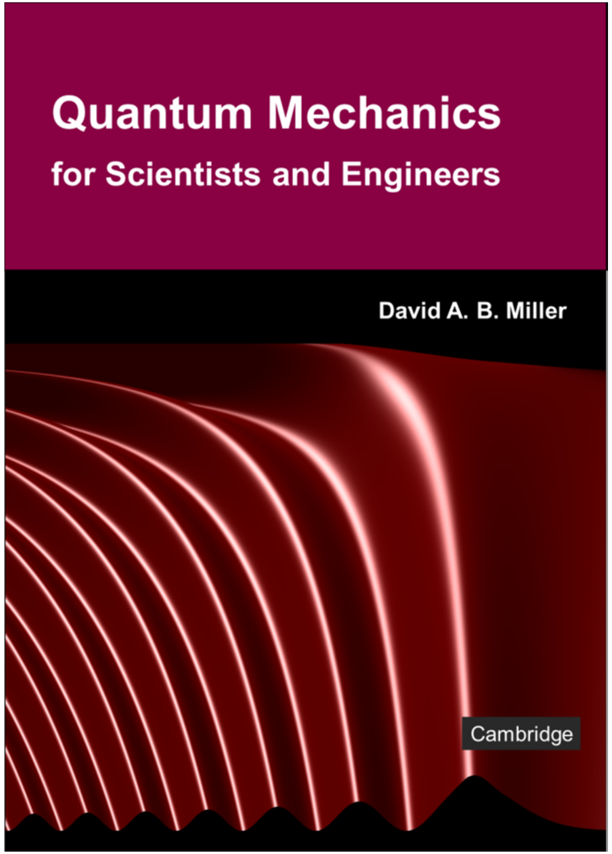
4.2 Wavepackets

Slides: Video 4.2.1 Introduction to wavepackets

Text reference: Quantum Mechanics for Scientists and Engineers

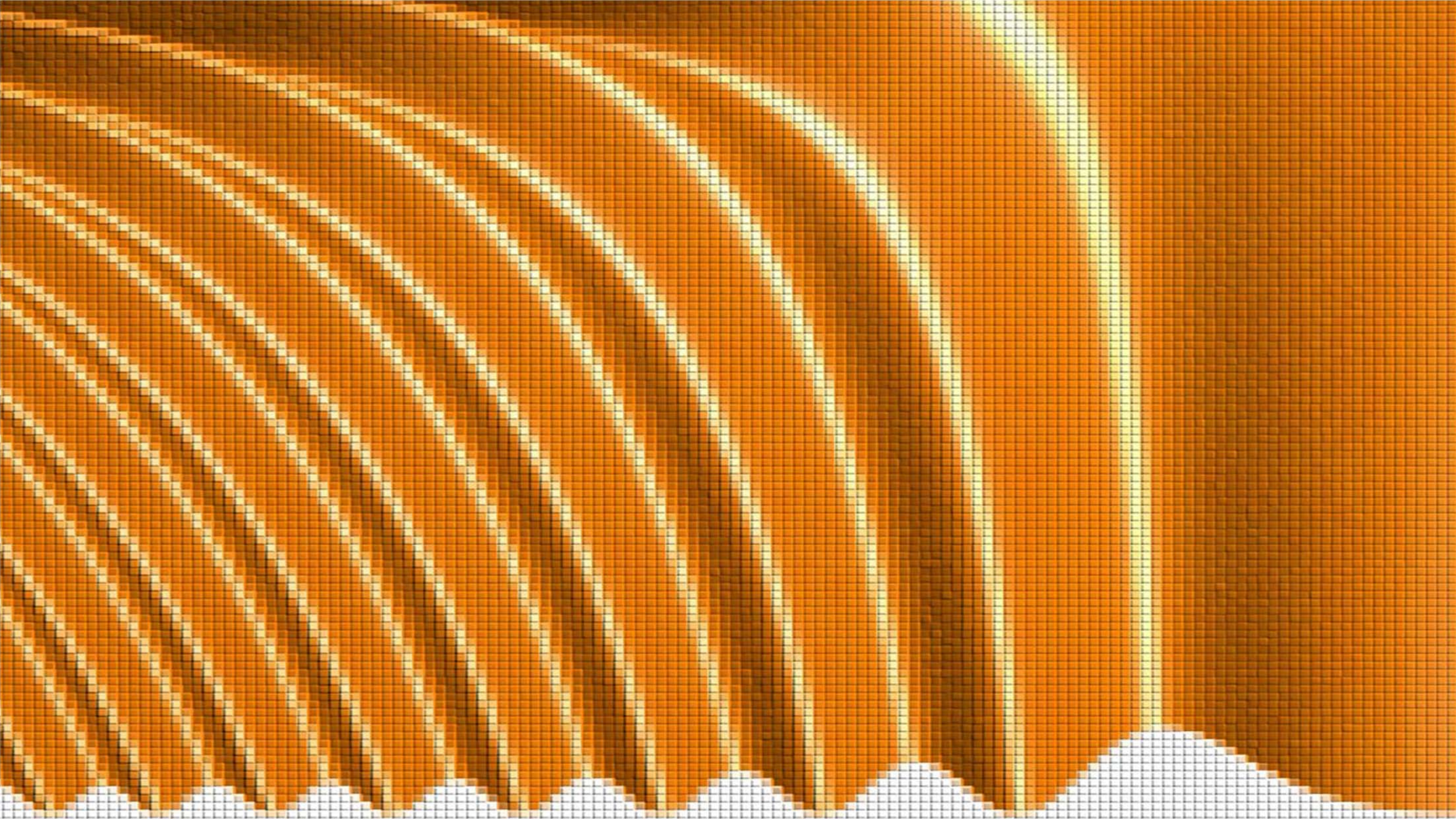
Section 3.7 introduction



Wavepackets

Quantum mechanics for scientists and engineers

David Miller

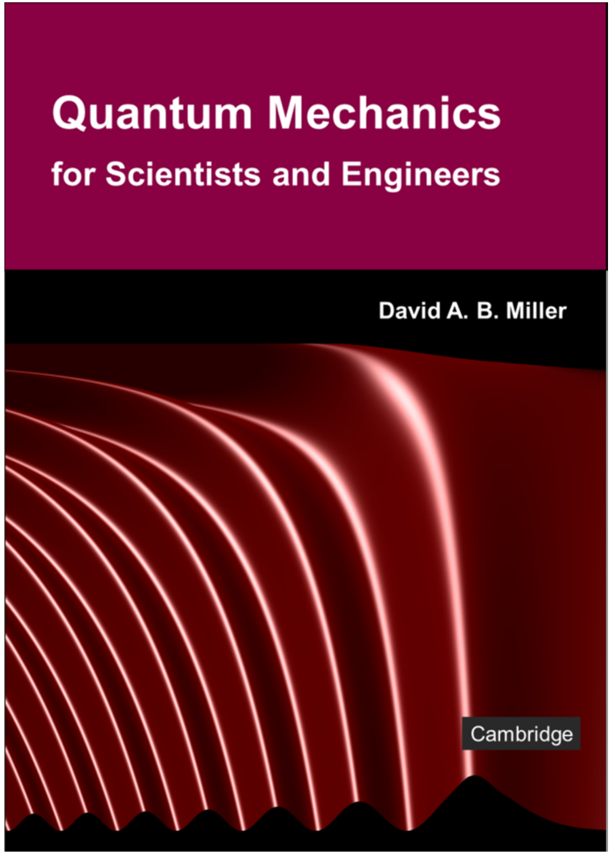


4.2 Wavepackets

Slides: Video 4.2.2 Group velocity

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.7 (“Group velocity” first part)



Wavepackets

Group velocity

Quantum mechanics for scientists and engineers

David Miller

Group velocity

Consider two waves at different frequencies ω_1 and ω_2

and suppose that the wave velocity v is the same independent of frequency

Then the corresponding wavevector magnitude

$$k = \omega / v$$

is the same for both waves

i.e., $k_1 = \omega_1 / v \qquad k_2 = \omega_2 / v$

Group velocity

If we take two such waves

of equal amplitudes

and add them together

then we get

spatial beats

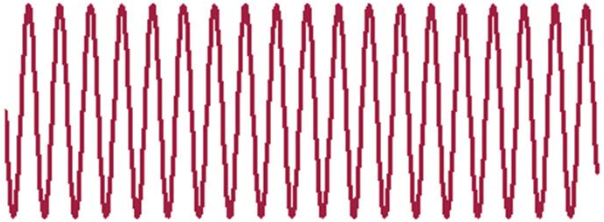
a "spatial envelope"

The "envelope" moves at the same speed as the wave

here we chose $v = 1$ for illustration

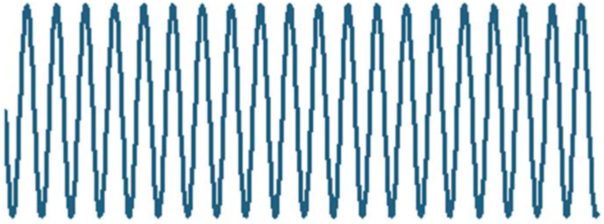
$\omega_1 = 0.4$

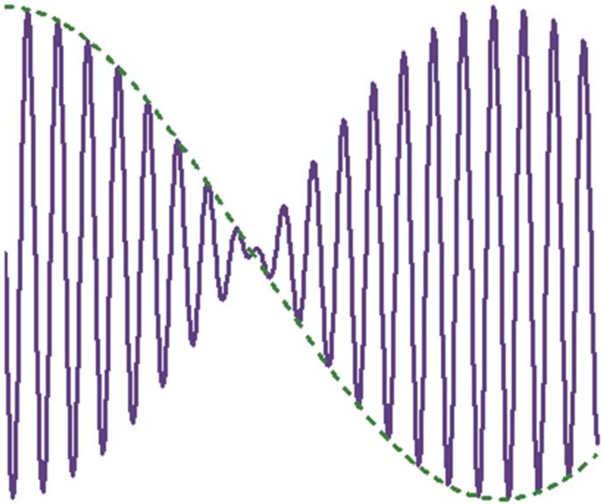
$k_1 = 0.4$



$\omega_2 = 0.425$

$k_2 = 0.425$





Group velocity

Algebraically, for two waves at different frequencies

one at frequency $\omega+\delta\omega$ and wavevector $k+\delta k$

one at frequency $\omega-\delta\omega$ and wavevector $k-\delta k$

using complex exponential waves, we get a total wave

$$f(z,t)$$

$$=\exp\left\{-i\left[(\omega+\delta\omega)t-(k+\delta k)z\right]\right\}+\exp\left\{-i\left[(\omega-\delta\omega)t-(k-\delta k)z\right]\right\}$$

$$=\exp\left[-i(\omega t-kz)\right]\left\{\exp\left[-i(\delta\omega t-\delta kz)\right]+\exp\left[+i(\delta\omega t-\delta kz)\right]\right\}$$

$$=2\cos(\delta\omega t-\delta kz)\exp\left[-i(\omega t-kz)\right]$$

Group velocity

The algebraic form

$$f\left(z,t\right)=$$

$$2\cos(\delta\omega t-\delta kz)\exp\left[-i\left(\omega t-kz\right)\right]$$

describes a cosine envelope

multiplying the wave

(here we show the real part)

Note here, because $k=\omega/v$ and $v=\omega/k$

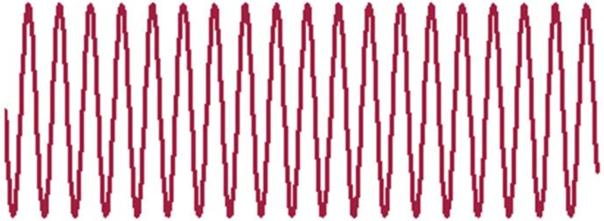
then $\delta k=\delta\omega/v$ and $v=\delta\omega/\delta k$

so the envelope and the wave

move at the same speed

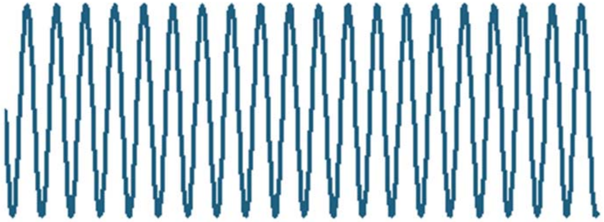
$\omega_1=0.4$

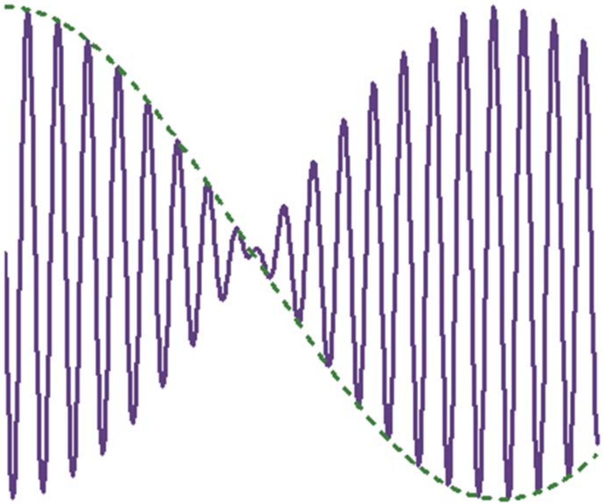
$k_1=0.4$



$\omega_2=0.425$

$k_2=0.425$





Group velocity

But suppose the wave velocity is different for different frequencies

e.g., suppose the higher frequency wave has a slower velocity

so a more than proportionately larger k

Then the “envelope velocity”

$$v_g = \delta\omega / \delta k$$

which we will call the **group velocity**

is not the same as the underlying wave velocity

Group velocity

If the higher frequency wave has a lower wave velocity, e.g.,

$$v_2 = \frac{\omega_2}{k_2} = \frac{0.425}{0.4375} = \frac{34}{35} \simeq 0.97$$

then the "envelope" moves at

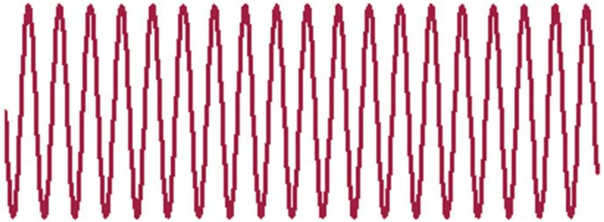
$$v_g = \delta\omega / \delta k \equiv 0.025 / 0.0375 = 2/3$$

The underlying wave moves at the average speed

$$\frac{\omega_1+\omega_2}{2} \Bigg/ \frac{k_1+k_2}{2} = \frac{\omega_1+\omega_2}{k_1+k_2} = \frac{66}{67} \simeq 0.985$$

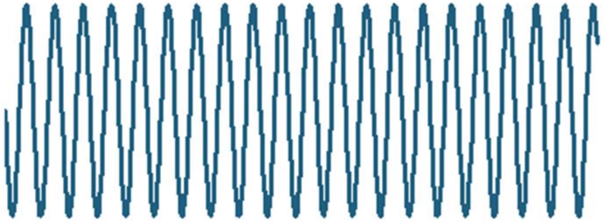
$\omega_1 = 0.4$

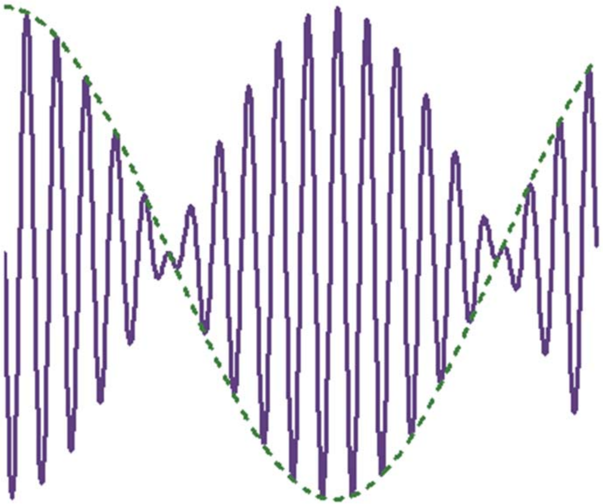
$k_1 = 0.4$



$\omega_2 = 0.425$

$k_2 = 0.4375$





Group velocity and phase velocity

We define group velocity as the limit as δk and $\delta\omega$ go to zero

$$v_g = \frac{d\omega}{dk}$$

This concept applies generally for the effective velocity of pulses or "wavepackets" in dispersive media

For clarity, we call

$$v_p = \frac{\omega}{k}$$

for a given frequency ω

the "phase velocity"

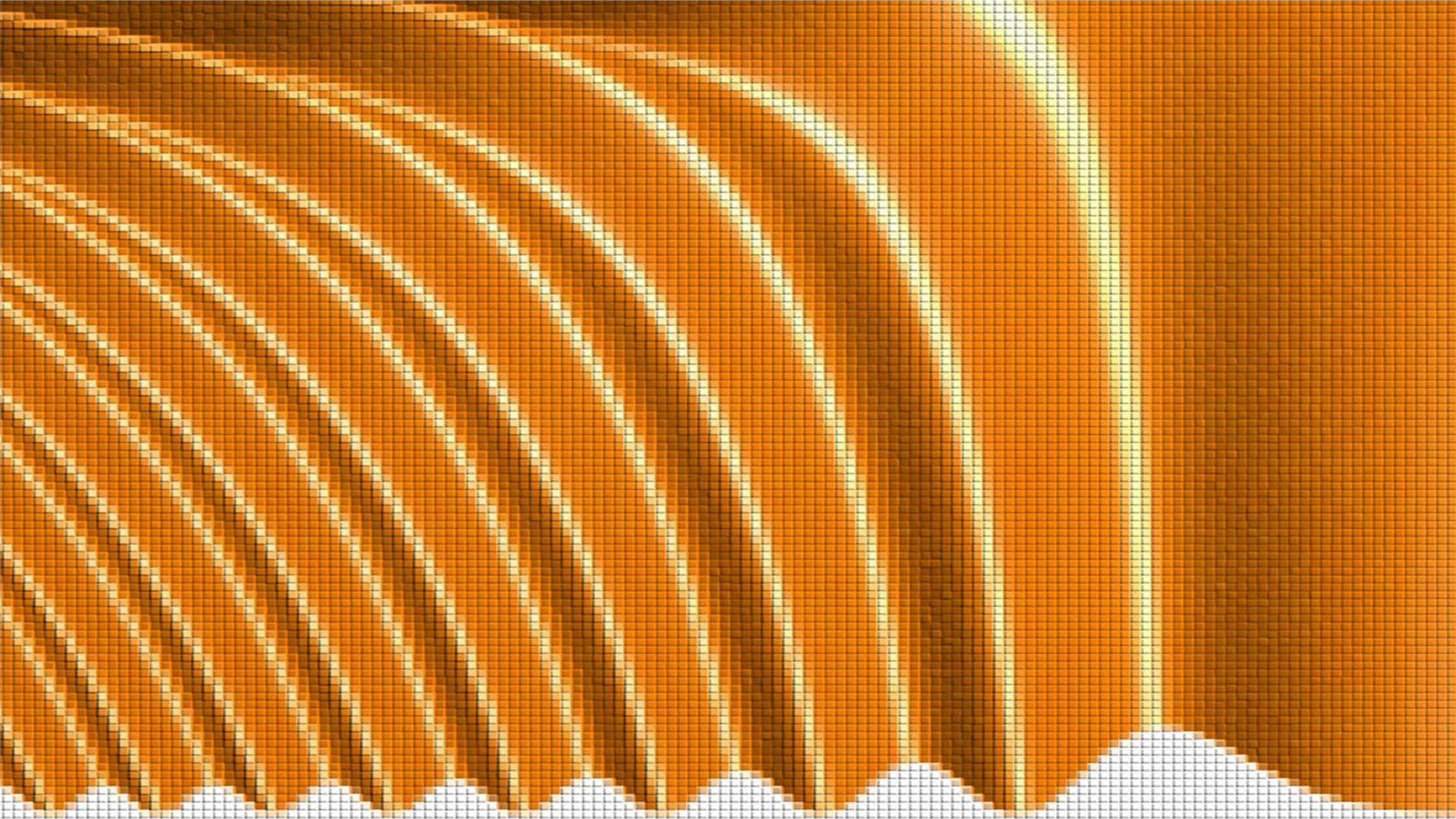
Group velocity and phase velocity

$$v_g = \frac{d\omega}{dk}$$

group velocity

$$v_p = \frac{\omega}{k}$$

phase velocity

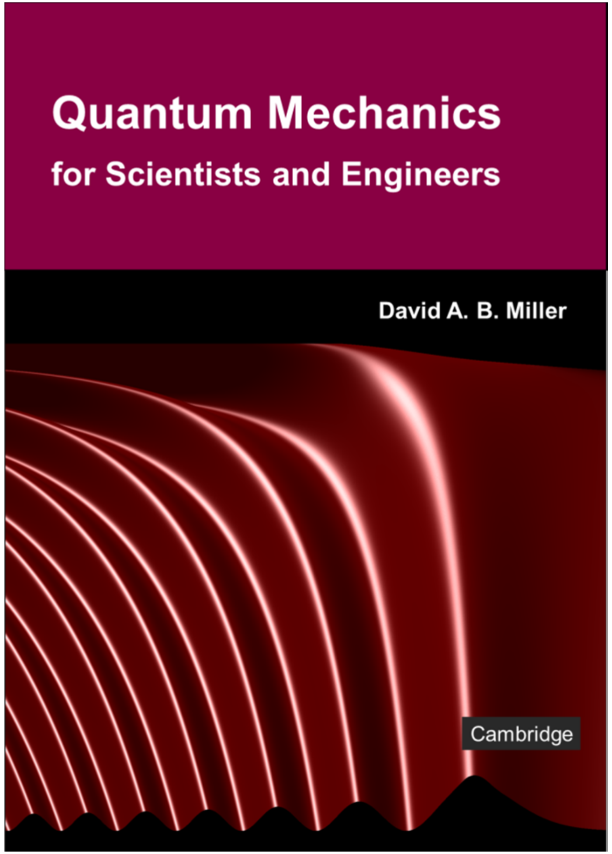


4.2 Wavepackets

Slides: Video 4.2.4 Group velocity for a free electron

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.7 (“Group velocity” second part)



Wavepackets

Group velocity for a free electron

Quantum mechanics for scientists and engineers

David Miller

Group velocity in optics

The small dispersion in glass gives significant effects in long fibers

Large dispersions are found near absorption lines

In waveguides, different spatial forms (modes) propagate at different velocities

- dispersion from geometry or structure

Any structure whose physical properties

- such as refractive index
  - change on a scale comparable with a wavelength
    - will also show strong "structural" dispersion

Group velocity for a free electron

For a free electron

the frequency ω is not proportional to the wavevector magnitude k

For a free electron,

i.e., one for which the potential $V(z)=0$

in one direction z the Schrödinger equation is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dz^2}=E\psi$$

with solutions $\psi(z)\propto\exp(\pm ikz)$ and $E=\dfrac{\hbar^2k^2}{2m}$

Group velocity for a free electron

But this means that

$$\omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}$$

so

$$\omega \propto k^2$$

not $\omega \propto k$

So the free electron group velocity is

$$v_g = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} = \frac{\hbar k}{m} = \sqrt{\frac{\hbar^2 k^2}{m^2}} = \sqrt{\frac{2}{m}\frac{\hbar^2 k^2}{2m}} = \sqrt{\frac{2E}{m}}$$

Group velocity of a free electron

This group velocity $v_g = \sqrt{\dfrac{2E}{m}}$

does give us $E = \dfrac{1}{2} m v_g^2$

which corresponds with our classical ideas of velocity and kinetic energy

This suggests it is meaningful to think of the electron as moving at the group velocity

Phase velocity and energy

Note that the phase velocity $v_p = \omega / k$ does not give us this kind of relation

With $E \equiv \hbar\omega = \hbar^2 k^2 / 2m$, we have $\dfrac{\omega}{k} \equiv v_p = \dfrac{\hbar k}{2m}$

i.e.,

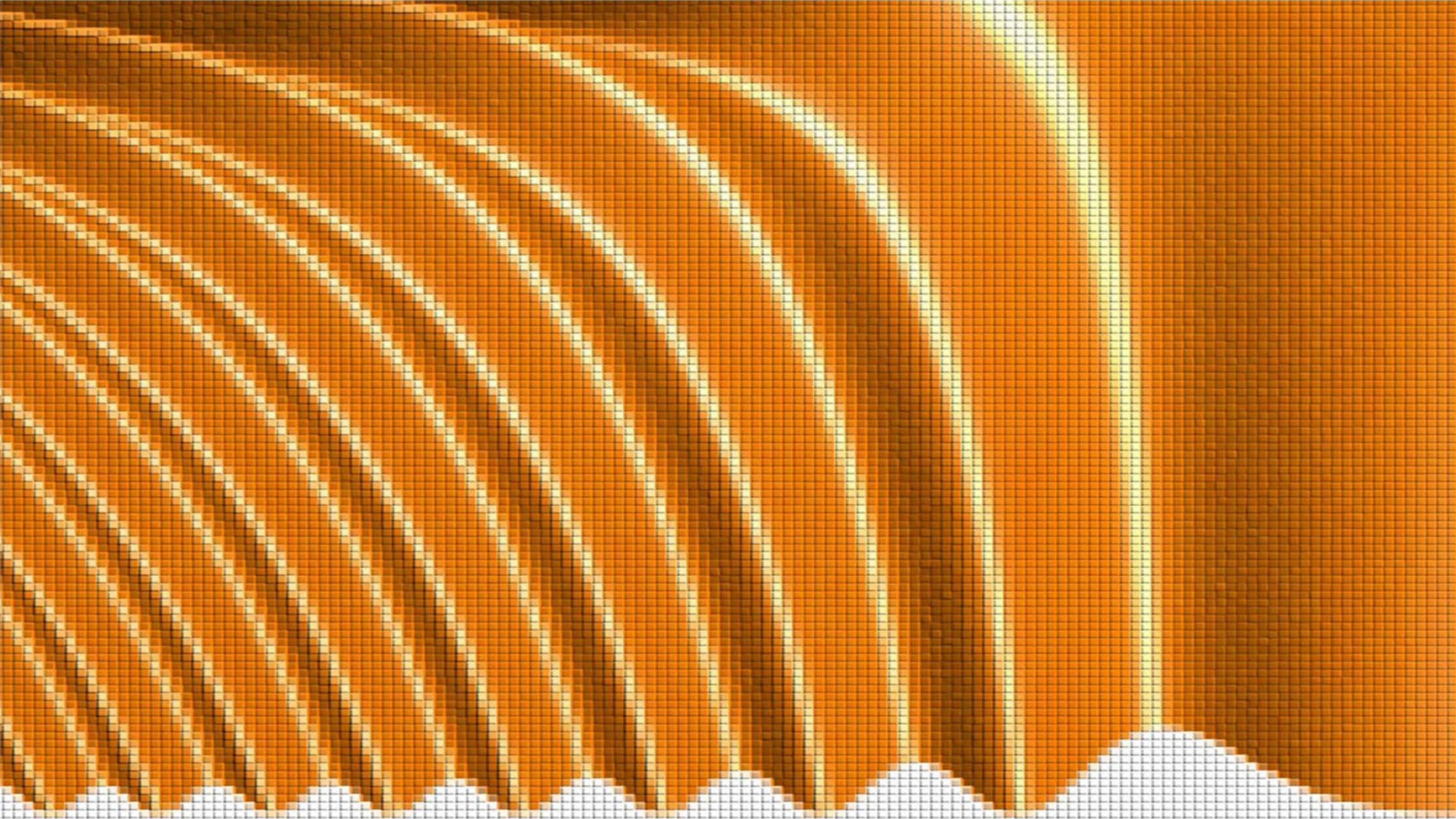
$$v_p^2 = \left(\frac{\hbar k}{2m}\right)^2 = \frac{1}{2m}\frac{\hbar^2 k^2}{2m} = \frac{1}{2m}E$$

i.e.,

$$E = 2mv_p^2$$

which does nor correspond to the classical relation between energy and velocity

The electron does not move at the phase velocity

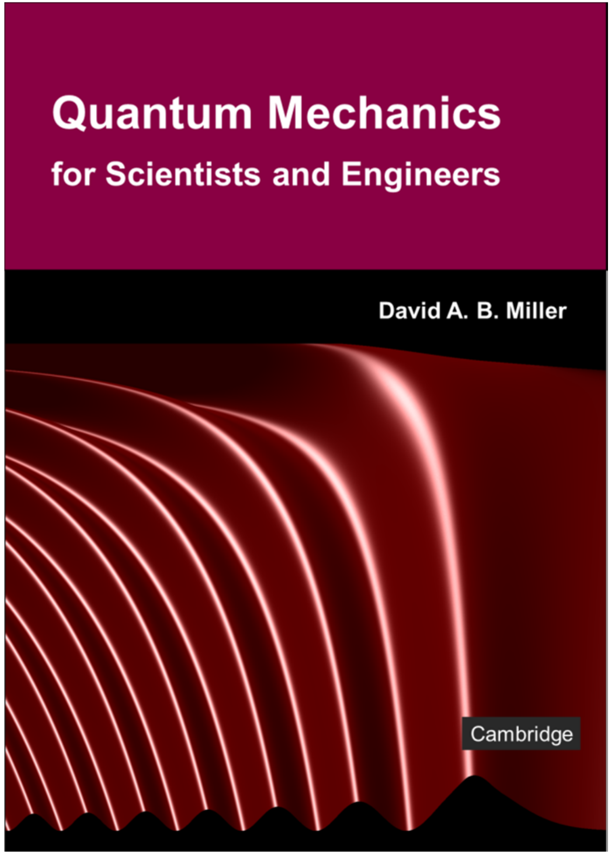


4.2 Wavepackets

Slides: Video 4.2.6 Electron wavepackets

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.7 ("Examples of motion of wavepackets")



Wavepackets

Electron wavepackets

Quantum mechanics for scientists and engineers

David Miller

Constructing a wavepacket

We can construct a "wavepacket" by putting together a linear superposition of energy eigensolutions

For a free electron or a similar particle of mass m

the individual eigensolutions are plane waves

For propagation in the z direction, these are of the form

$$\Psi_k(z,t) \propto \exp\left\{-i\left[\frac{E(k)}{\hbar}t - kz\right]\right\} = \exp\{-i[\omega(k)t - kz]\}$$

for some chosen value of k, and hence of

energy $E(k) = \dfrac{\hbar^2 k^2}{2m}$ and frequency $\omega(k) = \dfrac{E(k)}{\hbar}$

Constructing a wavepacket

Since

a linear superposition of such plane wave solutions of the time-dependent Schrödinger equation

is also a solution

we can have a "wavepacket"

$$\Psi_{WP}(z,t) \propto \sum_k a_k \Psi_k(z,t) = \sum_k a_k \exp\left\{-i\left[\omega(k)t - kz\right]\right\}$$

for some set of values of k in our sum

and some chosen amplitudes a_k for each such plane wave

Gaussian wavepacket

One convenient and useful set of k values and amplitudes a_k to choose is

a set of equally spaced k values

with Gaussian amplitudes or "weights" for a_k

$$\Psi_G(z,t) \propto \sum_k \exp\left[-\left(\frac{k-\bar{k}}{2\Delta k}\right)^2\right]\exp\left\{-i\left[\omega(k)t-kz\right]\right\}$$

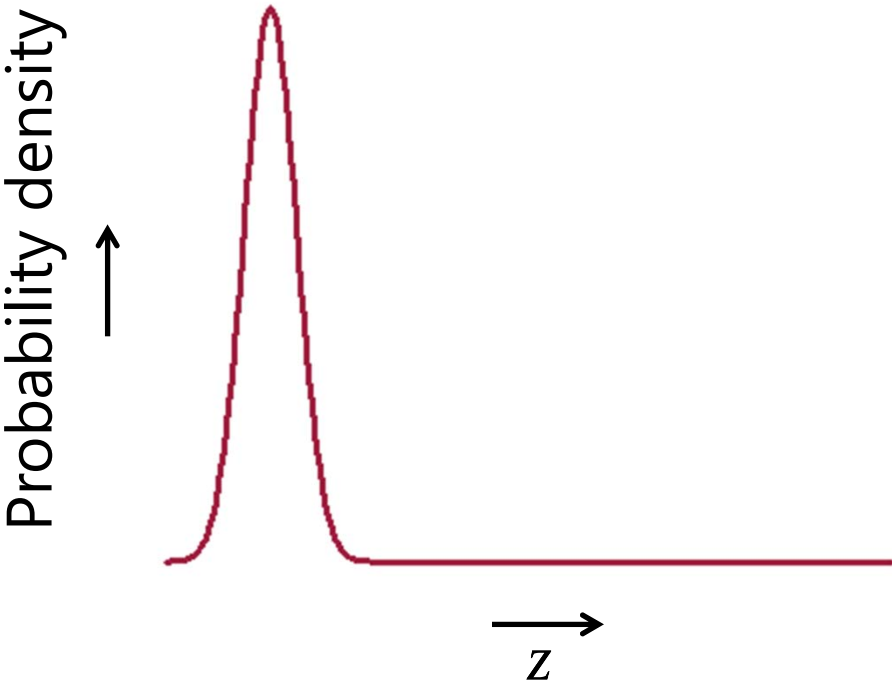
Here $\bar{k}$ is the center of the distribution of k values

Δk is a width parameter for the Gaussian function

Note this gives a "pulse" that is also Gaussian in space

Gaussian wavepacket

- Our Gaussian wavepacket is also Gaussian in space
  - As we let time evolve
    - simply adding up the terms in our wavepacket sum at each time
      - we can see the wavepacket propagate
        - moving to the right
          - and getting wider



Gaussian wavepacket

A wavepacket that increases in width as it propagates

is said to be "dispersing"

It gets wider because

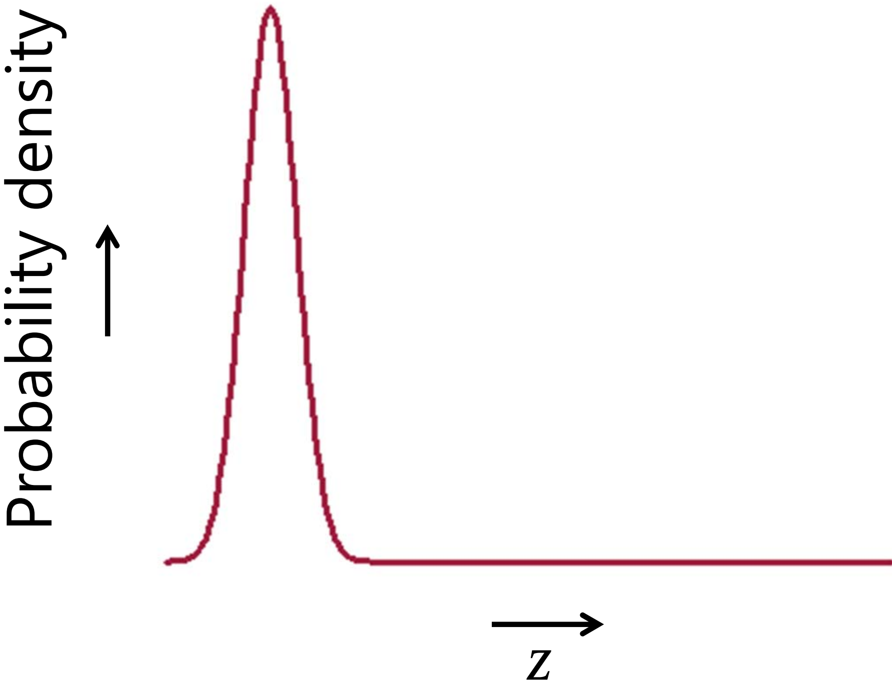
the change in ω with k

is not even linear

(here it is quadratic)

an effect known as

group velocity dispersion



Wavepacket at a barrier

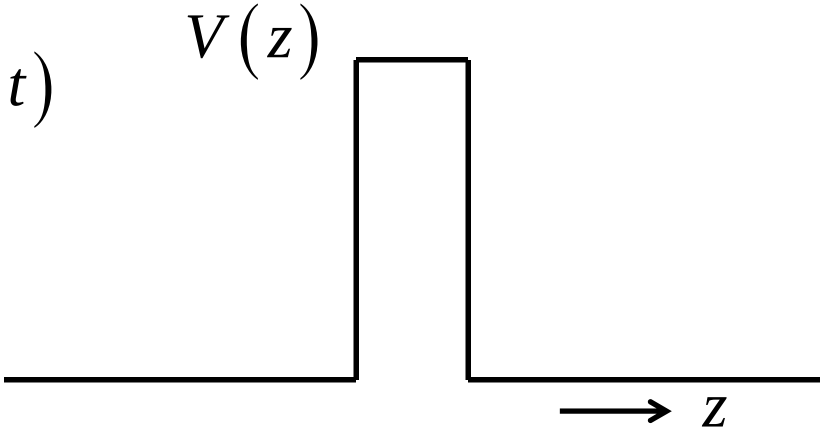
Suppose we want to understand a wavepacket hitting a barrier from the left

We proceed in the same way

but now we use

a superposition of the energy eigenfunctions $\Psi_{Bk}(z,t)$ of the Schrödinger equation

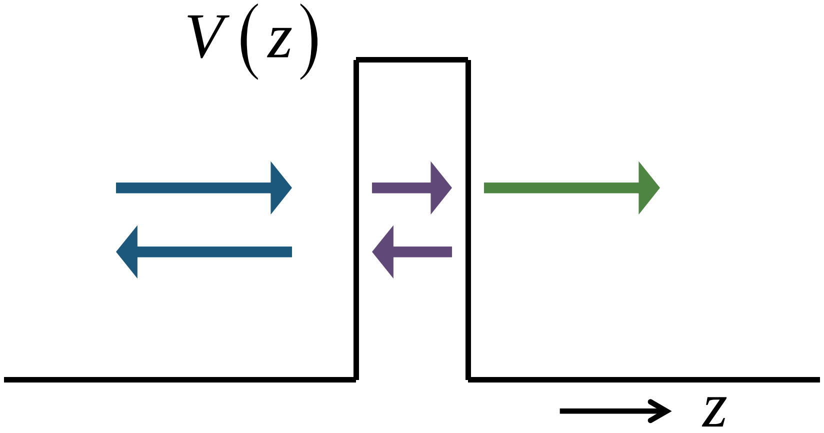
with a barrier potential $V(z)$



Eigensolutions with a barrier

The energy eigensolutions $\Psi_{Bk}(z,t)$

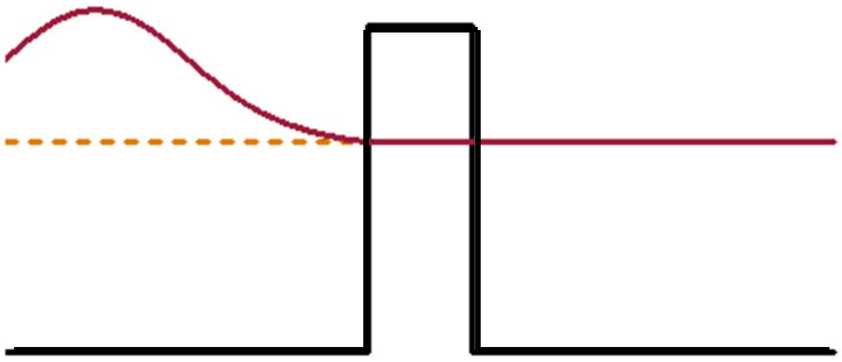
- for a particle incident from the left are
  - forward and backward propagating waves on the left
  - "forward" and "backward" exponentials inside the barrier
  - forward propagating waves on the right



Wavepacket at a barrier

Constructing a Gaussian-weighted linear superposition of solutions

- with equally-spaced k-values on the left
  - here centered round the k-value corresponding to the dashed orange line
    - gives an approximately Gaussian "pulse" on the left to start with



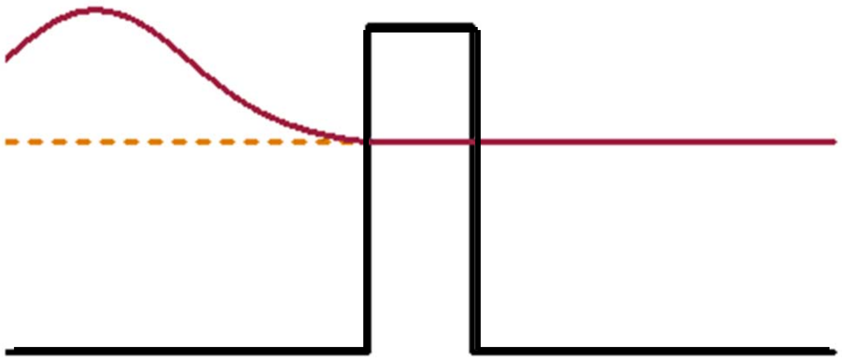
Wavepacket at a barrier

Now as time evolves, the "pulse" moves to the right

- where it partially bounces off
  - and partially transmits

Note that there is a significant probability of

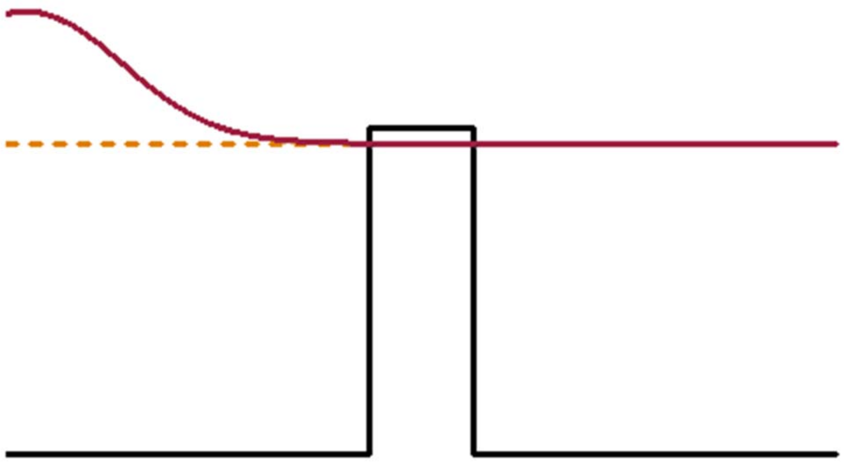
- finding the particle in the barrier
  - while the pulse is "hitting" it



Wavepacket at a barrier

With the particle incident at a higher average energy

- the transmitted pulse is stronger
- and the reflected pulse is weaker



Wavepacket at a barrier

Even with energies above the barrier

- there is still significant reflection of the pulse
  - wave are generally reflected off of any changes in the potential