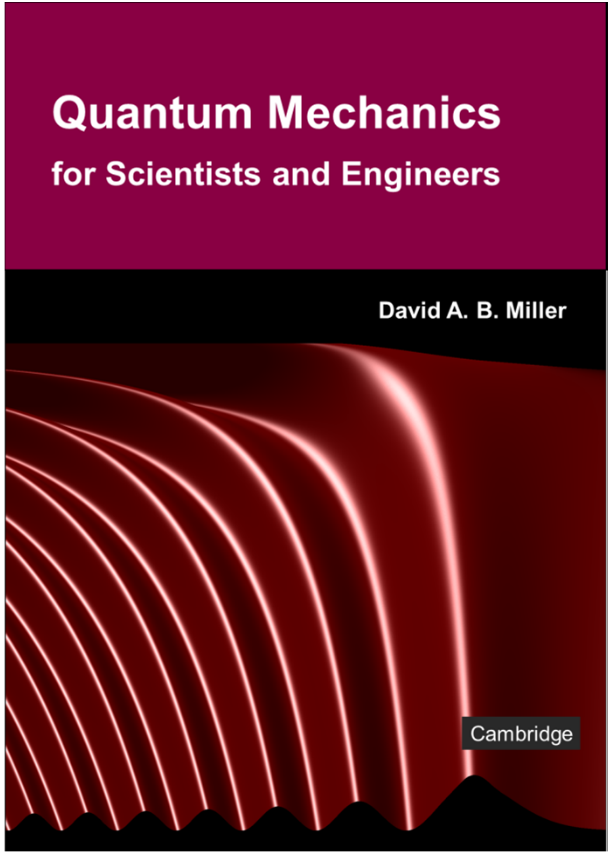
2.3 Particle in a box

Slides: Video 2.3.2 Linearity and normalization

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.4 – 2.5



The particle in a box

Linearity and normalization

Quantum mechanics for scientists and engineers

David Miller

Linearity and Schrödinger's equation

We see that Schrödinger's equation is linear

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi = E\psi$$

The wavefunction ψ appears only in first order

there are no second or higher order terms

such as ψ^2 or ψ^3

So, if ψ is a solution, so also is $a\psi$

this just corresponds to multiplying both sides by the constant a

Normalization of the wavefunction

Born postulated

- the probability $P(\mathbf{r})$ of finding a particle near a point $\mathbf{r}$ is $\propto |\psi(\mathbf{r})|^2$

Specifically let us define $P(\mathbf{r})$ as a

- "probability density"
  - For some very small (infinitesimal) volume $d^3\mathbf{r}$ around $\mathbf{r}$
    - the probability of finding the particle in that volume is $P(\mathbf{r})d^3\mathbf{r}$

Normalization of the wavefunction

The sum of all such probabilities should be 1

So

$$\int P(\mathbf{r})\, d^3\mathbf{r} = 1$$

Can we choose $\psi(\mathbf{r})$ so that we can use $|\psi(\mathbf{r})|^2$ as the probability density

not just proportional to probability density?

Unless we have been lucky

our solution to Schrödinger's equation did not give a $\psi(\mathbf{r})$ so that

$$\int |\psi(\mathbf{r})|^2\, d^3\mathbf{r} = 1$$

Normalization of the wavefunction

Generally, this integral would give some other real positive number

- which we could write as $1/|a|^2$
  - where a is some (possibly complex) number
    - That is, $\int |\psi(\mathbf{r})|^2 \, d^3\mathbf{r} = \frac{1}{|a|^2}$

But we know that if $\psi(\mathbf{r})$ is a solution of Schrödinger's equation

- so also is $a\psi(\mathbf{r})$

Normalization of the wavefunction

So

if we use the solution $\psi_N = a\psi$ instead of ψ

then

$$\int \left|\psi_N(\mathbf{r})\right|^2 d^3\mathbf{r} = 1$$

and we can use $\left|\psi_N(\mathbf{r})\right|^2$ as the probability density, i.e.,

$$P(\mathbf{r}) = \left|\psi_N(\mathbf{r})\right|^2$$

$\psi_N(\mathbf{r})$ would then be called a "normalized wavefunction"

Normalization of the wavefunction

So, to summarize normalization

we take the solution ψ we have obtained from Schrödinger's wave equation

we integrate $|\psi(\mathbf{r})|^2$ to get a number we call $1/|a|^2$

then we obtain the normalized wavefunction $\psi_N = a\psi$ for which

$$\int |\psi_N(\mathbf{r})|^2 \, d^3\mathbf{r} = 1$$

and we can use $|\psi_N(\mathbf{r})|^2$ as the probability density

Technical notes on normalization

Note that normalization only sets the magnitude of a

- not the phase
  - we are free to choose any phase for a
    - or indeed for the original solution ψ
      - a phase factor $\exp(i\theta)$ is just another number by which we can multiply the solution
        - and still have a solution

Technical notes on normalization

If we think of space as infinite

- functions like $\sin(kx)$, $\cos(kz)$, and $\exp(i\mathbf{k}\cdot\mathbf{r})$
  - cannot be normalized in this way
    - Technically, their squared modulus is not “Lebesgue integrable”
      - They are not “L2” functions

This difficulty is mathematical, not physical

- It is caused by over-idealizing the mathematics to get functions that are simple to use

Technical notes on normalization

There are "work-arounds" for this difficulty

1 - only work with finite volumes in actual problems

this is the most common solution

2 - use "normalization to a delta function"

introduces another infinity to compensate for the first one

This can be done

but we will try to avoid it