

Quantized Energies

Arnav Gupta

April 17, 2024

Contents

1	Spectroscopy	1
2	Energy Eigenvalue Equation	2
3	The Wave Function	2
4	Infinite Square Well	4
5	Finite Square Well	5
6	Observations	5
7	Superposition States and Time Dependence	5

1 Spectroscopy

Quantized energy levels arise from particle interactions that lead to bound systems (nuclei, atoms, etc).

Lowest energy state at $n = 1$ is called the **ground state**, and levels above are the **excited states**.

For energy eigenvalues E_i and energy eigenstates $|E_i\rangle$, the probability of a particular energy measurement is

$$\mathcal{P}_{E_i} = |\langle E_i | \psi \rangle|^2$$

and the energy eigenvalue equation is

$$\hat{H} |E_i\rangle = E_i |E_i\rangle$$

2 Energy Eigenvalue Equation

The quantum mechanical Hamiltonian operator for a particle moving in 1 dimension (from classical energy of such a particle) is

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

The wave function is a representation of the abstract quantum state so in position representation:

$$|\psi\rangle \doteq \psi(x)$$

For the energy eigenstates in position representation:

$$|E_i\rangle \doteq \varphi_{E_i}(x)$$

Similarly, the operators in position representation are:

$$\hat{x} \doteq x, \hat{p} = -i\hbar \frac{d}{dx}$$

The energy eigenvalue equation in position representation becomes:

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \varphi_E(x) = E \varphi_E(x)$$

Operator equations turn into differential equations.

3 The Wave Function

The wave function is a representation of a quantum state using the eigenstates of the position operator \hat{x} as the basis states, where position is not quantized (continuous).

State in position basis cannot be represented as a column vector since it is continuous, so instead must use quantum mechanical wave function.

Wave function is equivalent to probability amplitude (in Dirac notation) so

$$\psi(x) = \langle x | \psi \rangle$$

which gives the probability distribution function:

$$\mathcal{P}(x) = |\psi(x)|^2$$

and so $\mathcal{P}(x) dx$ is the infinitesimal probability of detecting a particle at x within an infinitesimal region of width dx . $\mathcal{P}(x)$ has dimensions of inverse length.

Measuring $\mathcal{P}(x)$ does not give $\psi(x)$, similar to the discrete case.

To find the probability that a particle is in a finite interval $a < x < b$:

$$\mathcal{P}_{a < x < b} = \int_a^b |\psi(x)|^2$$

and so the normalization condition is also an integral over all x .

Rules for translating bracket formulas to wave function formulas:

1. Replace ket with wave function.
2. Replace bra with wave function conjugate.
3. Replace bracket with integral over all space.
4. Replace operator with position representation.

The probability that the state $\psi(x)$ is measured to have the physical observable for which $\phi(x)$ is the eigenstate is

$$\mathcal{P}_{\psi \rightarrow \varphi} = |\langle \varphi | \psi \rangle|^2 = \left| \int_{-\infty}^{\infty} \varphi^*(x) \psi(x) dx \right|^2$$

For energy this becomes:

$$\mathcal{P}_{E_n} = |\langle E_n | \psi \rangle|^2 = \left| \int_{-\infty}^{\infty} \varphi_n^*(x) \psi(x) dx \right|^2$$

where $\varphi_n(x)$ is the energy eigenstate with energy E_n .

The expectation value of position in wave function notation is

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx$$

The expectation value of momentum in wave function notation is

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(-i\hbar \frac{d}{dx} \right) \psi(x) dx$$

4 Infinite Square Well

Potential energy functions that have a minimum are called **potential wells**. Particle energy is conserved, so kinetic energy is $T(x) = E - V(x)$.

Particles that have their motion constrained by the potential well are in **bound states**. Particles with energies beyond potential well do not have motion constrained, so they are in **unbound states**.

The **particle in a box** exists in a well with

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 < x < L \\ \infty & x > L \end{cases}$$

Infinite square well illustrates most important features of a particle bound to a limited region of space.

Solving the infinite square well gives a **quantization condition** with **quantum number** n , which is used to label quantized states and energies. Using these gives the energy quantization for the system:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

which are the allowed energies with $n = 1$ as the ground state. Further, the energy eigenstates are:

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

Here, the energy and the wavelength are related, as opposed to classical where energy and amplitude are.

A system exhibits properties similar to classical particles and classical waves, so there is **wave-particle duality**.

The probability density is

$$\mathcal{P}_n(x) = \frac{2}{L} \sin^2 \frac{n\pi x}{L}$$

Probability of finding the particle outside the well is 0, but also 0 at some places inside the well.

5 Finite Square Well

The potential energy of a finite square well is

$$V(x) = \begin{cases} V_0 & x < -a \\ 0 & -a < x < a \\ V_0 & x > a \end{cases}$$

In the regions outside the well, the wave function must be a decaying exponential. Boundary conditions to solve this are:

1. $\varphi_E(x)$ is continuous
2. $\frac{d\varphi_E(x)}{dx}$ is continuous unless $V = \infty$

Symmetry condition can also be used to solve, giving even and odd solutions.

Using these conditions gives transcendental equations that must be solved graphically or numerically for each different well.

Finite well eigenstates extend into the classically forbidden region (unlike infinite well), referred to as **barrier penetration**.

6 Observations

For higher energy states, the wave function penetrates further into the classically forbidden region, evident in finite well states.

A given finite well energy eigenvalue lies below the corresponding infinite well energy eigenvalue.

7 Superposition States and Time Dependence

The Schrödinger equation in energy eigenstate basis can be used to find the time evolution.

Probability and expectation value of energy are time-independent.