3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

3.23 Fall 2007 – Lecture 2

THINK OUTSIDE THE BOX

More practical info

- Problem sets – out on Wed (and posted on Stellar), due by 5pm of the following weekend (after that 75%, after Thu 5pm 50%, after Fri 5pm 25%)
- ~11 in total, 30% of the grade
- Sometimes I mention homework – it's not the "Problem Set" @ Poilvert, Bonnet

Homework

- Take notes
- Revise posted lecture
- Study posted or assigned material (TEXTBOOKS – do you have them ?)
- Meet with TAs or Instructor:

Last time: Wave mechanics

1. Particles, fields, and forces
2. Dynamics – from Newton to Schroedinger
3. De Broglie relation $\lambda \bullet p = h$
4. Waves and plane waves
5. Harmonic oscillator

Time-dependent Schrödinger's equation

(Newton's 2nd law for quantum objects)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

1925-onwards: E. Schrödinger (wave equation), W. Heisenberg (matrix formulation), P.A.M. Dirac (relativistic)

Plane waves as free particles

Our free particle $\Psi(\vec{r},t) = A\exp[i(\vec{k}\cdot\vec{r}-\omega t)]$ satisfies the wave equation:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

(provided $E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$)

Stationary Schrödinger's Equation (I)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

*

Stationary Schrödinger's Equation (II)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$

Stationary Schrödinger's Equation (III)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$

1. It's not proven – it's postulated, and it is confirmed experimentally
2. It's an "eigenvalue" equation: it has a solution only for certain values (discrete, or continuum intervals) of E
3. For those eigenvalues, the solution ("eigenstate", or "eigenfunction") is the complete descriptor of the electron in its equilibrium ground state, in a poteinitial V(r).
4. As with all differential equations, boundary conditions must be specified
5. Square modulus of the wavefunction = probability of finding an electron

Free particle: $\Psi(x,t)=\varphi(x)f(t)$

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(x)=E\varphi(x)$$

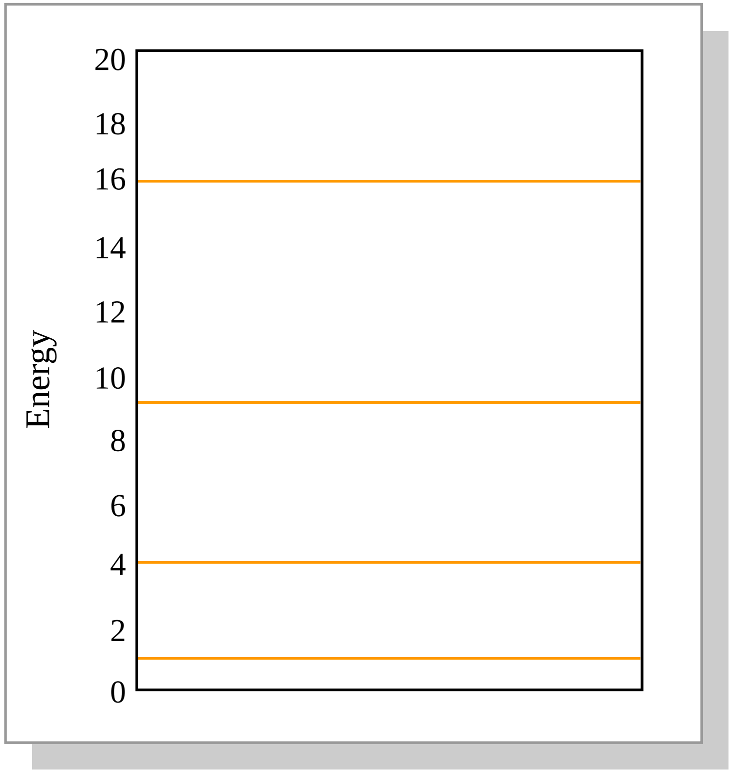
$$i\hbar\frac{d}{dt}f(t)=E\,f(t)$$

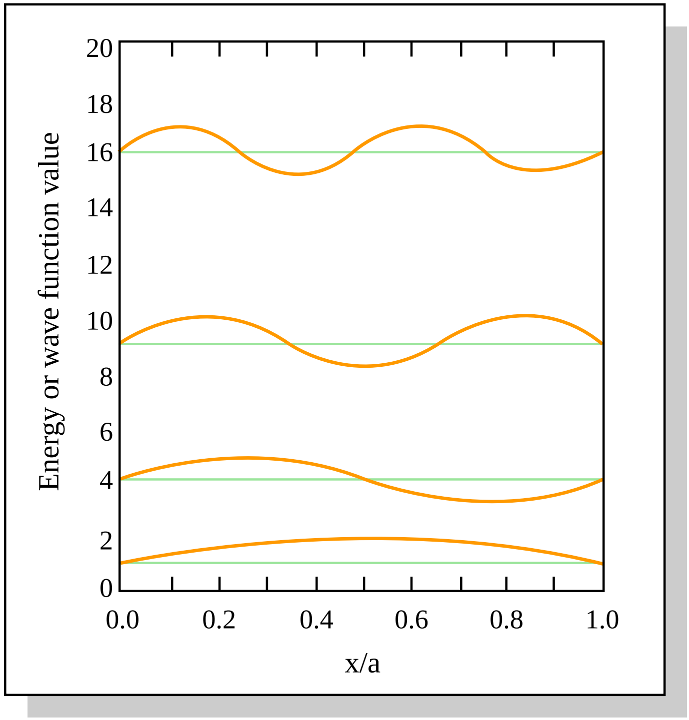
Infinite Square Well (I)
(particle in a 1-dim box)

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} = E\varphi(x)$$

Infinite Square Well (II)

Infinite Square Well (III)

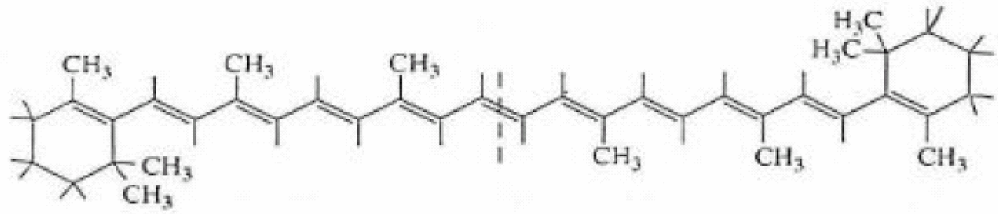




Figures by MIT OpenCourseWare.

The power of carrots

- β-carotene



Images removed due to copyright restrictions. Please see any spectrum of beta carotene, such as http://www.chm.bris.ac.uk/motm/carotene/beta-carotene_colourings.html.

Physical Observables from Wavefunctions

- Eigenvalue equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\varphi(x)=E\varphi(x)$$

- Expectation values for the operator (energy)

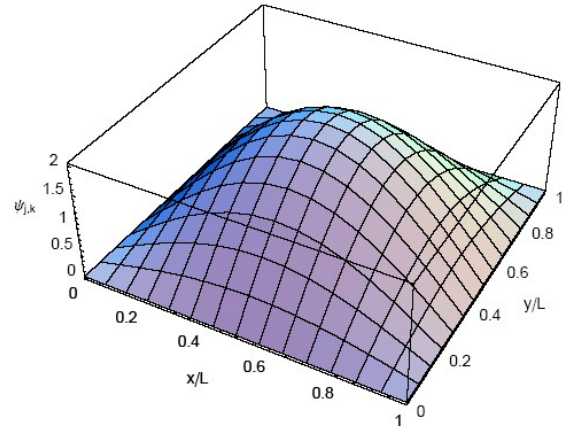
$$E=\int\varphi^*(x)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\varphi(x)\,dx$$

Particle in a 2-dim box

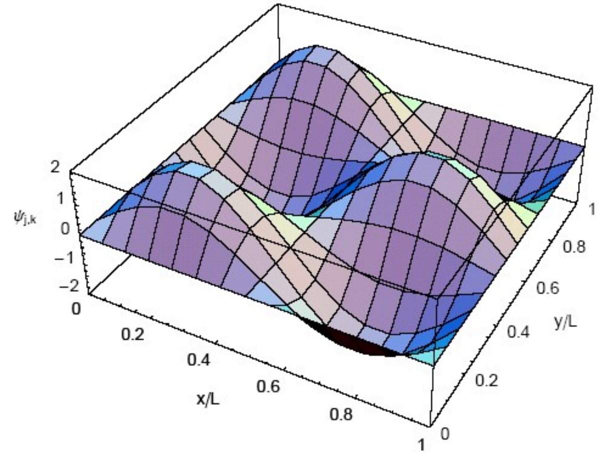
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi(x,y)=E\,\varphi(x,y)$$

Particle in a 2-dim box

$$\varphi(x,y) = C \sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)$$



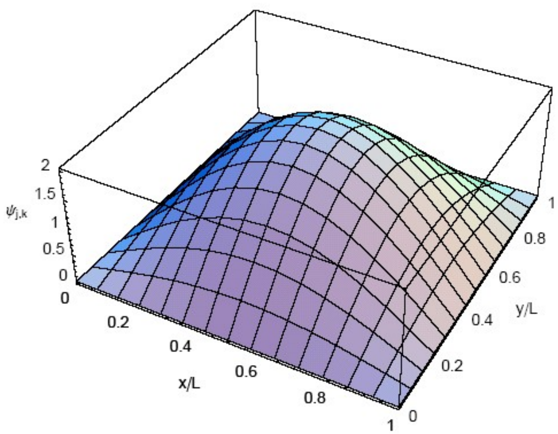
$$E = \frac{h^2}{8m}\left(\frac{l^2}{a^2} + \frac{m^2}{b^2}\right)$$

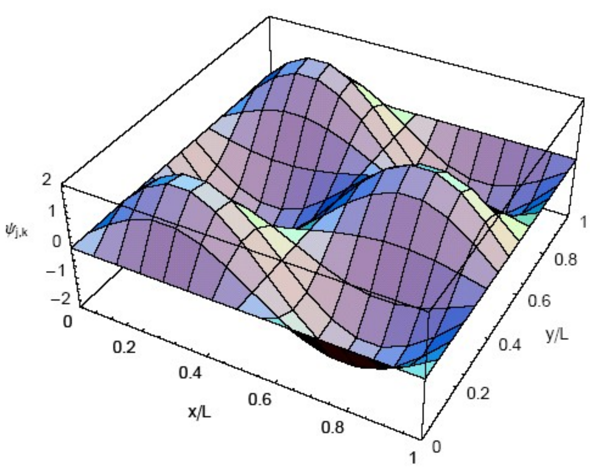


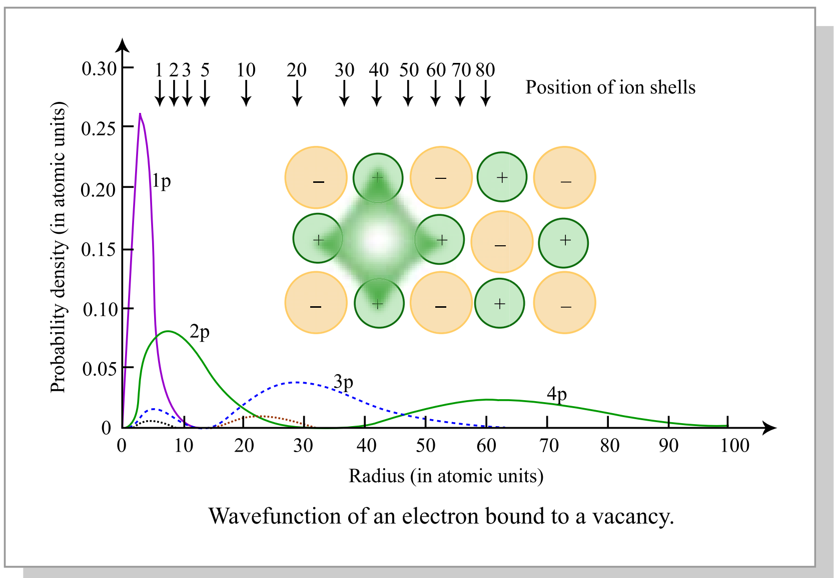
Particle in a 3-dim box

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z)=E\,\varphi(x,y,z)$$

Particle in a 3-dim box: *Farbe* defect in halides (e^- bound to a negative ion vacancy)







Wavefunction of an electron bound to a vacancy.

Figure by MIT OpenCourseWare.

From Carl Zeiss to MIT…

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Please see Avakian, P., and Smakula, A. "Color Centers in Cesium Halide Single Crystals." *Physical Review* 120 (December 1960): 2007.

Light absorption/emission

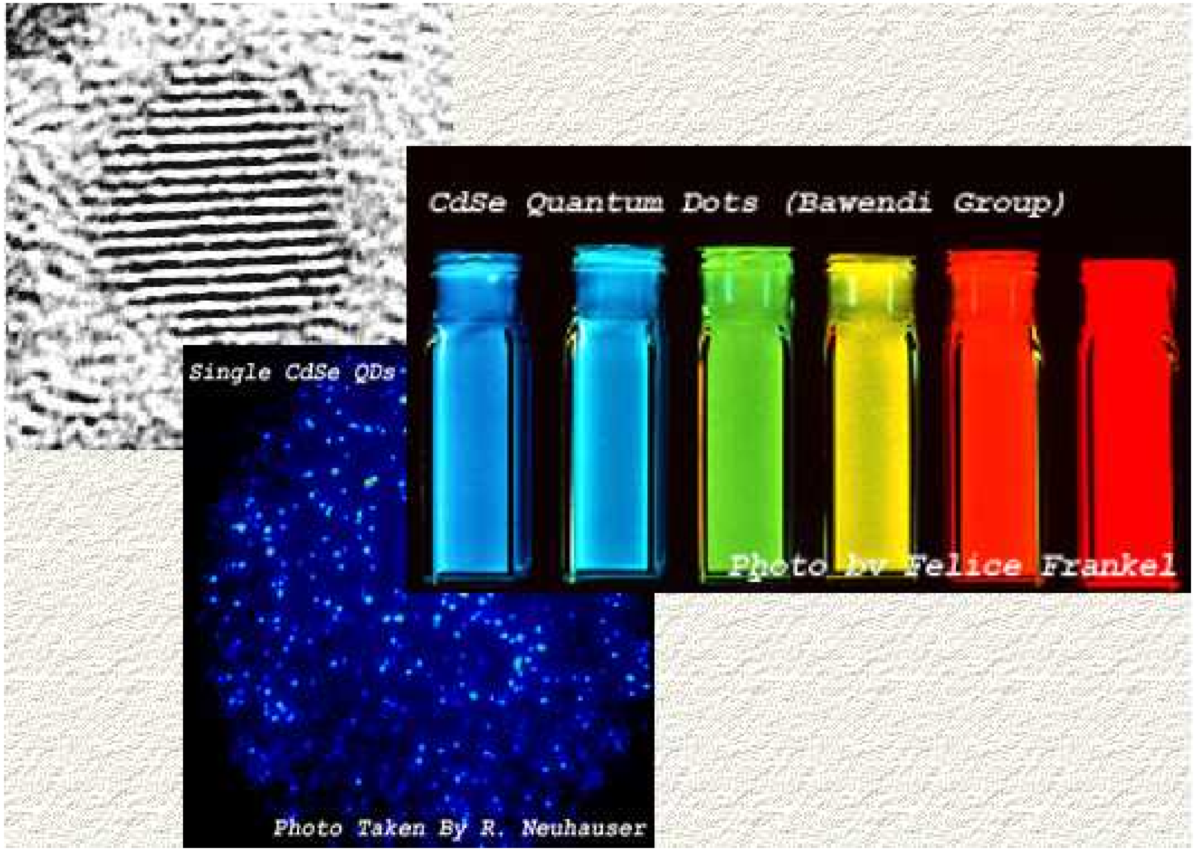
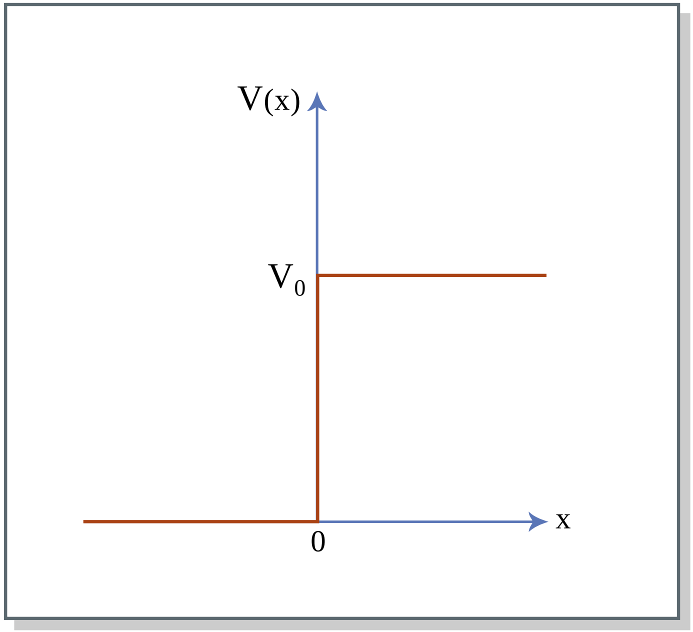


Image and text removed due to copyright restrictions. Please see:
Abstract and Fig. 1 in Willey, T. M., et al. "Molecular Limits to the Quantum Confinement Model in Diamond Clusters." *Physical Review Letters* 95 (2005): 113401.

Metal Surfaces (I)

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\varphi(x)=E\varphi(x)$$



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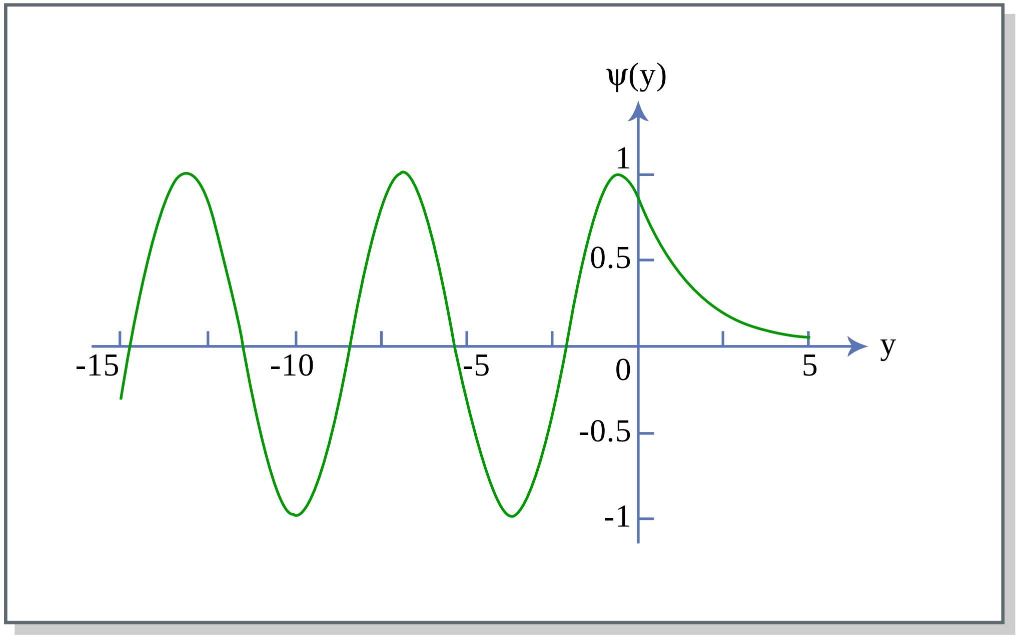
Metal Surfaces (II)



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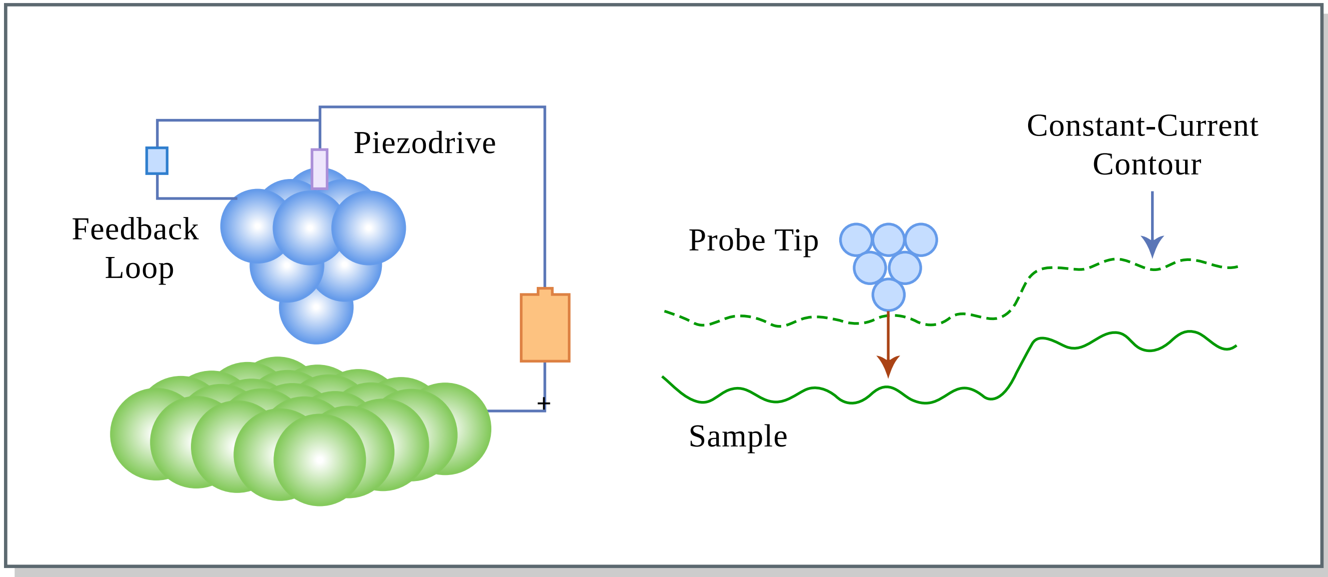
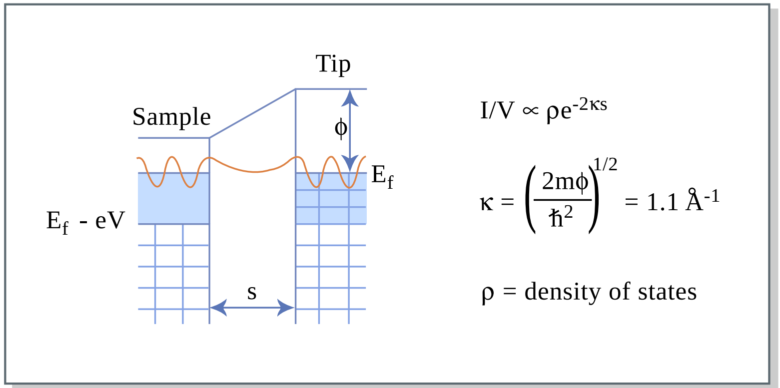
Scanning Tunnelling Microscopy





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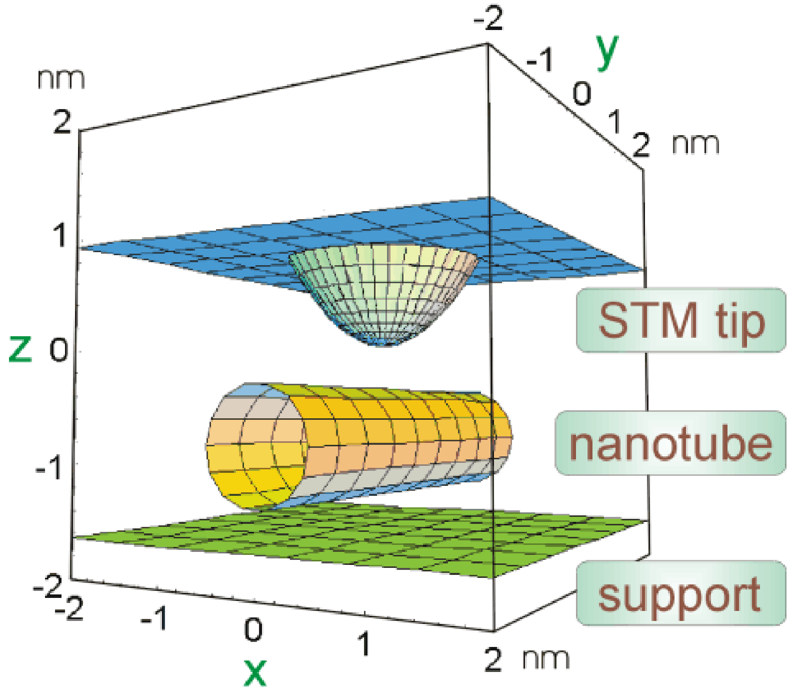
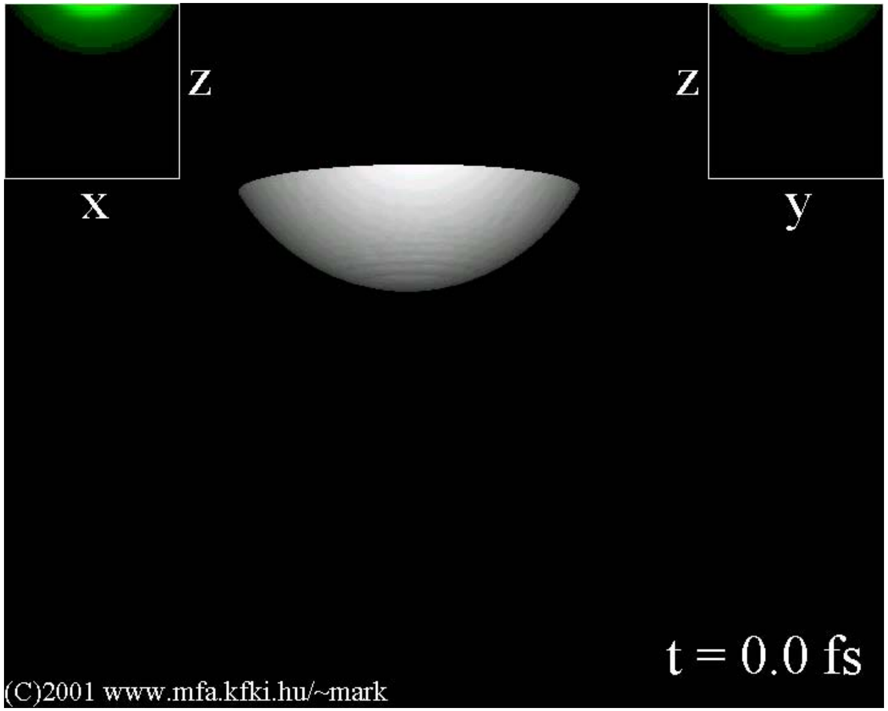
Wavepacket tunnelling through a nanotube





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http://newton.phy.bme.hu/education/schrd/index.html http://www.quantum-physics.polytechnique.fr