

QUANTUM MECHANICAL OPERATORS AND THE HARMONIC OSCILLATOR

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Introduction and Importance

In this poster we'll be deriving the Hamiltonian operator used in quantum mechanics from its classical roots, and using it in the problem of the quantum harmonic oscillator. The Q.H.O. is very important in physics as, given an energy potential $V(x)$, we can Taylor expand it to 2nd order in x - the resulting Hamiltonian operator can then be solved as a harmonic oscillator to give powerful solutions close to an equilibrium point.

Classical Mechanics

We begin with a brief overview of classical mechanics by mentioning the Lagrangian and Hamiltonian formalisms.

Lagrange's Equations¹

Given a **Lagrangian** $L(q, \dot{q}, t) = T - V$, a mechanical system *evolves* based on the the following Euler-Lagrange equation:

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0$$

We will now consider a Lagrangian which does not depend explicitly on time (this happens in all closed systems). By considering the rate of change of the Lagrangian, we can work to find a conserved quantity¹:

$$\begin{aligned} \frac{dL}{dt} &= \sum \dot{q} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) + \sum \frac{\partial L}{\partial \dot{q}} \ddot{q} \equiv \sum \frac{d}{dt} \left(\dot{q} \frac{\partial L}{\partial \dot{q}} \right) \\ \Rightarrow \frac{d}{dt} \left(\sum \dot{q} \frac{\partial L}{\partial \dot{q}} - L \right) &= 0. \end{aligned}$$

Therefore the quantity inside the parentheses is conserved! In general we call this the **Hamiltonian** but for most systems this is equivalent to the *total energy* of the system.

Hamilton's Equations²

First we define the *generalized momentum conjugate* p

$$p = \frac{\partial L}{\partial \dot{q}},$$

and by exchanging this into our previous definition of the Hamiltonian we can get the usual form of the Hamiltonian:

$$H(q, p) = \sum (\dot{q}p) - L.$$

Finally by considering time derivatives, we can write Hamilton's Equations:

$$\frac{\partial H}{\partial p} = \dot{q}, \quad \frac{\partial H}{\partial q} = -\dot{p}.$$

References

- (1) Landau LD, Lifshitz EM. *Mechanics*. Course of Theoretical Physics, volume 1. 3rd edition. Oxford: Pergamon Press; 1976.
- (2) Susskind L, Hrabovky G. *Classical Mechanics: The Theoretical Minimum*. The Theoretical Minimum, volume 1. London: Penguin Books; 2014.
- (3) Susskind L, Friedman A. *Quantum Mechanics: The Theoretical Minimum*. The Theoretical Minimum, volume 2. London: Penguin Books; 2014.
- (4) Griffiths DJ. *Introduction to Quantum Mechanics*. 1st edition. New Jersey: Prentice Hall; 1995.

Linear and Hermitian Operators³

Now we consider a Hilbert space of state-vectors, usually written $|\Psi\rangle$, which are represented in terms of functions $\psi: \mathbb{R} \rightarrow \mathbb{C}$ depending on the basis. We begin by introducing a linear operator, \mathbf{D} , defined by:

$$\mathbf{D}\psi(x) = \frac{d\psi(x)}{dx}.$$

We define the inner product between two elements of our hilbert space Ψ and Φ as follows:

$$\langle \Psi | \Phi \rangle = \int_{-\infty}^{\infty} \psi^*(x) \phi(x) dx$$

For a wavefunction $\psi(x)$, the probability of finding a particle within the interval (a, b) is given by

$$P(a, b) = \int_a^b \psi^*(x) \psi(x) dx \Rightarrow \int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = 1.$$

This is called the normalization constraint. Given an operator \mathbf{L} we can write the inner product of $\psi(x)$ and $\mathbf{L}(\phi(x))$ as $\langle \Psi | \mathbf{L} | \Phi \rangle$. We can then say \mathbf{L} is **Hermitian**, usually written $\mathbf{L}^\dagger = \mathbf{L}$, if and only if

$$\langle \Psi | \mathbf{L} | \Phi \rangle = \langle \Phi | \mathbf{L} | \Psi \rangle^*.$$

We can now check whether the differential operator \mathbf{D} is Hermitian using our definition from the inner product. Using integration by parts we obtain the identity:

$$\langle \Psi | \mathbf{D} | \Phi \rangle = -\langle \Phi | \mathbf{D} | \Psi \rangle^*.$$

In other words, \mathbf{D} is **anti-Hermitian** - however there is an easy way to transform a Hermitian operator into an anti-Hermitian operator and vice-versa!

If \mathbf{M} is anti-Hermitian then $\pm i\mathbf{M}$ is Hermitian.

With this information we can now introduce another linear - and now Hermitian - operator \mathbf{P} ,

$$\mathbf{P} = -i\hbar\mathbf{D} = -i\hbar\frac{d}{dx}.$$

We call this our **momentum operator** in one dimension. Now we can create an analog to our classical Hamiltonian.

The Hamiltonian Operator³

We first express the classical Hamiltonian as the sum of kinetic and potential energies,

$$H = T + V = \frac{p^2}{2m} + V(x, t)$$

and by considering the momentum operator we can define the Hamiltonian operator \mathcal{H}

$$\mathcal{H} = \frac{\mathbf{P}^2}{2m} + \mathbf{V}(x, t) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x, t)$$

This leads us to define the following eigenvalue problem:

The Time-Independant Schrödinger Equation

$$\mathcal{H}|\Psi\rangle = -\frac{\hbar^2}{2m} \frac{d^2|\Psi\rangle}{dx^2} + V(x, t)|\Psi\rangle = E|\Psi\rangle$$

The Quantum Harmonic Oscillator⁴

In this section we focus on a particular eigenvalue problem, that of the harmonic oscillator. Classically the harmonic oscillator comes from a potential $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$. Plugging this potential into the Schrödinger equation:

$$\mathcal{H}\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi.$$

To find the energy levels (eigenvalues) of this system we will first have to rewrite our Hamiltonian operator. First we consider the following two adjoint operators⁴,

$$\begin{aligned} a^+ &= \frac{1}{\sqrt{2m}} \left(\frac{\hbar}{i} \frac{d}{dx} + im\omega x \right), \\ a^- &= \frac{1}{\sqrt{2m}} \left(\frac{\hbar}{i} \frac{d}{dx} - im\omega x \right). \end{aligned}$$

These two operators are often called the *creation operator* and the *annihilation operator* respectively, for reasons we will see soon. Now we consider the product of these two operators - after some rearranging we arrive at:

$$\begin{aligned} a^- a^+ &= \mathcal{H} + \frac{1}{2}\hbar\omega, \\ a^+ a^- &= \mathcal{H} - \frac{1}{2}\hbar\omega, \end{aligned}$$

which also gives us the commutator relation between a^- and a^+

$$[a^-, a^+] = a^- a^+ - a^+ a^- = \hbar\omega.$$

We can use the form of $a^+ a^-$ above to rewrite the Schrödinger equation as

$$(a^+ a^- + \frac{1}{2}\hbar\omega)\psi = E\psi(*)$$

The Essential Lemma⁴:

If ψ is an eigenfunction to our Schrödinger equation with eigenvalue (energy) E , then $a^+\psi$ is another eigenfunction with eigenvalue $(E + \hbar\omega)$.

Proof:

$$\begin{aligned} \mathcal{H}(a^+\psi) &= (a^+ a^- + \frac{1}{2}\hbar\omega)a^+\psi \\ &= a^+(a^- a^+ + \frac{1}{2}\hbar\omega)\psi = a^+(\mathcal{H} + \hbar\omega)\psi \\ &= a^+(E\psi + \hbar\omega\psi) = (E + \hbar\omega)a^+\psi. \quad \square \end{aligned}$$

We could similarly prove that for an eigenfunction ψ with energy E , $a^-\psi$ is an eigenfunction with energy $(E - \hbar\omega)$. The fact that these operators can find wavefunctions with higher and lower energies is the reason for their names (creation and annihilation). Hence by finding a wavefunction $\psi_0(x)$ with the lowest possible non-zero energy (such that $a^-\psi_0 = 0$), we can find the rest of the wavefunctions by continuously applying a^+ ! Using the definition of a^- and the normalization constraint we can find:

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

And with this information we can calculate the rest of the wavefunctions by hand.

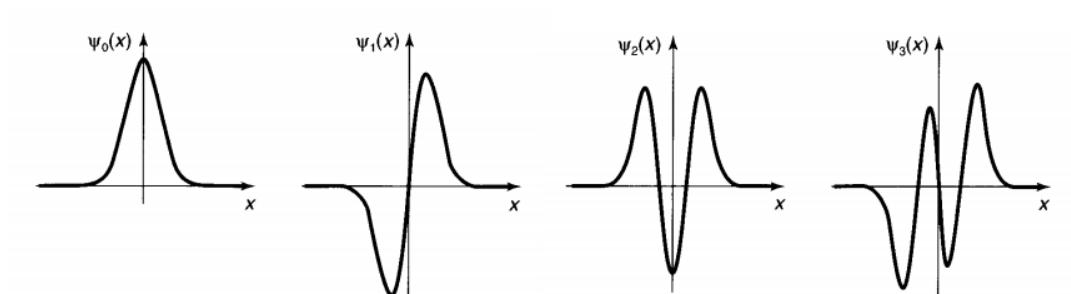


Fig. 1: The shape of the first four wavefunctions (4: p.42).