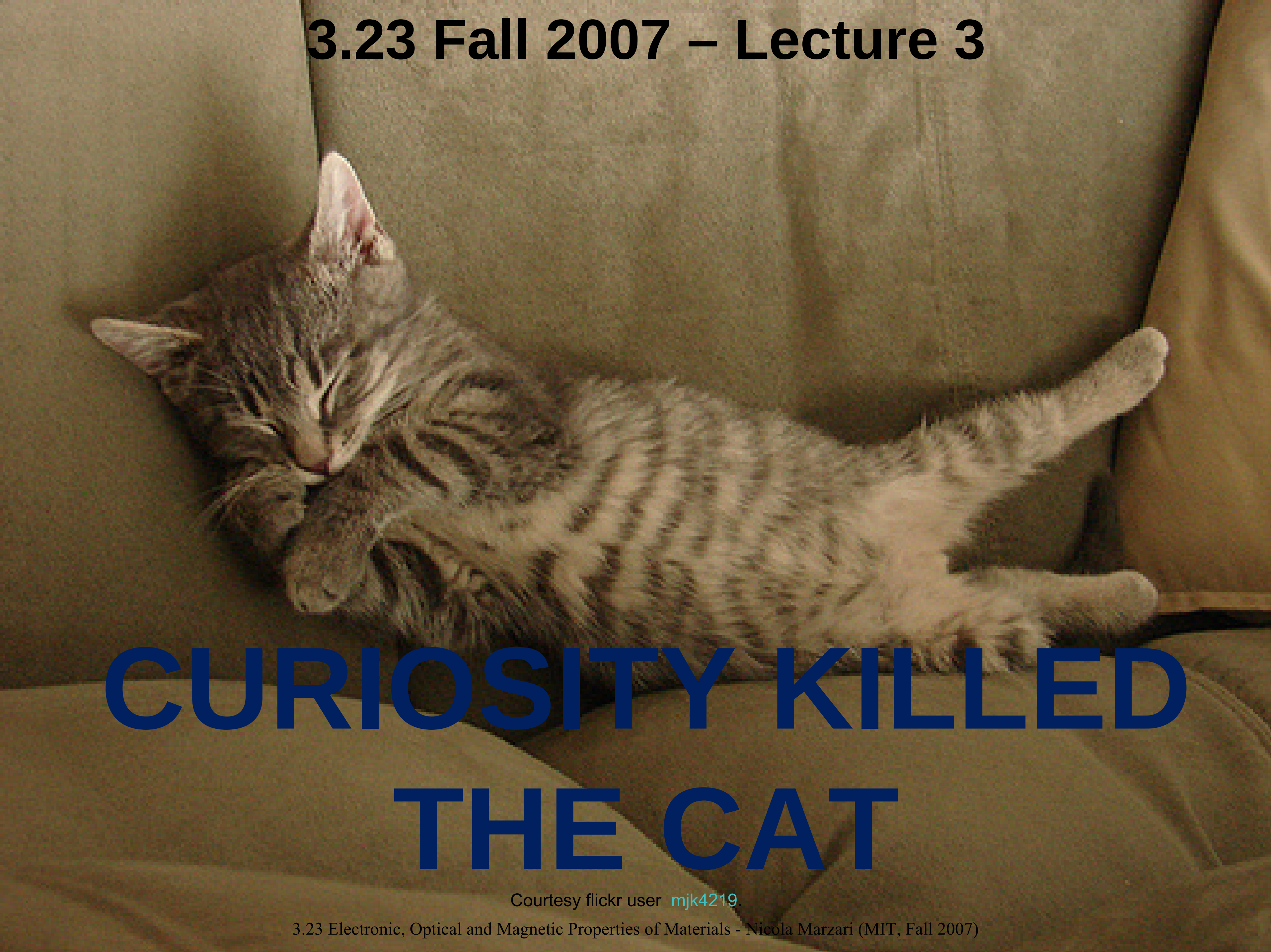
3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

# 3.23 Fall 2007 – Lecture 3




Courtesy flickr user mjk4219.

# Last time: Wave mechanics

1. Time-dependent Schrödinger equation
2. Separation of variables – stationary Schrödinger equation
3. Wavefunctions and what to expect from them
4. Free particle and particle in a 1-d, 2-d, 3-d box
5. Scanning tunnelling microscope
6. (Applets)

# Good news

- Study material: Prof Fink QM notes (uploaded on Stellar)

# First postulate

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

- The ket can also be a geometrical vector (e.g. spin); in truth, wavefunctions are objects that satisfy vector algebra, and the space of wavefuncitons is a Hilbert space (instead of being 3-d, it's infinite-d)

# Normalization, scalar products

# Second Postulate

- For every physical observable there is a corresponding Hermitian operator

# From classical mechanics to operators

- Total energy is T+V (Hamiltonian is kinetic + potential)

- classical momentum $\vec{p} \rightarrow$
  $\rightarrow$ gradient operator $-i\hbar\vec{\nabla}$

- classical position $\vec{r} \rightarrow$
  $\rightarrow$ multiplicative operator $\hat{r}$

# Operators and operator algebra

- Examples: derivative, multiplicative

# Linear and Hermitian

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

- $$\left\langle\varphi\middle|\hat{A}\psi\right\rangle=\left\langle\hat{A}\varphi\middle|\psi\right\rangle$$

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

# 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

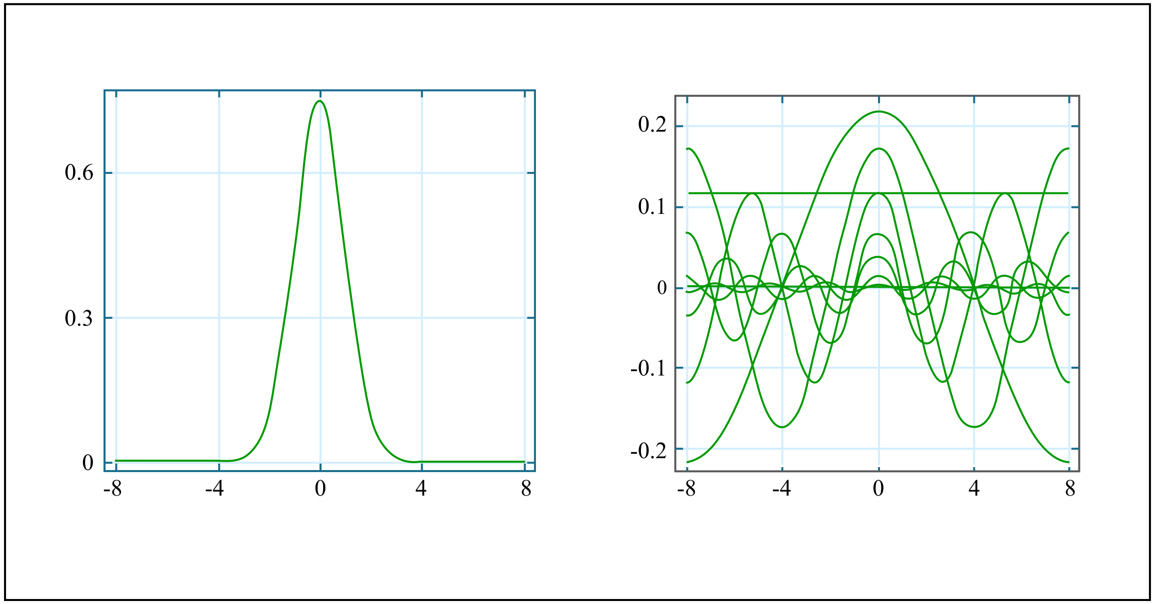
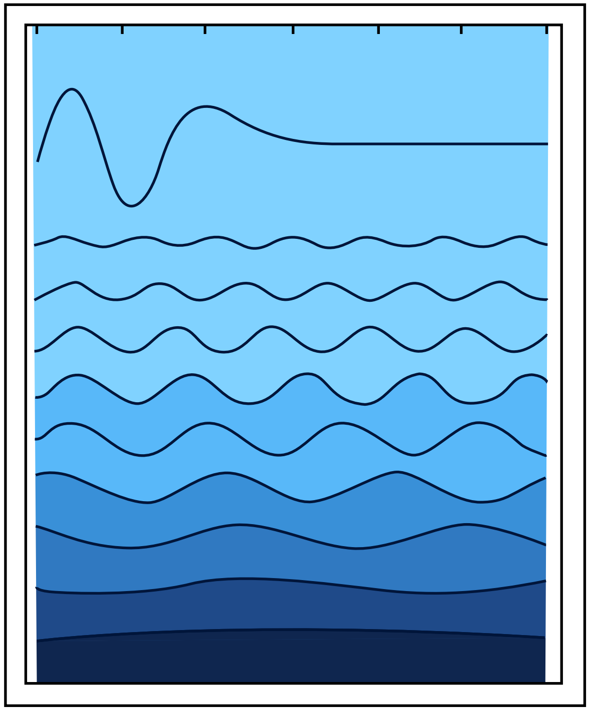



Figure by MIT OpenCourseWare.

# The set of eigenfunctions of a Hermitian operator is complete



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# Product of operators, and commutators

- $\hat{A}\hat{B}$

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

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

# Third Postulate

- In any single measurement of a physical quantity that corresponds to the operator A, the only values that will be measured are the eigenvalues of that operator.

# Fourth Postulate

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

  i.e. the probabiliy of obtaining an eigenvalue $a_n$ is $P(a_n) = \left| \langle \varphi_n | \Psi \rangle \right|^2$

# Dirac Notation

- Eigenvalue equation:

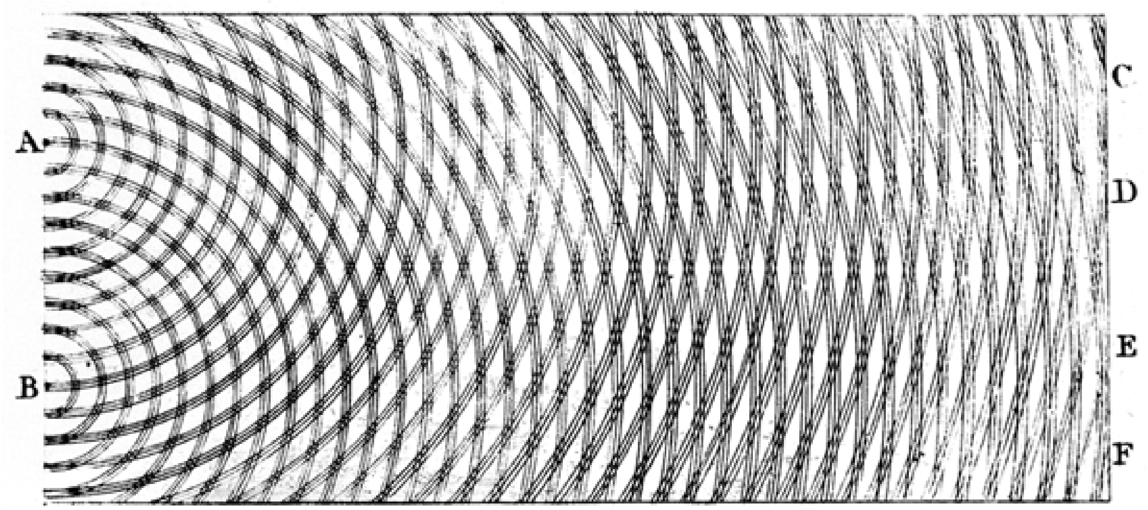
$$\hat{A}\left|\psi_i\right\rangle = a_i\left|\psi_i\right\rangle \qquad \left( \Rightarrow \left\langle \psi_i \middle| \psi_j \right\rangle = \delta_{ij} \right)$$

- Expectation values:

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

# Commuting Hermitian operators have a set of common eigenfunctions

# Quantum double-slit

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# Fifth postulate

- If the measurement of the physical quantity A gives the result $a_n$ , the wavefunction of the system immediately after the measurement is the eigenvector

$$\left|\varphi_n\right\rangle$$

# Position and probability

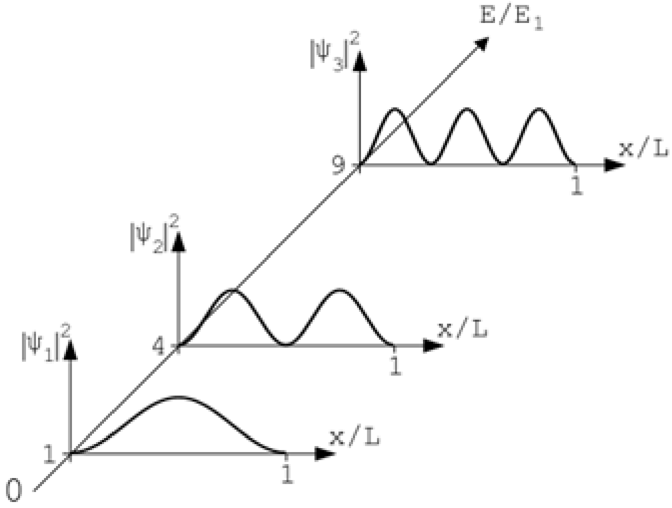


Fig: Diagram showing the probability densities of the first 3 energy states in a 1D quantum well of width L.

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, page 555, Figure 15.3.

# Quantum double-slit

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Please see any experimental verification of the double-slit experiment, such as
http://commons.wikimedia.org/wiki/Image:Doubleslitexperiment_results_Tanamura_1.gif

Image of a double-slit experiment simulation removed due to copyright restrictions.
Please see "Double Slit Experiment." in Visual Quantum Mechanics.

# 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!”*