Physics 438A – Lecture #7
Quantum Harmonic Oscillator

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Introduction

The harmonic oscillator plays a central role in quantum mechanics and appears, in one form or another, across nearly every area of physics. In atomic and molecular physics, the harmonic oscillator describes small oscillations of atoms about equilibrium configurations, governing vibrational spectra and setting the energy scales relevant for infrared absorption and emission. In condensed matter physics, collective excitations such as lattice vibrations (phonons) and charge-density fluctuations can be modeled as quantized harmonic oscillators, providing the foundation for understanding thermal properties, electrical transport, and superconductivity. Similarly, electromagnetic modes in cavities and waveguides are described by harmonic oscillators, a fact that underlies much of quantum optics and quantum information science.

The harmonic oscillator also appears naturally in modern experimental platforms. The motion of trapped ions and neutral atoms in optical traps is well approximated by harmonic potentials, making the oscillator an essential ingredient in precision metrology and quantum simulation. In superconducting circuits, effective harmonic oscillator modes form the starting point for the design of qubits and resonators used in quantum computing. Even in high-energy physics and quantum field theory, each mode of a free field behaves as an independent harmonic oscillator, with particle excitations emerging from the quantization of these modes.

In many of these contexts the harmonic oscillator description is only approximate, but it provides a controlled starting point for systematic improvements. Perturbation theory, semiclassical methods, and numerical techniques often rely on the harmonic oscillator as a reference system around which more realistic interactions are introduced. For this reason, a thorough understanding of the quantum harmonic oscillator is indispensable, both as an exactly solvable model and as a conceptual framework that extends far beyond the specific system it was originally introduced to describe. In these notes we focus primarily on the quantum mechanics of a single harmonic oscillator.

1 The Classical Harmonic Oscillator

A particle of mass m, constrained to move along the x axis, is interacting with some larger system that is essentially fixed. The force of interaction is conservative, and the system is in stable equilibrium at the point $x = 0$. For small displacements, $|x| \ll 1$, and we can Taylor expand the potential energy function about the equilibrium point:

$$V(x) = V(0) + \left(\frac{dV}{dx}\bigg|_{x=0}\right) x + \frac{1}{2}\left(\frac{d^2V}{dx^2}\bigg|_{x=0}\right) x^2 + O(x^3)$$

The leading term is quadratic because $V(0)$ can be defined to be zero without loss of generality and the linear term is zero because the first derivative of the potential energy function vanishes at an equilibrium point. Furthermore, since the equilibrium point is stable,

$$k \equiv \frac{d^2V}{dx^2}\bigg|_{x=0} > 0$$

By Newton's second law,

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

where the net force is $F = -dV/dx$. We can rewrite the equation of motion as

$$\frac{d^2x}{dt^2} + \omega^2 x = 0$$

which describes a simple harmonic oscillator with angular frequency $\omega = \sqrt{k/m}$. One valid way to write the solution to this differential equation is

$$x(t) = A\cos(\omega t + \phi)$$

where the amplitude of oscillations A and the phase constant ϕ are both determined by initial conditions. A prototypical example would be a simple mass-on-spring system.

In this situation, the total energy of the particle is conserved and corresponds to the system's classical Hamiltonian (covered in PHYS 304). The total energy is

$$H = T + V = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$$

and since $p = mv$ and $k = m\omega^2$,

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

2 Quantum Harmonic Oscillator

We define the 1D quantum harmonic oscillator by the Hamiltonian

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

where $x \to \hat{x}$ and $p_x \to \hat{p}_x$ are "promoted" to operators. This procedure–constructing a quantum Hamiltonian by replacing classical observables with operators–is known as **canonical quantization**. It should be emphasized that quantization is not a well-defined procedure: there is no general algorithm that takes a classical system and produces its quantum counterpart without ambiguity. Canonical quantization is a physically motivated heuristic that works remarkably well for simple systems like the harmonic oscillator, while more complicated systems often require additional principles or more sophisticated arguments.

The goal for this section is to find the energy eigenstates of the Hamiltonian, i.e. to find the states $|E\rangle$ such that $H|E\rangle = E|E\rangle$, where $E > 0$ (the minimum of the potential energy function) to have normalizable wave functions. This lower bound on the energy eigenvalues is our cue to find ladder operators similar to our treatment of angular momentum in lecture #4. Before we get started, the presentation will be much cleaner if we use dimensionless variables. Since $\hbar\omega$ has units of energy, we can write the Hamiltonian as

$$H = \frac{\hbar\omega}{2}\left(\frac{\hat{p}_x^2}{m\hbar\omega} + \frac{\hat{x}^2}{\hbar/m\omega}\right)$$

The quantity in parentheses must be dimensionless, so we can redefine units such that

$$[\text{energy}] = \hbar\omega, \qquad [\text{momentum}] = \sqrt{m\hbar\omega}, \qquad [\text{length}] = \sqrt{\hbar/m\omega}$$

In these units, the Hamiltonian becomes

$$H = \frac{1}{2}\left(\hat{p}_x^2 + \hat{x}^2\right),$$

which is the same as if we simply set $m = \omega = \hbar = 1$. Likewise, the commutator between $\hat{x}$ and $\hat{p}_x$ is now given by $[\hat{x}, \hat{p}_x] = i$. Notice the *classical Hamiltonian* can be easily factored as

$$H = \frac{1}{2}(x - ip_x)(x + ip_x)$$

since x and p_x "commute" in classical mechanics. Applying the same factorization to the

quantum operators, we find

$$\frac{1}{2}(\hat{x} - i\hat{p}_x)(\hat{x} + i\hat{p}_x) = \frac{1}{2}\left(\hat{x}^2 + \hat{p}_x^2 + i[\hat{x}, \hat{p}_x]\right) = H - \frac{1}{2}$$

Hence, due to the non-commutativity of the position and momentum operators,

$$H = \frac{1}{2}(\hat{x} - i\hat{p}_x)(\hat{x} + i\hat{p}_x) + \frac{1}{2}$$

We now define the operator a, called the "lowering operator," such that

$$a = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}_x)$$

and its Hermitian conjugate, $a^\dagger$, is the "raising operator" given by

$$a^\dagger = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p}_x)$$

Together, a and $a^\dagger$ are called *ladder operators* for reasons that will be clear very soon. They have the commutation relation

$$[a, a^\dagger] = 1$$

which follows from $[\hat{x}, \hat{p}_x] = i$. The dimensionless Hamiltonian can be written as

$$H = a^\dagger a + \tfrac{1}{2} = N + \tfrac{1}{2}$$

where $N = a^\dagger a$ is the "number operator." Let $|n\rangle$ be a normalized eigenvector of N with eigenvalue n, i.e. $N|n\rangle = n|n\rangle$. Given that H and N commute, it follows that $|n\rangle$ is also an eigenvector of H. Since N is Hermitian, we know that n must be real. Also, we can use properties of the inner product to demonstrate that n must be positive:

$$n = \langle n|N|n\rangle = \|a|n\rangle\|^2 \geq 0$$

The number operator has following commutation relations:

$$[N, a] = -a, \quad \text{and} \quad [N, a^\dagger] = a^\dagger$$

from which it follows that

$$N\left(a|n\rangle\right) = aN|n\rangle + [N, a]|n\rangle = (n-1)(a|n\rangle)$$

$$N\left(a^\dagger|n\rangle\right) = a^\dagger N|n\rangle + [N, a^\dagger]|n\rangle = (n+1)(a^\dagger|n\rangle)$$

Together, these equations imply that if $a|n\rangle$ and $a^\dagger|n\rangle$ do not vanish, they are eigenstates of the number operator with eigenvalues $n-1$ and $n+1$ respectively. If they do vanish, then they reduce to the trivial case $0 = 0$. We normally require eigenstates to be nonzero. Consider the inner product of $a|n\rangle$ with itself:

$$\|a|n\rangle\|^2 = \langle n|a^\dagger a|n\rangle = n \geq 0$$

Hence, $a|n\rangle$ vanishes if and only if $n = 0$. On the other hand,

$$\left\|a^\dagger|n\rangle\right\|^2 = \langle n|aa^\dagger|n\rangle = \langle n|(N+1)|n\rangle = n+1$$

which never vanishes since $n \geq 0$, i.e. the state $a^\dagger|n\rangle$ never vanishes. Since the raising and lowering operators change the eigenvalue by ± 1, it follows that n must be an integer. The spectrum of N consists of all nonnegative integers, and since the Hamiltonian has the same eigenstates as N,

$$H|n\rangle = E_n|n\rangle$$

where, in ordinary units,

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

Note that the ground state does not have zero energy, in contrast to the classical harmonic oscillator. Rather, the quantum mechanical ground state has a **zero-point energy** of $\hbar\omega/2$. The structure of the quantum harmonic oscillator–particularly the commutation relations, the ladder operators, and the existence of a lowest energy state–forces the energy spectrum to be discrete. Furthermore, the energy levels are equally spaced:

$$E_{n+1} - E_n = \hbar\omega$$

This is Planck's famous hypothesis–that the energy of the radiation emitted by the *oscillating charges* must come only in bundles (quanta) that are integral multiples of $\hbar\omega$.

2.1 Ladder Operators

In this section we'll work out the raising and lowering operators in more detail. Since $a|n\rangle$ is an eigenstate with eigenvalue $n-1$ for $n > 0$, it must be proportional to the state $|n-1\rangle$.

Let c_n be the constant of proportionality such that

$$a|n\rangle = c_n|n-1\rangle$$

Computing the norm squared, we find

$$\|a|n\rangle\|^2 = n = |c_n|^2$$

since the eigenstates are normalized. Setting the overal phase equal to 1, we have

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

Likewise, $a^\dagger|n\rangle$ is an eigenstate with eigenvalue $n+1$, so

$$a^\dagger|n\rangle = d_n|n+1\rangle$$

where d_n is a complex constant. Computing the norm squared,

$$\left\|a^\dagger|n\rangle\right\|^2 = n+1 = |d_n|^2$$

Again, setting the overall phase equal to 1,

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

In summary, we have

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

Starting from the lowest energy state $n=0$, we can systematically determine all energy eigenstates by repeated application of the raising operator:

$$|1\rangle = a^\dagger|0\rangle$$

$$|2\rangle = \frac{1}{\sqrt{2}}a^\dagger|1\rangle = \frac{1}{\sqrt{2}}(a^\dagger)^2|0\rangle$$

$$|3\rangle = \frac{1}{\sqrt{3}}a^\dagger|2\rangle = \frac{1}{\sqrt{3!}}(a^\dagger)^3|0\rangle$$

$$\vdots$$

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$$

2.2 Energy Eigenfunctions

We can determine any eigenstate by successive applications of the operator $a^\dagger$ on the ground state, so we start by solving for the position space wave function of the ground state. Since the operator a "annihilates" the ground state,

$$\langle x|a|0\rangle = \langle x|\frac{1}{\sqrt{2}}\left(\hat{x} + i\hat{p}_x\right)|0\rangle = 0$$

or

$$\left(x + \frac{d}{dx}\right)\psi_0(x) = 0$$

where $\psi_0(x) = \langle x|0\rangle$ is the position-space wave function for the ground state. We seek a function whose derivative gives $-x$ times the original function. Clearly $e^{-x^2/2}$ satisfies that criterion, so the normalized energy eigenfunction in dimensionless units is given by

$$\psi_0(x) = \frac{1}{\pi^{1/4}}e^{-x^2/2}$$

In ordinary units, $\psi_0(x)$ has units of $[\text{length}]^{-1/2}$, so

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar^2}$$

The nth excited state in dimensionless units is given by repeated application of $a^\dagger$,

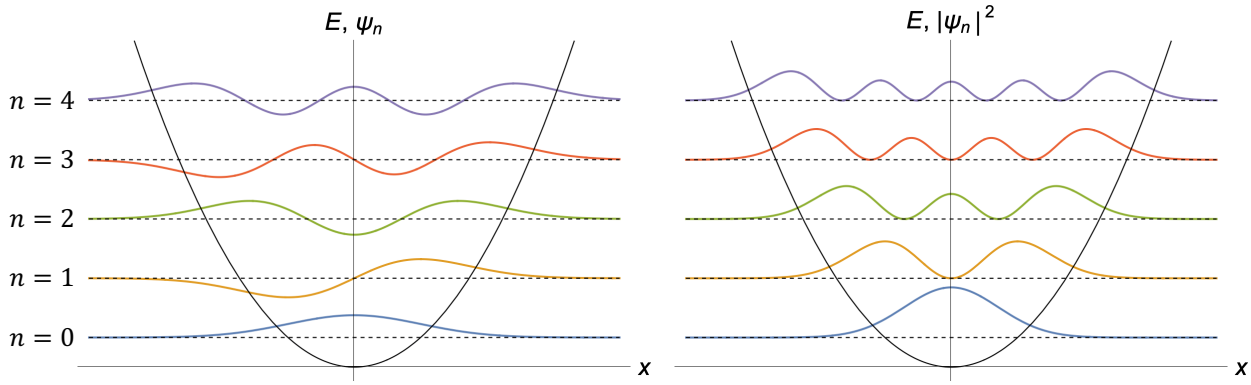
$$\psi_n(x) = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{n!2^n}}\left(x - \frac{d}{dx}\right)^n e^{-x^2/2}$$

We can "simplify" this equation by using a set of special functions called Hermite polynomials, which are a set of polynomials generated by the Rodriguez formula

$$H_n(x) = (-1)^n e^{x^2}\left(\frac{d}{dx}\right)^n e^{-x^2}$$

The excited states are then given by

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



or in ordinary units,

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

While it is nice to be able to write the eigenfunctions explicitly in terms of Hermite polynomials, for most practical purposes abstract operations involving kets and ladder operators are more useful than explicit representations in terms of wave functions.

3 Zero-Point Energy

In classical mechanics, the lowest energy state occurs when $p_x = 0$ and $x = 0$ (the spring is unstretched and the mass is at rest). This configuration is disallowed by the Heisenberg uncertainty relation–after repeated measurements on the system in its ground state, we will find a range of values for both position and momentum, so the expectation value of the energy will be nonzero. To see why, let $\Delta x^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle$ and $\Delta \hat{p}_x^2 = \langle \hat{p}_x^2 \rangle - \langle \hat{p}_x \rangle$. Then,

$$\langle E \rangle = \frac{1}{2}\left(\langle \hat{p}_x^2 \rangle + \langle \hat{x}^2 \rangle\right) = \frac{1}{2}\left(\Delta p_x^2 + \Delta x^2 - \langle \hat{p}_x \rangle - \langle \hat{x} \rangle\right)$$

The expectation values are easily computing using the ladder operators. Inverting the expressions for a and $a^\dagger$ in terms of $\hat{x}$ and $\hat{p}_x$, we find

$$\hat{x} = \frac{1}{\sqrt{2}}\left(a^\dagger + a\right)$$

$$\hat{p}_x = \frac{i}{\sqrt{2}}\left(a^\dagger - a\right)$$

It follows that for an energy eigenstate $|n\rangle$,

$$\langle n|\hat{x}|n\rangle = \frac{1}{\sqrt{2}}\langle n|(a^\dagger + a)|n\rangle = \frac{1}{\sqrt{2}}\left(\sqrt{n+1}\langle n|n+1\rangle + \sqrt{n}\langle n|n-1\rangle\right) = 0$$

$$\langle n|\hat{p}_x|n\rangle = \frac{i}{\sqrt{2}}\langle n|(a^\dagger - a)|n\rangle = \frac{i}{\sqrt{2}}\left(\sqrt{n+1}\langle n|n+1\rangle - \sqrt{n}\langle n|n-1\rangle\right) = 0$$

Hence,

$$\langle E\rangle = \frac{1}{2}\left(\Delta p_x^2 + \Delta x^2\right)$$

From the Heisenberg uncertainty relation $\Delta x \Delta p_x \geq 0$, it follows that $\langle E\rangle > 0$. Localizing the particle at the origin will create a spread in momentum, and likewise, trying to put the particle into a state with zero momentum creates a spread in position. Nature chooses a tradeoff in which the particle has both nonzero Δx and Δp_x and, therefore, nonzero energy.

Explicitly, for the ground state,

$$\begin{aligned}
\Delta p_x^2 = \langle \hat{p}_x^2\rangle &= -\frac{1}{2}\langle 0|(a^\dagger - a)^2|0\rangle \\
&= -\frac{1}{2}\langle 0|\left[a^\dagger a^\dagger - a^\dagger a - aa^\dagger + aa\right]|0\rangle \\
&= \frac{1}{2}\langle 0|aa^\dagger|0\rangle = \frac{1}{2}\langle 1|1\rangle = \frac{1}{2}
\end{aligned}$$

and

$$\begin{aligned}
\Delta x^2 = \langle \hat{x}^2\rangle &= \frac{1}{2}\langle 0|(a^\dagger + a)^2|0\rangle \\
&= \frac{1}{2}\langle 0|\left[a^\dagger a^\dagger + a^\dagger a + aa^\dagger + aa\right]|0\rangle \\
&= \frac{1}{2}\langle 0|aa^\dagger|0\rangle = \frac{1}{2}\langle 1|1\rangle = \frac{1}{2}
\end{aligned}$$

Hence, $\Delta x \Delta p_x \geq 1/2$ or $\hbar/2$ in ordinary units. Evidently, the ground state of the harmonic oscillator is a minimum uncertainty state, which we already knew since the position-space wave function is a Gaussian.