Physics at the Nanoscale

and applications

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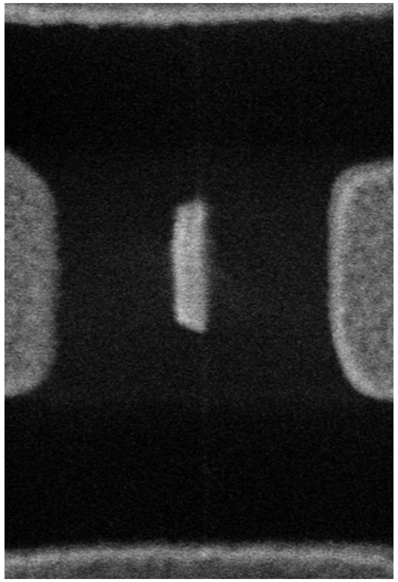
Nanoscience

Where Physics, Chemistry and Biology meet

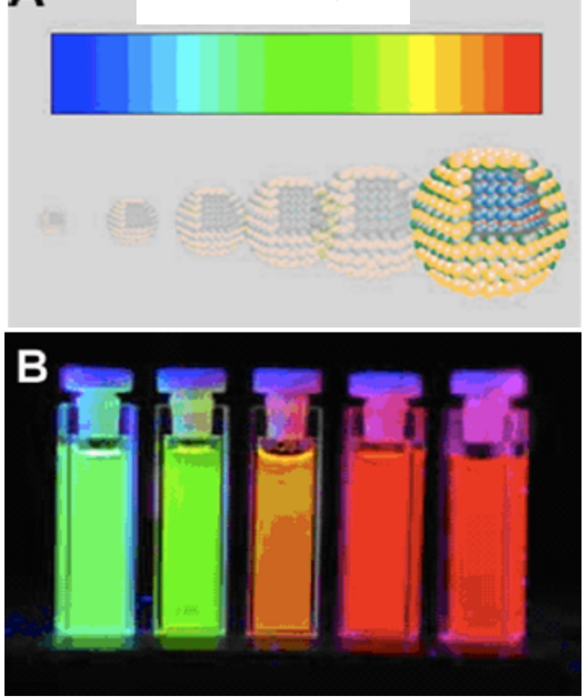
Nano-motor with Carbon nanotube bearing



(Courtesy of Professor Alex Zettl)

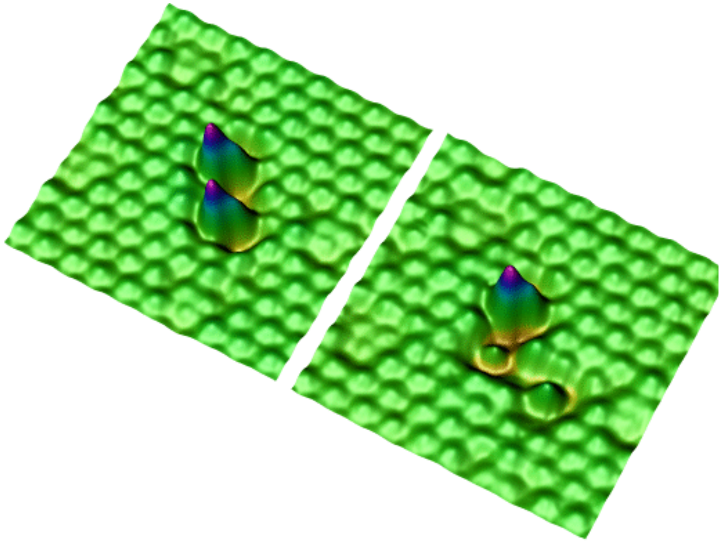
Tuning color via the size of nanoparticles

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$



(Source:D. Spencer / Philips)

Making chemistry by pushing atoms around



Single Molecule Chemistry

(Courtesy of Professor Wilson Ho)

Physics at the Nanoscale

Sources & Acknowledgements:

○ S. Lindsay, *Introduction to Nanoscience*, Oxford University Press, 2008. (textbook+slides)

○ H. Courtois, *Scanning Probe Microscopies*, Master lecture, Grenoble INP

○ T. Ouisse, *Electron Transport in Nanostructures and Mesoscopic Devices*, Wiley, 2008.

○ T. Ouisse, *Forces at the Nanoscale*, Nano Summerschool lecture, Grenoble INP, 2010.

Basic Principles of Quantum Mechanics:
Energy Quanta

Planck (1900, Nobel prize ‘18) explains black body radiation spectrum assuming

→ *Energy packets, « quanta »*

$$\Delta E = n \times h \times f_0 = n \times \hbar\omega_0 ,$$

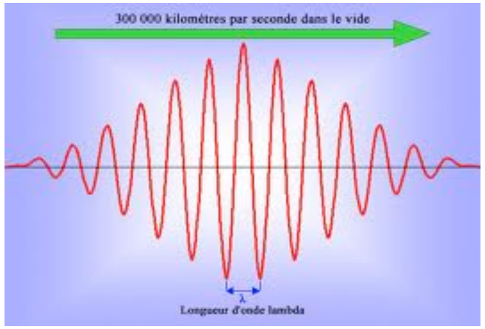
$$n \in N ,$$

$$\hbar = h/2\pi = 1.05 \times 10^{-34}\ J.s$$

Einstein (’05, Nobel prize ‘23) interprets energy quanta as particles carrying the electromagnetic field : the photon.

→ wave-particle duality

Wave packet



Basic Principles of Quantum Mechanics:

Momentum versus wave vector

Propagating waves

$$e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

$\propto \vec{p}$ $\propto E$

If waves behave like particles,
shouldn't particles behave like waves?

Every particle that has momentum, has a wave vector.
Every particle that has energy, oscillates in time.

de Broglie relation ('24, Nobel prize '29):

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

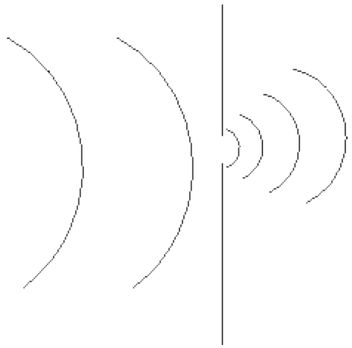
$$E = \hbar\omega$$

Basic Principles of Quantum Mechanics:

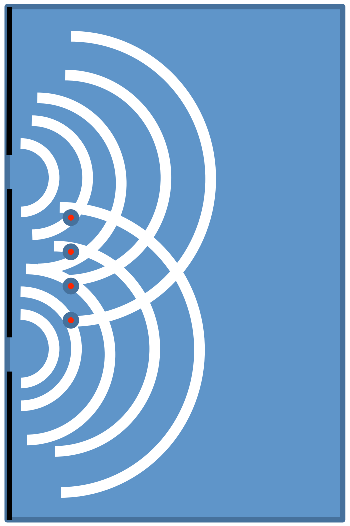
Wave diffraction and interference

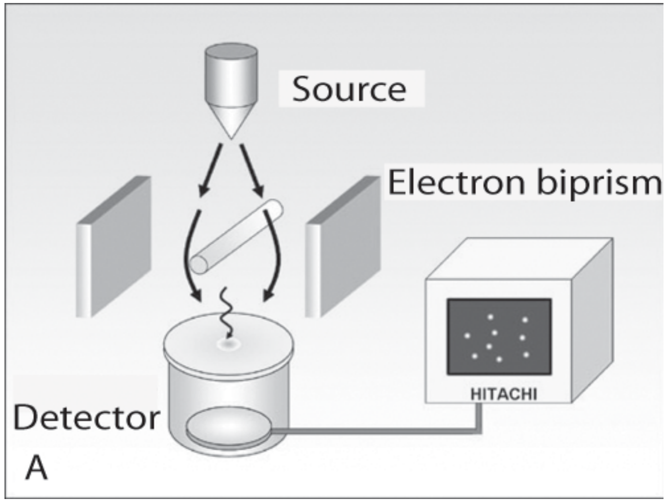
Young's double slit experiment with electrons

Diffraction



Interference





(Courtesy of Dr. Akira Tonomura / Hitachi)

Basic Principles of Quantum Mechanics:
The Schrödinger equation

« If there is a wave, there must be a wave equation » (Debye, Nobel prize '36)

In electromagnetism
(Maxwell's equations in free space)

$$\Delta\vec{E} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{E} = 0 \Rightarrow e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Schrödinger's guess ('26, Nobel prize '33):

In free space

$$i\hbar\frac{\partial}{\partial t} = \frac{-\hbar^2\Delta}{2m}$$

with a potential

$$i\hbar\frac{\partial}{\partial t} = \frac{-\hbar^2\Delta}{2m} + U$$

dispersion relation

$$E = \frac{\vec{p}^{\,2}}{2m} + V = E_c + E_p$$

$$\Delta = \vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Basic Principles of Quantum Mechanics:
Wave function

What do we apply Schrödinger's equation to?

→ What is the physical meaning of ψ ?

Mathematical constraint $$\int_{space} \left| \psi(\vec{r},t) \right|^2 d^3\vec{r} < +\infty$$

$|\psi|^2$ is similar to a probability distribution in space.

Basic Principles of Quantum Mechanics:
Wave function

What do we apply Schrödinger's equation to?

→ What is the physical meaning of ψ ?

Mathematical constraint $$\int_{space} \left|\psi(\vec{r},t)\right|^2 d^3\vec{r} < +\infty$$

IψI² is ~~similar to~~ a probability distribution in space.

Born ('26, Nobel prize '54)

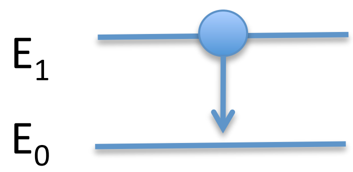
Basic Principles of Quantum Mechanics:
Did you say probability?

The square modulus of the wave function is the probility density to find the particle inside d^3r if measured at time t.

Philosophical issue:

- Is nature probabilistic by essence ?
  « God doesn't play dice! » (Einstein)
- What is the role of the measurement process ?
  objective observer?

...to go further: Einstein-Podolsky-Rosen paradox, Schrödinger's cat, ...



The decay of a given particle from energy state E_1 to state E_0 can only be predicted in terms of probabilities.

Basic Principles of Quantum Mechanics:

The Heisenberg uncertainty principle

1D plane wave

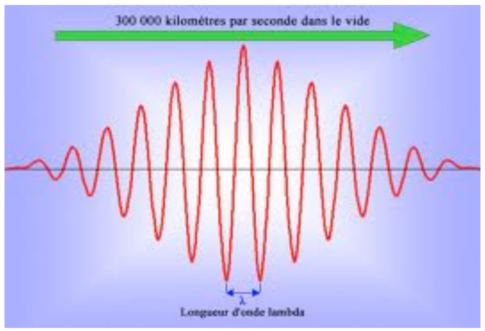
$$e^{i(kx-\omega t)}$$

p (=ħk) perfectly defined
position x perfectly undefined

Wave packet

$$\sum_k c_k e^{i(kx-\omega_k t)}$$

A wave packet is spatially localized with some region.
The cost for this: several p, that is an uncertainty on p.



Heisenberg

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$$\Delta t \Delta E \geq \frac{\hbar}{2}$$

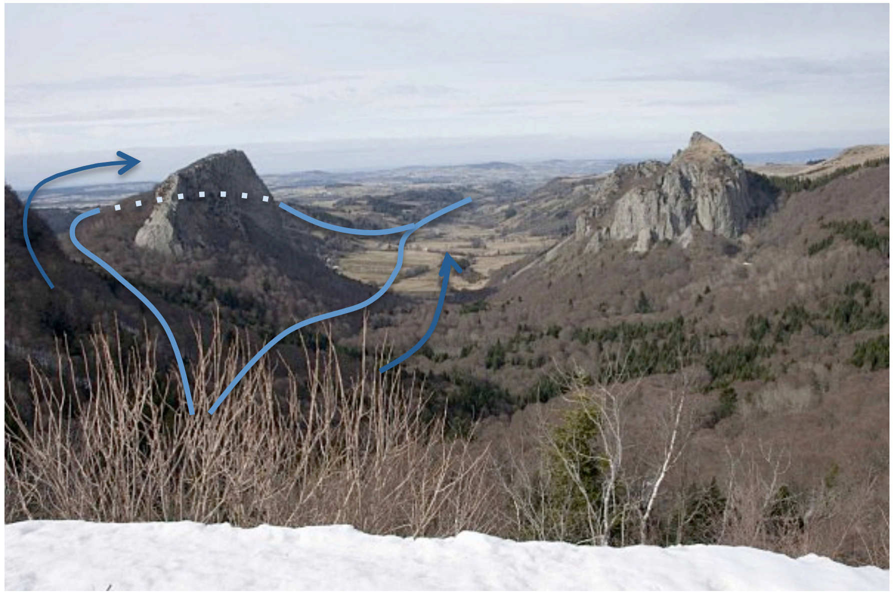
Basic Principles of Quantum Mechanics:

Phase, interference

$$\psi(\vec{r},t) = \left|\psi(\vec{r},t)\right| e^{i\varphi(\vec{r},t)}$$

$$\left|\psi_{transmitted}\right|^2 = \left|\psi_{left} + \psi_{right}\right|^2$$

$$\propto \left|e^{i\varphi_{left}} + e^{i\varphi_{right}}\right|^2$$



Maximum transmission if

$$\varphi_{left} = \varphi_{right} + 2n\pi$$

No transmission if

$$\varphi_{left} = \varphi_{right} + (2n+1)\pi$$

Basic Principles of Quantum Mechanics:
Tunneling

Time independent Schrödinger equation

$$E = \frac{-\hbar^2 \Delta}{2m} + U$$

Solution in free space (E > U=0):

$$\Psi(x,t) = A\exp\left(i\left[kx - \omega t\right]\right)$$

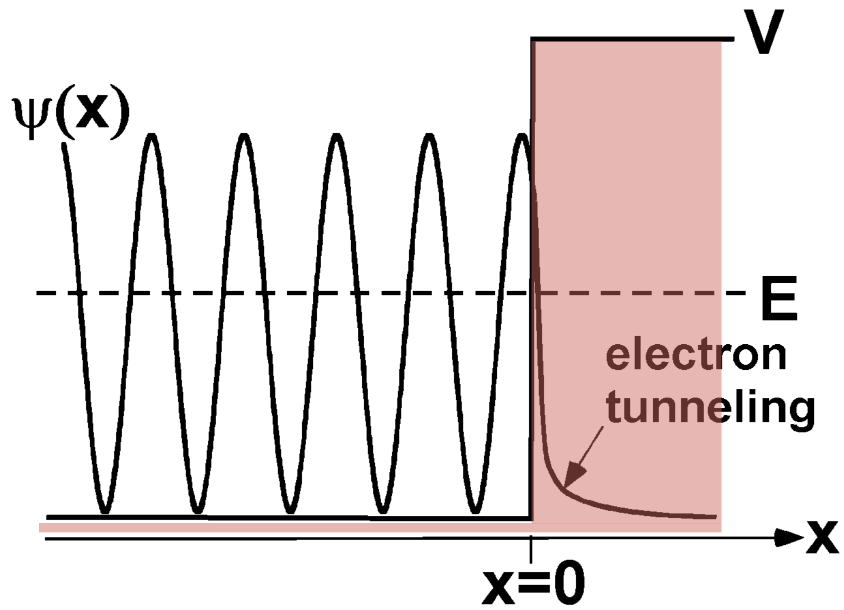
$$E - U = \hbar\omega = \frac{\hbar^2 k^2}{2m} > 0$$

For E < U:

$k^2<0$

k=ik', $k' = \sqrt{\frac{2m(V-E)}{\hbar^2}} \in R$

$$\Psi(x>0,t) = A\exp\left(-i\omega t\right)\exp\left(-k'x\right)$$



Basic Principles of Quantum Mechanics:
Transmission through a tunnel barrier

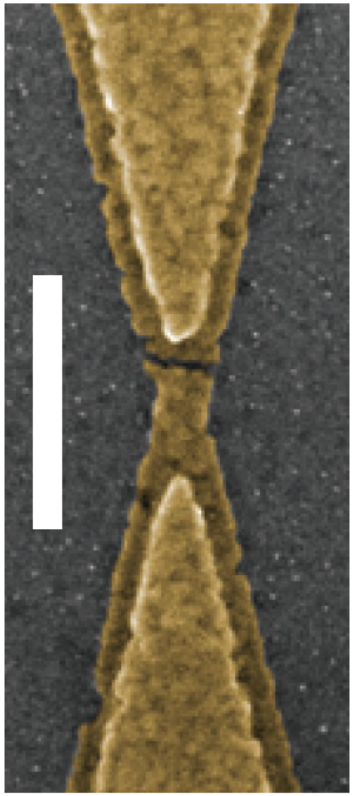
Probability of a tunneling event through a barrier of thickness d.

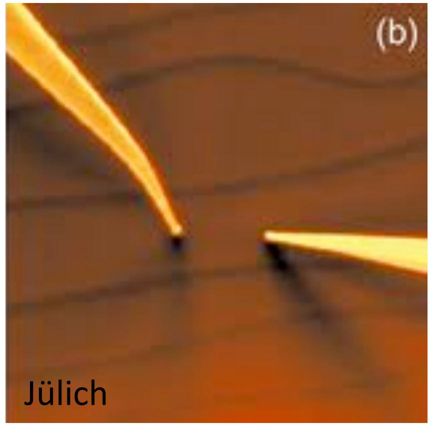
$$\left|\psi_{transmitted}\right|^2 \approx \left|\psi_{incident}\right|^2 \exp(-2k'\,d)$$

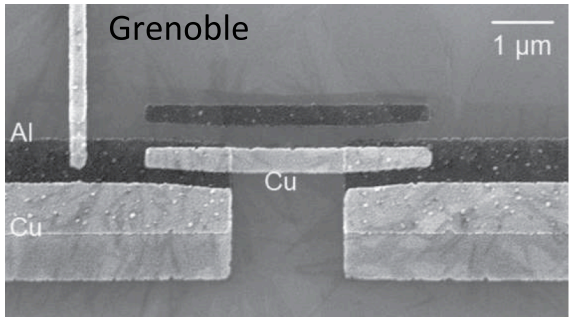
Tunneling simulator (U. Colorado)

Tunnel barrier acts like a resistor of resistance $R_t \propto \exp(2k'\,d)$

Grenoble







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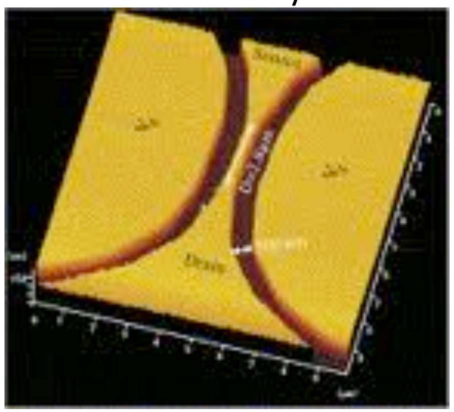


Basic Principles of Quantum Mechanics:

Particle in a 1D box : wavefunction

Time independent Schrödinger equation

$$E - U = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Solution E > U = 0

$$\Psi(x,t) = A\exp\big(i[kx - \omega t]\big)$$

$$\Rightarrow E - U = \hbar\omega = \frac{\hbar^2 k^2}{2m} > 0$$

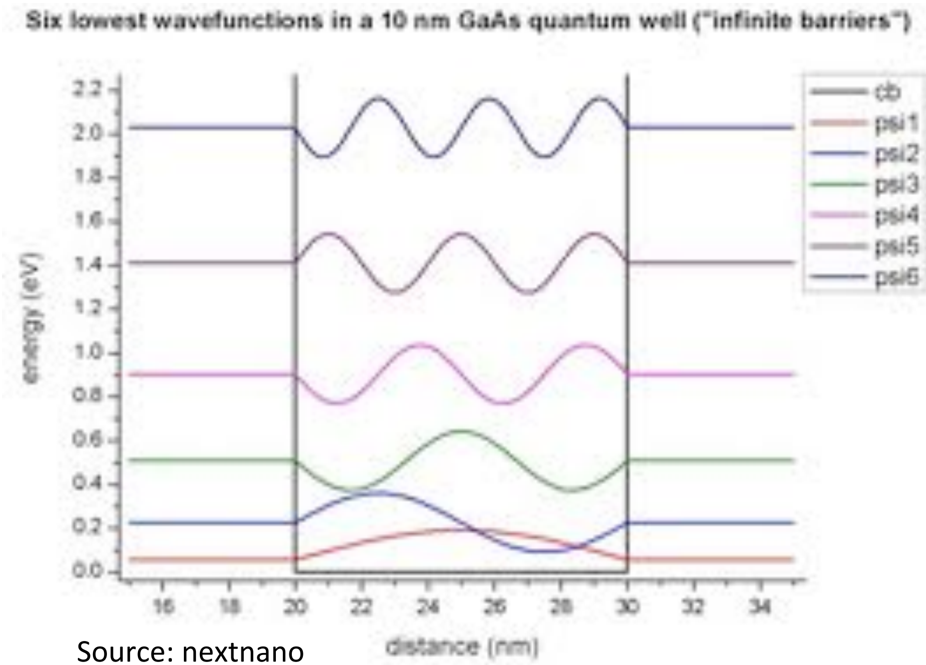
Outside [0,L]: U=+∞

$$\Psi(x<0,t) = \Psi(x>L,t) = 0$$

Fixed boundary conditions

$$\Rightarrow k = \frac{n\pi}{L}$$

$$n \in N^*$$

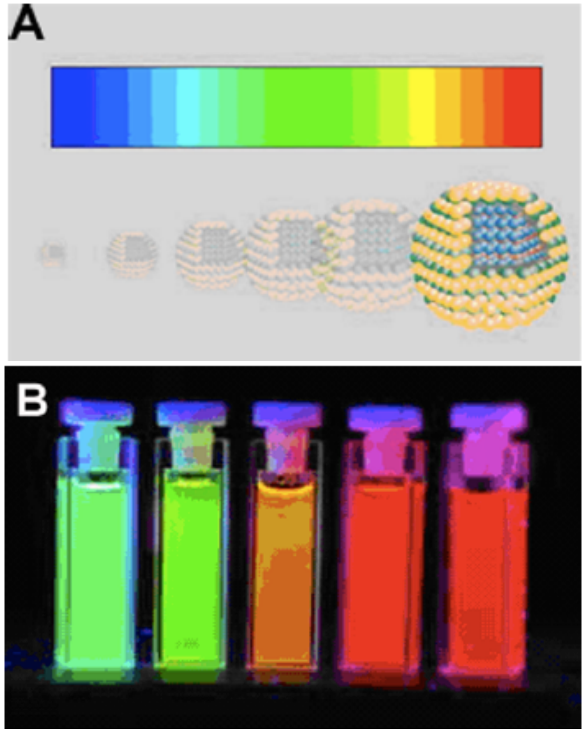


Source: nextnano

Basic Principles of Quantum Mechanics:
Energy spectrum of a confined particle

Square well

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

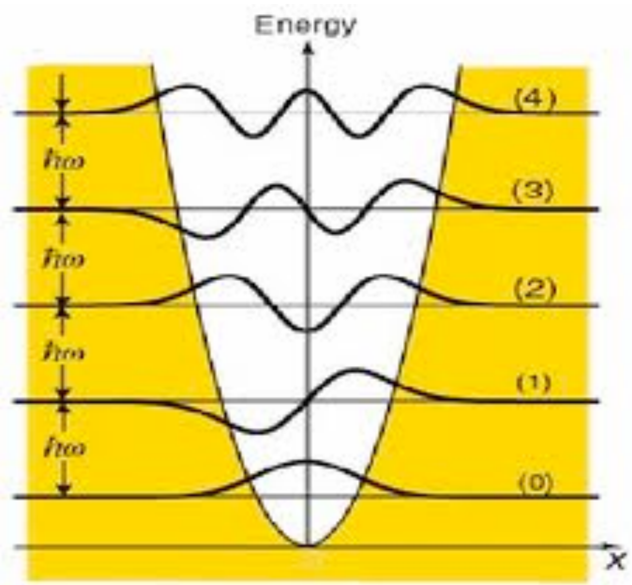


(Source:D. Spencer / Philips)

Harmonic potential

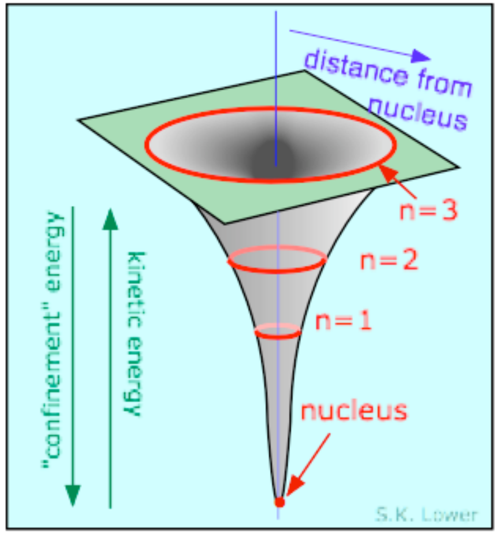
$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$$E_{n+1} - E_n = \hbar\omega$$



Coulomb potential
(Hydrogen atom)

$$E_n = -\frac{13{,}6eV}{n^2}$$



Basic Principles of Quantum Mechanics:
Main ideas

○ Quantum matter particles behave also as waves, waves behave also as quantum particles.

○ All physical information is contained in the wavefunction $\Psi(\vec{r},t)$

○ The spatial & time evolution of the wavefunction is governed by the Schrödinger equation.

○ Linearity of the Schrödinger equation: wavefunctions add up

⟹ Interference

○ Ψ and therefore the probability of presence may be non-zero even in regions where $E < U$

⟹ Tunnel effect

○ If the potential U forces confinement, the allowed energies are discrete.