Kwantumfysica I

2008-2009

Hoorcollege vrijdag 28 november 2008

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

Vandaag:

1. Wave packets

2. Formalisme:
   - Dirac notation
   - State vector space = Hilbert space
   - (Hermitian operators)

3. Particle in a box model and research

Wave packets

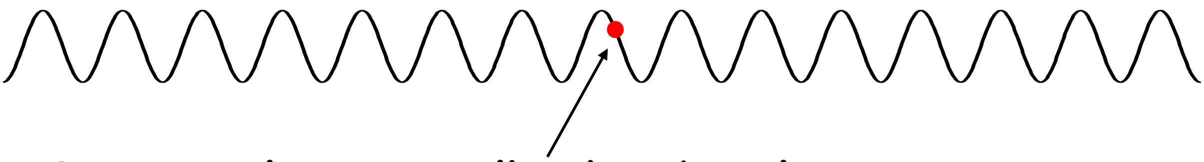
Velocity of wave packets (group velocity)

and Heisenberg

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.**

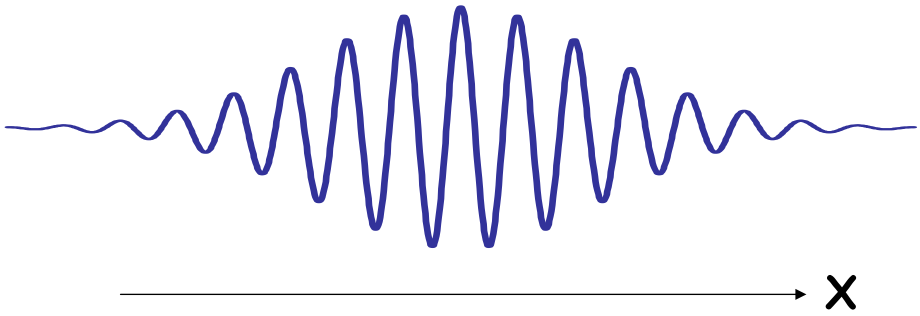
$$kx - \omega t = C$$

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

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

More realistic, a wave packet:

Velocity of a wave packet



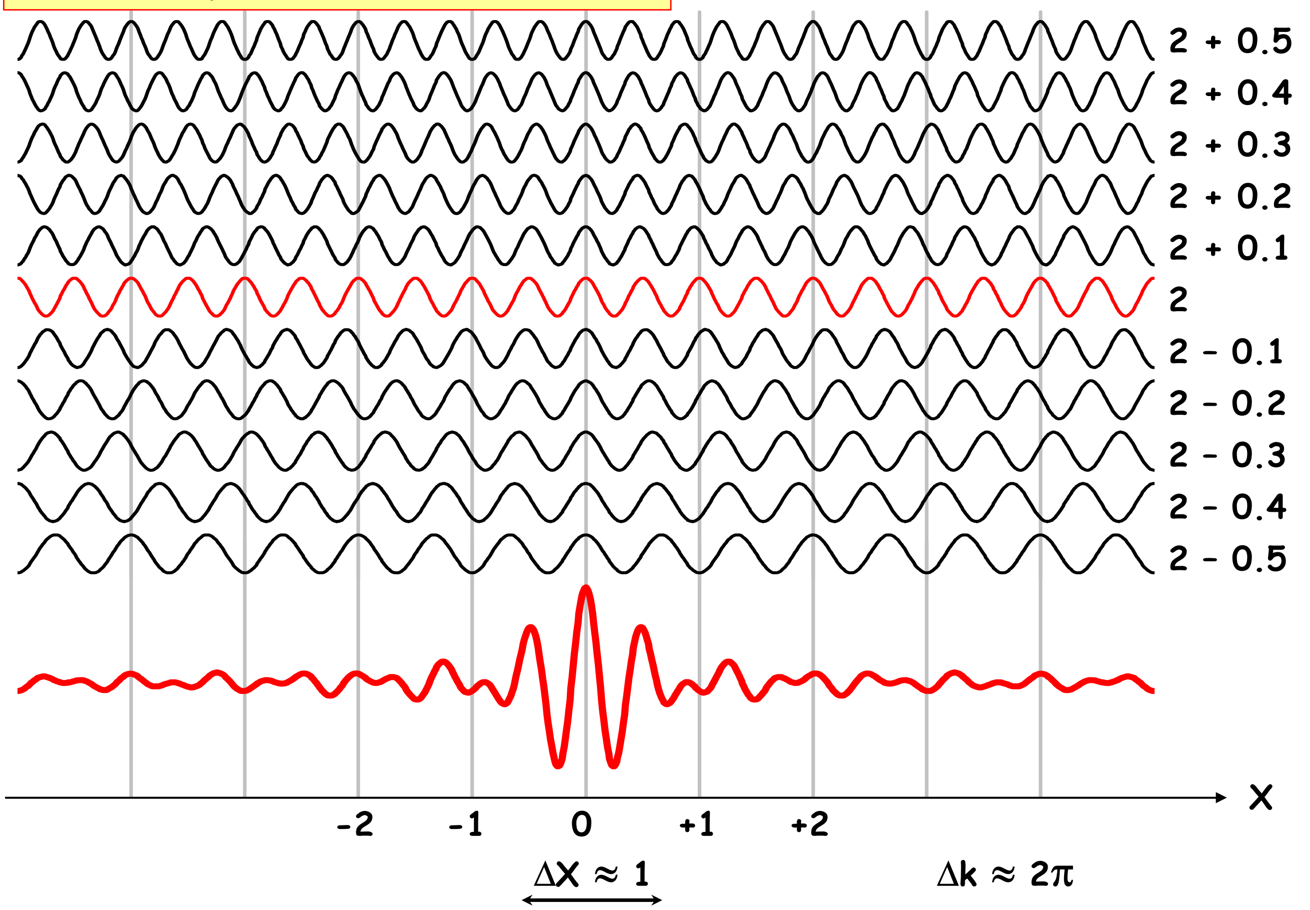
$$V_{PHASE}(k) = \frac{\hbar k}{2m}$$

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

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

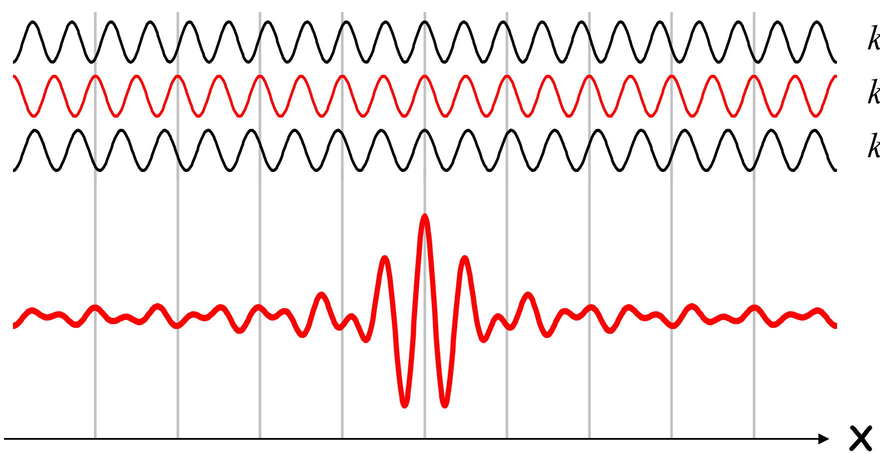
Komt door Fourier transform relatie voor golven:

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

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

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

Volgende week Fourier tutorial



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

k_0 $\quad \omega_0$

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

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

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

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

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

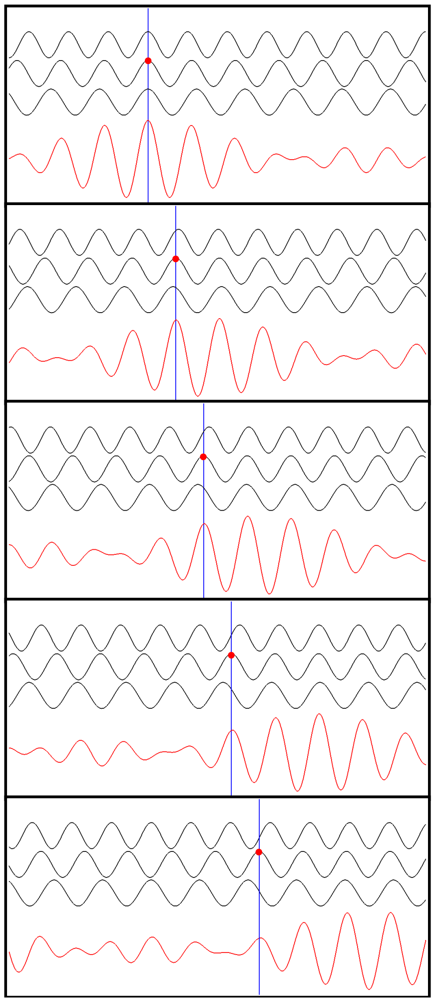
$$= \sqrt{\frac{1}{3}} e^{i(k_0 x - \omega_0 t)} \left(1 + 2\cos(\delta k x - \delta\omega t) \right)$$

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.



Filmpje

$t=t_0$

$t=t_1$

$t=t_2$

$t=t_3$

$t=t_4$

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 ⇒ They all have and keep the same phase (*k*x-ωt) for realizing this constructive interference maximum, whatever their *k*.

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

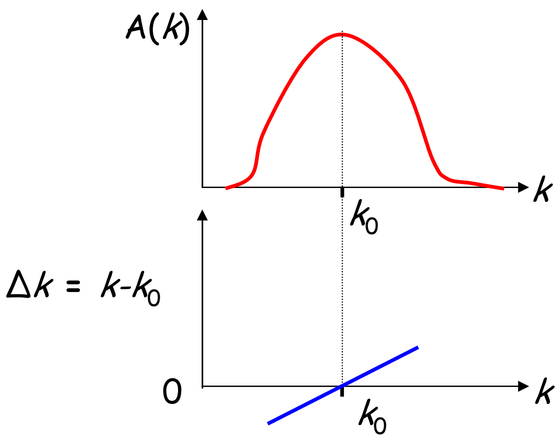
$$x-\frac{\partial \omega}{\partial k}t=0$$

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

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

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

Why use this notation?

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

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

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

→ 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

$\left\langle\Psi|\varphi\right\rangle$, $\left\langle\Psi\right|\hat{A}\left|\varphi\right\rangle$, $\left\langle\hat{A}\right\rangle$ → Between brackets

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

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

Dirac notation

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

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

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

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

Hilbert space

The <u>linear</u> vectorspace 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> 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 φ_a of $\hat{A}$.

The eigenvectors φ_a 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!

$$|\Psi\rangle \leftrightarrow \langle\Psi|$$

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

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

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

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

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

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

Hermitian operators

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

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

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

Hermitian operators (observables) have
- **real eigenvalues**
- **orthogonal eigenvectors**

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

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

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

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)

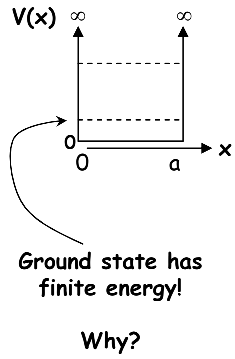
$$\hat{H} = \hat{H}_{kin} + \hat{H}_{pot}$$

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

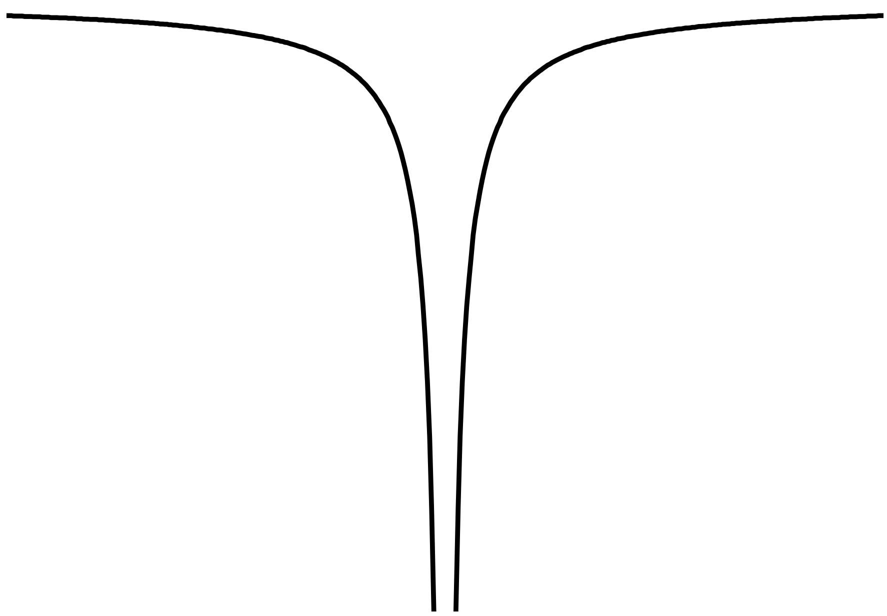
This gives the Hamiltonian of a free particle for the interval 0<x<a, but with boundary conditions.

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

Huiswerk voor H4

Theorie 1913

Studiestof:
Alles van H4
Appendix A, behalve laatste pagina

Leesstof:
geen

Oefeningen:

Thuis maken, vóór het werkcollege:
4.1, 4.2, 4.3, 4.4, 4.5, 4.11, 4.12, 4.13, 4.14, 4.16, 4.25, 4.29

Tijdens werkcollege, 1 opgave wordt uitgedeeld, en
4.6 (use p. 857), 4.9, 4.10 (only for <px>), 4.15, 4.17, 4.21, 4.22, 4.33, 4.35, 4.36

Extra voor zelf later verder oefenen: Zie webpagina voor dit vak

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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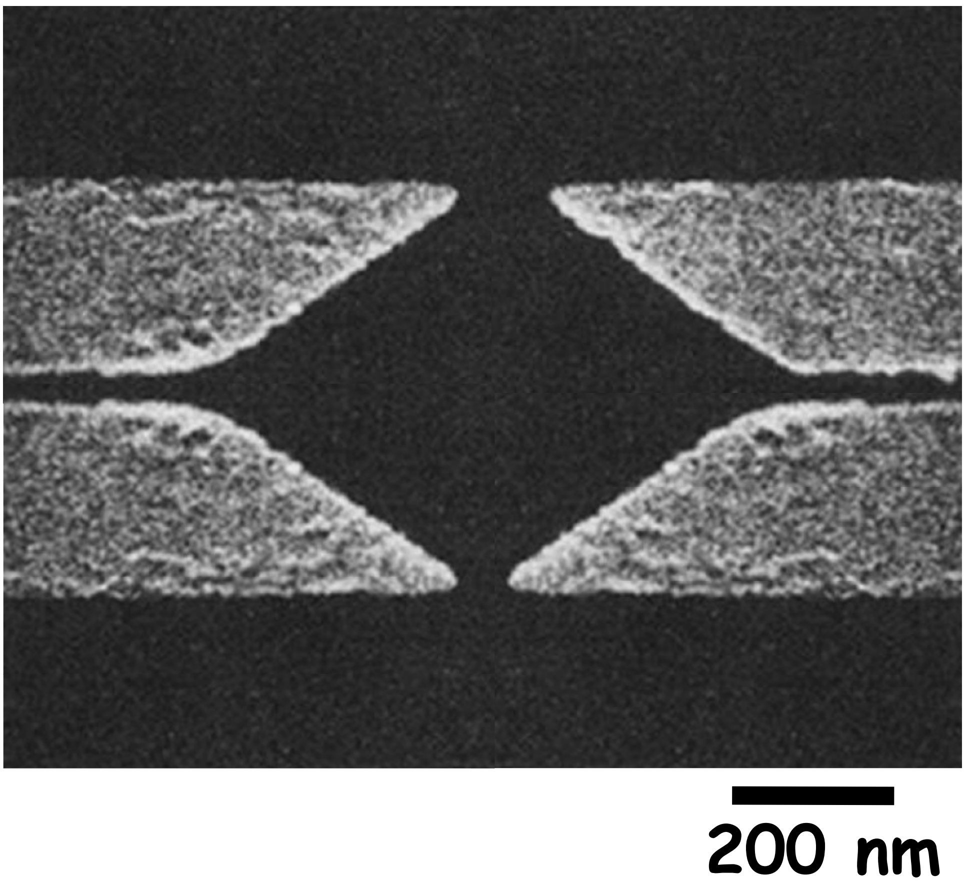
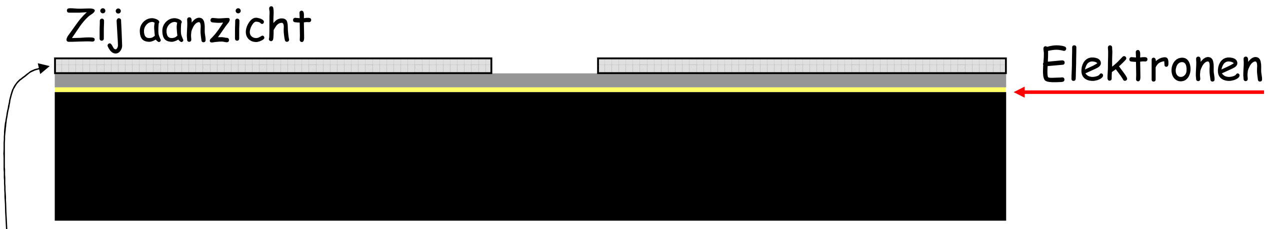
(Received 19 May 1992)

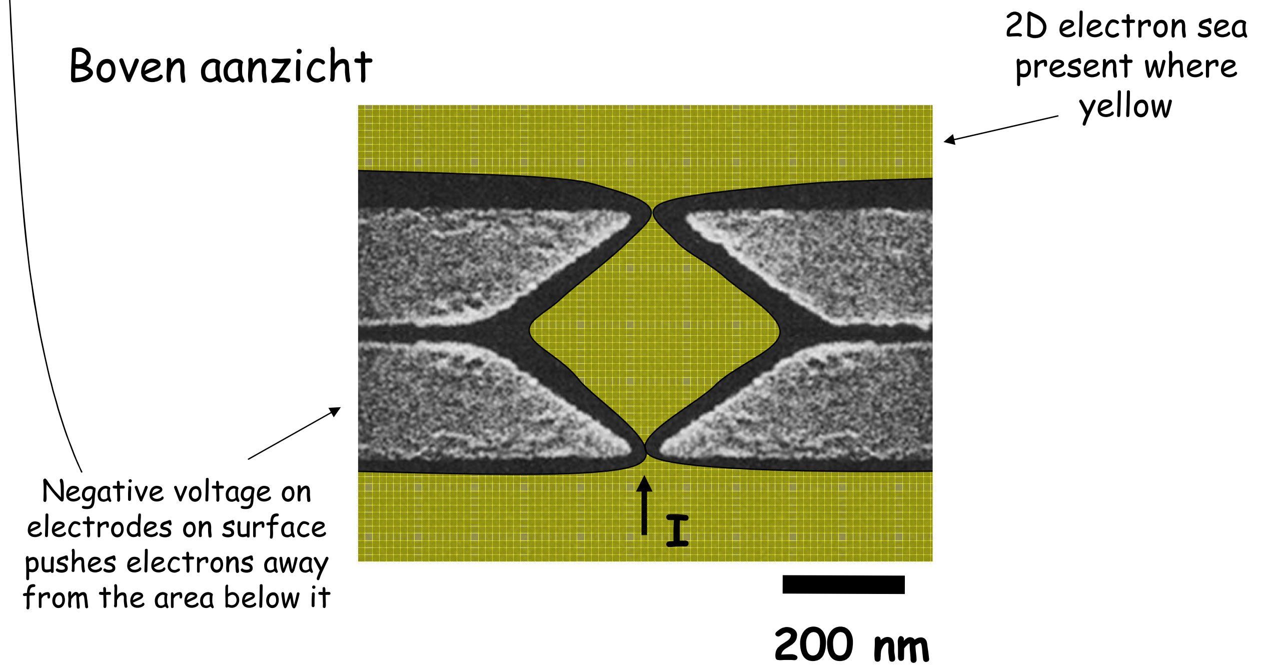
We observe new transport effects in lateral quantum dots where zero-dimensional (0D) states and single electron charging coexist. In linear transport we see *coherent* resonant tunneling, described by a Landauer formula despite the many-body charging interaction. In the nonlinear regime, Coulomb oscillations 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

QUANTUM DOT (Boven aanzicht)







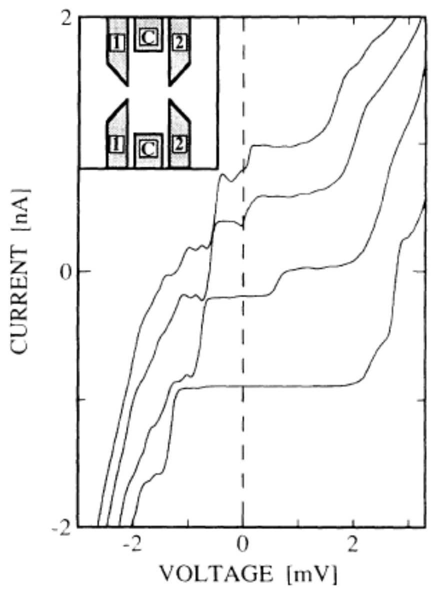


FIG. 3. Zero-field I-V curves at various center gate voltages for dot 2, showing the double-staircase structure. From the bottom, the center gate voltage is −920, −910, −907, and −905 mV. The curves are offset for clarity; all traces have $I=0$ when $V=0$. Inset: Sample 2 gate geometry. Transport is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

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

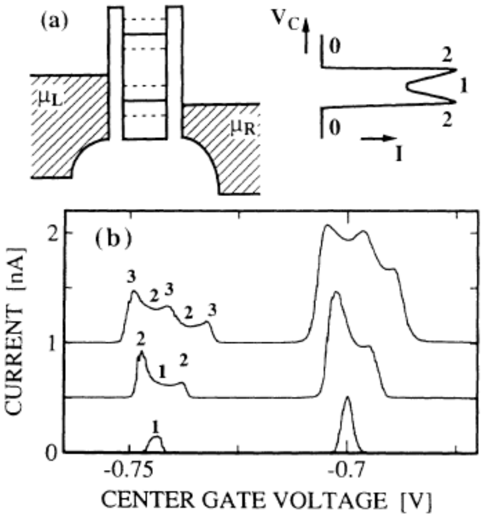


FIG. 2. (a) Potential energy landscape (left) and Coulomb oscillation with 0D shoulders (right) for a quantum dot with bias voltage $eV = \mu_L - \mu_R = 1.8\,\delta E$. Solid lines in the dot are the electrochemical potentials $\mu_d(N)$ and $\mu_d(N+1)$. Dashed lines show excitations with splitting 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.

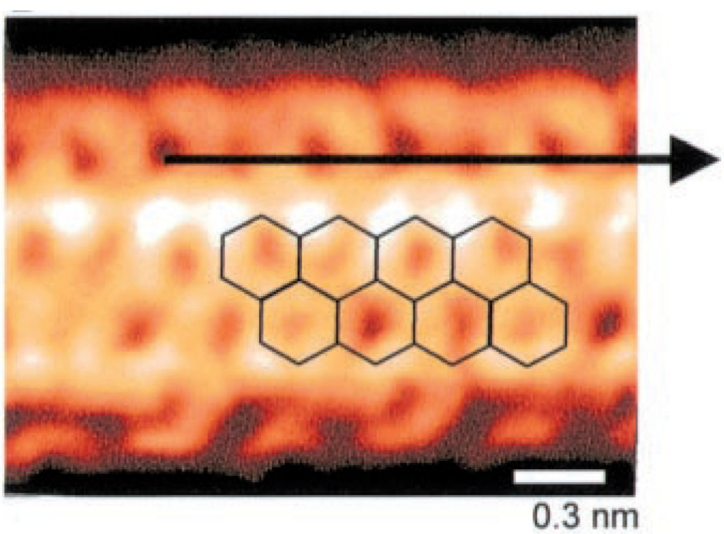
1 JANUARY 1999 VOL 283 SCIENCE www.sciencemag.org

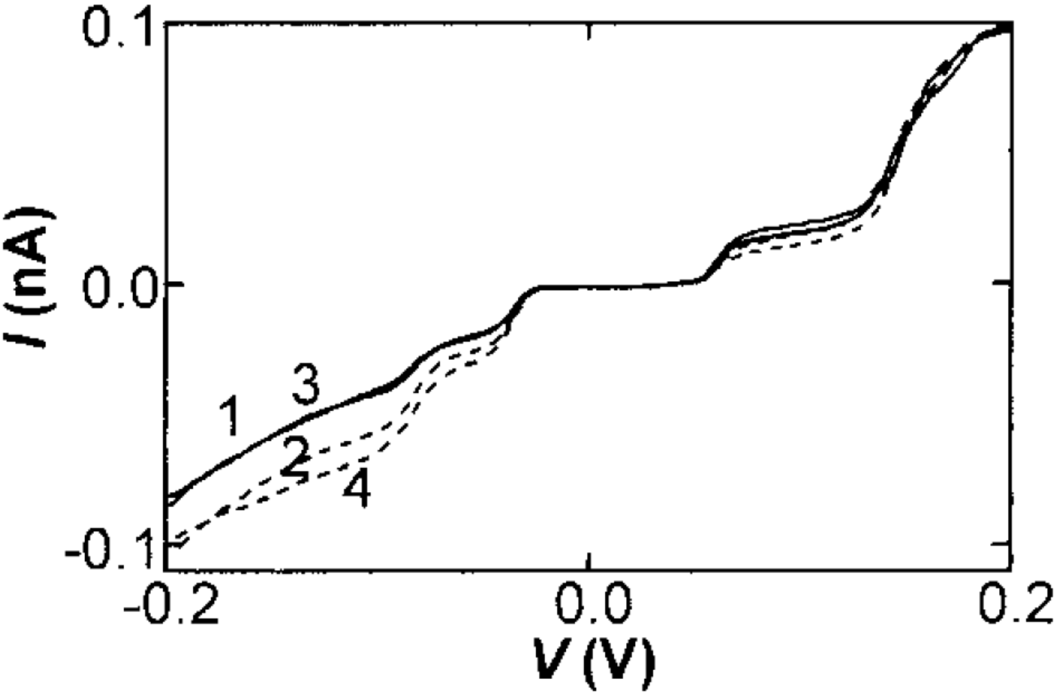
Imaging Electron Wave Functions of Quantized Energy Levels in Carbon Nanotubes

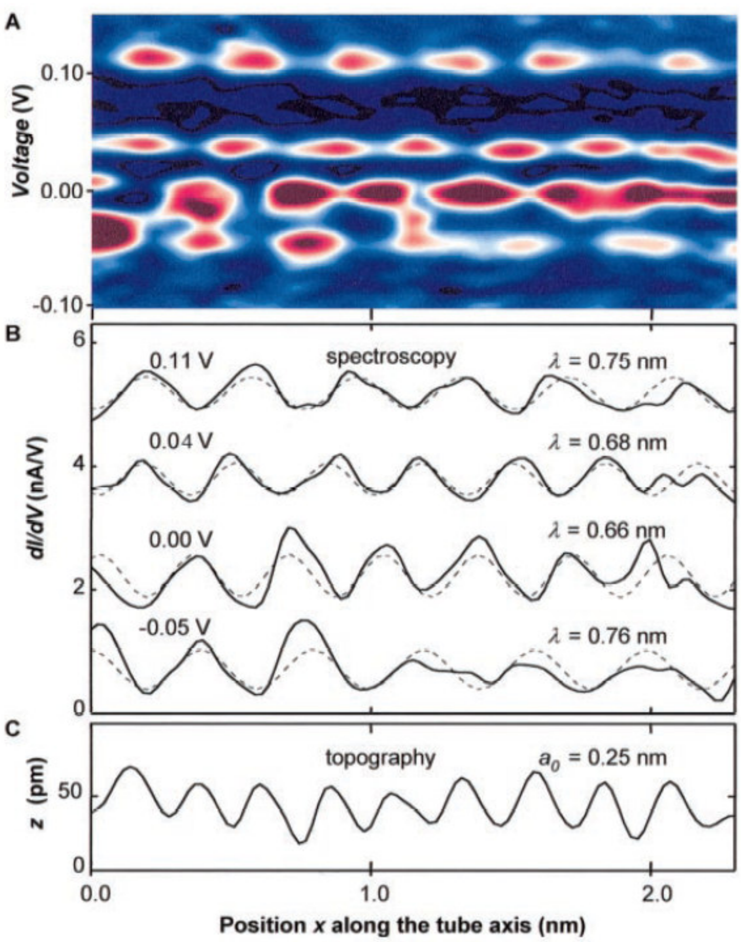
Liesbeth C. Venema, Jeroen W. G. Wildöer, Jorg W. Janssen, Sander J. Tans, Hinne L. J. Temminck Tuinstra, Leo P. Kouwenhoven, Cees Dekker*

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
Lateral melt migration
Building immunity
The T-cell repertoire


0.3 nm


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


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