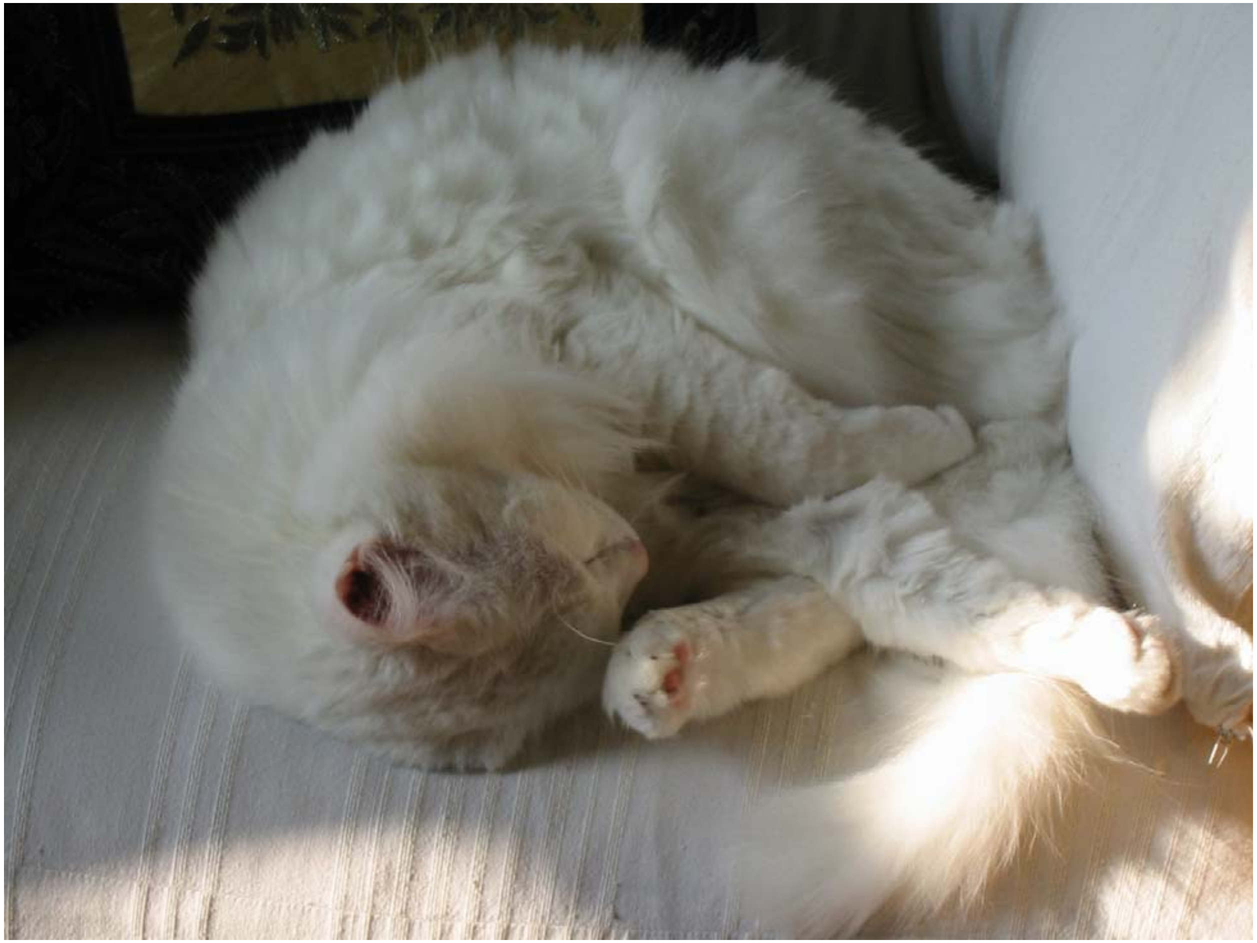
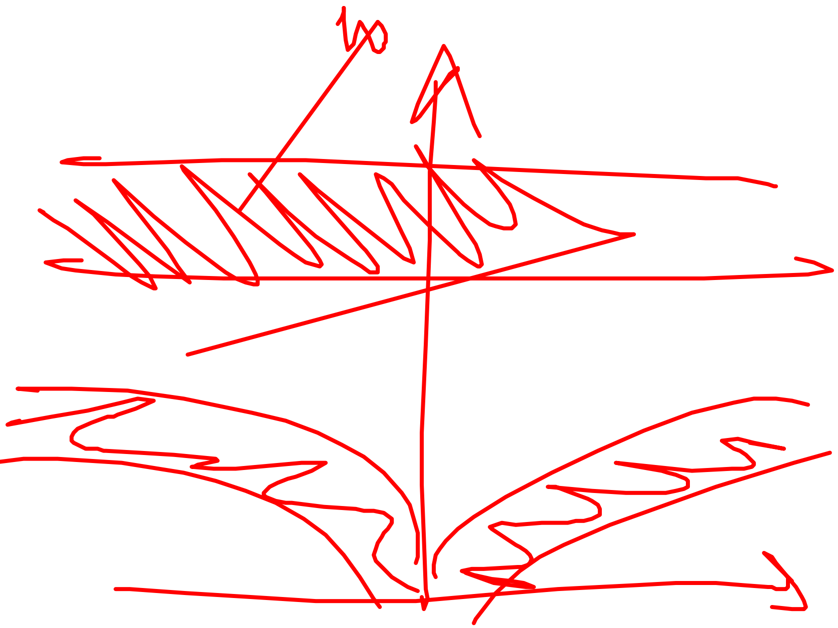
3.012 Fund of Mat Sci: Bonding – Lecture 4

CURIOSITY KILLED THE CAT



Specific Heat of Graphite (Dulong and Petit)



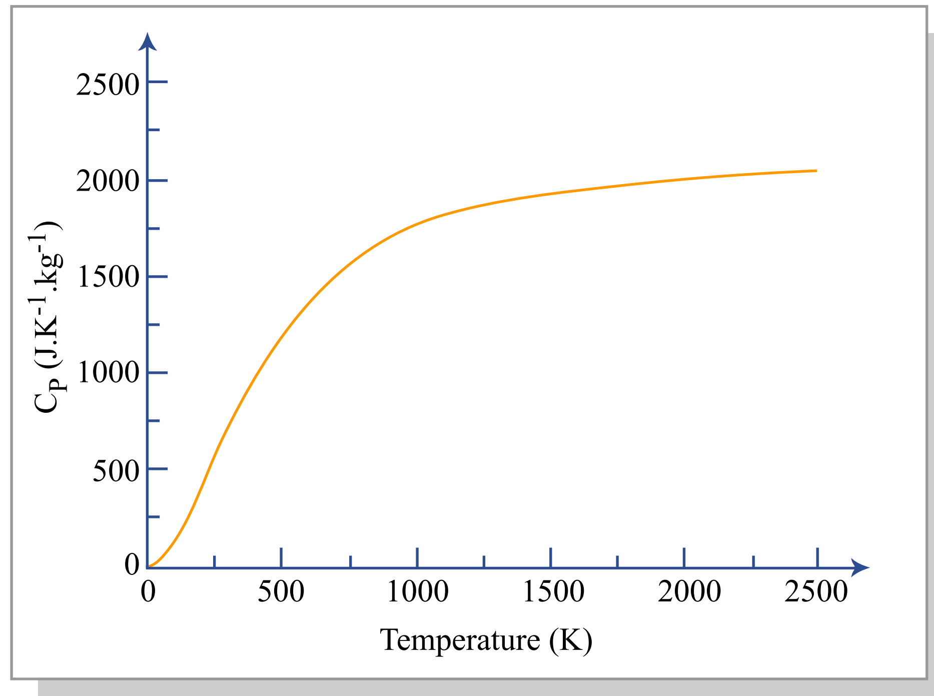


Figure by MIT OCW.

Last Time

$$\frac{h^2}{8m}\left(\frac{n^2}{a^2}\right)$$

- Expectation values of the energy in an infinite well (particle-in-a-box)
- Absorption lines (linear conjugated molecules)
- Particles in 3-dim box (quantum dots, “Farbe” defects)

Homework for Fri 23

- Study: 14.1, 14.2, 14.3
- Read: 14.4

Metal Surfaces (I)

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

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

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) = (E-V_0)\varphi(x)$$

~~e^{kx}~~ e^{-kx}

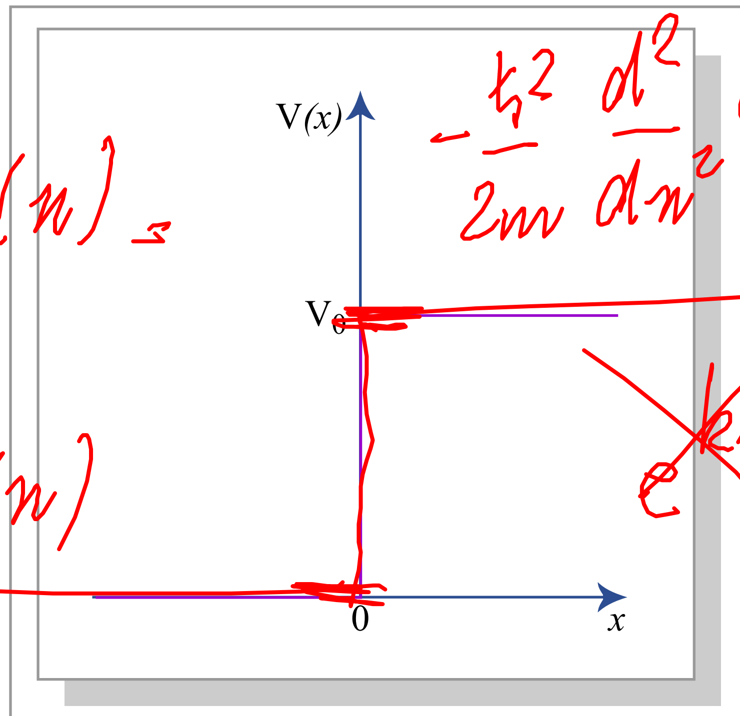


Figure by MIT OCW.

Metal Surfaces (II)

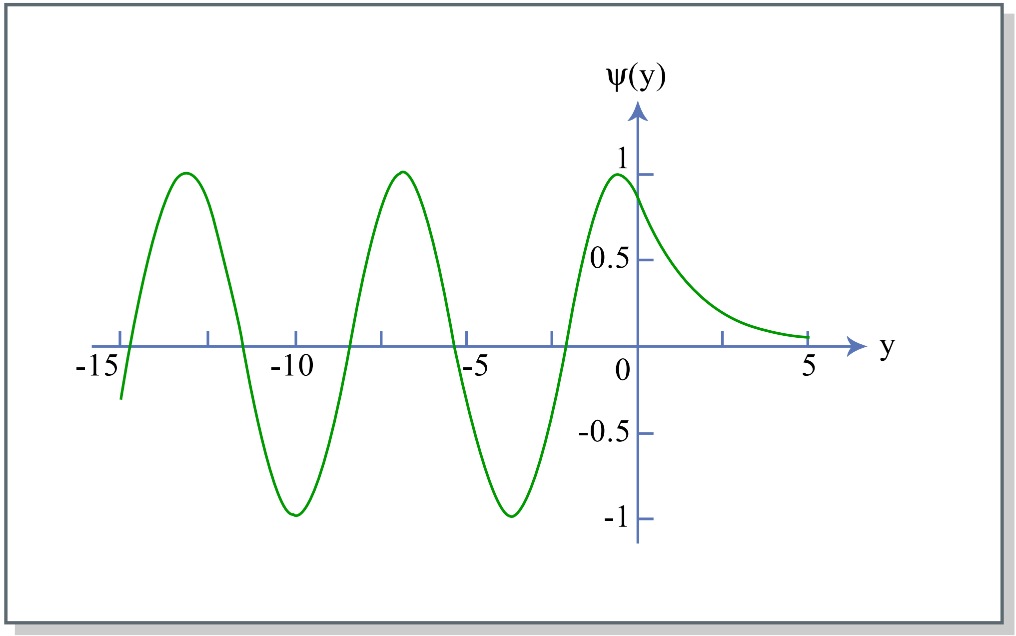
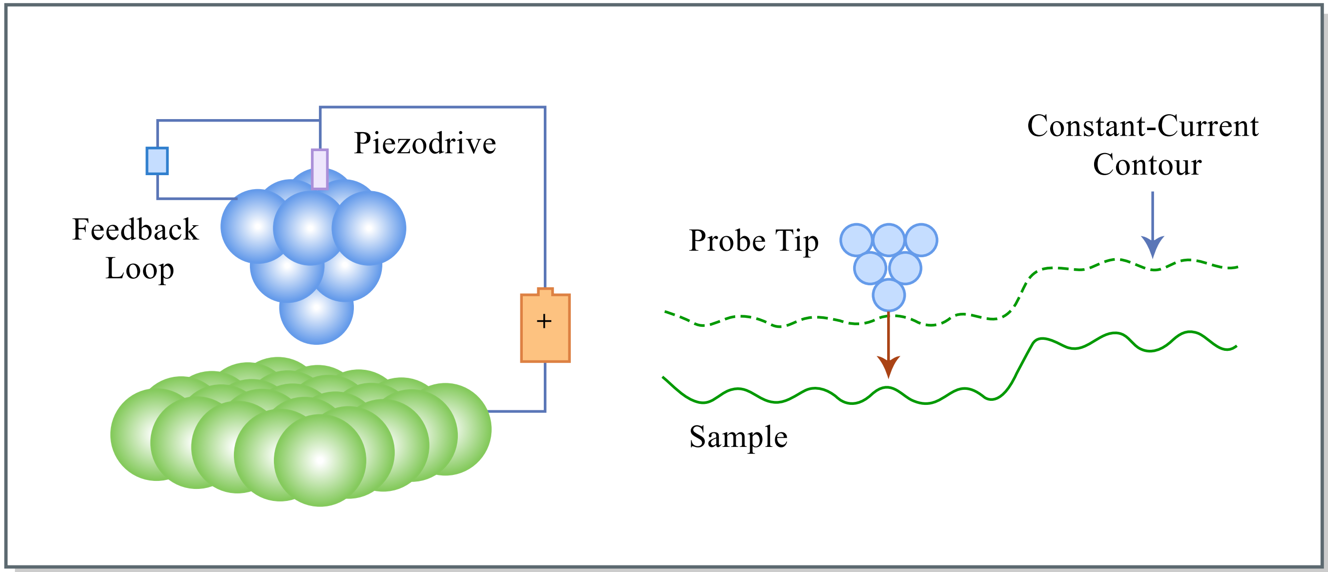


Figure by MIT OCW.

Scanning Tunnelling Microscopy



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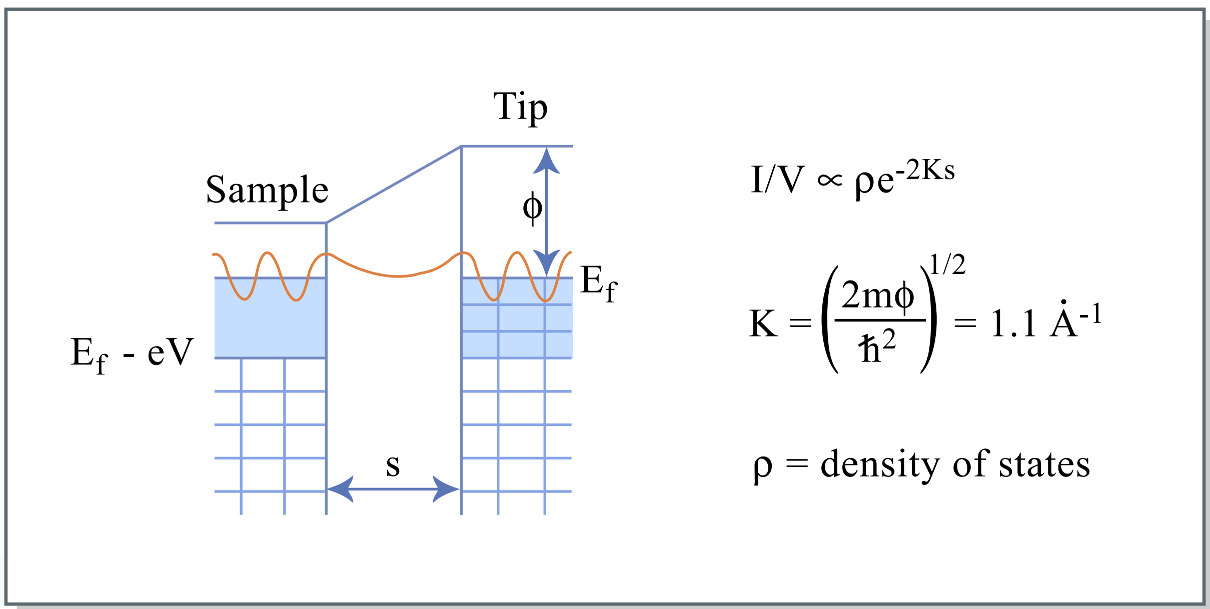


Figure by MIT OCW.

Wavepacket tunnelling through a nanotube

Images removed for copyright reasons. See http://www.mfa.kfki.hu/int/nano/online/kirchberg2001/index.html

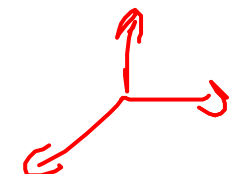
Dirac Notation

- Eigenvalue equation:

$$\hat{A}\left|\psi_i\right\rangle = a_i\left|\psi_i\right\rangle \qquad \left(\Rightarrow \left\langle \psi_i \middle| \psi_j \right\rangle = \delta_{ij} \right)$$

$\int \psi_i^* \psi_j = 1$ if $i=j$, 0 if $i \neq j$

BRA KET



$b_1 = (1,0,0)$

$b_2 = (0,1,0)$

$b_3 = (0,0,1)$

$\vec{b}_i \cdot \vec{b}_j = \delta_{ij}$

- Expectation values:

$$\left\langle \psi_i \middle| \hat{H}\psi_i \right\rangle = \left\langle \psi_i \middle| \hat{H} \middle| \psi_i \right\rangle = \int \psi_i^*(\vec{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \right] \psi_i(\vec{r})\, d\vec{r} = E_i$$

Operators and operator algebra

- Examples: derivative, multiplicative

$\vec{\nabla} \varphi(x)$ $\qquad$ $V(x)\psi(x)$

Product of operators, and commutators

- $\hat{A}\hat{B}\,\varphi$ $\qquad \hat{A}\left(\hat{B}\varphi\right)$

- $\left[\hat{A},\hat{B}\right] = \hat{A}\cdot\hat{B} - \hat{B}\cdot\hat{A}$

  $\left[x,\frac{d}{dx}\right] f(x) = x\frac{df(x)}{dx} - \frac{d}{dx}\left(x f(x)\right)$

  $= x\frac{df}{dx} - x\frac{df}{dx} - f\frac{dx}{dx} = -f$

- $\left[x,\frac{d}{dx}\right] = -1$

Linear and Hermitian

- $\hat{A}\left[\alpha|\varphi\rangle+\beta|\psi\rangle\right]=\alpha\hat{A}|\varphi\rangle+\beta\hat{A}|\psi\rangle$

$$\frac{d}{dx}\left(\alpha f(x)+\beta g(x)\right)=\alpha\frac{df}{dx}+\beta\frac{dg}{dx}$$

- $\left\langle\varphi\middle|\hat{A}\psi\right\rangle=\left\langle\hat{A}\varphi\middle|\psi\right\rangle=\int\varphi^{*}A\psi=\int(A\varphi)^{*}\psi$

OPERATORS THAT CORRESPOND TO PHYS. VARIAB. ARE HERMITIAN

Examples: (d/dx) and i(d/dx)

First postulate

- All information of an ensemble of identical physical systems is contained in the wavefunction $\Psi(x,y,z,t)$, which is complex, continuous, finite, and single-valued; square-integrable. $\left(\text{i.e.} \int \|\varphi\|^2 d\vec{r} \text{ is finite}\right)$

Second Postulate

- For every physical observable there is a corresponding Hermitian operator

$$\vec{p} \rightarrow -i\hbar\vec{\nabla}$$

$$\vec{r} \rightarrow \vec{r}$$

Hermitian Operators

1. The eigenvalues of a Hermitian operator are real

2. Two eigenfunctions corresponding to different eigenvalues are orthogonal

3. The set of eigenfunctions of a Hermitian operator is complete

4. Commuting Hermitian operators have a set of common eigenfunctions

The set of eigenfunctions of a Hermitian operator is complete

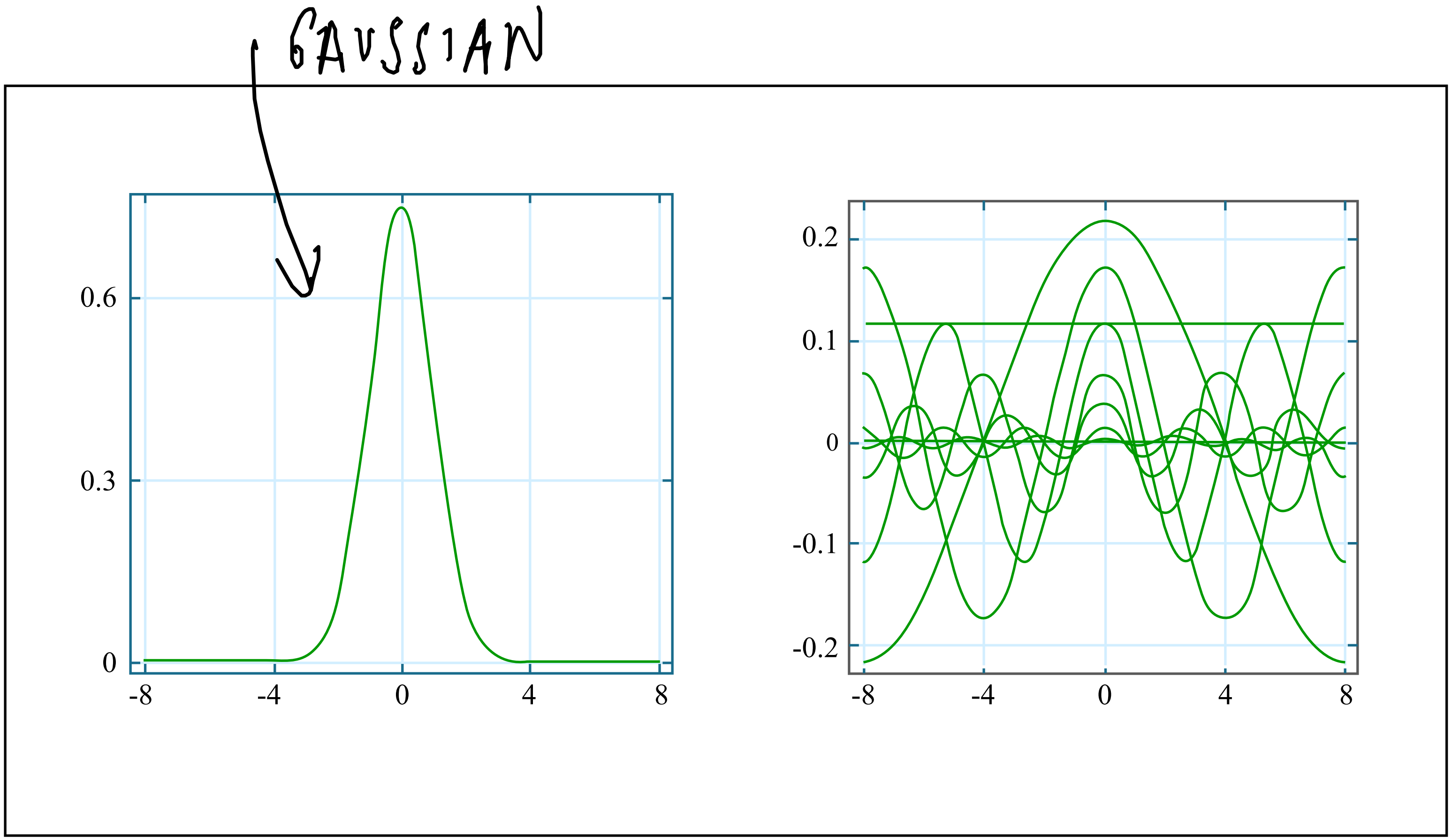


Figure by MIT OCW.

Position and probability

Graph of the probability density for positions of a particle in a one-dimensional hard box removed for copyright reasons.

See Mortimer, R. G. *Physical Chemistry*. 2nd ed. San Diego, CA: Elsevier, 2000, p. 554, figure 15.2.

Graphs of the probability density for positions of a particle in a one-dimensional hard box according to classical mechanics removed for copyright reasons.

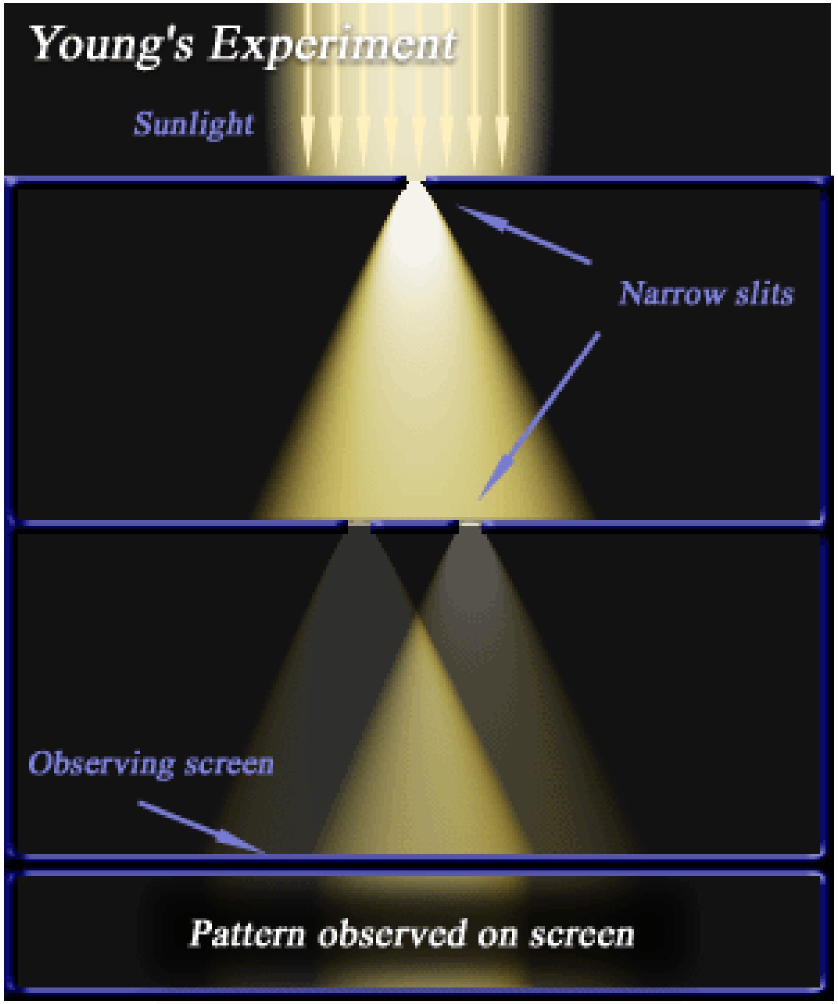
See Mortimer, R. G. *Physical Chemistry*. 2nd ed. San Diego, CA: Elsevier, 2000, p. 555, figure 15.3.

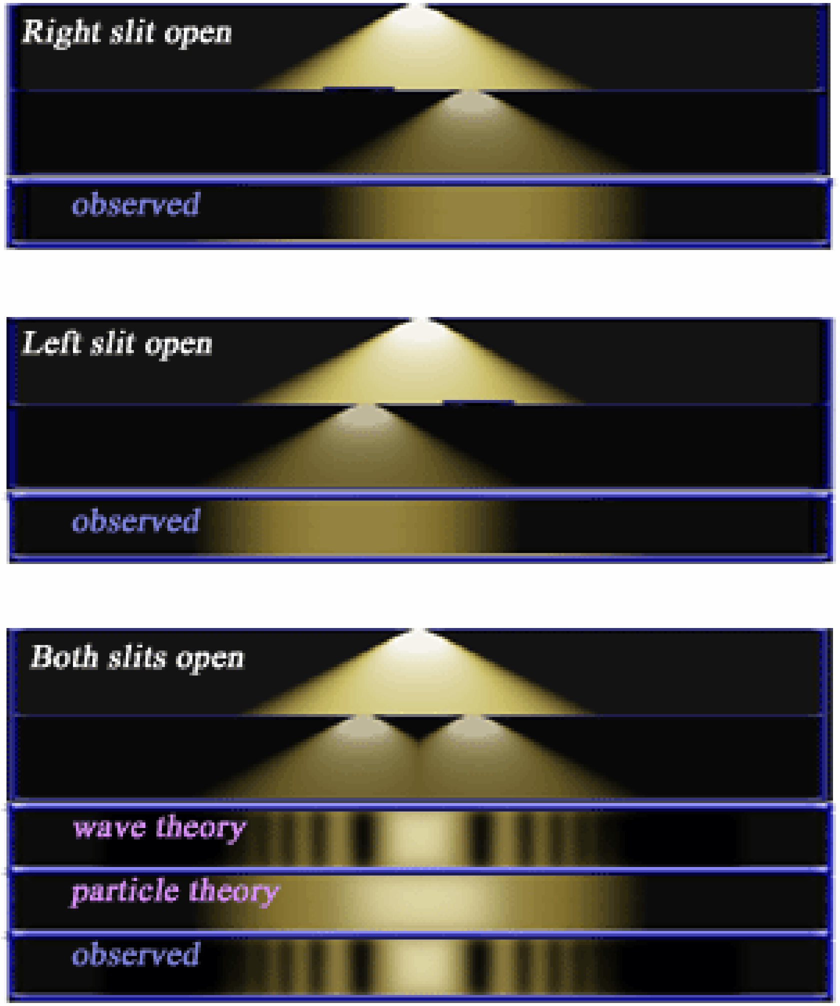
Commuting Hermitian operators have a set of common eigenfunctions

Fourth Postulate

- If a series of measurements is made of the dynamical variable A on an ensemble described by Ψ, the average ("expectation") value is $\langle A \rangle = \dfrac{\langle \Psi | \hat{A} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$

Quantum double-slit





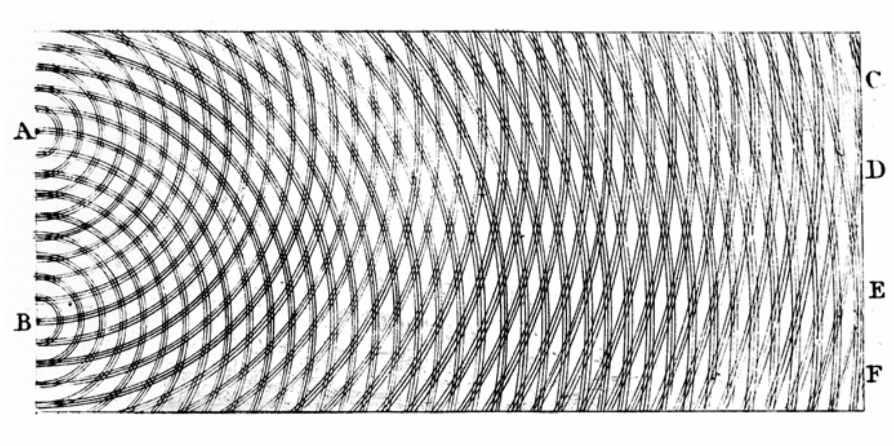
Source: Wikipedia

Quantum double-slit

Image of the double-slit experiment removed for copyright reasons.

See the simulation at http://www.kfunigraz.ac.at/imawww/vqm/movies.html:

"Samples from *Visual Quantum Mechanics*": "Double-slit Experiment."



Above: Thomas Young's sketch of two-slit diffraction of light. Narrow slits at A and B act as sources, and waves interfering in various phases are shown at C, D, E, and F. Source: Wikipedia

Deterministic vs. stochastic

- Classical, macroscopic objects: we have well-defined values for all dynamical variables at every instant (position, momentum, kinetic energy…)

- Quantum objects: we have well-defined probabilities of measuring a certain value for a dynamical variable, when a large number of identical, independent, identically prepared physical systems are subject to a measurement.

Top Three List

- ***Albert Einstein:* "*Gott wurfelt nicht!" [God does not play dice!]*
- ***Werner Heisenberg*** *"I myself . . . only came to believe in the uncertainty relations after many pangs of conscience. . ."*
- **Erwin Schrödinger:** *"Had I known that we were not going to get rid of this damned quantum jumping, I never would have involved myself in this business!"*