Quantum Physics 1

2015-2016

Lectures of the 3rd and 4th week of the course

Question about anything till now (lectures, problem sets)?

At start of 2nd lecture this week:
Quick test/check and reminders mid-term exam

Homework for week 3 of the course

Study: **Chapters 2 and 3,**
emphasis on sections 2.4, 3.1, 3.2, 3.6
and Eqs. [2.111]-[2.113] (Dirac delta function in Sec. 2.5,)
(2.1, 2.2, 2.3 was last week)

See **http://www.quantumdevices.nl/teaching/**

Problems:

To be made <u>before</u> the tutorial session
Chapter 2 - 2.18, 2.19, and 2.21
Chapter 3 - 3.1, 3.3, and 3.22

Slides for week 3 and 4:

1. Dirac delta function
2. Fourier basics
3. Role Fourier in quantum mechanics
4. Dirac notation

And also this or next week (not for midterm exam):

5. Group and phase velocity of wave packets
6. Research examples particle in a box

What on these slides should you know for the mid-term exam?

The set of slides includes the topics:

- **the Dirac delta function**
- **the Fourier transform and its role in quantum physics**
- **basics of wave packets**
- **Dirac notation**

This is part of week 3 (and must be known for the midterm exam).

These topics are also needed for problem W3.1.

Some topics on these slides are presented in week 4 (not for mid term exam). These are:

- **group velocity and phase velocity for wave packets (and any wave phenomenon),**
- **some research topics related to a particle-in-a-box system**

Delta function

Kronecker delta

(Eq. [2.31] in Griffiths book)

$$\boxed{\delta_{nm} = \begin{cases} 1 \ , \ for \ \ n = m \\ 0 \ , \ for \ \ n \neq m \end{cases}}$$

Dirac-delta function δ(x)

Fourier transformation

....same as from the course that introduced Fourier Theory

(this was in recent years the course *Calculus 3* or *Mathematical Physics*)

Dirac-delta function δ(x)

$$\boxed{\delta(x)=\lim_{\varepsilon\to 0}\begin{cases}0, & |x|>\dfrac{\varepsilon}{2}\\[2ex] \dfrac{1}{\varepsilon}, & |x|\le\dfrac{\varepsilon}{2}\end{cases}}$$

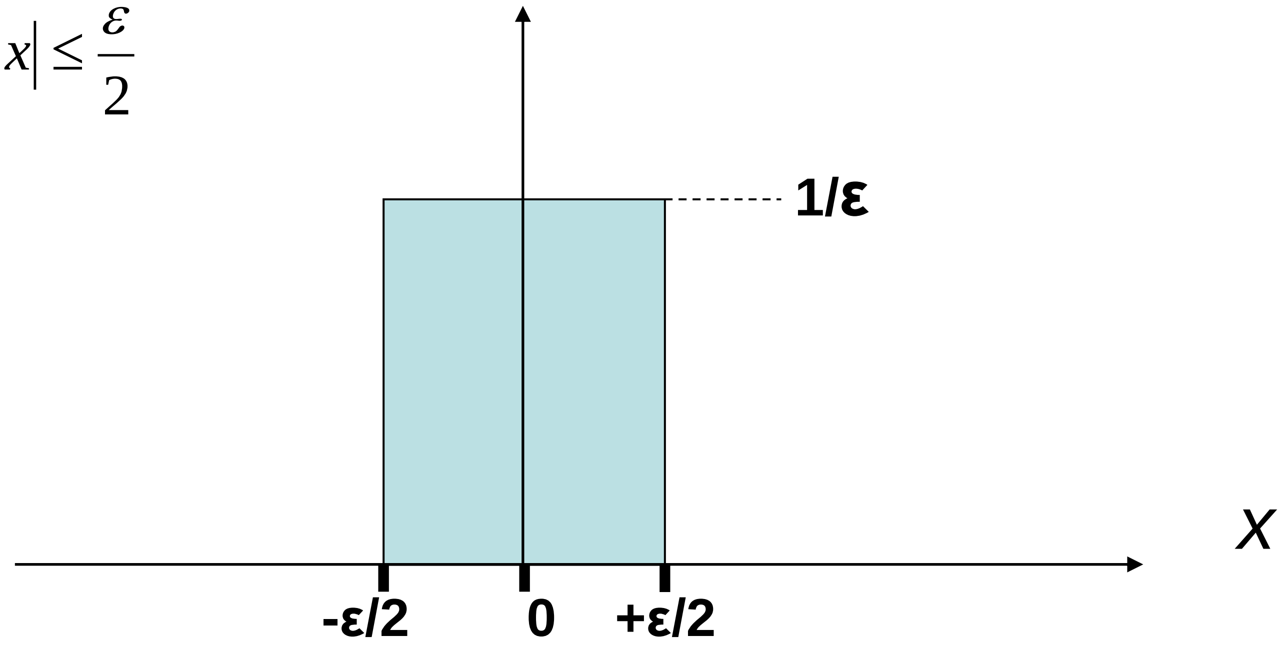
$$\boxed{\int_{-\infty}^{\infty}\delta(x)\,dx=1}$$

$$\boxed{\int_{-\infty}^{\infty}f(x)\delta(x-a)\,dx=f(a)}$$

Dirac-delta function δ(x) from block function

$$\delta(x)=\lim_{\varepsilon\to 0}\begin{cases}0, & |x|>\dfrac{\varepsilon}{2}\\[2ex] \dfrac{1}{\varepsilon}, & |x|\le\dfrac{\varepsilon}{2}\end{cases}$$

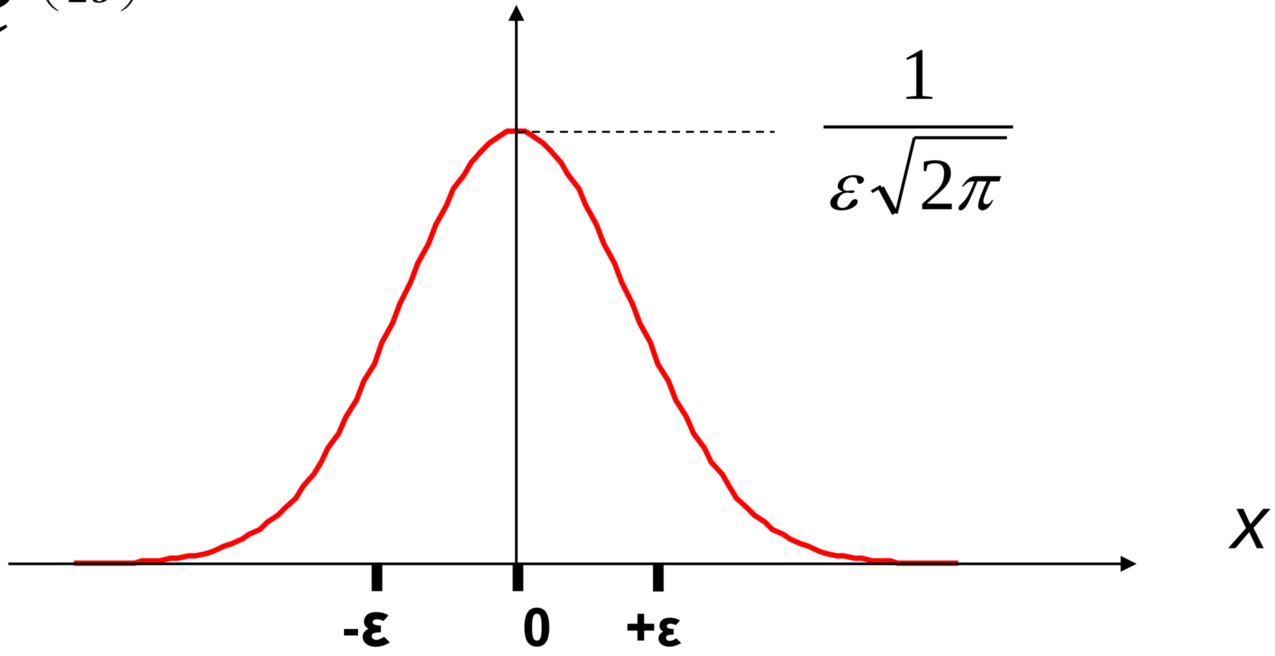
$$\boxed{\int_{-\infty}^{\infty}\delta(x)\,dx=1}$$



Dirac-delta function δ(x) from a Gaussian

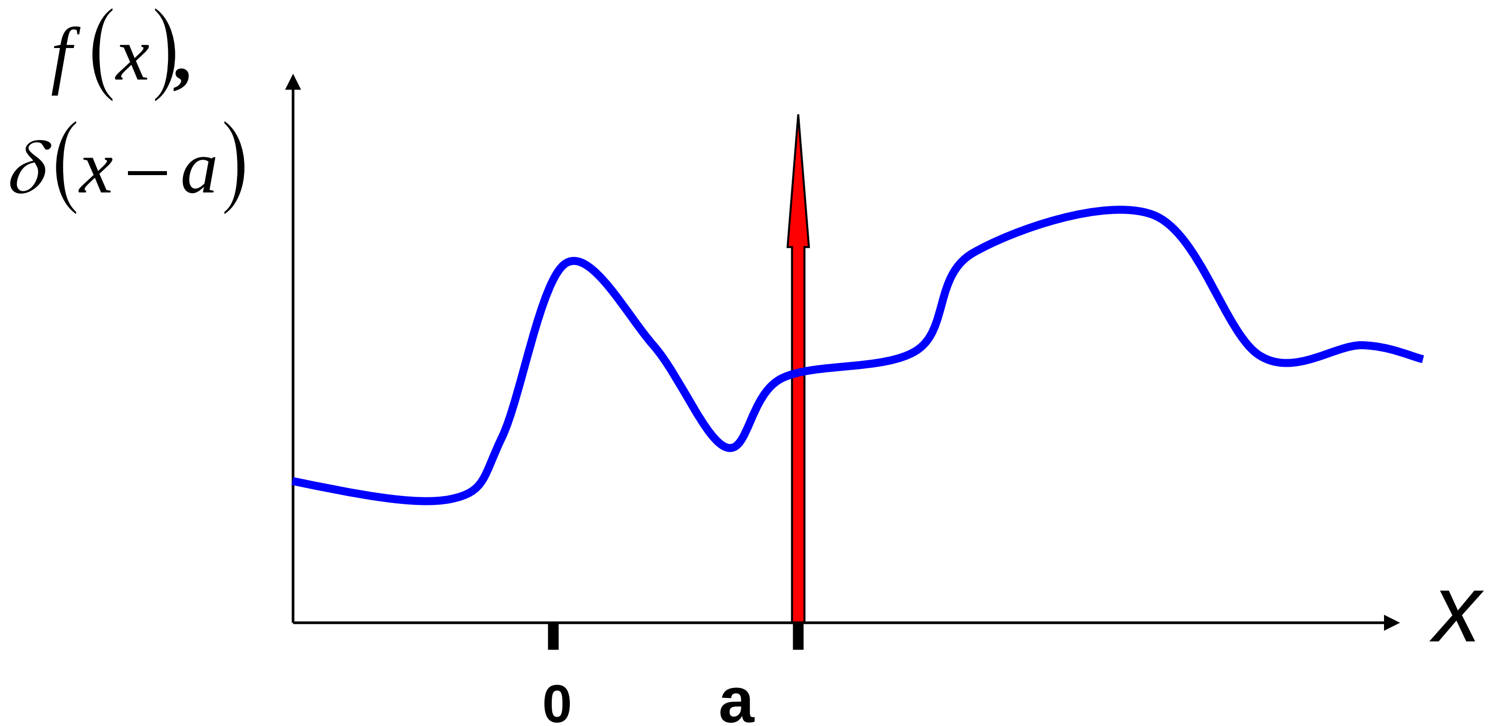
$$\delta(x) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon\sqrt{2\pi}} e^{-\left(\frac{x}{2\varepsilon}\right)^2}$$

$$\boxed{\int_{-\infty}^{\infty} \delta(x)\,dx = 1}$$



Dirac-delta function δ(x)

$$\int_{-\infty}^{\infty} f(x)\delta(x-a)\,dx = f(a)$$



Dirac-delta function δ(x)

$$\int_{-\infty}^{\infty} \delta(x-a)\,\delta(x-a)\,dx = \delta(a-a) = \delta(0) = \infty$$

Wave functions in the form of a Dirac delta function cannot be normalized.

The fact that a wave functions $\delta(x\text{-}a)$ cannot be normalized, is because in quantum mechanics the uncertainty Δx in the position of the particle can never be really zero (see also Griffiths near Eqs. [2.90]-[2.99]). Physically, the state $\delta(x\text{-}a)$ cannot exist. However, the Dirac delta function is a very useful mathematical tool for calculations with wave functions. The same is true for plane waves as in Griffiths near Eqs. [2.90]-[2.99], [3.32]-[3.35] and Liboff p. 72, that run by definition from -∞ to +∞, and which also do not exist in practice.

Fourier

In the lecture, first ask students to work out a regular inner product for 2 simple 3D vectors.

Goal for today:

At the end of this lecture, these equations should be very familiar and natural to you

$$x(t) \overset{\mathfrak{F}}{\leftrightarrow} X(\omega)$$

$$x(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} X(\omega)\, d\omega$$

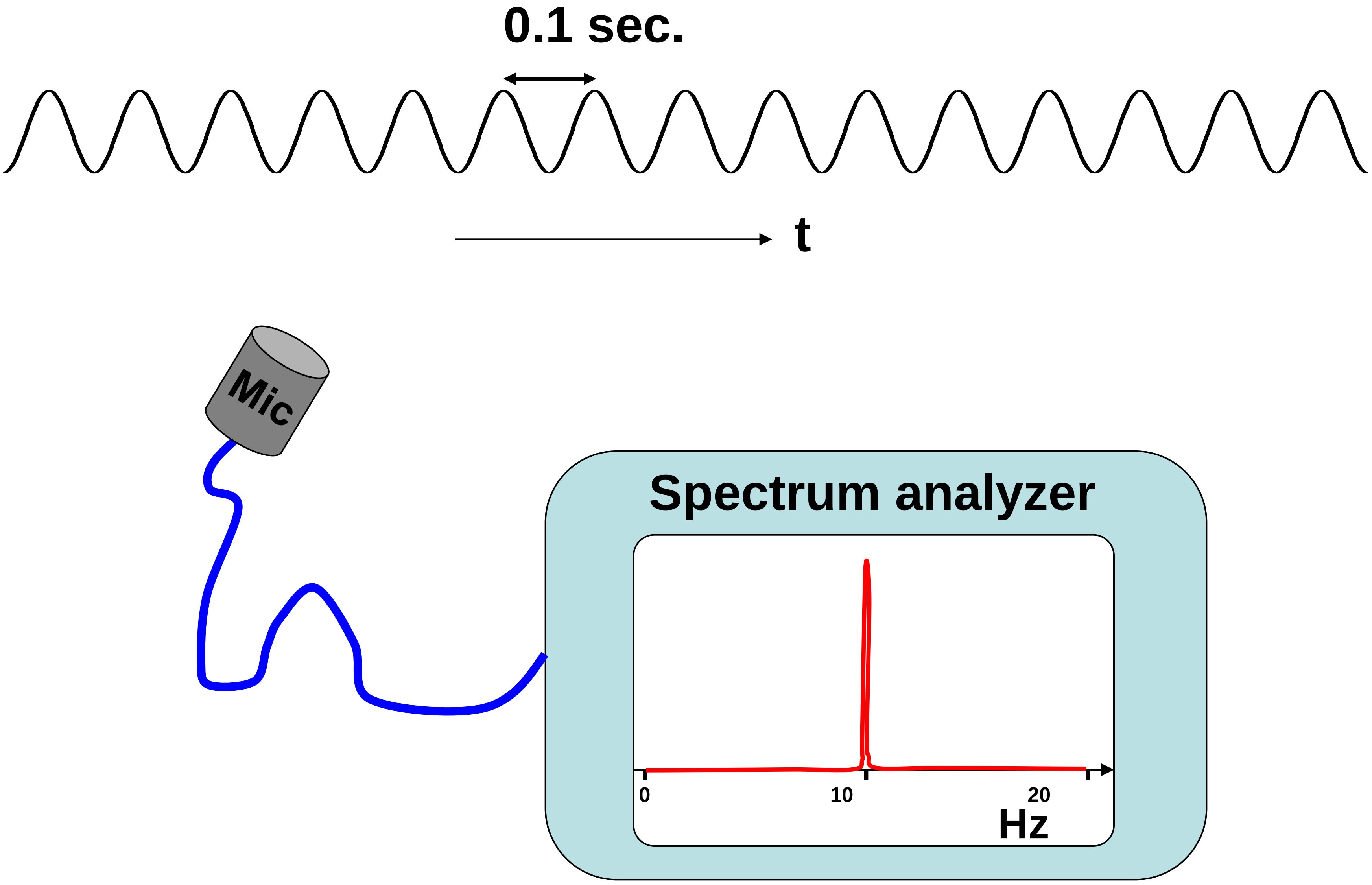
$$X(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} x(t)\, dt$$

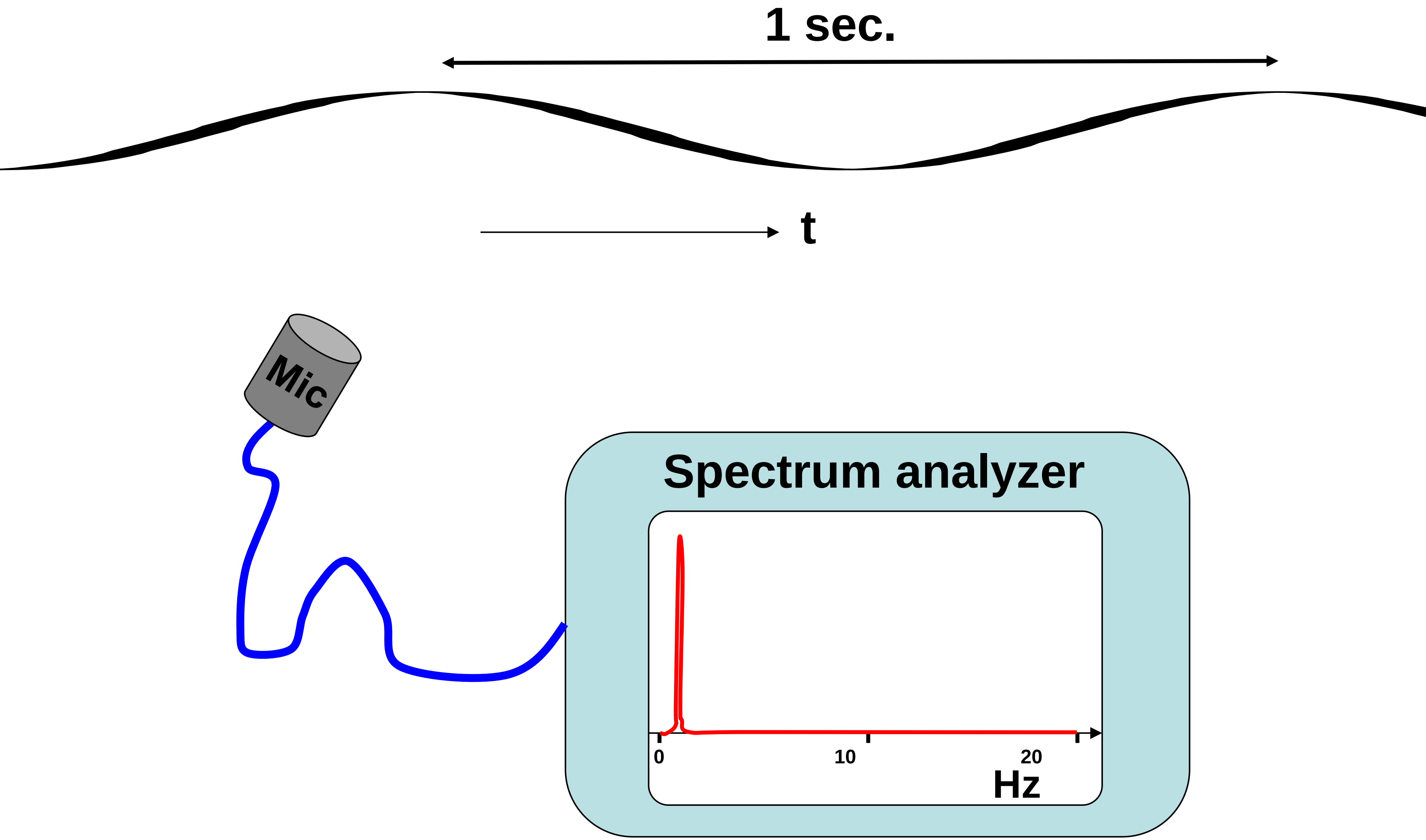
Tutorial on Fourier theory

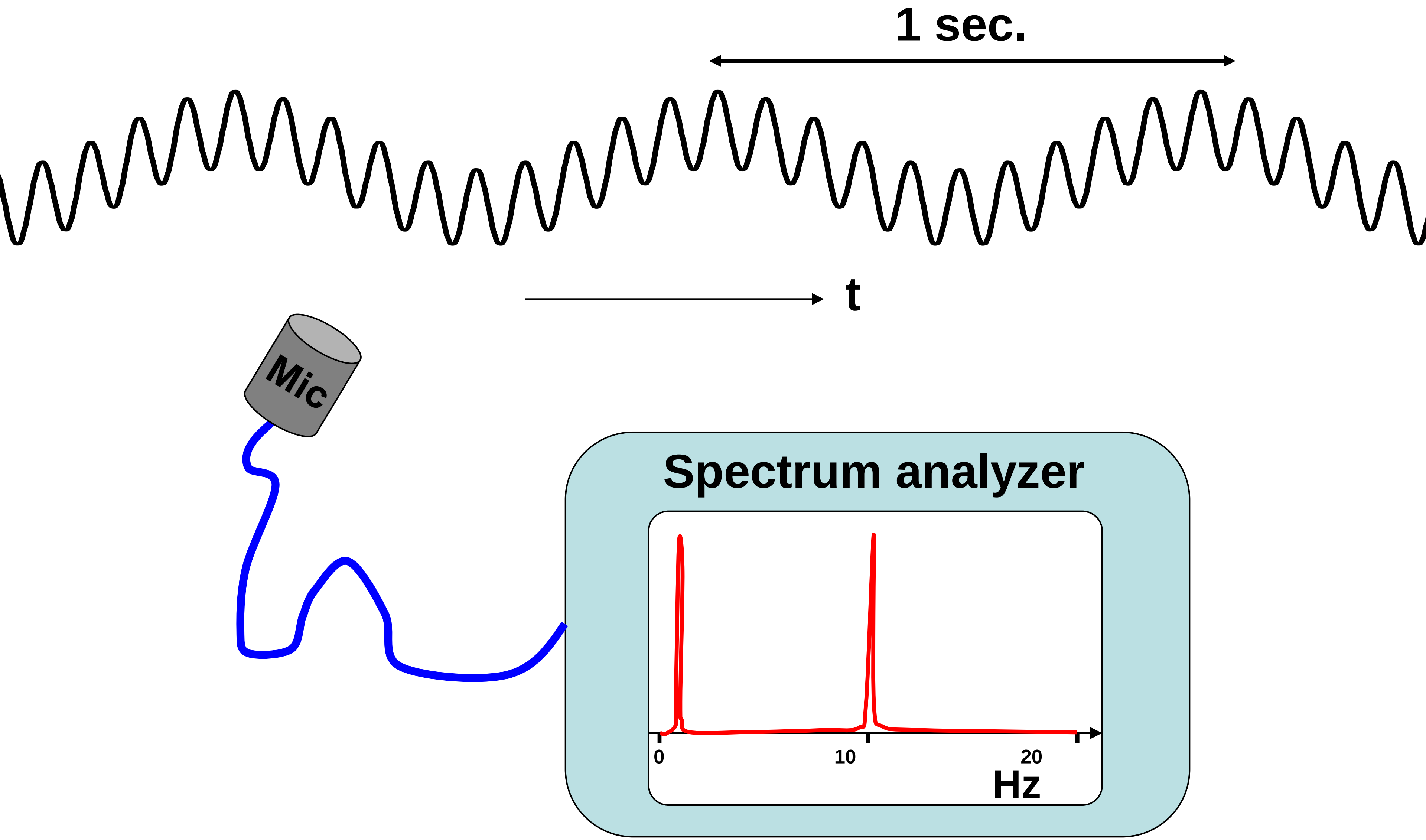
and its role in quantum mechanics

FOURIER IS VERY WIDELY USED IN PHYSICS

First very basic:




1 sec.
t
Mic
Spectrum analyzer
0
10
20
Hz


1 sec.
t
Mic
Spectrum analyzer
0
10
20
Hz

Idea behind Fourier transformation:

Every physical signal as a function of time can be written in a unique (and therefore invertible) manner as a linear combination of sines and cosines of various frequencies.
Thus, it can be represented as a amplitude-spectrum and a phase-spectrum.

$$x(t) = \sum_{\omega} A_{\omega} \cos(\omega t) + B_{\omega} \sin(\omega t)$$

$$= \sum_{\omega} C_{\omega} \cos(\omega t + \phi_{\omega})$$

$$\text{with} \quad \omega = 2\pi f$$

“Physical signal ” means continuous, differentiable, integrable from –∞ to +∞.

But then we also must have:

Every physical signal as a function of frequency can be written in a unique (and therefore invertible) manner as a linear combination of sines and cosines of various dependencies on time.

Paired variables with a Fourier relation

Time versus frequency, in time

$$x(t) \leftrightarrow X(\omega) \qquad \text{with} \quad \omega = 2\pi\, f$$

Position versus frequency, in space

$$g(x) \leftrightarrow G(k) \qquad \text{with} \quad k = \frac{2\pi}{\lambda}$$

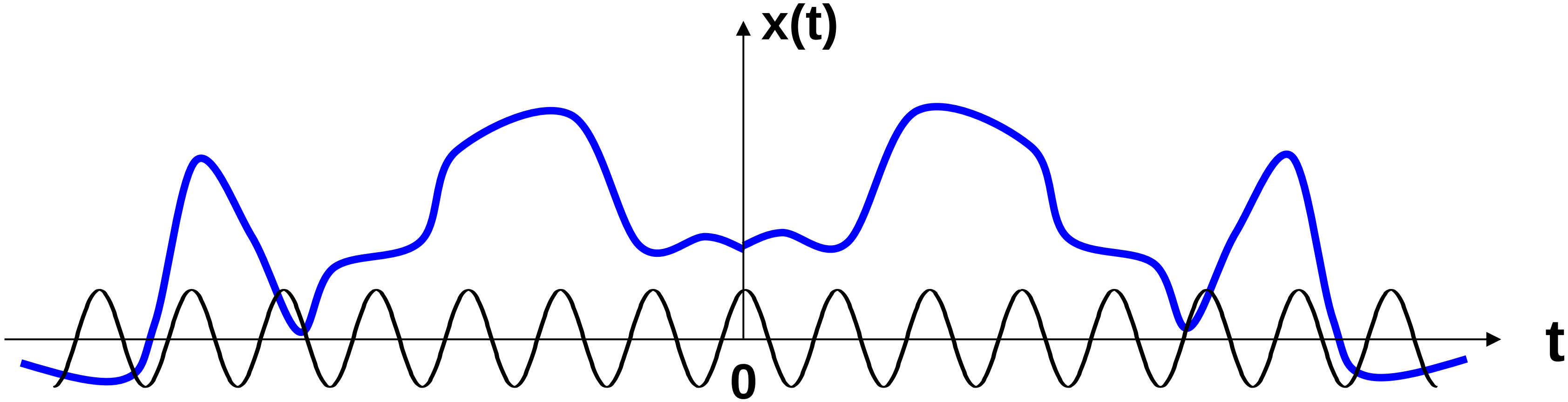
Wave function $\Psi(x)$ **versus wave function** $\overline{\Psi}(p_x)$

$$\Psi(x) \leftrightarrow \overline{\Psi}(p_x) \qquad \text{with} \quad p_x = \hbar k \;\; \text{en} \;\; k = \frac{2\pi}{\lambda}$$

Say x(t) is even: $$x(t)=\sum_{\omega} A_{\omega}\cos(\omega t)$$

What is a good measure for A_{ω} **?**

$$\boxed{A_{\omega} \propto \int_{-\infty}^{\infty} \cos(\omega t)\cdot x(t)\, dt}$$



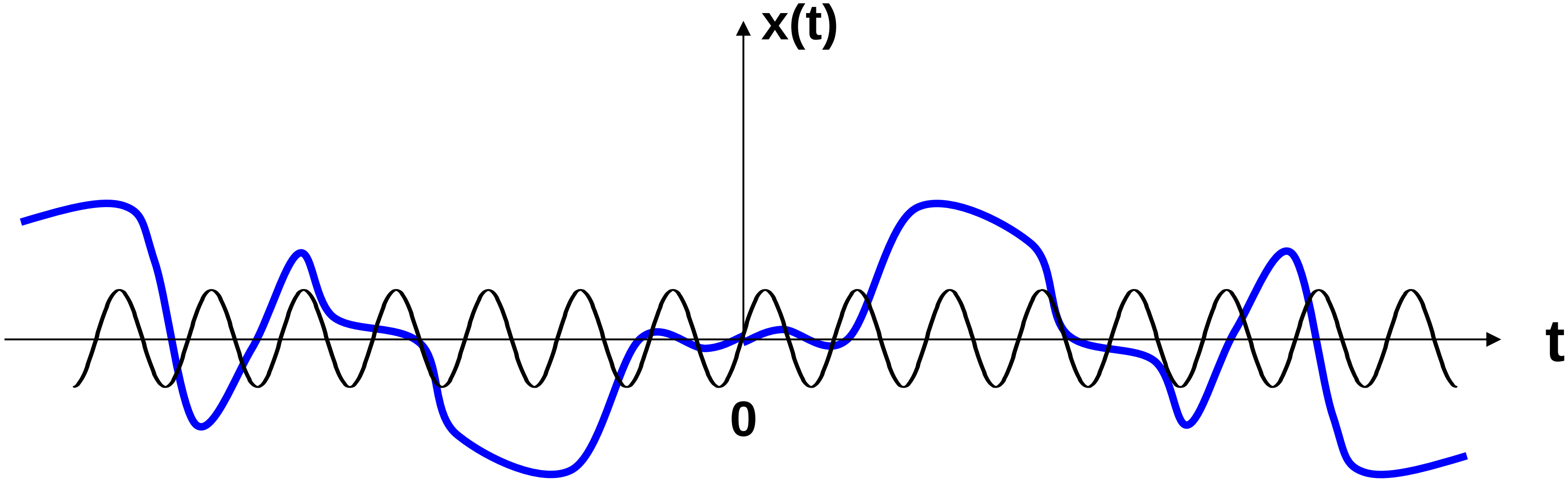
Note: Solve the integral graphically on the board.

Say x(t) is odd:

$$x(t) = \sum_{\omega} B_{\omega} \, \mathbf{sin}(\omega t)$$

What is a good measure for B_{ω} **?**

$$\boxed{B_{\omega} \propto \int_{-\infty}^{\infty} \sin(\omega t) \cdot x(t)\, dt}$$



Say x(t) is real and a sum of even and odd:

$$x(t) = \sum_{\omega} A_{\omega} \cos(\omega t) + B_{\omega} \sin(\omega t)$$
$$= \sum_{\omega} C'_{\omega} \cos(\omega t + \phi_{\omega})$$

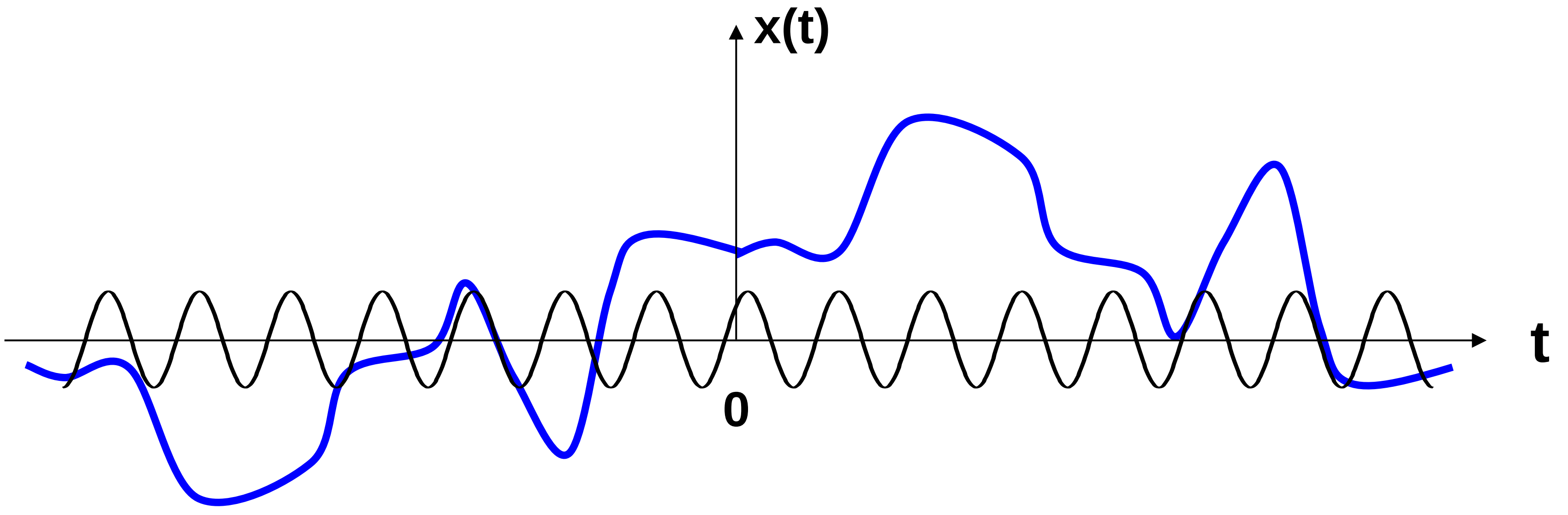
What is a good measure for C'_{ω} ?

Easier with complex spectrum:

$$x(t) = \sum_{\omega} \mathrm{Re}\left(C_{\omega} e^{i\omega t}\right)$$

$$\boxed{C_{\omega} \propto \int_{-\infty}^{\infty} e^{-i\omega t} \cdot x(t)\, dt}$$

C_{ω} **has amplitude and phase**



Say x(t) is complex and a sum as (with various phase values):

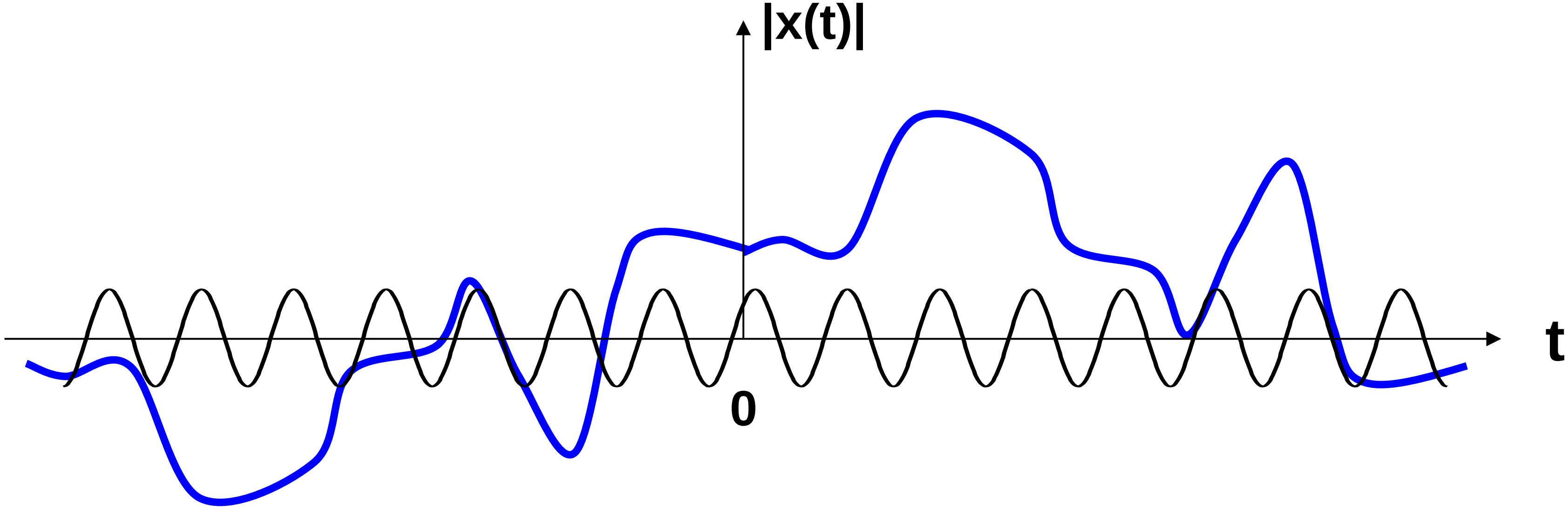
$$x(t) = \sum_{\omega} C_\omega e^{i\omega t}$$

What is a good measure for the (complex!) C_ω **?**

Again a complex spectrum:

$$\boxed{C_\omega \propto \int_{-\infty}^{\infty} e^{-i\omega t} \cdot x(t)\, dt}$$

C_ω **Has an amplitude and phase**



General presentation Fourier and inverse Fourier transformation:

$$x(t) \overset{\mathcal{F}}{\leftrightarrow} X(\omega)$$

$$X(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t}\, x(t)\ dt$$

$$x(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t}\, X(\omega)\, d\omega$$

The factor 1/2*π* is sometimes distributed differently,
a matter of definition:

(engineers vs physicists, but in both cases you get back where you started if you do two transforms in sequence)

$$X(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t}\, x(t)\, dt$$

$$x(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t}\, X(\omega)\, d\omega$$

or

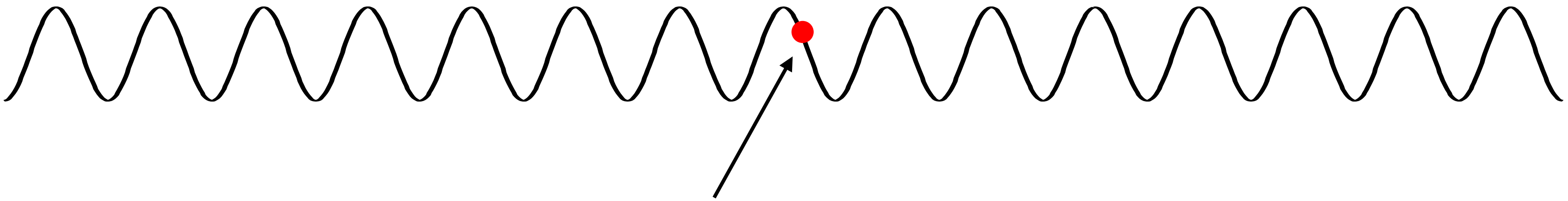
$$x(t) = \int_{-\infty}^{\infty} e^{i\omega t}\, X(\omega)\, d\omega$$

$$X(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t}\, x(t)\, dt$$

Velocity of a plane wave

Propagation of a plane wave

$$\Psi(x,t) = e^{ikx} \cdot e^{-i\omega t} = e^{i(kx-\omega t)}$$

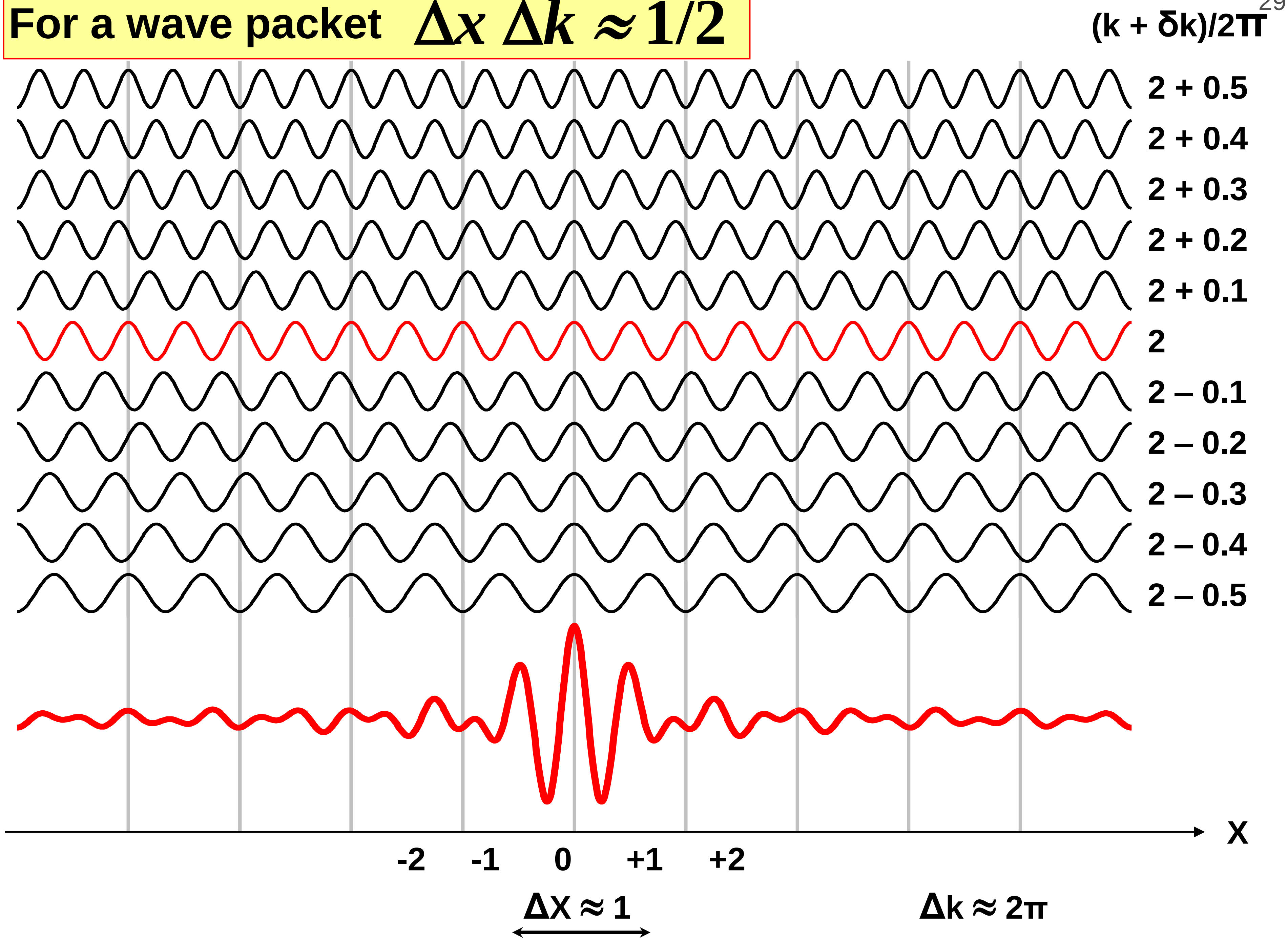


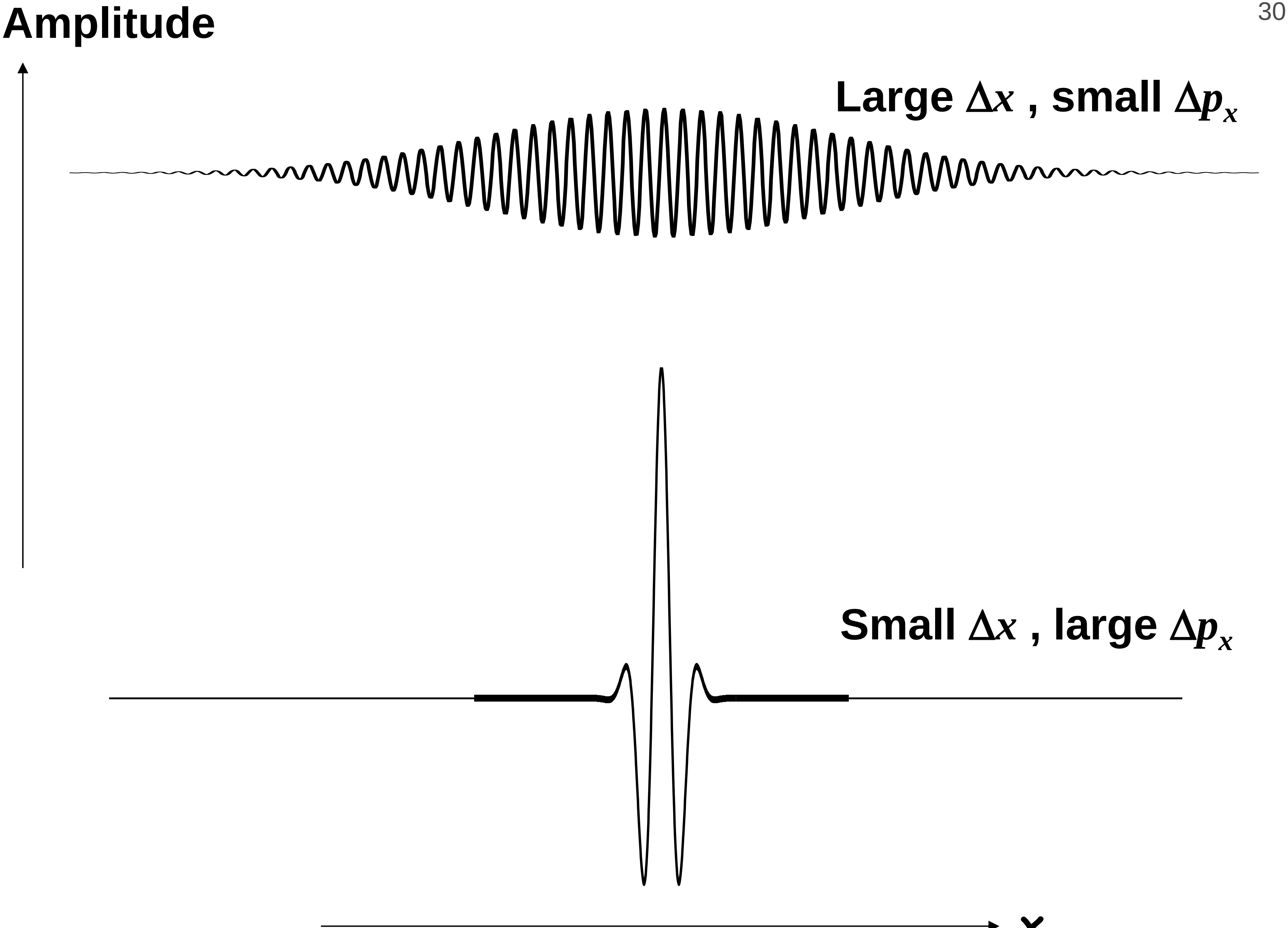
To determine the propagation speed, follow a point of constant phase $kx-\omega t$.

$$kx-\omega t = C$$

$$\frac{dx}{dt} = +\frac{\omega}{k}$$ **= PHASE velocity**

For a wave packet $\Delta x \, \Delta k \approx 1/2$




Amplitude
Large Δx , small Δp_x
Small Δx , large Δp_x
x

For this wave packet $\boxed{\Delta x\, \Delta k \approx 1/2}$

Smaller Δx is only possible with larger Δk.

Smaller Δk is only possible with larger Δx.

This is in fact a consequence of the Fourier transform relation for waves:

$$\Psi_x(x) \quad \overset{\mathfrak{F}}{\leftrightarrow} \quad \overline{\Psi}_p(p)$$

$$\overline{\Psi}_p(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\, \Psi_x(x)\, dx$$

$$\Psi_x(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar}\, \overline{\Psi}_p(p)\, dp$$

Fourier in Quantum

Fourier transformation between *x*-representation
and *k*-representation (or p-representation) of a state

Fourier in Griffiths book (2nd ed.) is around Eqs. [2.100]-[2.102] and [2.33]-[2.36]

$$\Psi(x) \quad \overset{\mathfrak{F}}{\longleftrightarrow} \quad \overline{\Psi}(k)$$

$$\overline{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx}\, \Psi(x)\, dx$$

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx}\, \overline{\Psi}(k)\, dk$$

$$\boxed{p = \hbar k}$$

Summary Fourier and wave packets:

1. The state of a quantum particle is often in a the form of a wave packet.
2. The wave function in terms of $\boldsymbol{x}$ and the wave function in terms of $\boldsymbol{p_x}$ are each others Fourier transform.
3. Heisenberg uncertainty relation follows directly from the wave character of Fourier-relation for states.

To be continued on the topic:
Group and phase velocity of a wave packet

Example representations, Fourier

The <u>same</u> *state* of a quantum system can be *represented* in many different ways.

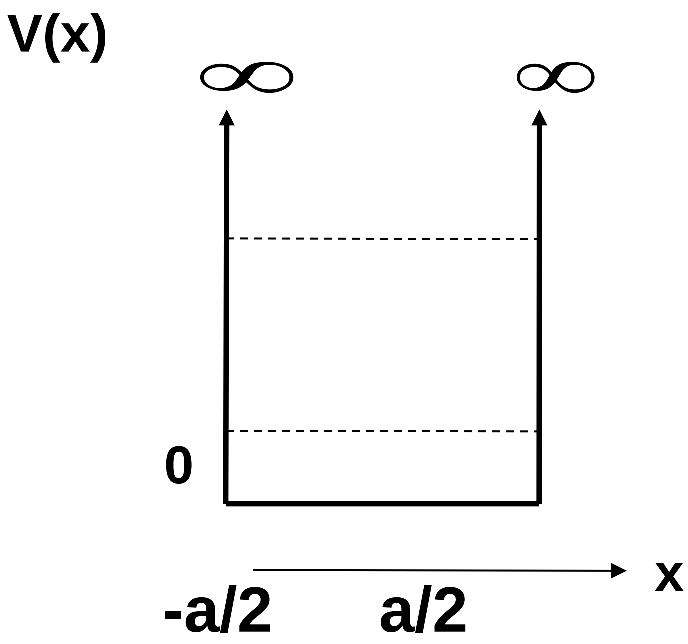
- **a wave function that is a function of position *x***

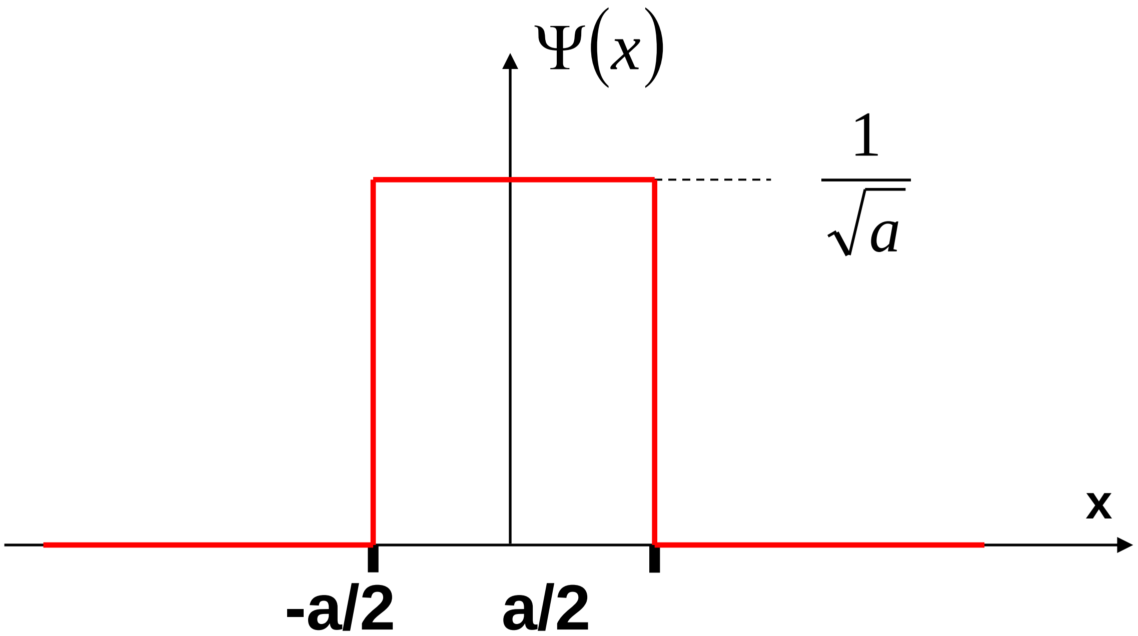
- **a wave function that is a function of wave number *k* (or, $p_x=\hbar k$)**

- **a superposition of energy eigenstates**

- **x-or p-representation versus Dirac notation**

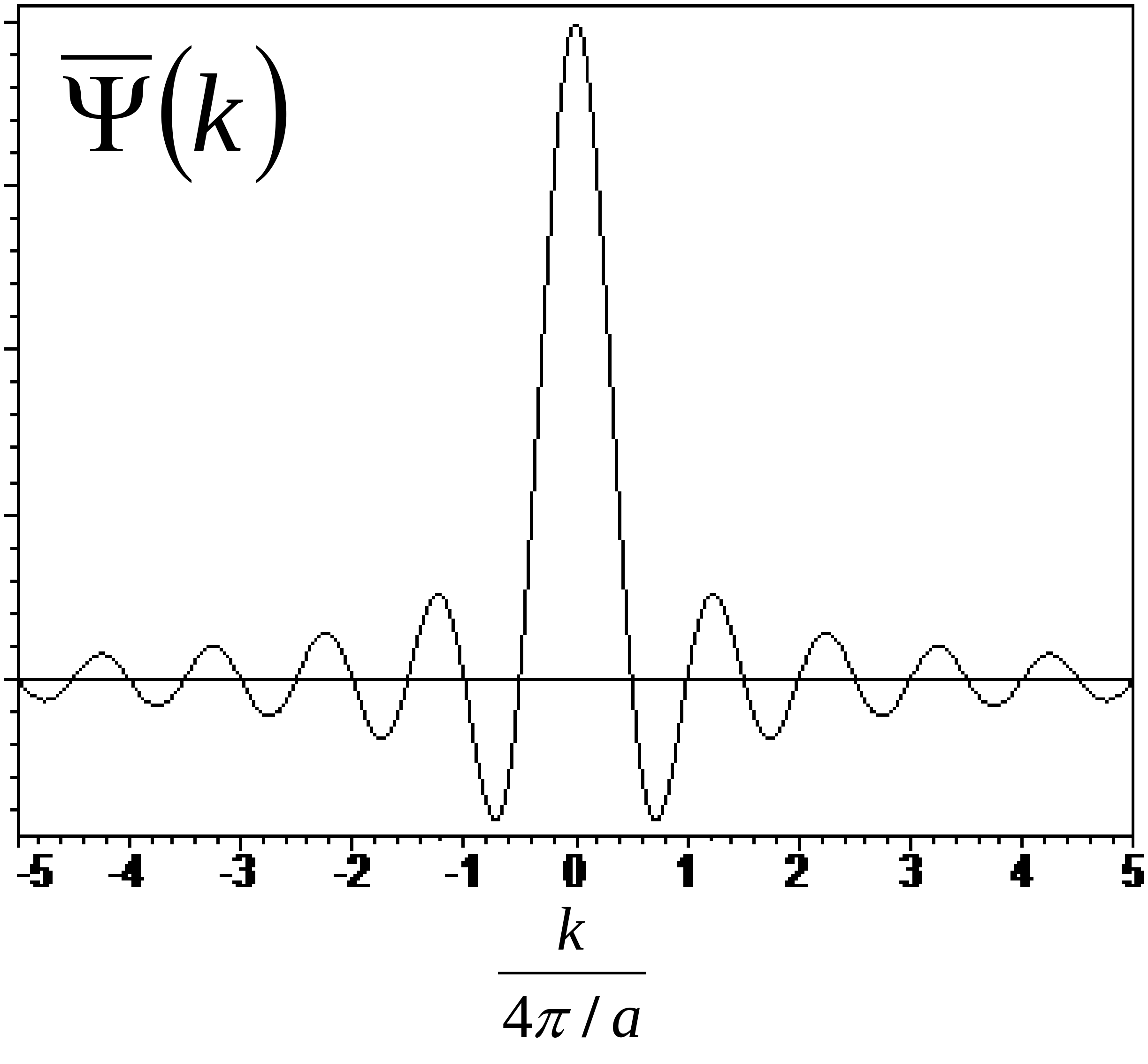
- **more………**


V(x)
∞
∞
0
x
-a/2
a/2


$\Psi(x)$
$\frac{1}{\sqrt{a}}$
x
-a/2
a/2

See problem W3.1

$$\overline{\Psi}(k) = \frac{\sqrt{a}}{\sqrt{2\pi}} \frac{\sin\left(\frac{a}{2}k\right)}{\frac{a}{2}k}$$



See problem W3.1

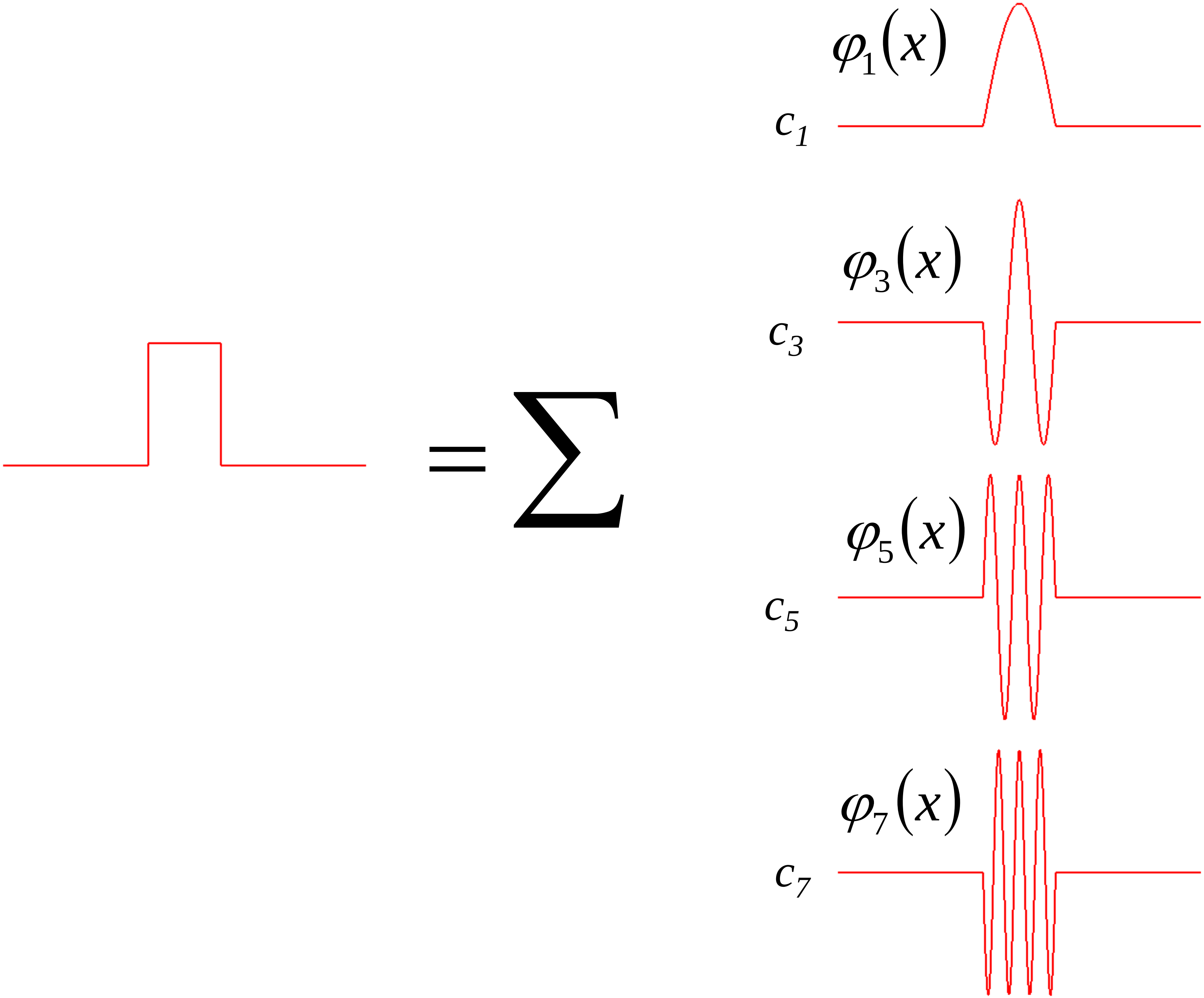
$$\left|\Psi\right\rangle = \sum_n c_n \left|\varphi_n\right\rangle$$

What are the $\left|\varphi_n\right\rangle$ **?**

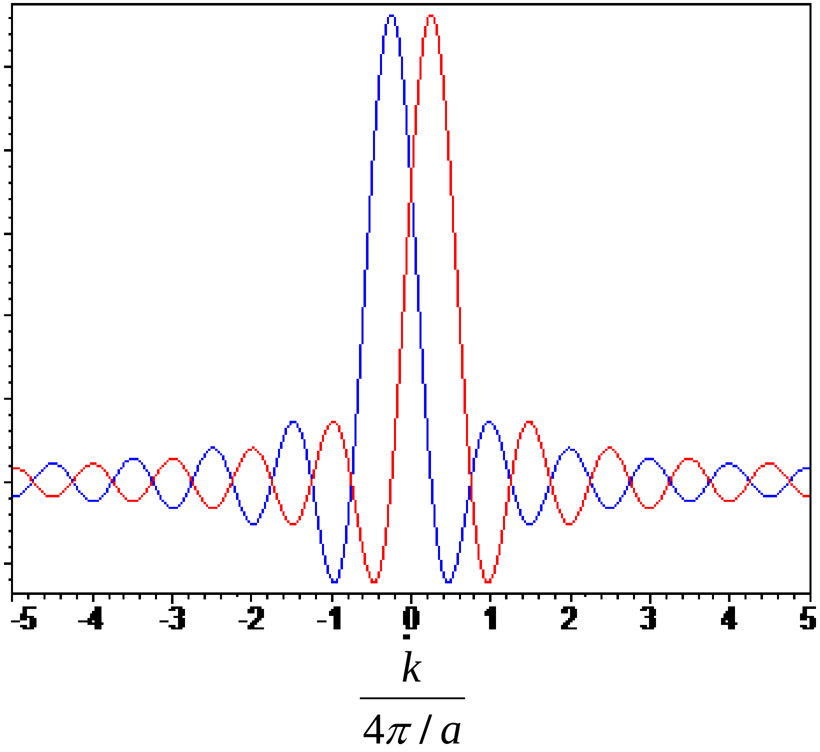
What are the c_n **?**

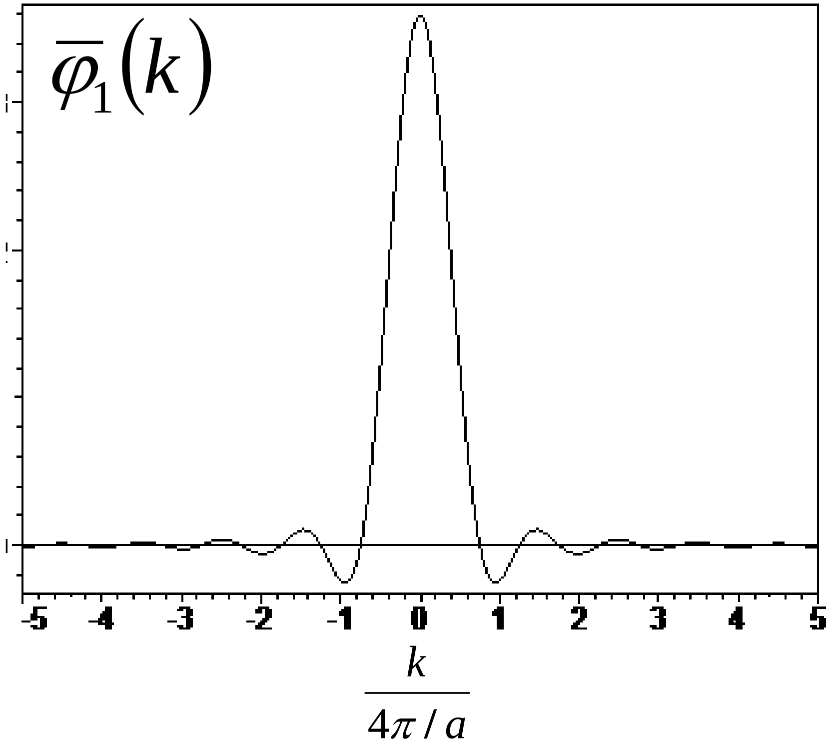
$$\begin{cases} \varphi_n(x) = \sqrt{\frac{2}{a}}\,\mathbf{sin}\left(\frac{n\pi x}{a}\right), & n \text{ even} \\ \varphi_n(x) = \sqrt{\frac{2}{a}}\,\mathbf{cos}\left(\frac{n\pi x}{a}\right) & n \text{ odd} \end{cases}$$

$$c_n = \left\langle \varphi_n \middle| \Psi \right\rangle$$

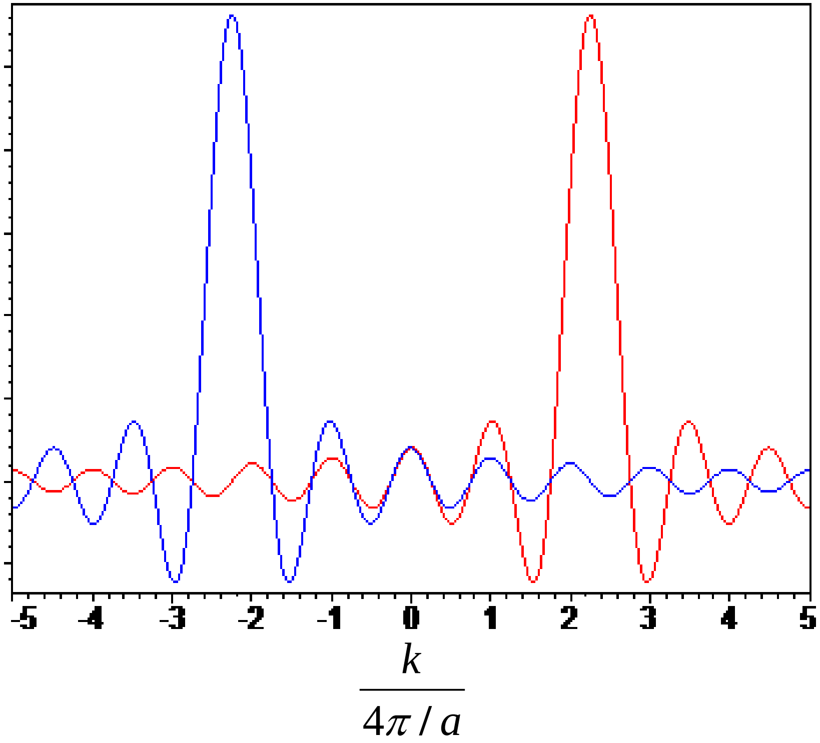

=Σ
φ1(x)
c1
φ3(x)
c3
φ5(x)
c5
φ7(x)
c7

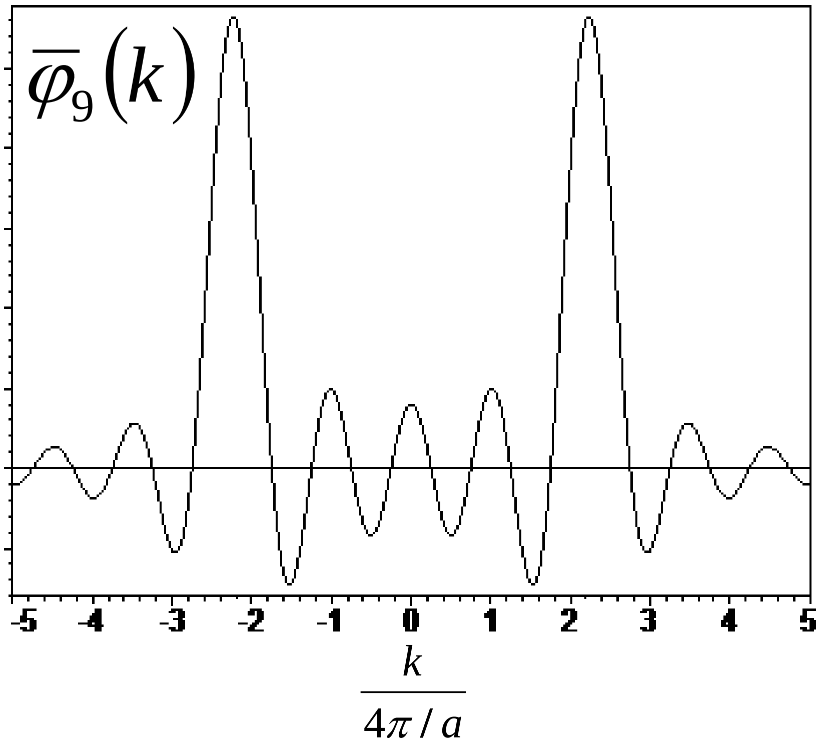
See problem W3.1

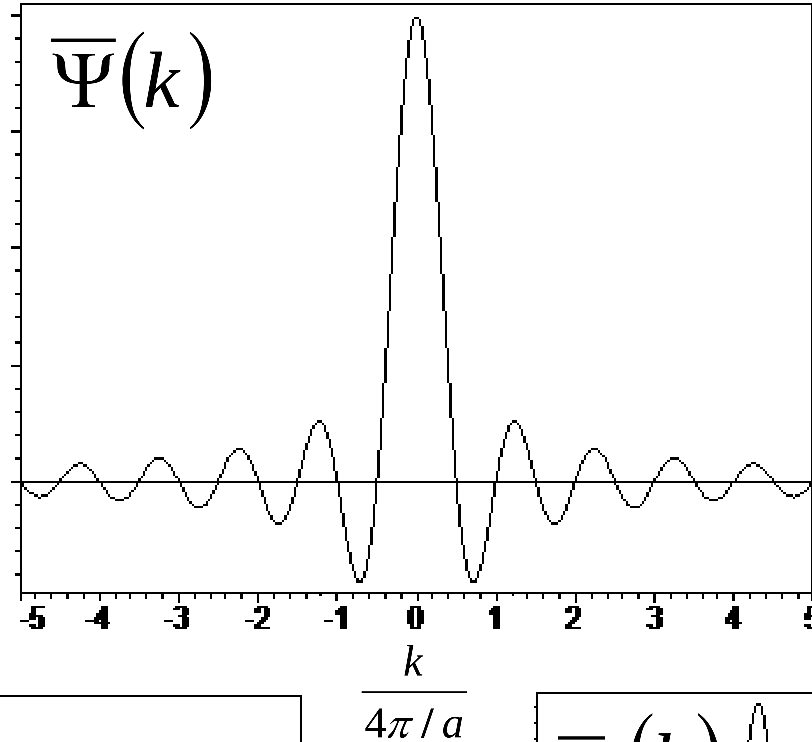


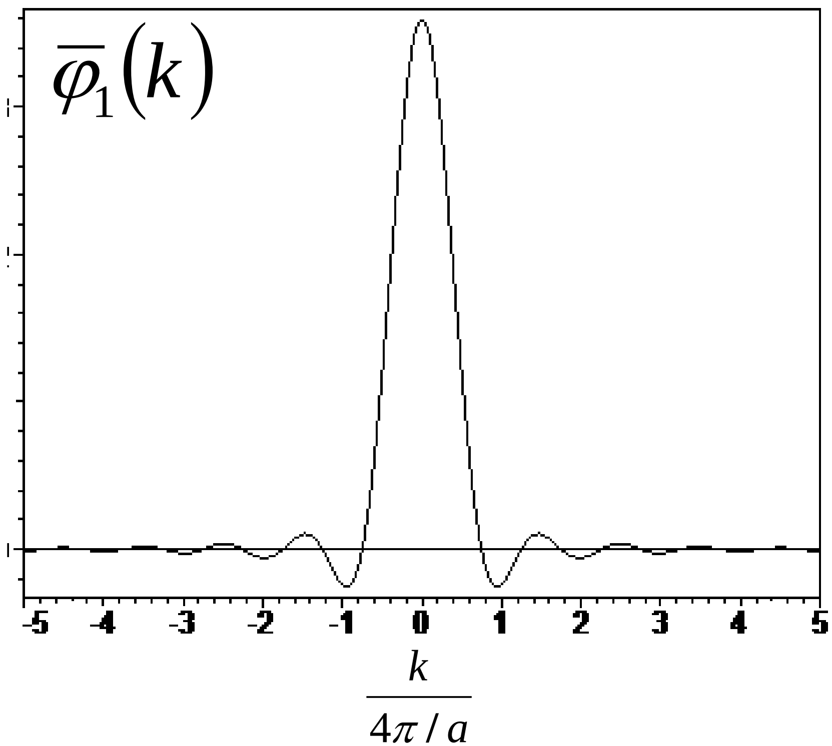


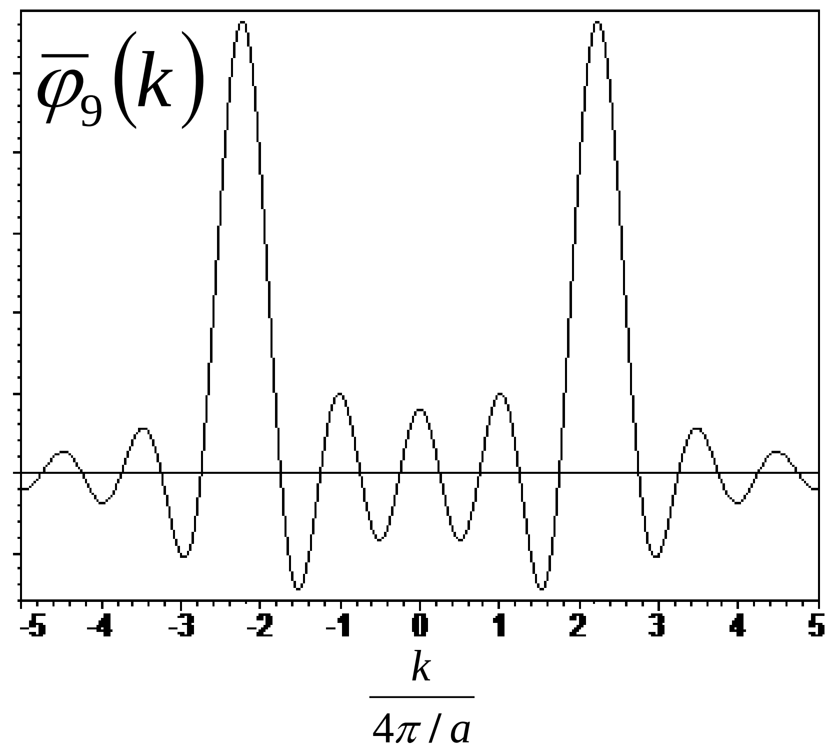
See problem W3.1

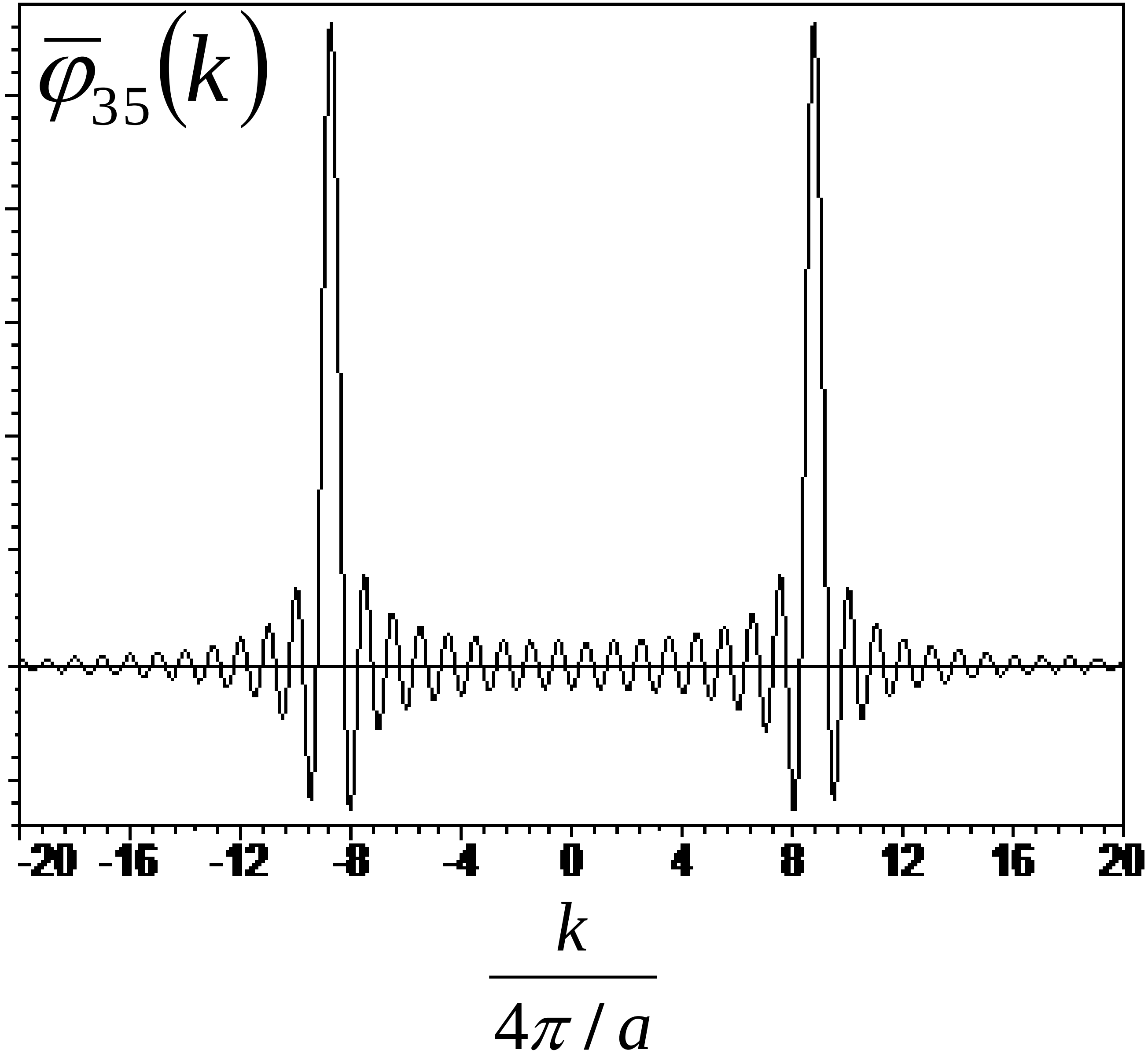





$\overline{\Psi}(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi / a}$

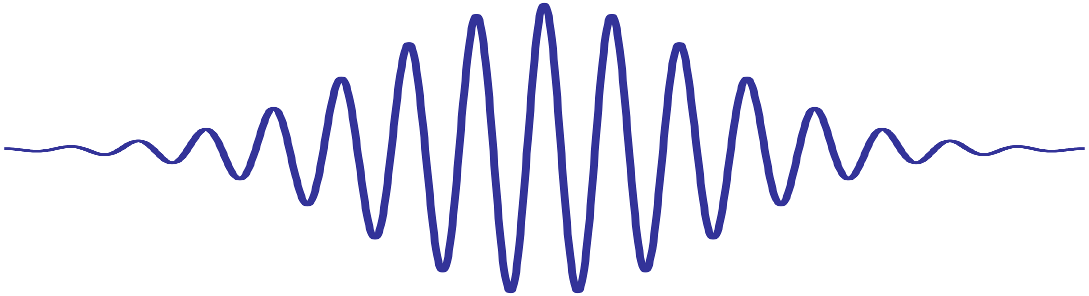

$\overline{\varphi}_1(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi / a}$


$\overline{\varphi}_9(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi / a}$


$\overline{\varphi}_{35}(k)$
-20 -16 -12 -8 -4 0 4 8 12 16 20
$\frac{k}{4\pi / a}$

Heisenberg game

Wave packets and Heisenberg



Size (e.g. in space)

Velocity PHASE velocity (details later)

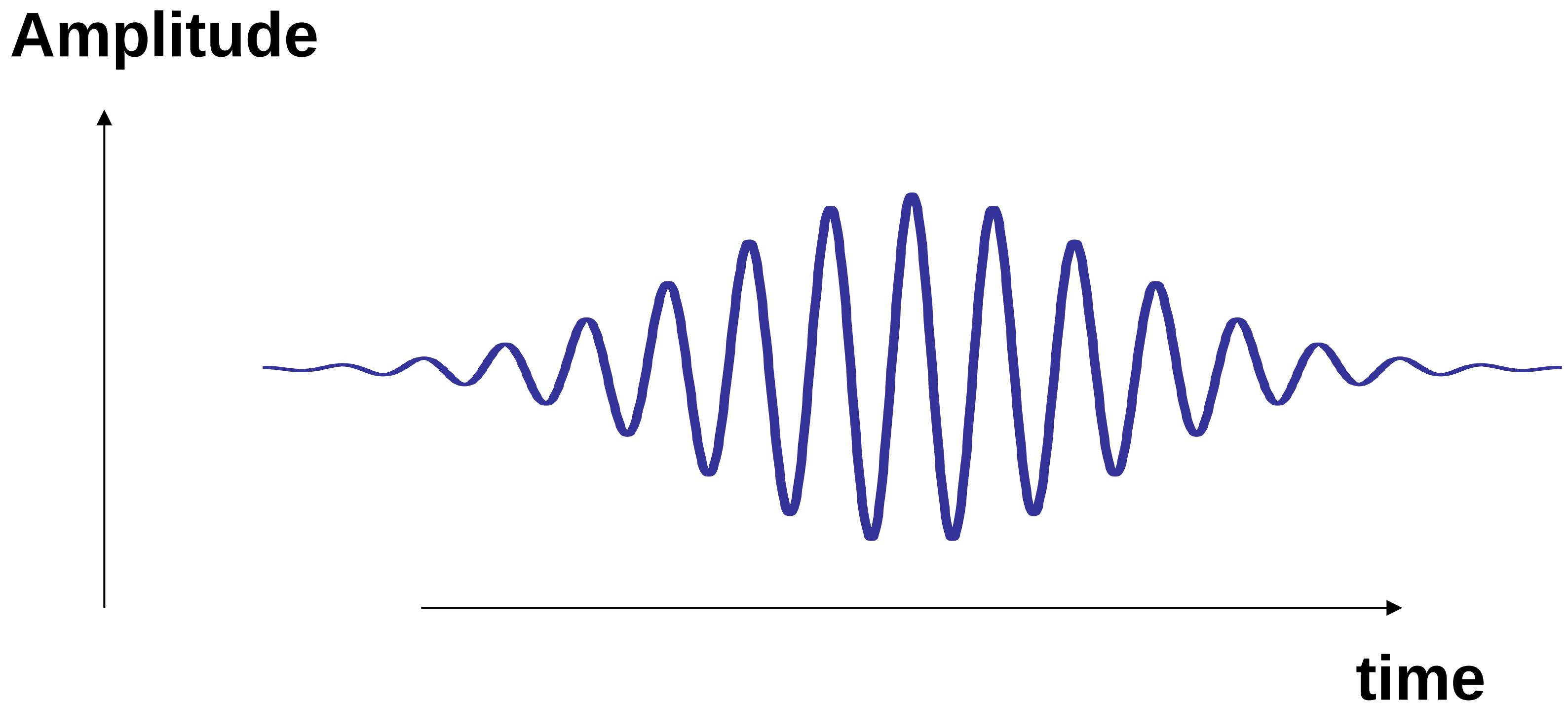
GROUP velocity (details later)

Shows that Heisenberg uncertainty relation follows

from wave nature of quantum states

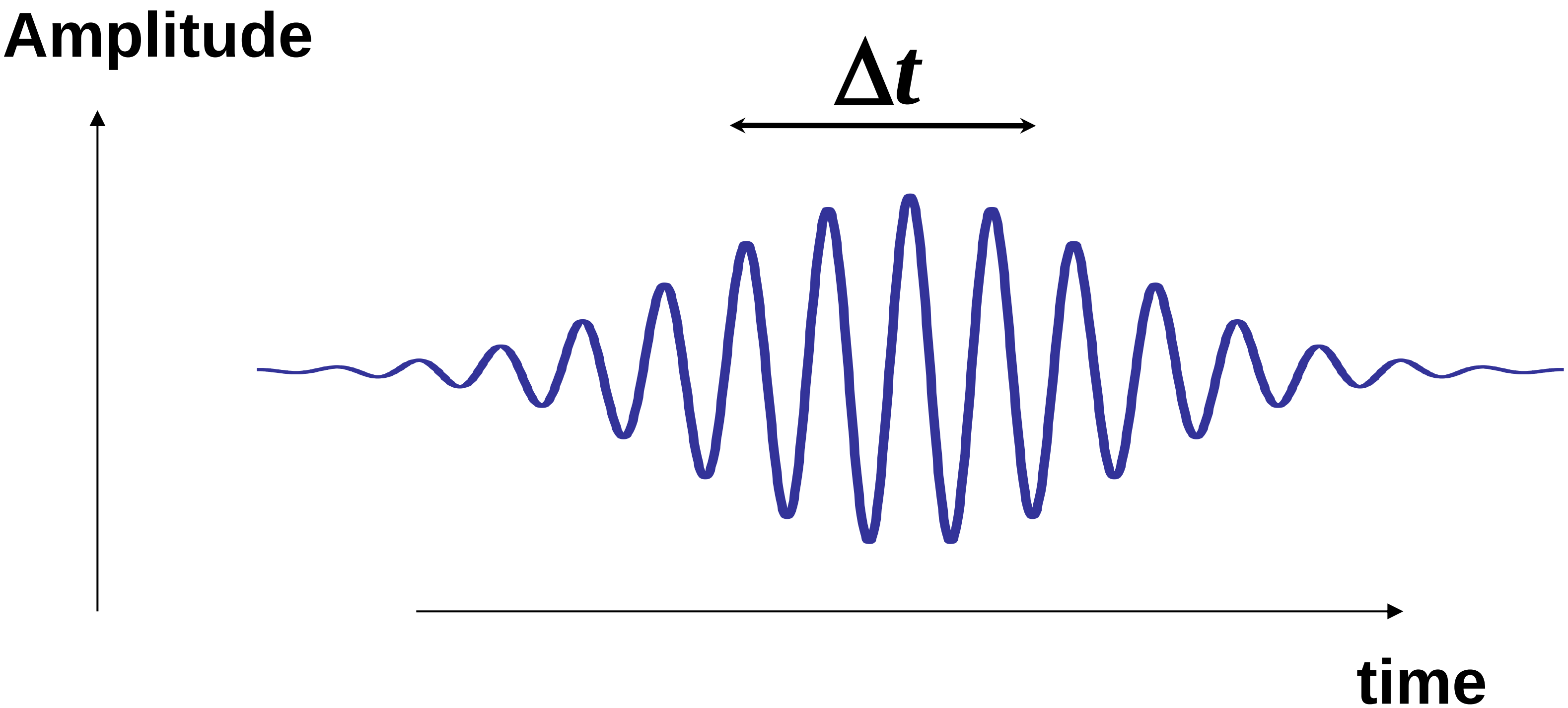
First: the Heisenberg uncertainty game

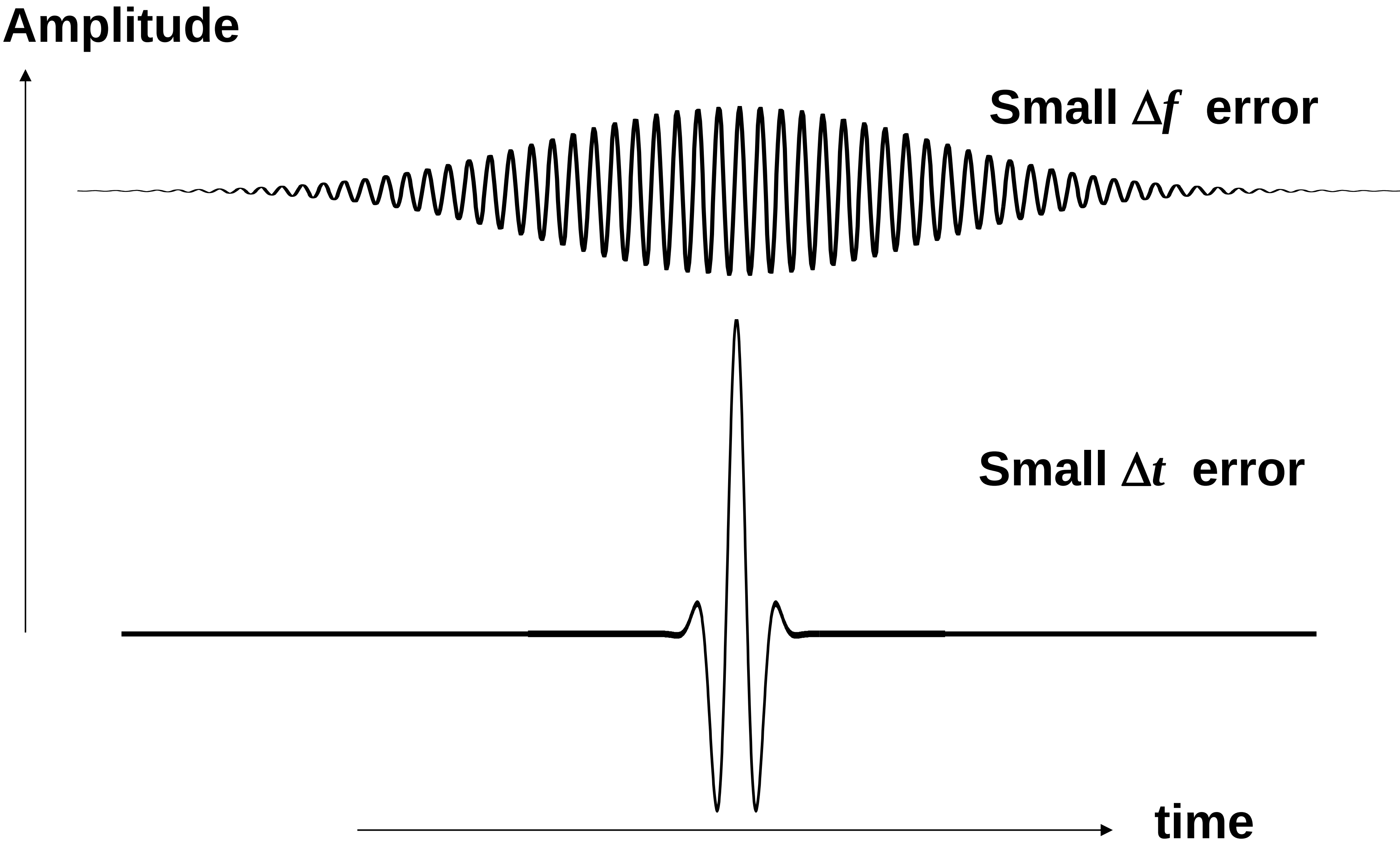
Say, you have a system for making an acoustic tone of finite duration. These tones always have a smooth envelope function. You can control the frequency of the tone and the moment of emission.



This is the question to the listening party:

Determine as accurately as possible
-When do you hear the tone?
-What is the frequency of the tone?





Δt error is the FWHM of the Gaussian envelope

Δf error is $\dfrac{(N_{period}+1) - N_{period}}{\Delta t} = 1/\Delta t$

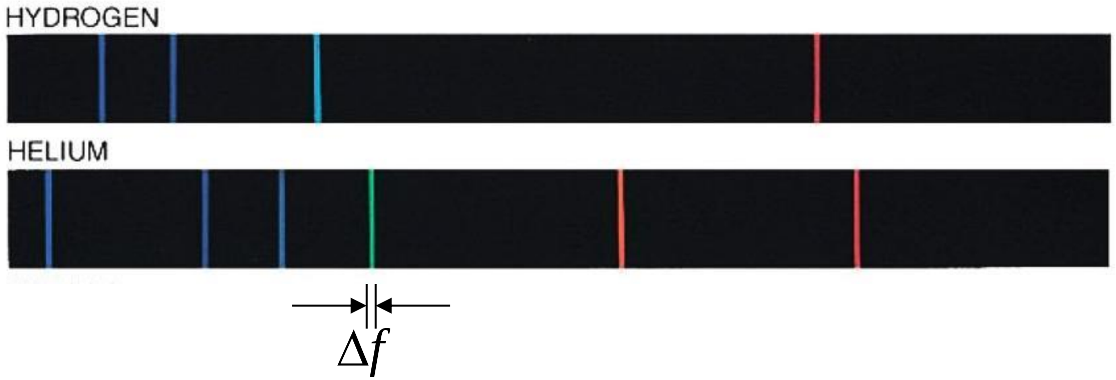
$$\boxed{\Delta f\,\Delta t \approx 1}$$

Heisenberg uncertainty relation for energy - time

$$\Delta f\, \Delta t \approx 1$$

$$h\Delta f\, \Delta t \approx h$$

$$\boxed{\Delta E\, \Delta t \geq \hbar/2}$$



This determines, for example, the width Δf of spectral lines. An electron in an atom that decays from an excited state to the ground sate emits optical wave, but only for a short duration Δt (because of electric dipole oscillation of the atom). The frequency of these oscillation can therefor not exist (or be observed) more precisely than the uncertainty Δf.

Dirac notation

Formalism:

Dirac notation

Dirac notation

Describe the state of a system as some abstract

state vector $\left|\Psi\right\rangle$

Why use this notation?

→ **Compact** $\left\langle\Psi\middle|\varphi\right\rangle = \int_{-\infty}^{\infty}\Psi(x)^{*}\varphi(x)\,dx$

→ **More general, abstract, also for systems (e.g.spin) whose state cannot be written as**

$$\boxed{\left|\Psi\right\rangle = \frac{\left|\uparrow\right\rangle + \left|\downarrow\right\rangle}{\sqrt{2}}}$$

$$\left|\Psi\right\rangle \leftrightarrow \Psi(x)$$

→ **Basis (presentation) independent** $\Psi(x)$ vs $\overline{\Psi}(p_x)$

Dirac notation

State vector $\left|\Psi\right\rangle$ **"Ket"-vector**

$\left\langle\Psi\right|$ **"Bra"-vector**

$$\left\langle\Psi\middle|\varphi\right\rangle, \quad \left\langle\Psi\middle|\hat{A}\middle|\varphi\right\rangle, \quad \left\langle\hat{A}\right\rangle \quad \rightarrow$$ **Between <u>bra</u>c<u>ket</u>s**

$$\left\langle\Psi\middle|\hat{A}\middle|\Psi\right\rangle \Rightarrow$$

$$\begin{pmatrix} c_1^* & c_2^* & c_3^* \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \sum_{i=1}^{3} \sum_{j=1}^{3} c_i^* c_j A_{ij} = \text{a real scalar number}$$

Dirac notation

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

<u>Inner product</u> – as in linear algebra

$$\langle \Psi | \hat{A} | \varphi \rangle = \int_{-\infty}^{\infty} \Psi(x)^* \hat{A} \varphi(x) dx$$

Term for expectation value

$$\langle \Psi | \varphi \rangle = \langle \varphi | \Psi \rangle^*$$

$$\langle a\Psi | \varphi \rangle = a^* \langle \Psi | \varphi \rangle$$

$$| a\Psi + b\varphi \rangle = a | \Psi \rangle + b | \varphi \rangle$$

Etc., as in linear algebra, see also Griffiths around Eqs. [3.2]-[3.10] and Eqs. [A.19]-[A.28]

Dirac notation (needs delta function)

Relation with previous notation $|\Psi\rangle \leftrightarrow \Psi(x)$

$$\langle x_0|\Psi\rangle = \int_{-\infty}^{\infty} \delta(x - x_0)^* \Psi(x)\,dx = \Psi(x_0)$$

Basis (eigen) vector of x-basis

But also, for example,

$$\langle \varphi_{k0}|\Psi\rangle = \int_{-\infty}^{\infty} \delta(p_x - p_{x0})^* \,\overline{\Psi}(p_x)\,dp_x = \overline{\Psi}(p_{x0})$$

Basis (eigen) vector of p_x-basis

There was a short blackboard presentation on a few examples of common mistakes with using Dirac notation (or better said, mixed up notation which is very wrong). Only one example here.

It is by now clear what we mean with:

$$\left|\Psi\right\rangle \leftrightarrow \Psi\left(x\right)$$

$$\left\langle\Psi\right| \leftrightarrow \Psi\left(x\right)^*$$

In this context it is really nonsense and wrong to write things like

$$\left|\Psi(x)\right\rangle \quad , \quad \left\langle\Psi\right|^* \quad , \quad \left\langle\Psi^*\right|$$

$$\int_{x_1}^{x_2} \left|\Psi\right\rangle dx \qquad \left|\Psi\right\rangle = \Psi(x)$$

WRONG !!

Hilbert space

(Griffiths section 3.1)

The <u>linear</u> vector space where the <u>state vectors</u> $|\varphi\rangle$ live.

It is the space that contains all the possible state for a system.

Say the state of some system can be <u>completely</u> characterized by the physical property A, with associated observable Â.

Then, every possible state Ψ of the system can be described as a superposition of eigenvectors $|\varphi_a\rangle$ of Â .

The eigenvectors $|\varphi_a\rangle$ of Â then span the Hilbert space of this system.

$$|\Psi\rangle = \sum_a c_a |\varphi_a\rangle \qquad with \quad \langle\varphi_a|\varphi_{a'}\rangle = \delta_{a,a'}$$

$$c_a = \langle\varphi_a|\Psi\rangle \qquad P(a) = |\langle\varphi_a|\Psi\rangle|^2$$

Hermitian adjoint (NOT MID-TERM exam, but study for final exam)

Note order!

$$\left|\Psi\right\rangle \leftrightarrow \left\langle\Psi\right|$$

$$\hat{A} \leftrightarrow \hat{A}^{+}$$

$$\left|\Psi'\right\rangle = \hat{A}\left|\Psi\right\rangle \leftrightarrow \left\langle\Psi'\right| = \left\langle\Psi\right|\hat{A}^{+}$$

$$\left(\hat{A}\hat{B}\right)^{+} = \hat{B}^{+}\hat{A}^{+}$$

$$\left(\hat{A}^{+}\right)^{+} = \hat{A}$$

$$\left(c\hat{A}\right)^{+} = c^{*}\hat{A}^{+}$$

In general $\hat{A} \neq \hat{A}^{+}$

Hermitian operators

$$|\Psi'\rangle = \hat{A}|\Psi\rangle \quad \leftrightarrow \langle\Psi'| = \langle\Psi|\hat{A}^+$$

Hermitian if $$\hat{A}^+ = \hat{A}$$

and then $$\langle\Psi|\hat{A}|\varphi\rangle = \langle\varphi|\hat{A}|\Psi\rangle^*$$

Hermitian operators (observables) have
•<u>real</u> eigenvalues
•<u>orthogonal</u> eigenvectors

$$\hat{A}\varphi_n(x) = a_n\varphi_n(x)$$

$$\langle\varphi_n|\varphi_m\rangle \quad = \delta_{n,m} = \begin{cases} 1 \text{ , } for \;\; n = m \\ 0 \text{ , } for \;\; n \neq m \end{cases} \qquad \Rightarrow$$

$$\langle\varphi_n|\hat{A}|\varphi_m\rangle = a_n\delta_{n,m} = \begin{cases} a_n \text{ , } for \;\; n = m \\ 0 \text{ , } for \;\; n \neq m \end{cases}$$

Postulate 5

Generalized and in Dirac notation

Postulate 5 – General formulation using Dirac notation

(not treated very well in the book)

Probability P_a for a measurement outcome with result a

$$\boxed{P_a = \left| \langle \varphi_a | \Psi \rangle \right|^2}$$

$|\varphi_a\rangle$ **Eigenstate associated with eigenvalue a**

$|\Psi\rangle$ **The state before the measurement**

Group velocity

(Griffiths near Eqs. [2.104]-[2.105])

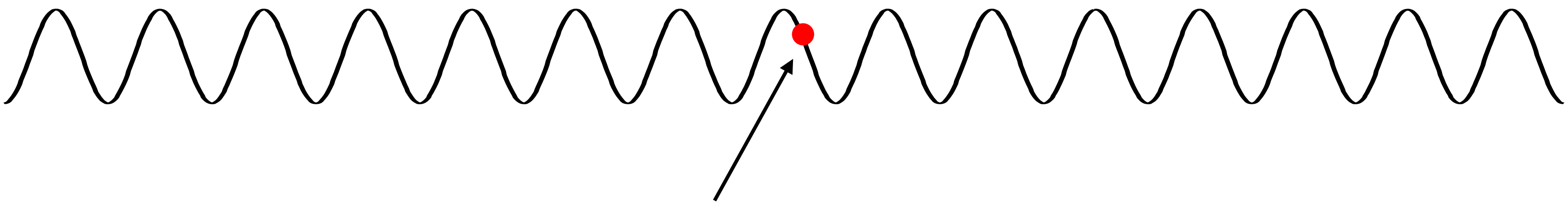
More on wave packets:

Velocity of wave packets (group velocity)

Velocity of a plane wave

Propagation of a plane wave

$$\Psi(x,t) = e^{ikx} \cdot e^{-i\omega t} = e^{i(kx - \omega t)}$$



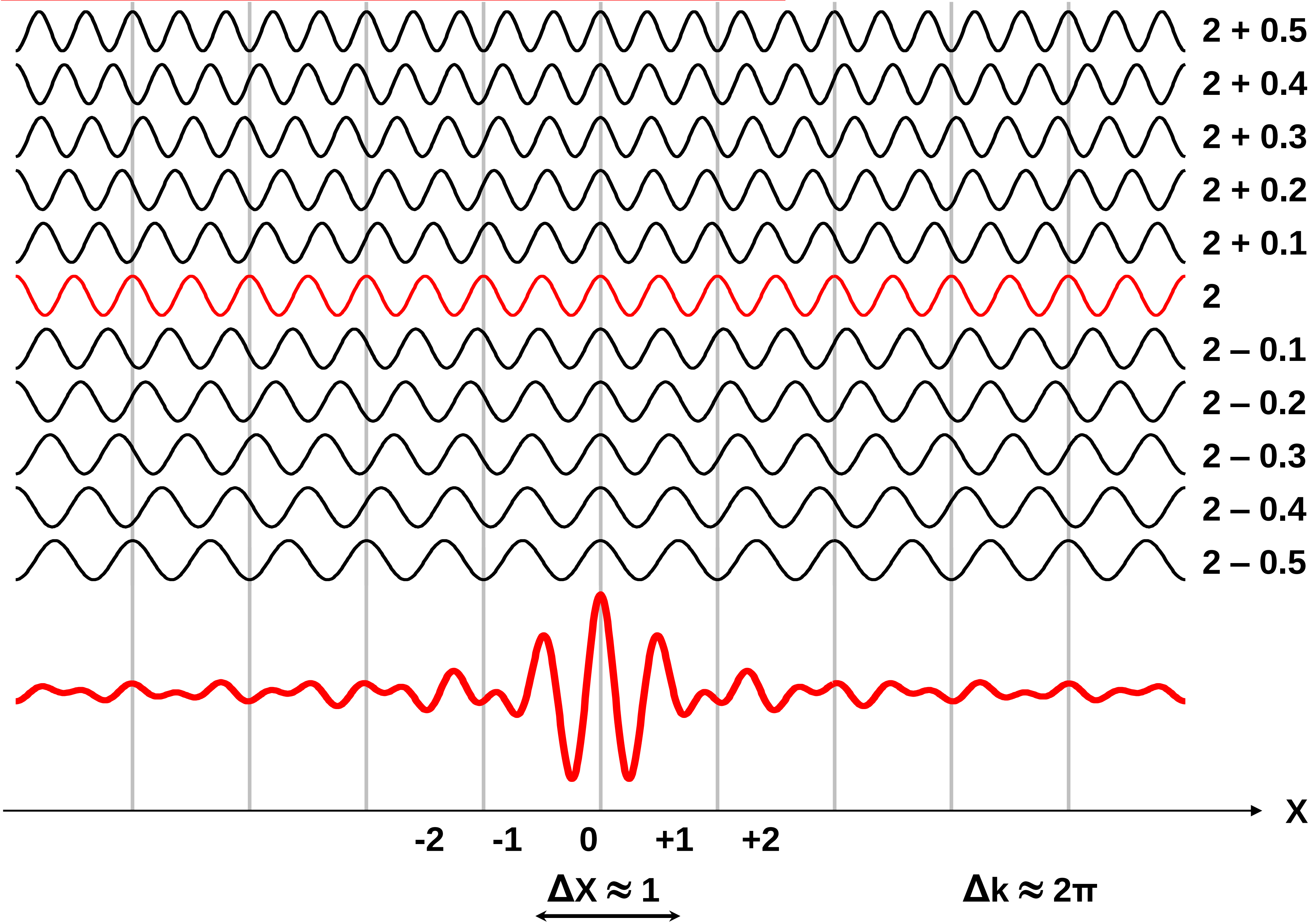
To determine the propagation speed, follow a point of constant phase $kx - \omega t$**.**

$$kx - \omega t = C$$

$$\frac{dx}{dt} = +\frac{\omega}{k}$$ **= PHASE velocity**

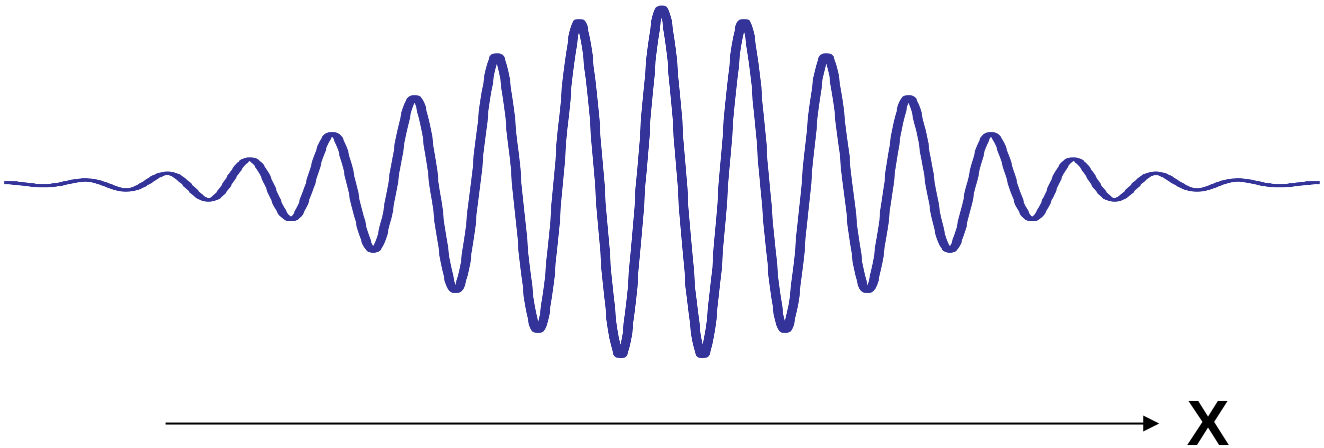
But $$\frac{dx}{dt} = +\frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{p^2/2m}{p} = \frac{p}{2m} = \frac{\mathrm{v}_{CL}}{2}$$ **???**

For a wave packet $\Delta x \, \Delta k \approx 1/2$



More realistic, a wave packet:

Velocity of a wave packet

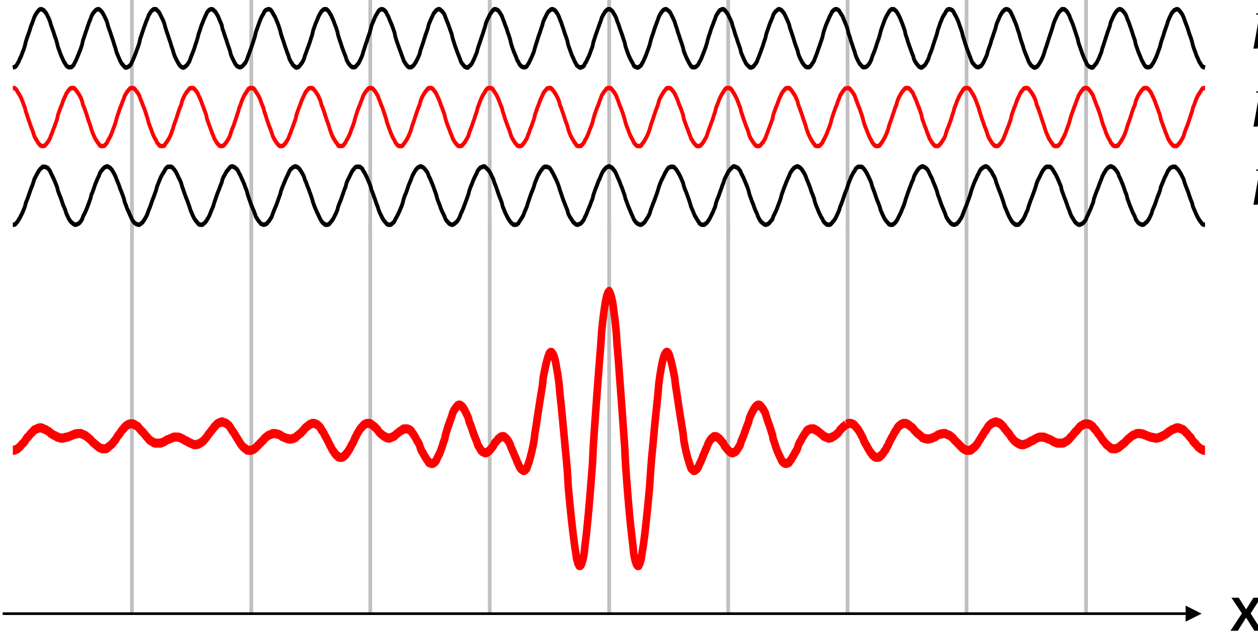


$$\mathrm{V}_{PHASE}(k)=\frac{\hbar k}{2m}$$

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

$$\frac{dx}{dt}=+\frac{\partial\omega}{\partial k}=\mathrm{V}_{CL}$$ **GROUP velocity**

$$\mathrm{V}_{GROUP}(k)=\frac{\partial}{\partial k}\left(\frac{\hbar k^2}{2m}\right)=\frac{\hbar k}{m}=\mathrm{V}_{CL}$$



$k_0 + \delta k \qquad \omega_0 + \delta\omega$

$k_0 \qquad \omega_0$

$k_0 - \delta k \qquad \omega_0 - \delta\omega$

$$V_{PHASE}(k) = \frac{\hbar k}{2m}$$

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

Say $$\Psi(x,t) = \sqrt{\frac{1}{3}}\left(e^{i([k_0+\delta k]x-[\omega_0+\delta\omega]t)} + e^{i(k_0x-\omega_0 t)} + e^{i([k_0-\delta k]x-[\omega_0-\delta\omega]t)}\right)$$

$$= \sqrt{\frac{1}{3}}e^{i(k_0x-\omega_0 t)}\left(e^{i(\delta kx-\delta\omega t)} + 1 + e^{-i(\delta kx-\delta\omega t)}\right)$$

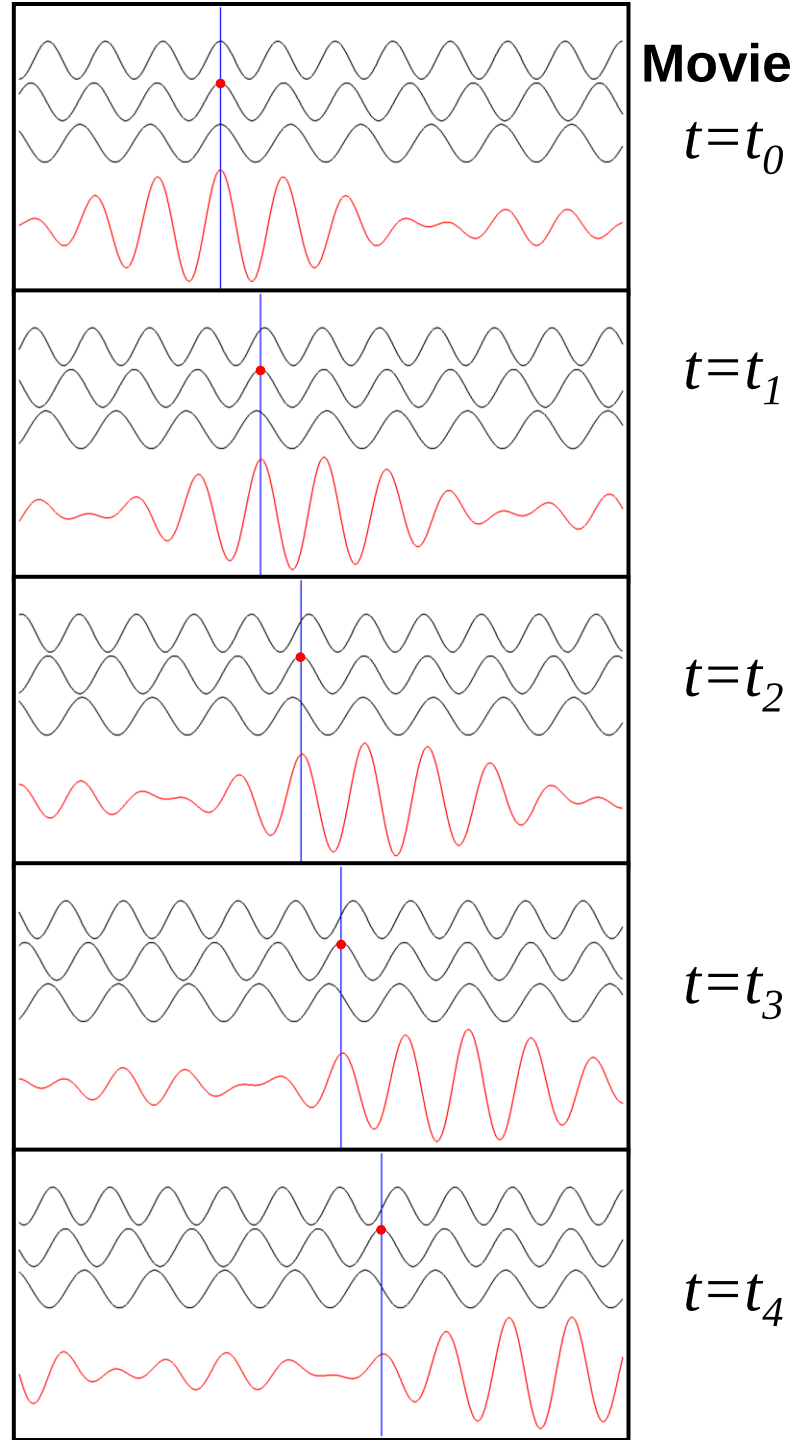
$$= \sqrt{\frac{1}{3}}e^{i(k_0x-\omega_0 t)}\left(1 + 2\cos(\delta kx - \delta\omega t)\right)$$

Interference maximum propagates at $$V_{GROUP} = \frac{\delta\omega}{\delta k} \neq \frac{\omega_0}{k_0}$$

For the case of matter waves, the ω-k relation gives

$$v_{group} = 2\ v_{phase}.$$

In the movie snap shots here, the blue line moves with the phase velocity of the middle plane wave (black), attached at a point with constant phase (red dot). The three plane waves have a different phase velocity. This causes that the velocity of the constructive interference of the three plane waves (velocity of the red wave packet) is in this case twice as fast.



Another way to describe this:

Maximum of wave packet is a point where many plane ways $e^{i(kx-\omega t)}$ with different *k* interfere constructively $\Rightarrow$ They all have and keep the same phase (*k*x - *ωt*) for realizing this constructive interference maximum, whatever their *k*.

$$\frac{\partial}{\partial k}\left(kx-\omega t\right)=0$$

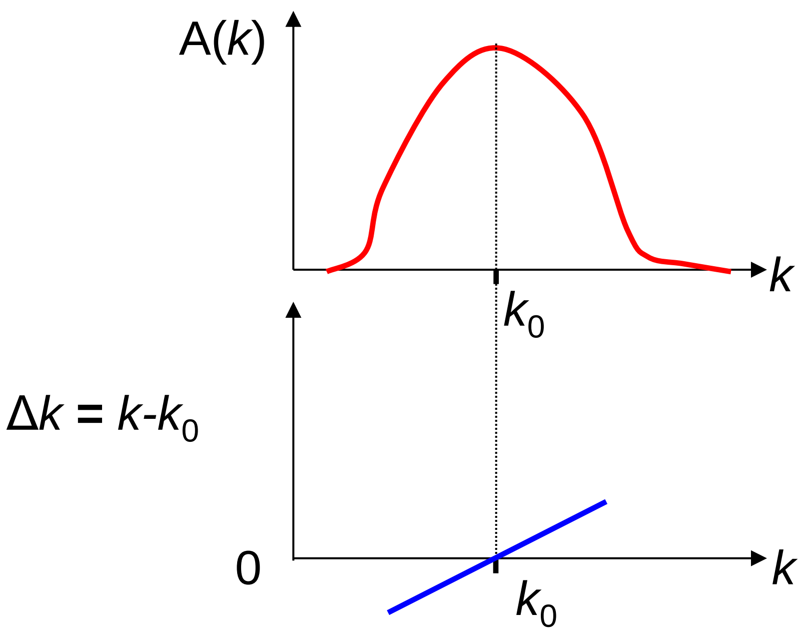
$$x-\frac{\partial\omega}{\partial k}t=0$$

$$\frac{dx}{dt}=\frac{\partial\omega}{\partial k}$$

Group velocity more general:

A wave packet has a maximum due to interference of many plane waves $e^{i(kx-\omega t)}$ with amplitudes A(k).

The velocity of this maximum (group velocity) is determined by the variation of ω (around a central ω_0) with respect to changes Δk in k around the average $k = k_0$



Group velocity: depends on dispersion (*ω*-*k* relation):

For Electro Magnetic wave packets (optical pulses)
in free space (no dispersion):

$$\mathrm{V}_{\mathrm{PHASE}}(k) = \mathrm{V}_{\mathrm{GROUP}}(k) = \frac{\partial \omega}{\partial k} = c \qquad \omega = ck \qquad k = \frac{2\pi}{\lambda}$$

For quantum waves of massive particles
(de Broglie matter waves)

$$\mathrm{V}_{GROUP} = \frac{\partial \omega}{\partial k} = \frac{\hbar k}{m}$$

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

Commutator

Commutator bracket:

$\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$ **Commutator (in general an operator)**

$\left[\hat{A},\hat{B}\right]=0$ $\hat{A}$ **and** $\hat{B}$ **commute, same eigenvectors**

$\left[\hat{x},\hat{p}_x\right]=i\hbar\cdot\hat{I} \quad \Rightarrow \quad \Delta x\Delta p_x>\hbar/2$

$$\hat{H}_V\hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}\begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}=\begin{pmatrix} 0 & V_1T \\ V_2T & 0 \end{pmatrix}$$

$$\hat{H}_T\hat{H}_V \leftrightarrow \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}\begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}=\begin{pmatrix} 0 & V_2T \\ V_1T & 0 \end{pmatrix}$$

$$f\left(\hat{H}_V\right)=f\left(\begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}\right)=\begin{pmatrix} g_1(V_1,V_2) & 0 \\ 0 & g_2(V_1,V_2) \end{pmatrix}$$

Commutator bracket:

$\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$ **Commutator (in general an operator)**

$\left[\hat{A},\hat{B}\right]=0$ $\hat{A}$ **and** $\hat{B}$ **commute, same eigenvectors**

$\left[\hat{x},\hat{p}_x\right]=i\hbar\cdot\hat{I}$ $\Rightarrow$ $\Delta x\Delta p_x>\hbar/2$

Measure A with result a_1, then B, then again A

$\Rightarrow\hat{A}$ **and** $\hat{B}$ **commute, measurement gives again result a_1**

$\Rightarrow\hat{A}$ **and** $\hat{B}$ **do not commute, gives arbitrary outcome**

Particle in a box

Particle in a box: important model system.

For example, very simple model for electron trapped around nucleus.

To characterize system: First solve time-independent Schrodinger Eq.
(this system has time-independent Hamiltonian)

$$\hat{H} = \hat{H}_{kin} + \hat{H}_{pot}$$

$$V(x) = 0, \qquad 0 < x < a$$
$$V(x) = \infty, \qquad \textit{all other } x$$

This gives the Hamiltonian of a free particle for the interval $0<x<a$, but with boundary conditions.

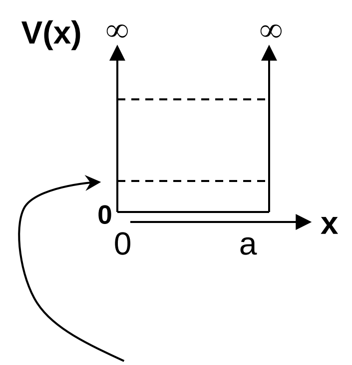
Some additional assumptions needed to find eigenstates:

$\varphi(x) = 0$ outside interval $0<x<a$

$\varphi(0) = \varphi(a) = 0$ <u>continuous</u> at x=0 and x=a

solving gives that $\varphi(x)$ can be taken real over $0<x<a$

See Griffiths Chapter 2



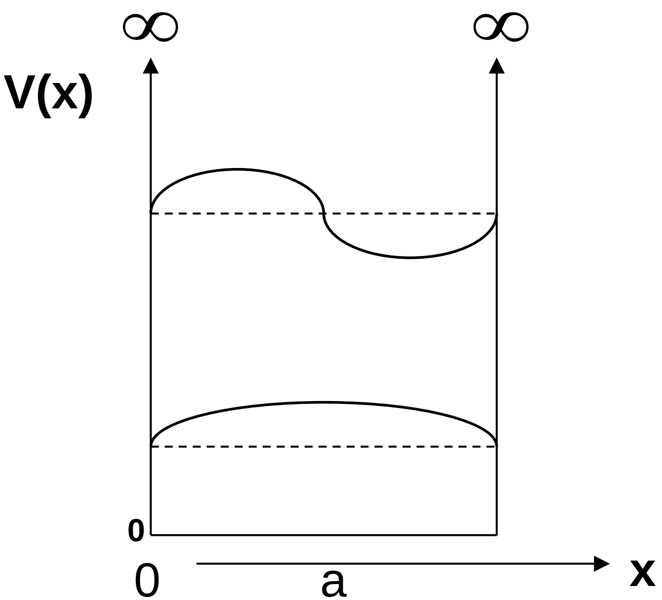
Ground state has finite energy!

Why?

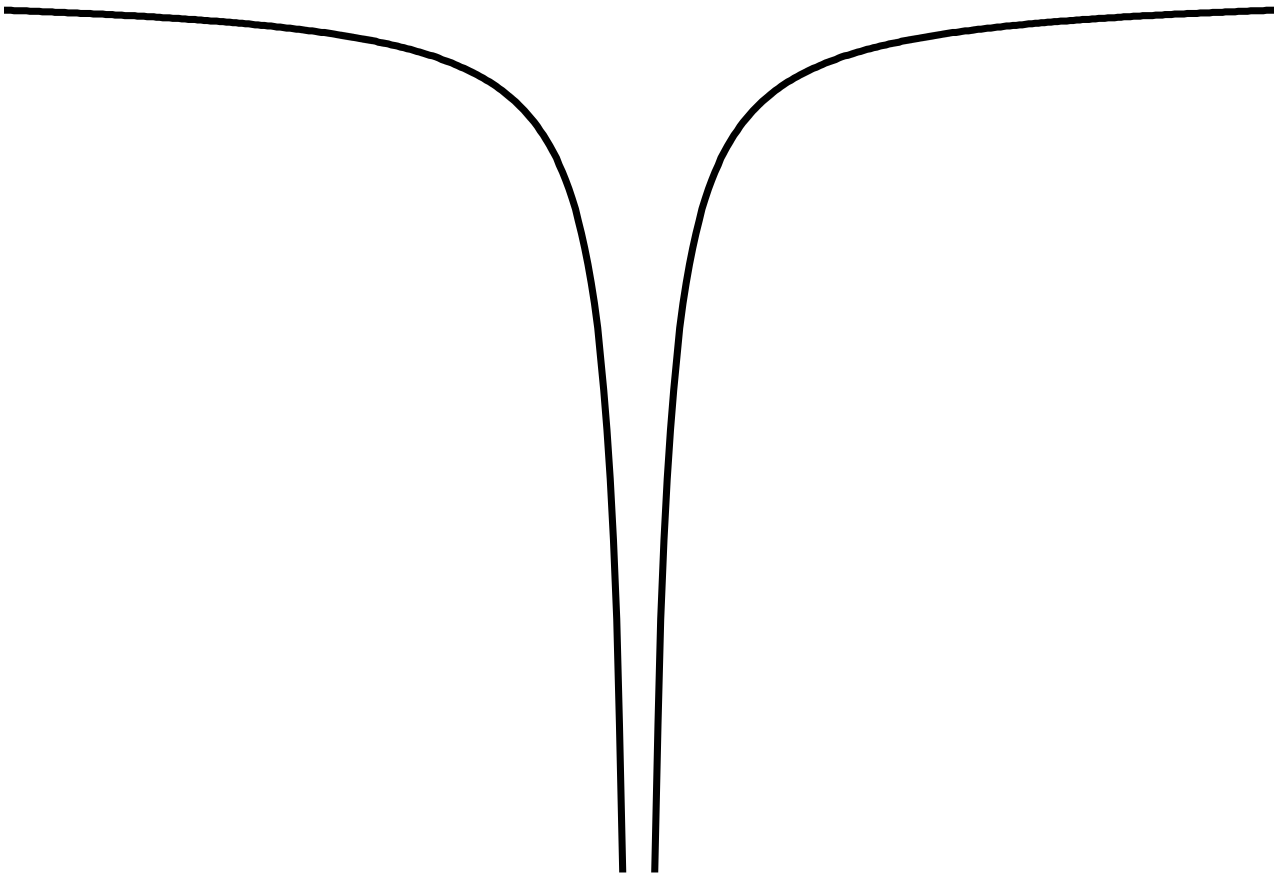
Peer instruction question

How many graphs do you see at the same time here?

A 1
B 2
C 3
D 4



Very simple model for V(r) for potential for electron in Hydrogen atom



Summary

Summary:

- Formalism and notation
- Dirac notation
- State vector space = Hilbert space
- Hermitian operators
- Wave packets and Heisenberg
- Particle in a box

Some extra’s on current research topics:

Particle in a box

Experiments on electron in a box

VOLUME 69, NUMBER 10 PHYSICAL REVIEW LETTERS 7 SEPTEMBER 1992

Zero-Dimensional States and Single Electron Charging in Quantum Dots

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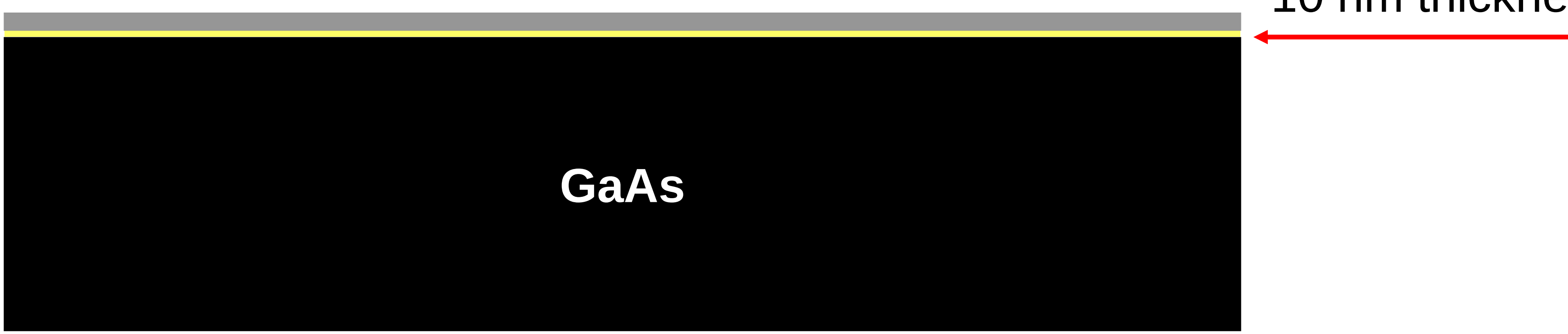
(Received 19 May 1992)

We observe new transport effects in lateral quantum dots where zero-dimensional (0D) states and single electron charging coexist. In linear transport we see *coherent* resonant tunneling, described by a Landauer formula despite the many-body charging interaction. In the nonlinear regime, Coulomb oscillations of a qunatum dot with about 25 electrons show structure due to 0D excited states as the bias voltage increases, and the current-voltage characteristic has a double-staircase shape.

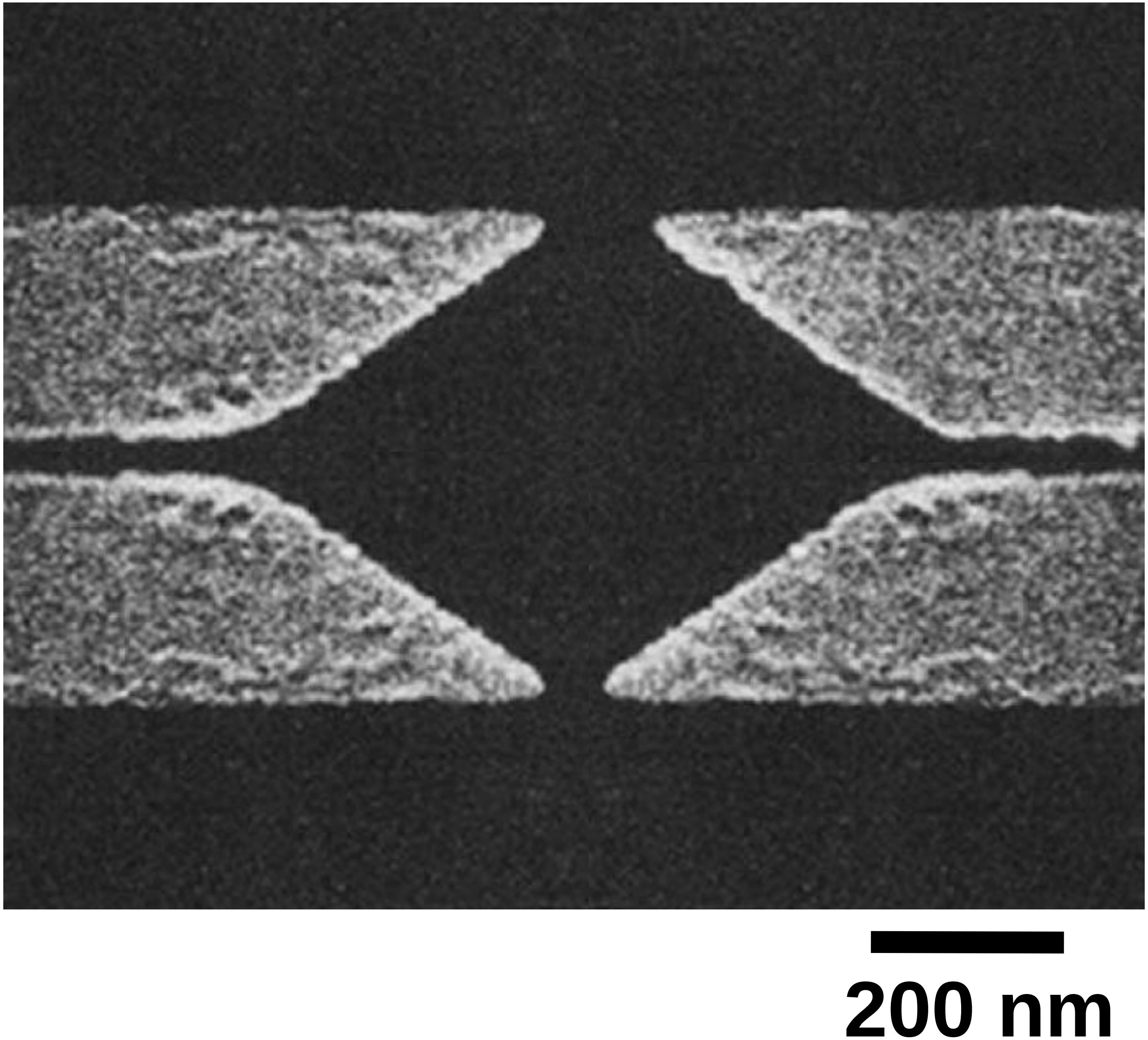
GaAs - $Al_xGa_{1-x}As$ hetero-structure

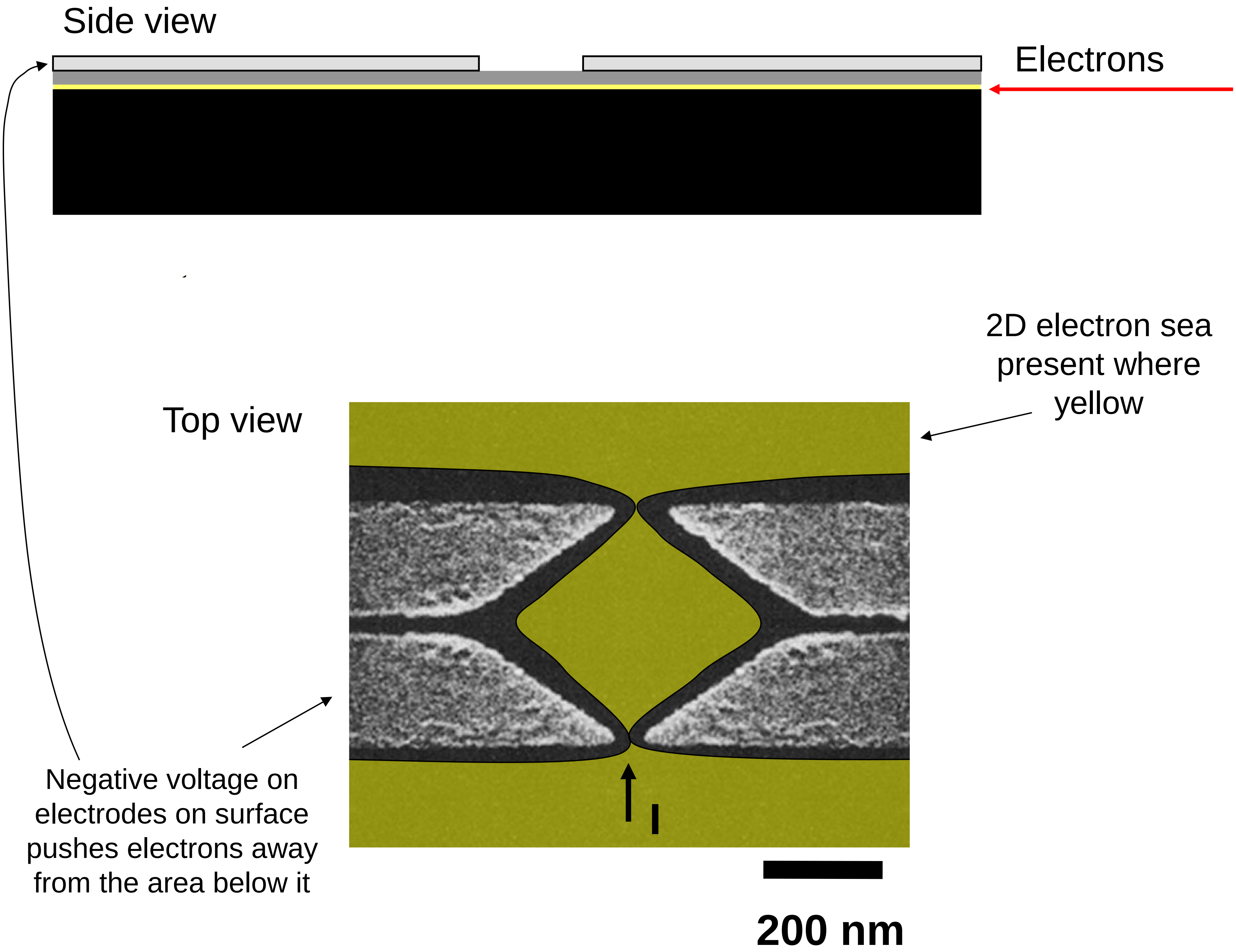
Side view

Electrons in a layer of about 10 nm thickness



QUANTUM DOT (top view)




Side view
Electrons
Top view
2D electron sea present where yellow
Negative voltage on electrodes on surface pushes electrons away from the area below it
I
200 nm

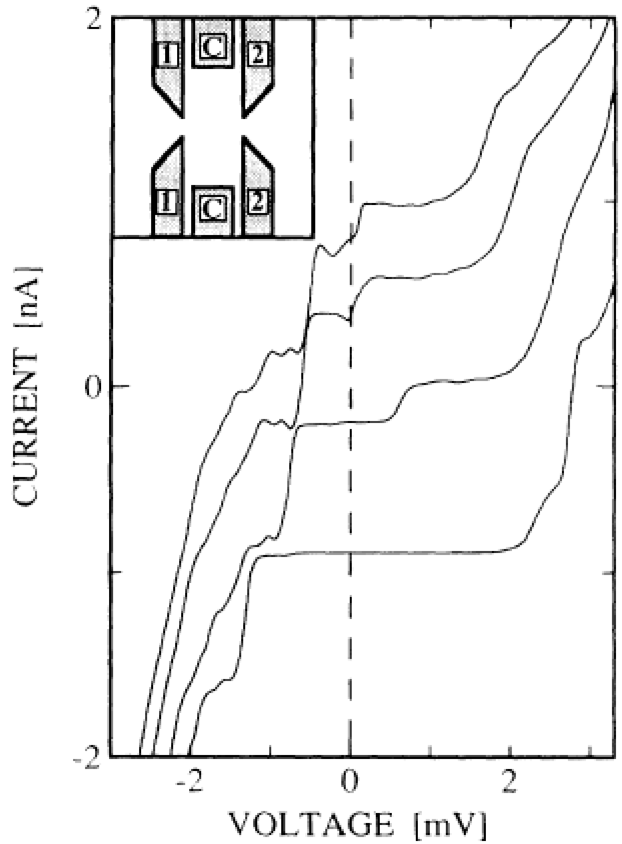


FIG. 3. Zero-field I-V curves at various center gate voltages for dot 2, showing the double-staircase structure. From the bottom, the center gate voltage is −920, −910, −907, and −905 mV. The curves are offset for clarity; all traces have $I=0$ when $V=0$. Inset: Sample 2 gate geometry. Transport is from left to right through QPCs 1 and 2.

Gate voltage controls the potential energy level that corresponds to the botton of the well.

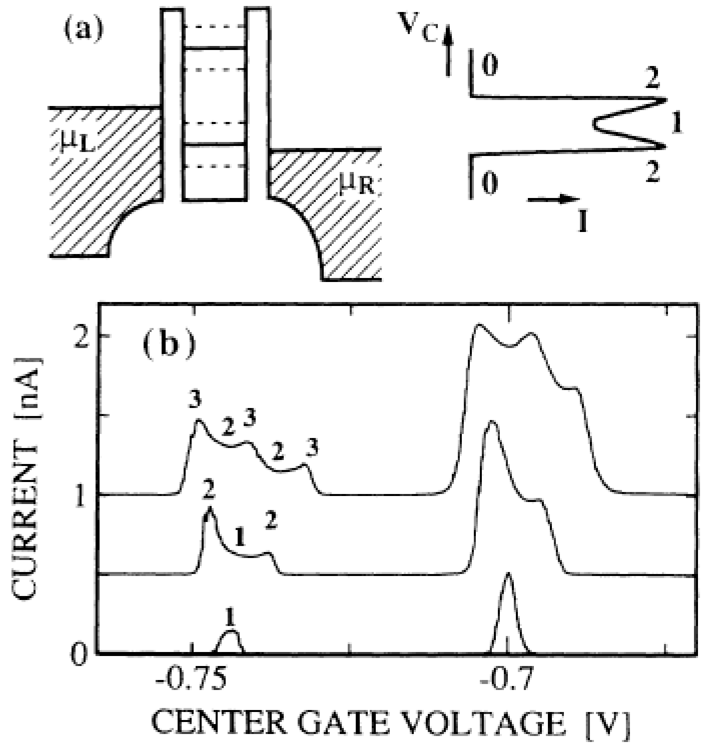


FIG. 2. (a) Potential energy landscape (left) and Coulomb oscillation with 0D shoulders (right) for a quantum dot with bias voltage $eV = \mu_L - \mu_R = 1.8\,\delta E$. Solid lines in the dot are the electrochemical potentials $\mu_d(N)$ and $\mu_d(N+1)$. Dashed lines show excitations with splitting δE. The number of states available for transport, noted by the peak, changes as 0-2-1-2-0 as V_C varies. (b) Evolution of 0D shoulders with increasing bias voltage in dot 2. The curves are offset for clarity. From the bottom, the bias voltages are 100, 400, and 700 μV. The magnetic field is 4 T.

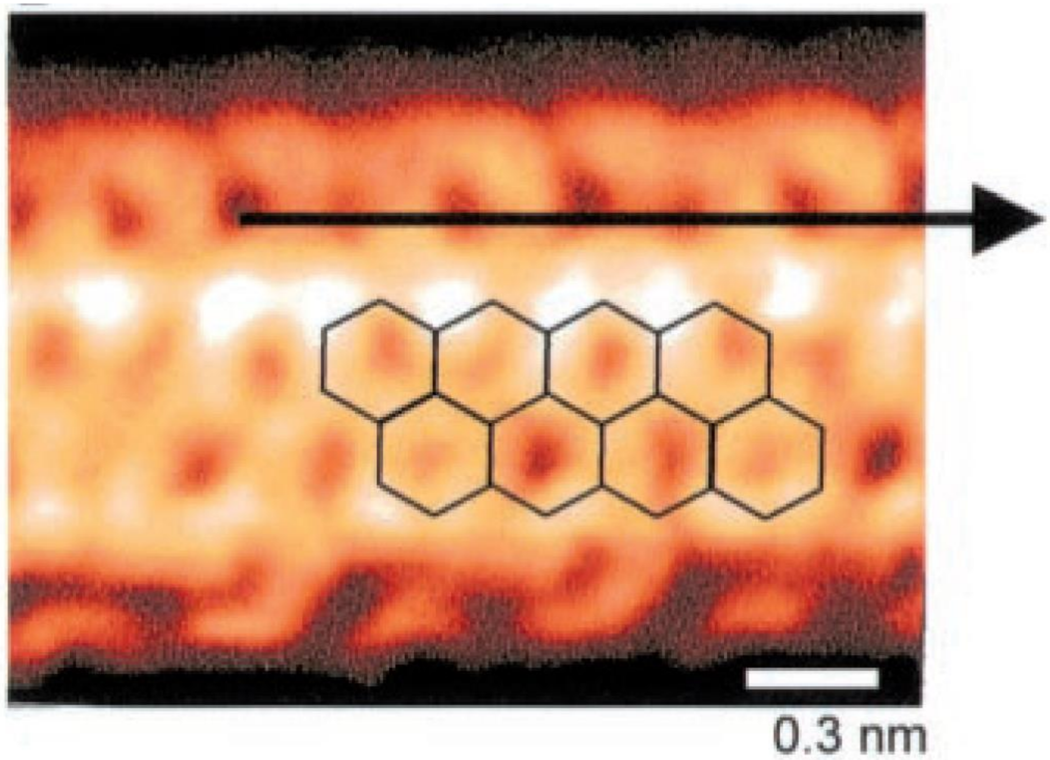
1 JANUARY 1999 VOL 283 SCIENCE www.sciencemag.org

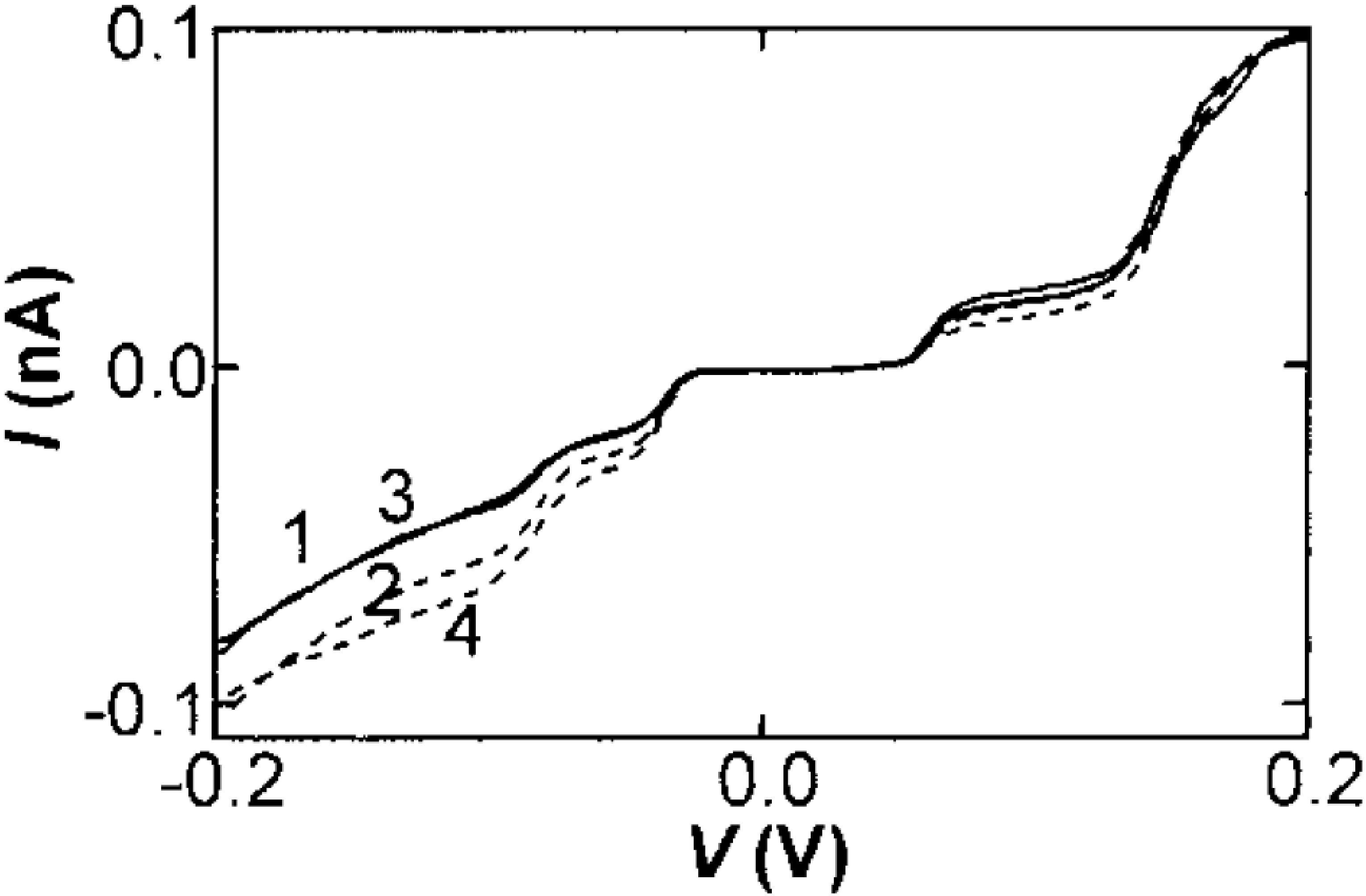
Imaging Electron Wave Functions of Quantized Energy Levels in Carbon Nanotubes

Liesbeth C. Venema, Jeroen W. G. Wildöer, Jorg W. Janssen, Sander J. Tans, Hinne L. J. Temminck Tuinstra, Leo P. Kouwenhoven, Cees Dekker*

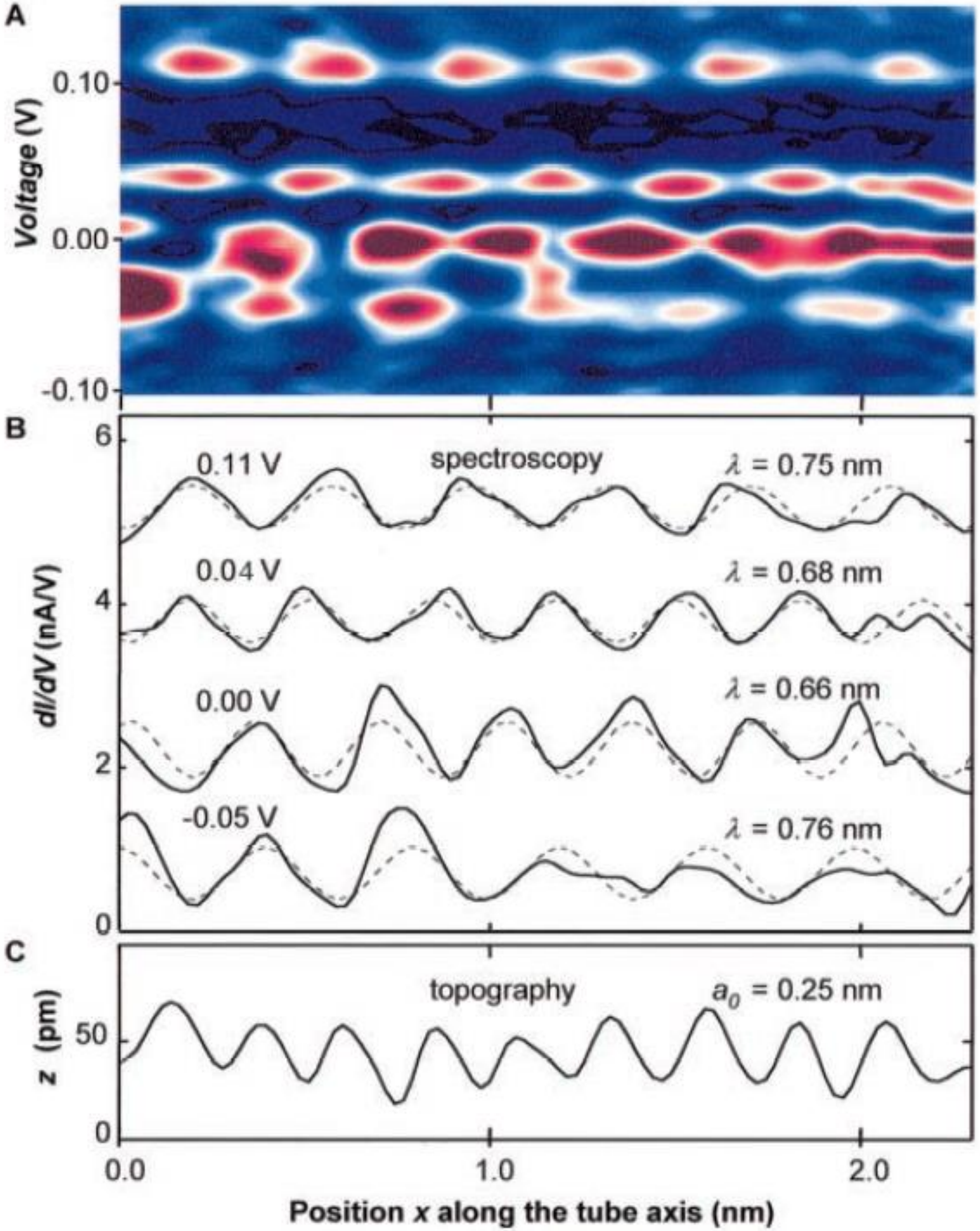
Carbon nanotubes provide a unique system for studying one-dimensional quantization phenomena. Scanning tunneling microscopy was used to observe the electronic wave functions that correspond to quantized energy levels in short metallic carbon nanotubes. Discrete electron waves were apparent from periodic oscillations in the differential conductance as a function of the position along the tube axis, with a period that differed from that of the atomic lattice. Wave functions could be observed for several electron states at adjacent discrete energies. The measured wavelengths are in good agreement with the calculated Fermi wavelength for armchair nanotubes.


nature
Carbon nanotube devices
Ageing
Ocean ridges
Lateral melt migration
Building immunity
The T-cell repertoire


0.3 nm



0.1
0.0
-0.1
I (nA)
-0.2
0.0
0.2
V (V)
1
2
3
4


A
B
C
Voltage (V)
0.10
0.00
-0.10
dI/dV (nA/V)
spectroscopy
0.11 V
λ = 0.75 nm
0.04 V
λ = 0.68 nm
0.00 V
λ = 0.66 nm
-0.05 V
λ = 0.76 nm
6
4
2
0
z (pm)
topography
a0 = 0.25 nm
50
0
0.0
1.0
2.0
Position x along the tube axis (nm)

To do

list for the teacher:

Example of determining velocity given a certain Psi(x)

Probability for a measurement outcome in a certain velocity range