Kwantumfysica I

2009-2010

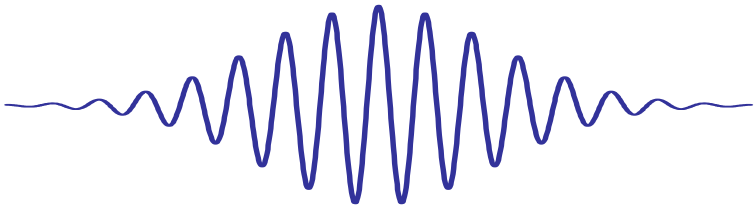
Hoorcollege dinsdag 1 december 2009

Vragen n.a.v. stof vorige week of werkcollege?

Vandaag:

1. Heisenberg
2. Wave packets
3. Formalisme:
   - Dirac notation
   - State vector space = Hilbert space
   - (Hermitian operators)
4. Particle in a box model (and research)

Wave packets and Heisenberg



Size (e.g. in space)

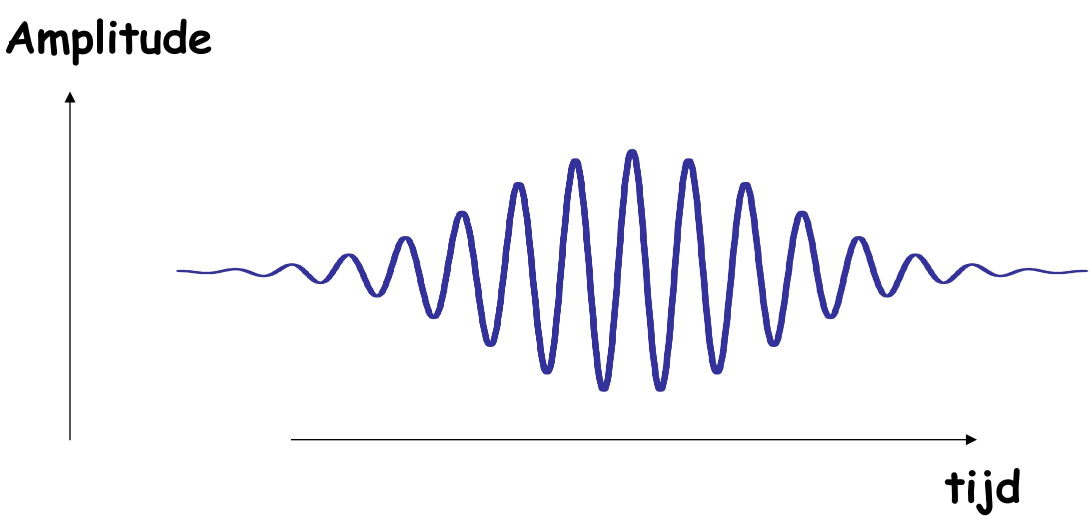
Velocity <u>PHASE</u> velocity

<u>GROUP</u> velocity

Shows that Heisenberg uncertainty relation
follows from wave nature of quantum states

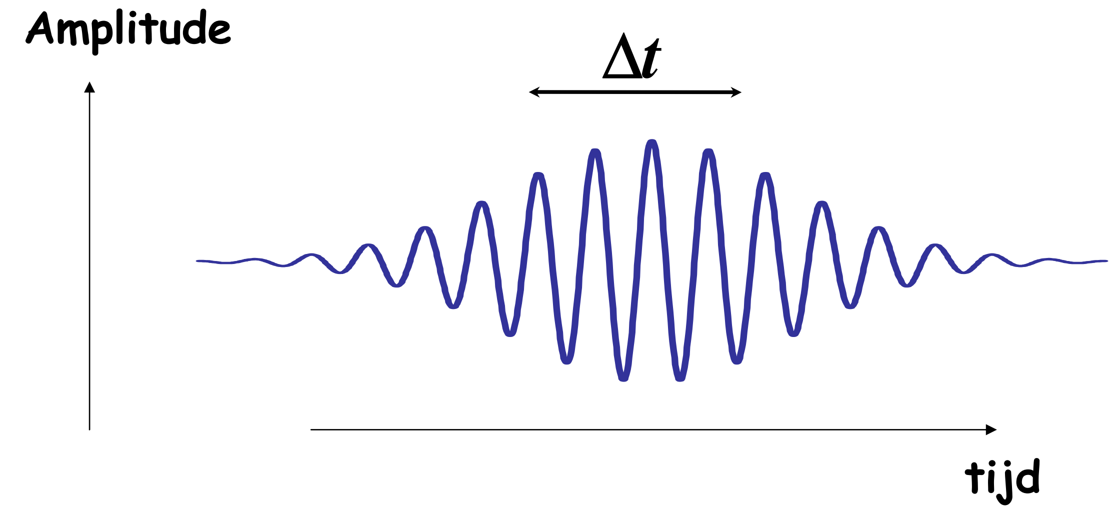
Eerst: Heisenberg onzekerheids-game

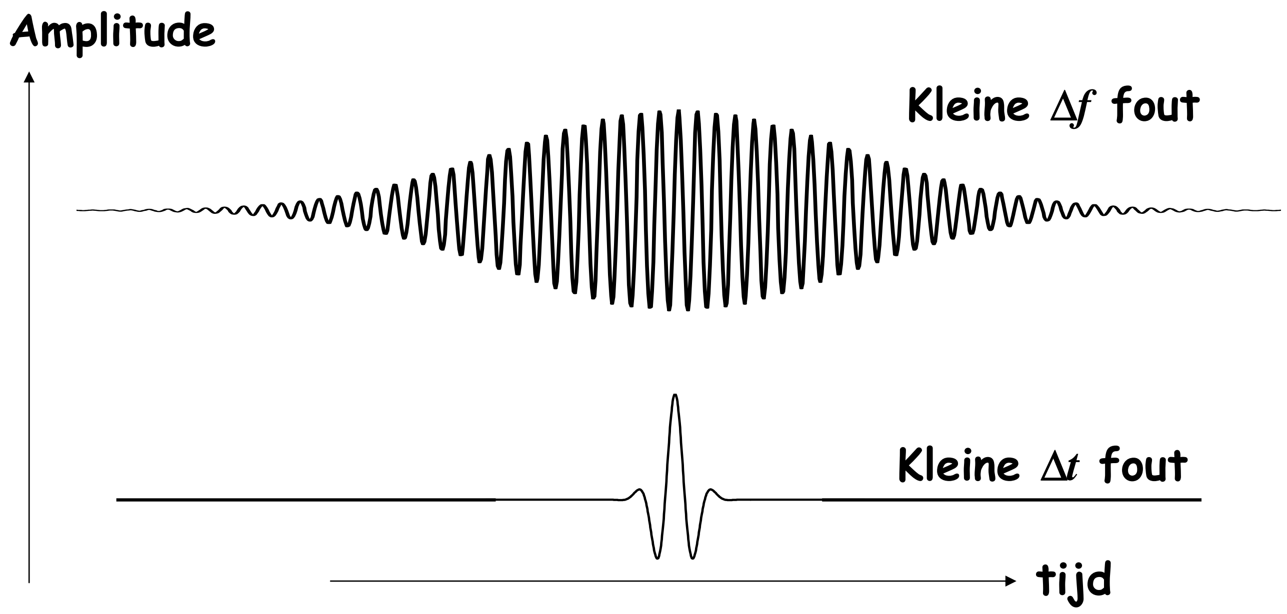
Stel, je hebt een systeem om fluit-tonen van eindige duur te maken, die altijd een "zachte" omhullende (envelope function) hebben. Je kunt de frequentie en het uitzend-tijdstip controleren.



Aan een luisterende partij de vraag:

Bepaal zo precies mogelijk
-Wanneer hoorde je de fluittoon?
-Wat is de frequentie van de fluittoon?





Δt fout is FWHM van Gaussian envelope

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

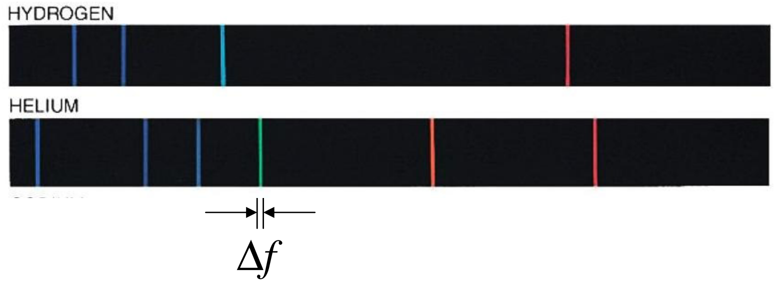
$$\Delta f \, \Delta t \approx 1$$

Heisenberg onzekerheidsrelatie voor Energie - tijd

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

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

$$\Delta E \, \Delta t \geq \hbar/2$$



Bepaalt b.v. breedte van spectraallijnen Δf.
Een electron in een atoom dat van een aangeslagen toestand naar de grondtoestand vervalt, zendt maar voor een korte tijdsduur Δt optische golven uit door oscillaties van het electrische dipool. De frequentie van deze oscillaties kan dus niet preciezer zijn dan Δf.

Samenvatting:

1. Toestand van quantum deeltje is vaak in de vorm van een golfpakket (wave packet)
2. Heisenberg onzekerheidsrelatie volgt direct uit golfkarakter van toestanden.

Vervolg:
Groep en fase snelheid van golfpakket
Deeltje opgesloten in een klein volume

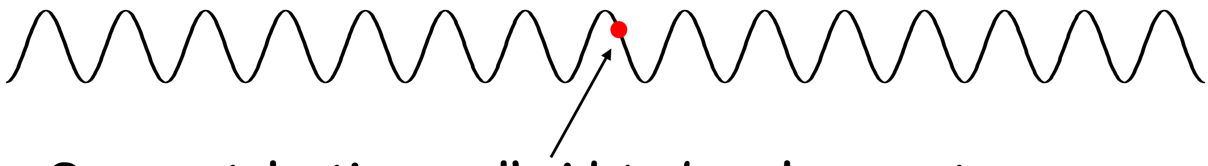
More on wave packets:

Velocity of wave packets (group velocity)

Velocity of a plane wave

Voorplanting van vlakke golf

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



Om voortplantingssnelheid te bepalen, punt van constante phase $kx - \omega t$ volgen.

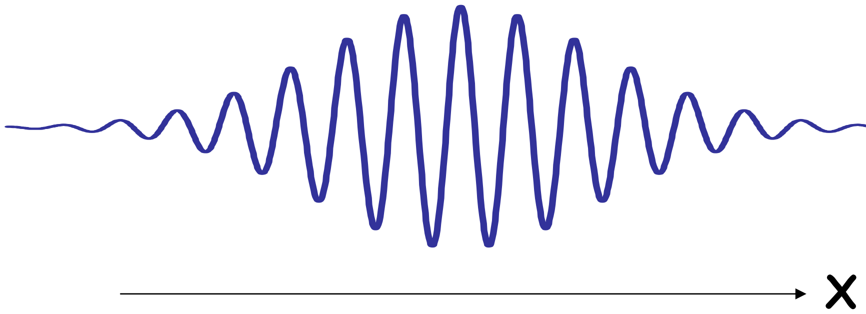
$$kx - \omega t = C$$

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

Maar $\frac{dx}{dt} = +\frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{p^2/2m}{p} = \frac{p}{2m} = \frac{v_{CL}}{2}$ **???**

More realistic, a wave packet:

Velocity of a wave packet



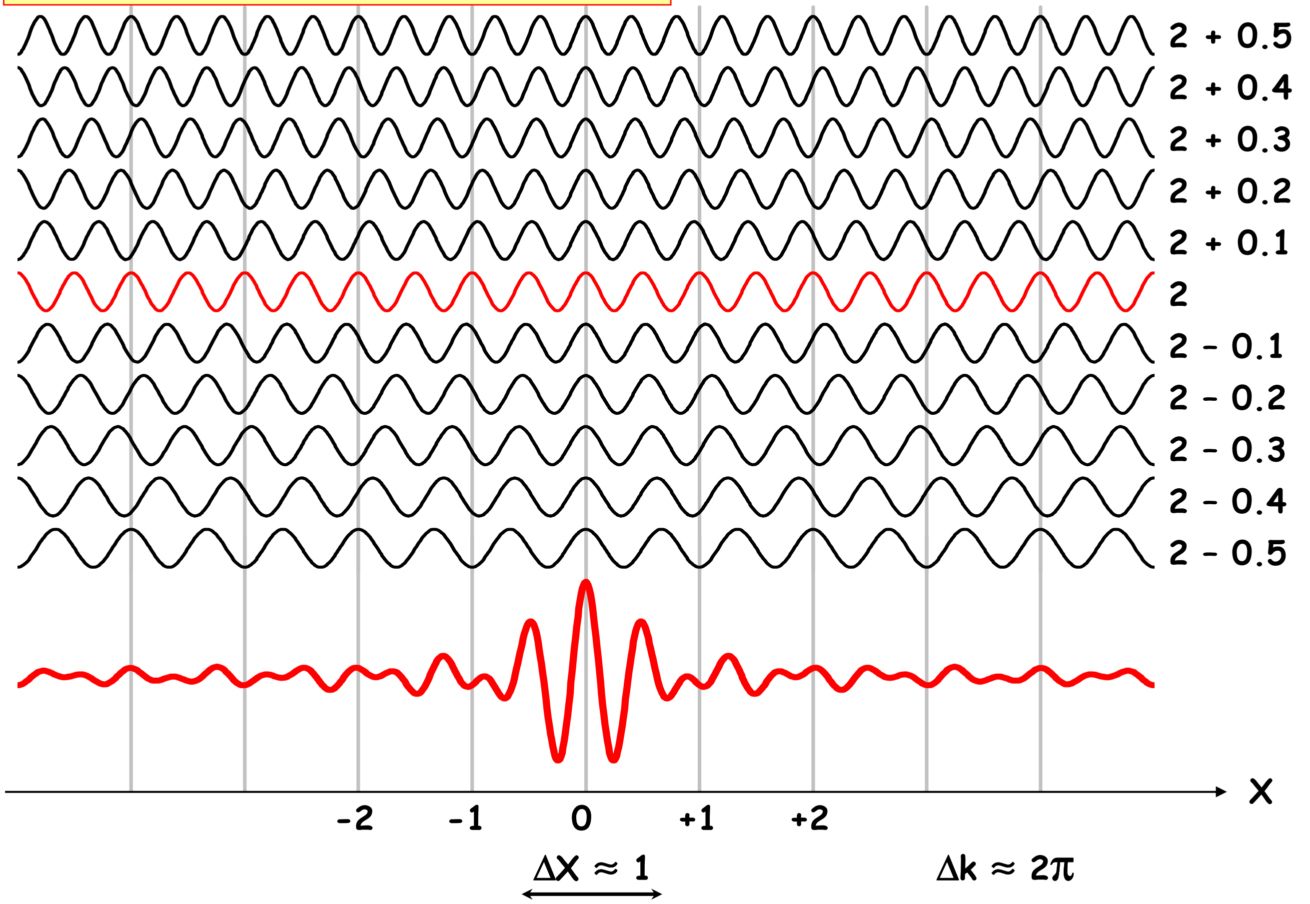
$$V_{PHASE}(k) = \frac{\hbar k}{2m}$$

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

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

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

Voor golfpakket $\Delta x \; \Delta k \approx 2\pi$



Voor dit golfpakket $\Delta x \, \Delta k \approx 2\pi$

Kleinere Δx kan alleen met grotere Δk.

Kleinere Δk kan alleen met grotere Δx

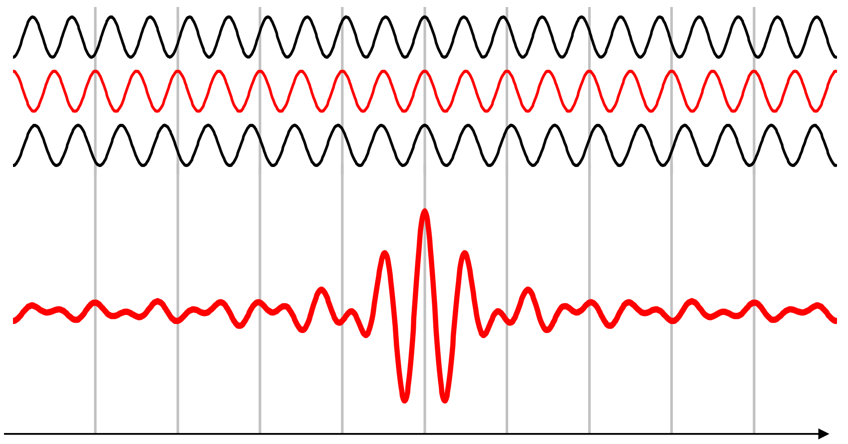
Komt door Fourier transform relatie voor golven:

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

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

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

Volgende week Fourier tutorial



$k_0 + \delta k$	$\omega_0 + \delta\omega$
k_0	ω_0
$k_0 - \delta k$	$\omega_0 - \delta\omega$

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

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

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

$$= \sqrt{\frac{1}{3}} e^{i(k_0x-\omega_0t)}\left(e^{i(\delta kx-\delta\omega t)} + 1 + e^{-i(\delta kx-\delta\omega t)}\right)$$

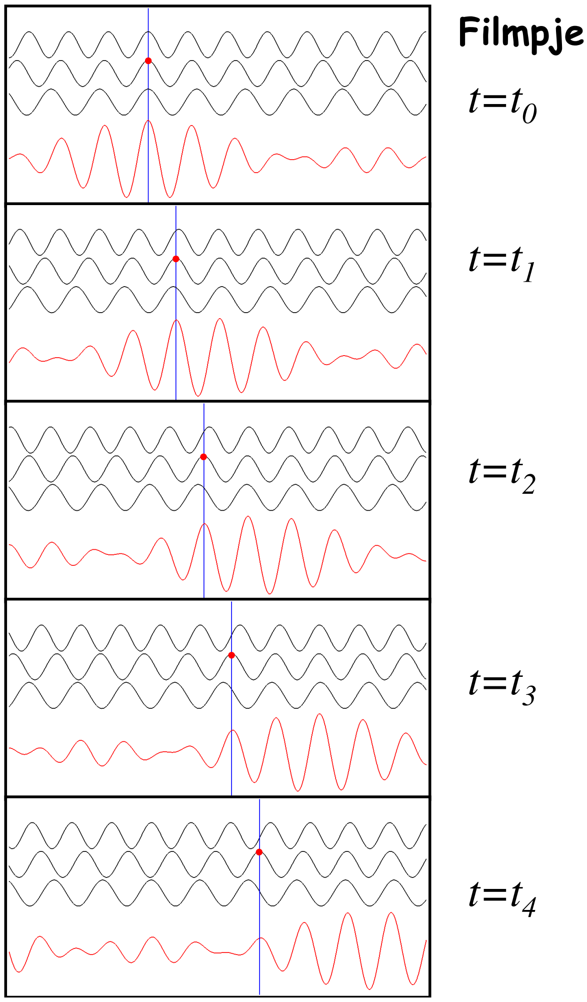
$$= \sqrt{\frac{1}{3}} e^{i(k_0x-\omega_0t)}\left(1 + 2\cos(\delta kx - \delta\omega t)\right)$$

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 wavepacket 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 ($kx-\omega t$) for realizing this constructive interference maximum, whatever their k.

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

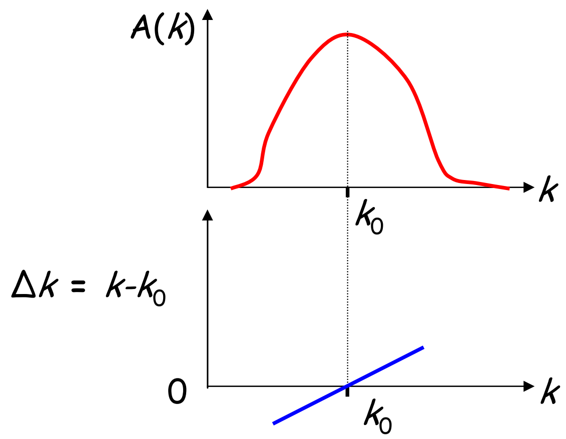
$$x-\frac{\partial \omega}{\partial k}t=0$$

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

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 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)

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

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

Dirac notation

Describe the state of a system as some abstract

<u>state vector</u> $|\Psi\rangle$

Why use this notation?

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

→ More general, abstract,
also for systems (e.g.spin) whose state cannot be written as $|\Psi\rangle \leftrightarrow \Psi(x)$

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

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

Formalism:

Dirac notation

Dirac notation

State vector $|\Psi\rangle$ "Ket"-vector

$\langle\Psi|$ "Bra"-vector

$\langle\Psi|\varphi\rangle,\quad \langle\Psi|\hat{A}|\varphi\rangle,\quad \langle\hat{A}\rangle \quad \rightarrow$ Between **br**ac**kets**

$$\langle\Psi|\hat{A}|\Psi\rangle \quad \Rightarrow$$

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

Dirac notation

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

Inner product – 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, on p. 97 (eq. 4.21 – 4.25)

Dirac notation

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

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

Basis (eigen) vector of x-basis

But also, for example,

$$\langle \varphi_k|\Psi\rangle = \int_{-\infty}^{\infty} \delta(p_x)\,\overline{\Psi}(p_x)\,dp_x = \overline{\Psi}(p_x)$$

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)

Hilbert space

The linear vectorspace where the state vectors $|\varphi\rangle$ live.

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

Say the state of some system can be completely characterizdd by the physical property A, with associated observable $\hat{A}$.

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

The eigenvectors $|\varphi_a\rangle$ of $\hat{A}$ 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 (NIET TOETS, wel tentamen)

Note order!

$$|\Psi\rangle \leftrightarrow \langle\Psi| \qquad (\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$$

$$\hat{A} \leftrightarrow \hat{A}^+ \qquad (\hat{A}^+)^+ = \hat{A}$$

$$|\Psi'\rangle = \hat{A}|\Psi\rangle \leftrightarrow \langle\Psi'| = \langle\Psi|\hat{A}^+ \qquad (c\hat{A})^+ = c^*\hat{A}^+$$

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

Hermitian operators

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

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**

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

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

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

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)

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

$V(x) = 0, \quad 0 < x < a$

$V(x) = \infty, \quad all\ other\ x$

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

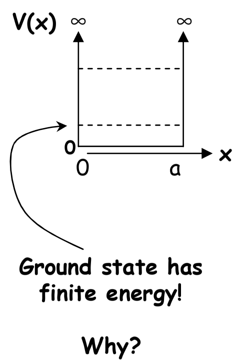
Some additional assumptions needed to find eigenstates:

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

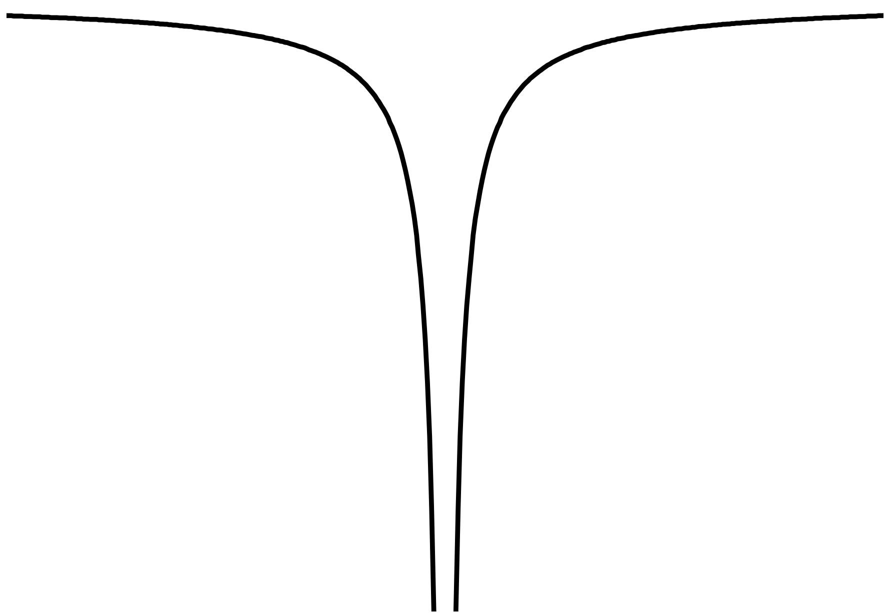
$\varphi(0) = \varphi(a) = 0$ continuous at x=0 and x=a

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

See book on p. 92



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



Samenvatting:

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

Volgende college:

Meer over wave packets en Fourier tutorial Fourier
Commutators
Some more research