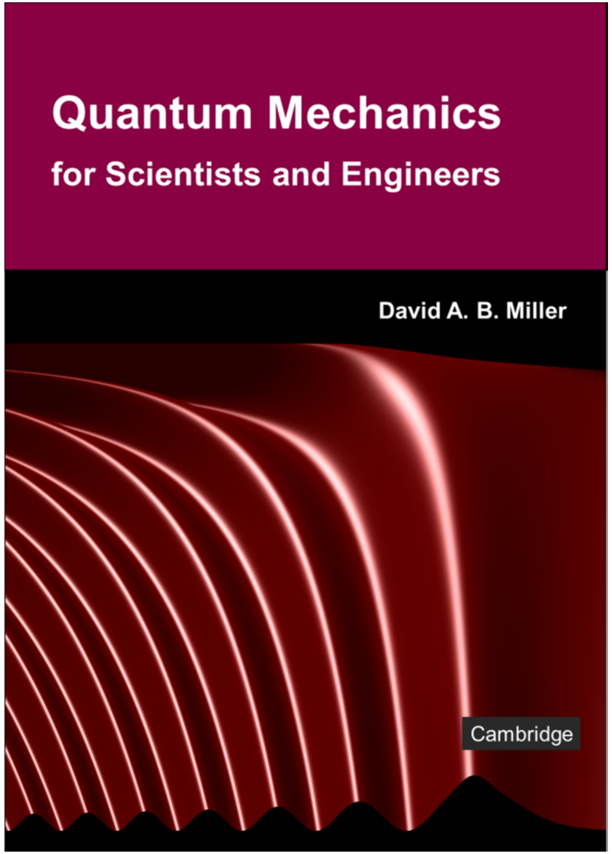
# 3.3 The time-dependent Schrödinger equation

Slides: Video 3.3.1 Introduction to the time-dependent Schrödinger equation

Text reference: Quantum Mechanics for Scientists and Engineers

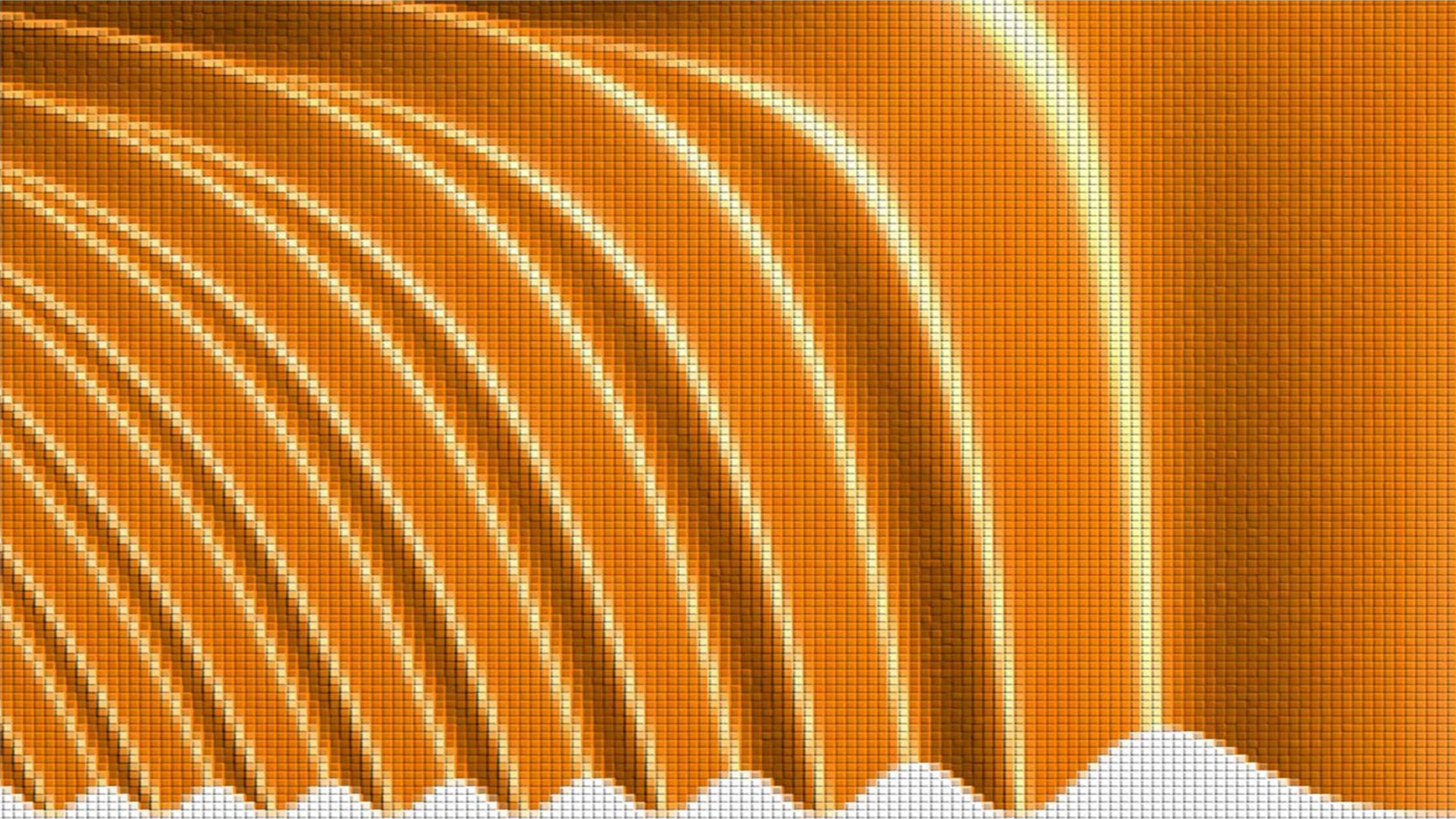
Chapter 3 introduction



# The time-dependent Schrödinger equation

Quantum mechanics for scientists and engineers

David Miller

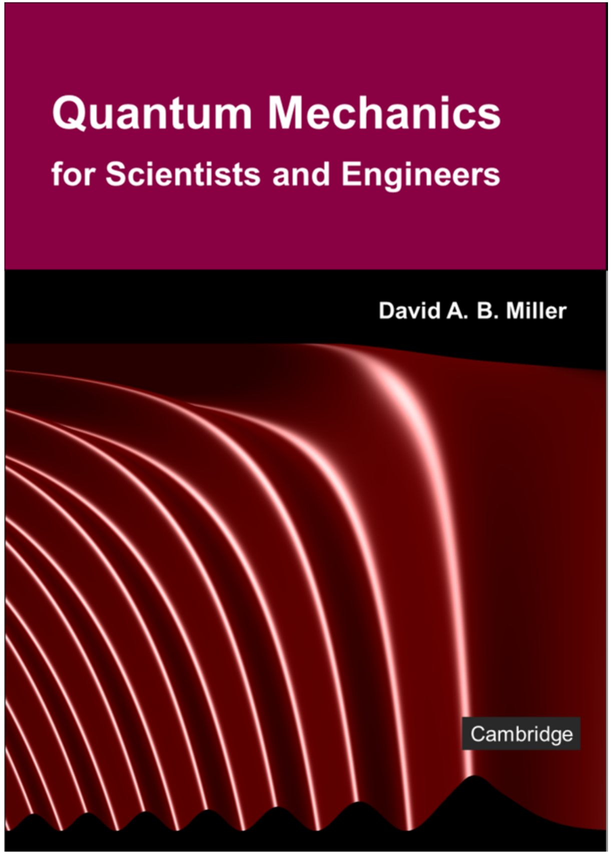


# 3.3 The time-dependent Schrödinger equation

Slides: Video 3.3.2 Rationalizing the time-dependent Schrödinger equation

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 3.1 – 3.2



# The time-dependent Schrödinger equation

## Rationalizing the time-dependent Schrödinger equation

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# Relation between energy and frequency

The relation between

energy

and

frequency

for

photons

is $$\boxed{E = h\nu = \hbar\omega}$$

# Relation between energy and frequency

The relation between

energy

and

frequency

for

**quantum mechanics**

is $\boxed{E = h\nu = \hbar\omega}$

# Rationalizing the time-dependent equation

We want a time-dependent wave equation

- for a particle with mass $m$
  - with this relation $E = h\nu = \hbar\omega$ between energy and frequency

We might also reasonably want it to have plane wave solutions

- e.g., of the form $\exp\left[i\left(kz - \omega t\right)\right]$
  - when we have some specific energy $E$
    - and when we are in a uniform potential

# Rationalizing the time-dependent equation

Schrödinger postulated the time-dependent equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r},t)\Psi(\mathbf{r},t)=i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$

Note that for a uniform potential

e.g., $V=0$ for simplicity

with $E=\hbar\omega$ and $k=\sqrt{2mE/\hbar^2}$

waves of the form

$$\exp\left[-i(\omega t\pm kz)\right]\equiv\exp\left[-i\left(\frac{Et}{\hbar}\pm kz\right)\right]\equiv\exp\left(-i\frac{Et}{\hbar}\right)\exp(\mp ikz)$$

are indeed solutions

# Rationalizing the time-dependent equation

In his time-dependent equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r},t)\Psi(\mathbf{r},t)=i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$

Schrödinger chose a sign for the right hand side

which means that a wave with a spatial part

$$\propto \exp(ikz)$$

is definitely going in the positive $z$ direction

That wave, including its time dependence

would be of the form (for $V=0$)

$$\exp\left[i\left(kz-Et/\hbar\right)\right]$$

# Compatibility with the time-independent equation

Before examining the time-dependent equation further

first we should check that it is compatible with the time-independent equation

The time-independent equation could apply if we had states of definite energy $E$, an eigenenergy

Suppose we had some corresponding eigenfunction $\psi(\mathbf{r})$

so that

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

# Compatibility with the time-independent equation

As it stands

this solution $\psi(\mathbf{r})$ is not a solution of the time-dependent equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r},t)\Psi(\mathbf{r},t)=i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$

Putting $\psi(\mathbf{r})$ in here for $\Psi(\mathbf{r},t)$ does not work

because $\psi(\mathbf{r})$ has no time-dependence

the right hand side is zero

whereas it should be $E\psi(\mathbf{r})$

how do we resolve this?

# Compatibility with the time-independent equation

Suppose that, instead of proposing the solution $\psi(\mathbf{r})$

we propose $\Psi(\mathbf{r},t)=\psi(\mathbf{r})\exp(-iEt/\hbar)$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r})\Psi(\mathbf{r},t)$$

$$=-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})\exp(-iEt/\hbar)+V(\mathbf{r})\psi(\mathbf{r})\exp(-iEt/\hbar)$$

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

$$=E\Psi(\mathbf{r},t)$$

so $\Psi(\mathbf{r},t)=\psi(\mathbf{r})\exp(-iEt/\hbar)$ solves the time-independent Schrödinger equation

# Compatibility with the time-independent equation

Similarly, knowing that $\psi(\mathbf{r})$ solves the time-independent equation with energy $E$

substituting $\Psi(\mathbf{r},t) = \psi(\mathbf{r})\exp(-iEt/\hbar)$

in the time-dependent equation gives

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = i\hbar\frac{\partial}{\partial t}\left[\psi(\mathbf{r})\exp(-iEt/\hbar)\right]$$

$$= i\hbar\psi(\mathbf{r})\frac{\partial}{\partial t}\left[\exp(-iEt/\hbar)\right] = i\hbar\psi(\mathbf{r})\left[-i\frac{E}{\hbar}\right]\exp(-iEt/\hbar) = E\,\Psi(\mathbf{r},t)$$

so $\Psi(\mathbf{r},t) = \psi(\mathbf{r})\exp(-iEt/\hbar)$ solves the time-dependent Schrödinger equation

# Compatibility with the time-independent equation

So every solution $\psi(\mathbf{r})$ of the time-independent Schrödinger equation, with eigenenergy $E$

is also a solution of the time-dependent equation

as long as we always multiply it by a factor $\exp(-iEt/\hbar)$

If $\psi(\mathbf{r})$ is a solution of the time-independent Schrödinger equation, with eigenenergy $E$

then $\Psi(\mathbf{r},t)=\psi(\mathbf{r})\exp(-iEt/\hbar)$

is a solution of both the time-independent

and the time-dependent Schrödinger equations

making these two equations compatible

# Oscillations and time-independence

If we propose a solution

$$\Psi(\mathbf{r},t)=\psi(\mathbf{r})\exp(-iEt/\hbar)$$

to a time-independent problem

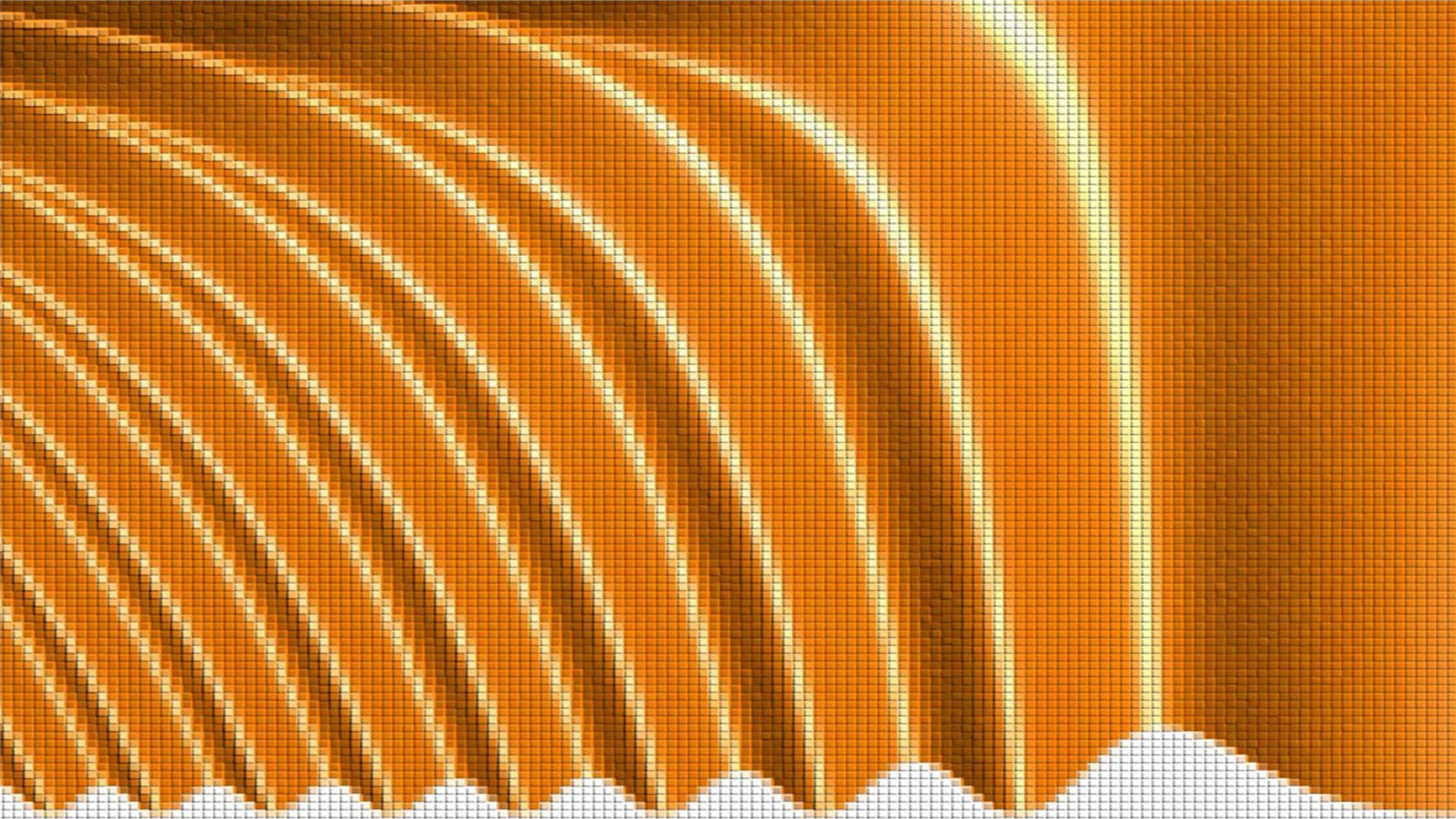
can this represent something that is stable in time?

Yes! - measurable quantities associated with this state

are stable in time!

e.g., probability density

$$|\Psi(\mathbf{r},t)|^2=\left[\exp(+iEt/\hbar)\psi^*(\mathbf{r})\right]\times\left[\exp(-iEt/\hbar)\psi(\mathbf{r})\right]=|\psi(\mathbf{r})|^2$$

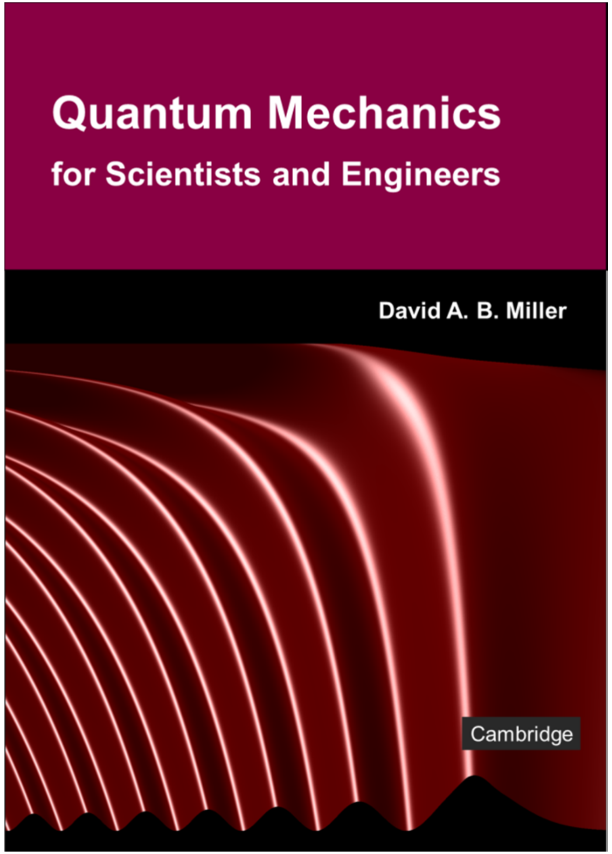


# 3.3 The time-dependent Schrödinger equation

Slides: Video 3.3.4 Solutions of the time-dependent Schrödinger equation

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.3



# The time-dependent Schrödinger equation

## Solutions of the time-dependent Schrödinger equation

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# Contrast to classical wave equation

The common classical wave equation has a different form

$$\nabla^2 f = \frac{k^2}{\omega^2}\frac{\partial^2 f}{\partial t^2}$$

for which

$$f \propto \exp\left[i\left(kz - \omega t\right)\right]$$

would also be a solution

Note the classical equation has a second time derivative

as opposed to the first time derivative in Schrödinger's time-dependent equation

# Schrödinger's complex waves

Note that Schrödinger's use of a complex wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r},t)\Psi(\mathbf{r},t)=i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$

with the "$i$" on the right hand side

means that generally the wave $\Psi$ is required to be a complex entity

For example, for $V=0$

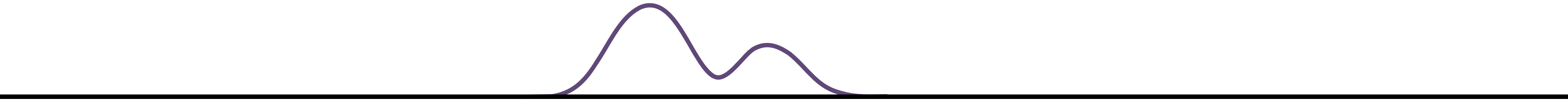
though $\exp\left[i\left(kz-Et/\hbar\right)\right]$ is a solution

$\sin\left(kz-Et/\hbar\right)$ is ***not*** a solution

# Wave equation solutions

With the classical wave equation

- if at some time we see a particular shape of wave
  - e.g., on a string



# Wave equation solutions

With the classical wave equation

if at some time we see a particular shape of wave

e.g., on a string

we do not know if it is going

to the right $f(z-ct)$

# Wave equation solutions

With the classical wave equation

if at some time we see a particular shape of wave

e.g., on a string

we do not know if it is going

to the right $f(z-ct)$

or to the left $g(z+ct)$

or even some combination of the two

# Time evolution from Schrödinger's equation

In Schrödinger's equation, for a known potential $V$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r},t)\Psi(\mathbf{r},t)=i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$

if we knew the wavefunction $\Psi(\mathbf{r},t_o)$ at every point in space at some time $t_o$

we could evaluate the left hand side of the equation at that time for all $\mathbf{r}$

so we would know $\partial\Psi(\mathbf{r},t)/\partial t$ for all $\mathbf{r}$

so we could integrate the equation to deduce $\Psi(\mathbf{r},t)$ at all future times

# Time evolution from Schrödinger's equation

Explicitly

knowing $\partial\Psi(\mathbf{r},t)/\partial t$ we can calculate

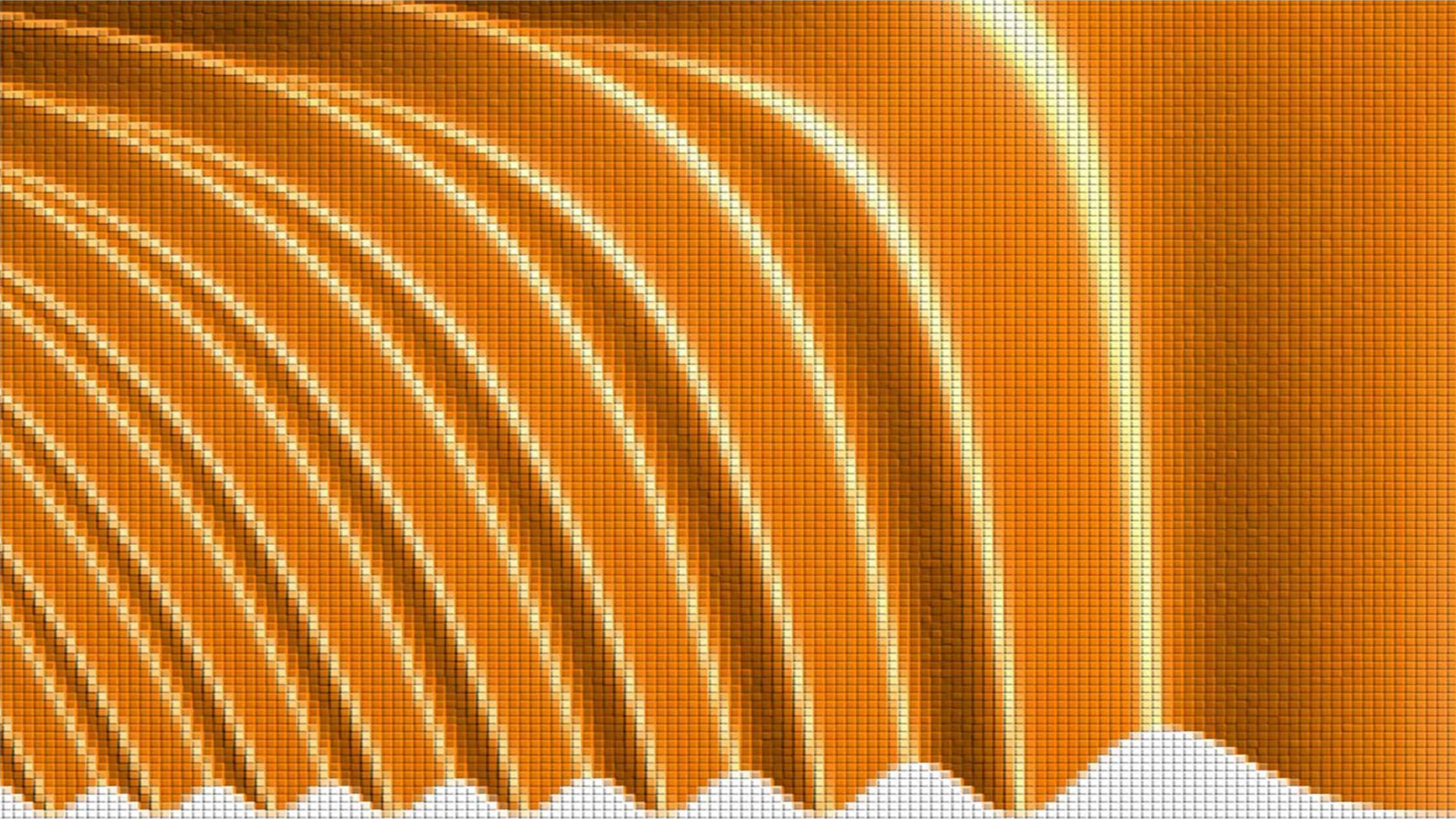
$$\Psi(\mathbf{r},t_o+\delta t)\simeq\Psi(\mathbf{r},t_o)+\left.\frac{\partial\Psi}{\partial t}\right|_{\mathbf{r},t_o}\delta t$$

that is, we can know the new wavefunction in space at the next instant in time

and we can continue on to the next instant

and so on

predicting all future evolution of the wavefunction

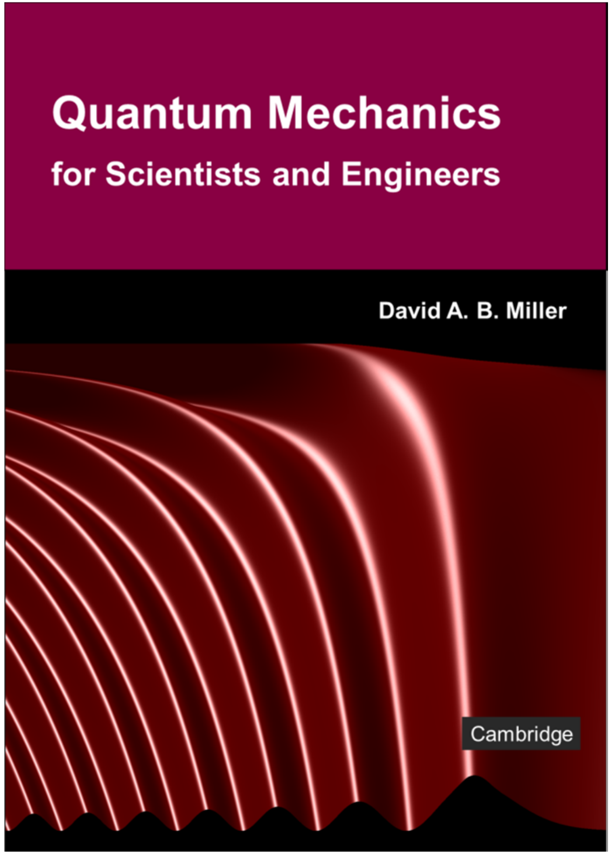


# 3.3 The time-dependent Schrödinger equation

Slides: Video 3.3.6 Linear superposition

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.4 – 3.5



# The time-dependent Schrödinger equation

## Linear superposition

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# Linearity of Schrödinger's equation

The time-dependent Schrödinger equation is linear in the wavefunction $\Psi$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r},t)\Psi(\mathbf{r},t)=i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$

One reason is that no higher powers of $\Psi$ appear anywhere in the equation

A second reason is that $\Psi$ appears in every term

there is no additive constant term anywhere

# Linearity of Schrödinger's equation

Linearity requires two conditions

obeyed by Schrödinger's time-dependent equation

1 - If $\Psi$ is a solution, then so also is $a\Psi$ , where $a$ is any constant

2 - If $\Psi_a$ and $\Psi_b$ are solutions, then so also is $\Psi_a + \Psi_b$

A consequence of these two conditions is that

$$\Psi_c(\mathbf{r},t) = c_a \Psi_a(\mathbf{r},t) + c_b \Psi_b(\mathbf{r},t)$$

where $c_a$ and $c_b$ are (complex) constants

is also a solution

# Linear superposition

The fact that

$$\Psi_c(\mathbf{r},t) = c_a \Psi_a(\mathbf{r},t) + c_b \Psi_b(\mathbf{r},t)$$

is a solution if $\Psi_a$ and $\Psi_b$ are solutions

is the property of

linear superposition

To emphasize

linear superpositions of solutions of the time-dependent Schrödinger equation

are also solutions

# Time-dependence and expansion in eigenstates

We know that

if the potential $V$ is constant in time

each of the energy eigenstates $\psi_n(\mathbf{r})$

with eigenenergy $E_n$

is separately a solution of the time-dependent Schrödinger equation

provided we remember to multiply by the right complex exponential factor

$$\Psi_n(\mathbf{r},t) = \exp(-iE_n t/\hbar)\psi_n(\mathbf{r})$$

# Time-dependence and expansion in eigenstates

Now we also know that the set of eigenfunctions of problems we will consider is a complete set

so the wavefunction at $t = 0$ can be expanded in them

$$\Psi(\mathbf{r},0) = \sum_n a_n \psi_n(\mathbf{r})$$

where the $a_n$ are the expansion coefficients

But we know that a function that starts out as $\psi_n(\mathbf{r})$

will evolve in time as $\Psi_n(\mathbf{r},t) = \exp(-iE_n t/\hbar)\psi_n(\mathbf{r})$

so, by linear superposition, the solution at time t is

$$\Psi(\mathbf{r},t) = \sum_n a_n \Psi_n(\mathbf{r},t) = \sum_n a_n \exp(-iE_n t/\hbar)\psi_n(\mathbf{r})$$

# Time-dependence and expansion in eigenstates

Hence, for the case where the potential V does not vary in time

$$\Psi(\mathbf{r},t) = \sum_n a_n \Psi_n(\mathbf{r},t) = \sum_n a_n \exp(-iE_n t/\hbar)\psi_n(\mathbf{r})$$

is the solution of the time-dependent equation

with the initial condition $\Psi(\mathbf{r},0) = \psi(\mathbf{r}) = \sum_n a_n \psi_n(\mathbf{r})$

Hence, if we expand the wavefunction at time $t = 0$ in the energy eigenstates

we have solved for the time evolution of the state just by adding up the above sum