position and momentum operators respectively.

so

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{X} - i\hat{P}) = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega}{\hbar}}\hat{x} - i\sqrt{\frac{1}{m\hbar\omega}}\hat{p}). \tag{7.42}$$

Since $\hat{x}^\dagger = \hat{x}$ and $\hat{p}^\dagger = \hat{p}$, $\hat{a}$ and $\hat{a}^\dagger$ are adjoints. So

$$\hat{a}^\dagger \hat{a} = \frac{1}{2}(\hat{X} - i\hat{P})(\hat{X} + i\hat{P})$$
$$= \frac{1}{2}(\hat{X}^2 + \hat{P}^2 - i\hat{P}\hat{X} + i\hat{X}\hat{P}) \tag{7.43}$$
$$= \frac{1}{2}(\hat{X}^2 + \hat{P}^2) + \frac{i}{2}[\hat{X}, \hat{P}].$$

What is $[\hat{x}, \hat{p}]$? We can calculate this from the canonical commutator relation in quantum mechanics.

$$[\hat{x}, \hat{p}] = i\hbar \quad \Rightarrow \quad [\hat{X}, \hat{P}] = i,$$

$$\hat{a}^\dagger \hat{a} = \frac{1}{2}(\hat{X}^2 + \hat{P}^2) - \frac{1}{2},$$

$$\therefore \hat{H} = \hbar\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2}).$$

The Hamiltonian can be conveniently rewritten by using $\hat{a}^\dagger \hat{a}$. We define

$$\hat{N} = \hat{a}^\dagger \hat{a}, \tag{7.44}$$

$\hat{N}$ is the "number operator", for reasons that will be clear soon. We notice a few important properties of $\hat{N}$:

1. N is Hermitian, $\hat{N}^\dagger = (\hat{a}^\dagger \hat{a})^\dagger = \hat{a}^\dagger \hat{a} = \hat{N}$.

2. $[\hat{H}, \hat{N}] = 0$, so $\hat{H}$ and $\hat{N}$ share the same eigenfunctions. We then convert solving T.I.S.E. into solving eigenvalues and eigenfunctions of $\hat{N}$. We want to solve

$$\hat{N}\psi_n = n\psi_n \text{ with } \int \psi_n^* \psi_m dx = \delta_{nm} \tag{7.45}$$

   and n is real!!

3. Eigenvalues of $\hat{N}$ is zero or positive, i.e. $n \geq 0$. This is because $\hat{N} = \hat{a}^\dagger \hat{a}$, given any eigenfunction ψ_n, we obtain

$$\int \psi_n^* \hat{N} \psi_n d\tau = \int \psi_n^* n \psi_n d\tau = n \cdot \int \psi_n^* \psi_n d\tau = n \tag{7.46}$$

   However,

$$\int \psi_n^* \hat{N} \psi_n d\tau = \int \psi_n^* \hat{a}^\dagger \hat{a} \psi_n d\tau$$

$$= \int (\hat{a}\psi_n)^* (\hat{a}\psi_n) d\tau \tag{7.47}$$

$$= \int |\hat{a}\psi_n|^2 d\tau \geq 0$$

   $\therefore n \geq 0$. n can't be negative.

4. If $n = 0$ (i.e. eigenvalue $= 0$), then $\hat{a}\psi_{n=0} = 0$ This follow directly from point 3

$$\int |\hat{a}\psi_n|^2 d\tau = 0 \text{ if and only if } \hat{a}\psi_{n=0}. \tag{7.48}$$

5. If $n > 0$, and $\hat{N}\psi_n = n\psi_n$. Then $a\psi_n$ is an eigenfunction of $\hat{N}$ with eigenvalue $n - 1$. To prove this we will need a few more commutator relations:

Given $[\hat{X}, \hat{P}] = i$.

$$\text{i. } [\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = -i[\hat{X}, \hat{P}] = 1 \tag{7.49}$$

$$\text{ii. } [\hat{a}, \hat{a}^\dagger] = 1 \Rightarrow \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1, \ \hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1 \tag{7.50}$$

$$\begin{aligned} \text{iii. } [\hat{N}, \hat{a}] = [\hat{a}^\dagger\hat{a}, \hat{a}] &= \hat{a}^\dagger\hat{a}\hat{a} - \hat{a}\hat{a}^\dagger\hat{a} \\ &= \hat{a}^\dagger\hat{a}\hat{a} - (\hat{a}^\dagger\hat{a} + 1)\hat{a} \\ &= \hat{a}^\dagger\hat{a}\hat{a} - \hat{a}^\dagger\hat{a}\hat{a} - \hat{a} = -\hat{a} \end{aligned} \tag{7.51}$$

$$\begin{aligned} \text{iv. } [\hat{N}, \hat{a}^\dagger] = [\hat{a}^\dagger\hat{a}] &= \hat{a}^\dagger\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}^\dagger\hat{a} \\ &= \hat{a}^\dagger(\hat{a}^\dagger\hat{a} + 1) - \hat{a}^\dagger\hat{a}^\dagger\hat{a} \\ &= \hat{a}^\dagger \end{aligned} \tag{7.52}$$

To show that $\hat{a}\psi_n$ is an eigenfunction of $\hat{N}$, we operate $\hat{N}$ onto $\hat{a}\psi_n$.

$$\begin{aligned} \hat{N}\hat{a}\psi_n = \hat{a}^\dagger\hat{a}\hat{a}\psi_n &= (\hat{a}\hat{a}^\dagger - 1)\hat{a}\psi_n \\ &= \hat{a}\hat{a}^\dagger\hat{a}\psi_n - \hat{a}\psi_n \\ &= (n - 1)\hat{a}\psi_n. \end{aligned} \tag{7.53}$$

So $\hat{a}\psi_n$ is an eigenfunction of $\hat{N}$ with the eigenvalue $(n - 1) \Rightarrow \hat{N}\psi_{n-1} = (n - 1) \cdot \psi_{n-1}$ That is, $\hat{a}\psi_n = c \cdot \psi_{n-1}$. We can calculate c using normalization condition. If ψ_n is normalized, then

$$\int \psi_n^* \hat{a}^\dagger\hat{a}\psi_n d\tau = \int |\hat{a}\psi_n|^2 d\tau = |c|^2 \int |\psi_n|^2 d\tau = |c|^2, \tag{7.54}$$

also

$$\int \psi_n^* \hat{a}^\dagger\hat{a}\psi_n d\tau = n \cdot \int \psi_n^* \psi_n d\tau = n, \tag{7.55}$$

therefore $|c|^2 = n$, and we choose the positive solution $c = \sqrt{n}$.

To now, we already obtain:

$$\hat{a}\psi_n = \sqrt{n}\psi_{n-1}. \tag{7.56}$$

Simlarly, one can show that

$$\hat{a}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}. \tag{7.57}$$

Check:

$$\hat{a}^\dagger \hat{a} \psi_n = \hat{a}(\sqrt{\psi}_{n-1}) = \sqrt{n}\hat{a}^\dagger \psi_{n-1} = n\psi_n, \tag{7.58}$$

we get a consistent result! So, eigenstate of $\hat{N}$ are quantized/discrete, and $\hat{a}^\dagger$(or $\hat{a}$) can raise(lower) the eigenstates. They are "ladder operators".

$$\hat{a} : \text{ lowering/annihilation operator,}$$

$$\hat{a}^\dagger : \text{ raising/creation operator.}$$

6. n are zero or positive integers. At this point we have not determine the values of n. We just know $\hat{a}$ and $\hat{a}^\dagger$ can allow us to create a different eigenstate from a "known" eigenstate. How do we determine the quantization condition for n? It's logical that we need a closure condition. If n is not an integer, then for

$$\hat{a}\psi_n = \sqrt{n}\psi_{n-1}, \tag{7.59}$$

let's say n is between two consecutive integers

$$j < n < j+1,$$

then $(\hat{a})^{j+1}\psi_n = \sqrt{n}\sqrt{n-1}\cdots\sqrt{n-j}\psi_{n-j-1}$. But $n - j - 1 < 0$, we will obtain negative eigenvalue for $\hat{N}$, this must be avoided!

If n is a positive integer

$$(\hat{a})^n\psi_n = \sqrt{n}\sqrt{n-1}\sqrt{n-2}\cdots\sqrt{1}\psi_0, \tag{7.60}$$

then $\hat{a}\psi_0 = 0$, $\psi_0 = 0$, it can't get lower! So the eigenvalues of $\hat{N}$ is determined:

$$\hat{N}\psi_n = n\psi_n, \ n = 0, 1, 2, 3, \cdots, \infty. \tag{7.61}$$

Then $\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$,

$$\hat{H}\psi_n = E_n\psi_n, \ E_n = (n + \frac{1}{2})\hbar\omega, \ n = 0, 1, 2, \cdots, \infty. \tag{7.62}$$

7. How about eigenfunctions ? start from $\hat{a}\psi_0 = 0$. Since,

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}) = \frac{1}{\sqrt{2}}[\sqrt{\frac{m\omega}{\hbar}}\hat{x} + i \cdot \sqrt{\frac{1}{m\hbar\omega}}\hat{p}]$$
$$= \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega}{\hbar}}x \cdot + \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\cdot), \tag{7.63}$$

and

$$\hat{a}\psi_0(x) = 0, \tag{7.64}$$

$$\Rightarrow (\frac{m\omega}{\hbar}x + \frac{d}{dx})\psi_0(x) = 0. \tag{7.65}$$

This first order differential equation can be solve to find $\psi_0(x)$, the ground state wavefunction!

Let's see

$$\frac{d}{dx}\psi_0(x) = -\frac{m\omega}{\hbar}x\psi_0(x). \tag{7.66}$$

Take the derivative of $\psi_0(x)$ yields $x \cdot \psi_0(x)$. What is $\psi_0(x)$? A Gaussian function!

$$\begin{aligned}\psi_0(x) &= C_0 \cdot e^{-\frac{\alpha x^2}{2}} \\ &= C_0 \cdot e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}.\end{aligned} \tag{7.67}$$

How to determine C_0? By normalization condition again:

$$\int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = 1 \quad \Rightarrow \quad C_0 = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}. \tag{7.68}$$

Here we come the ground state wavefunction of quantum harmonic oscillator and it is indeed a Gaussian function!

$$\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}e^{\frac{m\omega}{2\hbar}x^2}. \tag{7.69}$$

8. How to determine the excited state? $\rightarrow$ by ladder operators

$$\begin{aligned}\hat{a}^\dagger\psi_0(x) &= \sqrt{1}\psi_1(x), \\ \hat{a}^\dagger\psi_1(x) &= \sqrt{2}\psi_2(x), \\ &\cdots\end{aligned} \tag{7.70}$$

For instance

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}),$$

then to obtain first excited state wavefunction

$$\begin{aligned}\psi_1(x) &= \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx})(\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}e^{\frac{m\omega}{2\hbar}x^2} \\ &= \frac{1}{\sqrt{2}}(\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}(\sqrt{\frac{m\omega}{\hbar}}x + \sqrt{\frac{m\omega}{\hbar}}x)e^{\frac{m\omega}{2\hbar}x^2} \\ &= (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}(\frac{m\omega}{\hbar})^{\frac{1}{2}}\sqrt{2}xe^{\frac{m\omega}{2\hbar}x^2}.\end{aligned} \tag{7.71}$$

All eigenfunctions can be found in this way. Actually, we do not need to know these functions. All expectation values can be calculated from the algebra of $\hat{a}$ and $\hat{a}^\dagger$!

9. Since the ground state is non-degenerate and the creation operator $\hat{a}^\dagger$ is single valued. All eigenstate of the 1-D quatnum harmonic oscillator model is non-degenerate.

10. The wavefunctions and the corresponding probability density are ploted below. We can easily find that the energy is equal spaced and the zero point energy of quantum harmonic oscillator is $\frac{1}{2}\hbar\omega$.
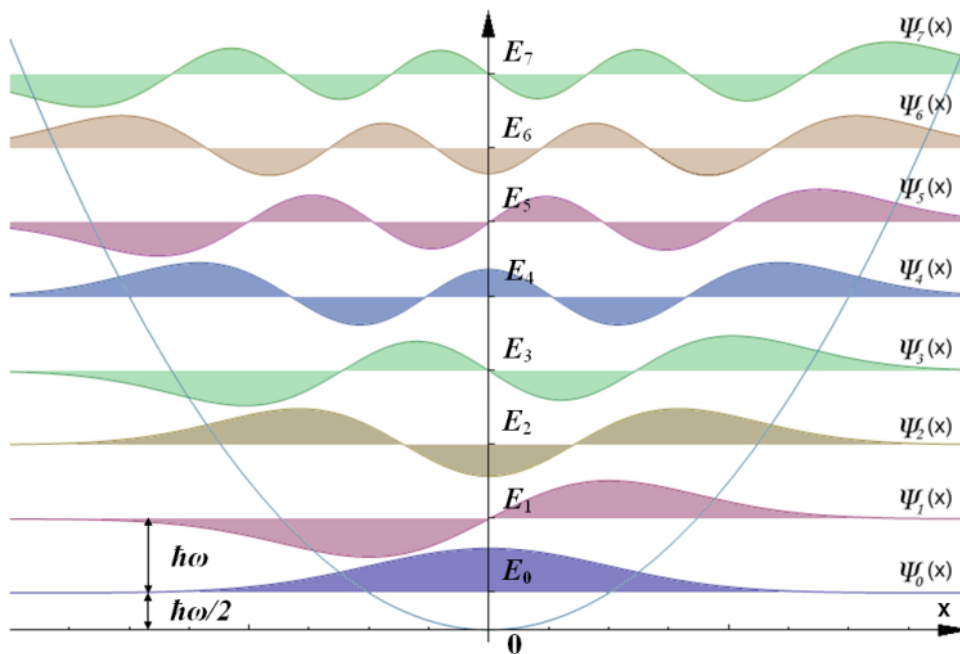

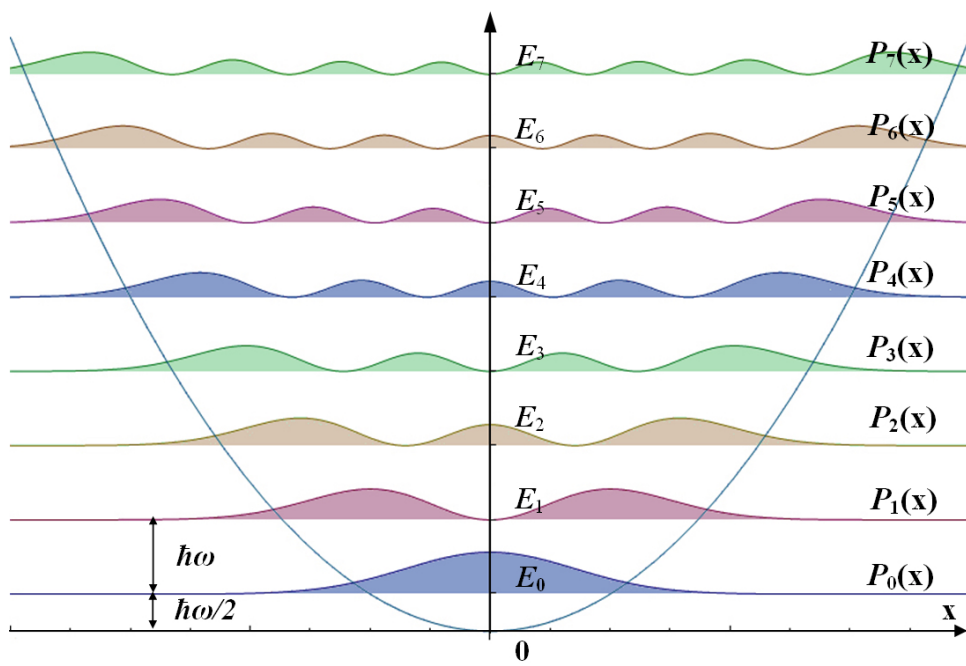Figure 7.4: Wavefunctions of a quantum harmonic oscillator. Figure's author: AllenMcC.

Figure 7.5: Probability density of quantum harmonic oscillator.