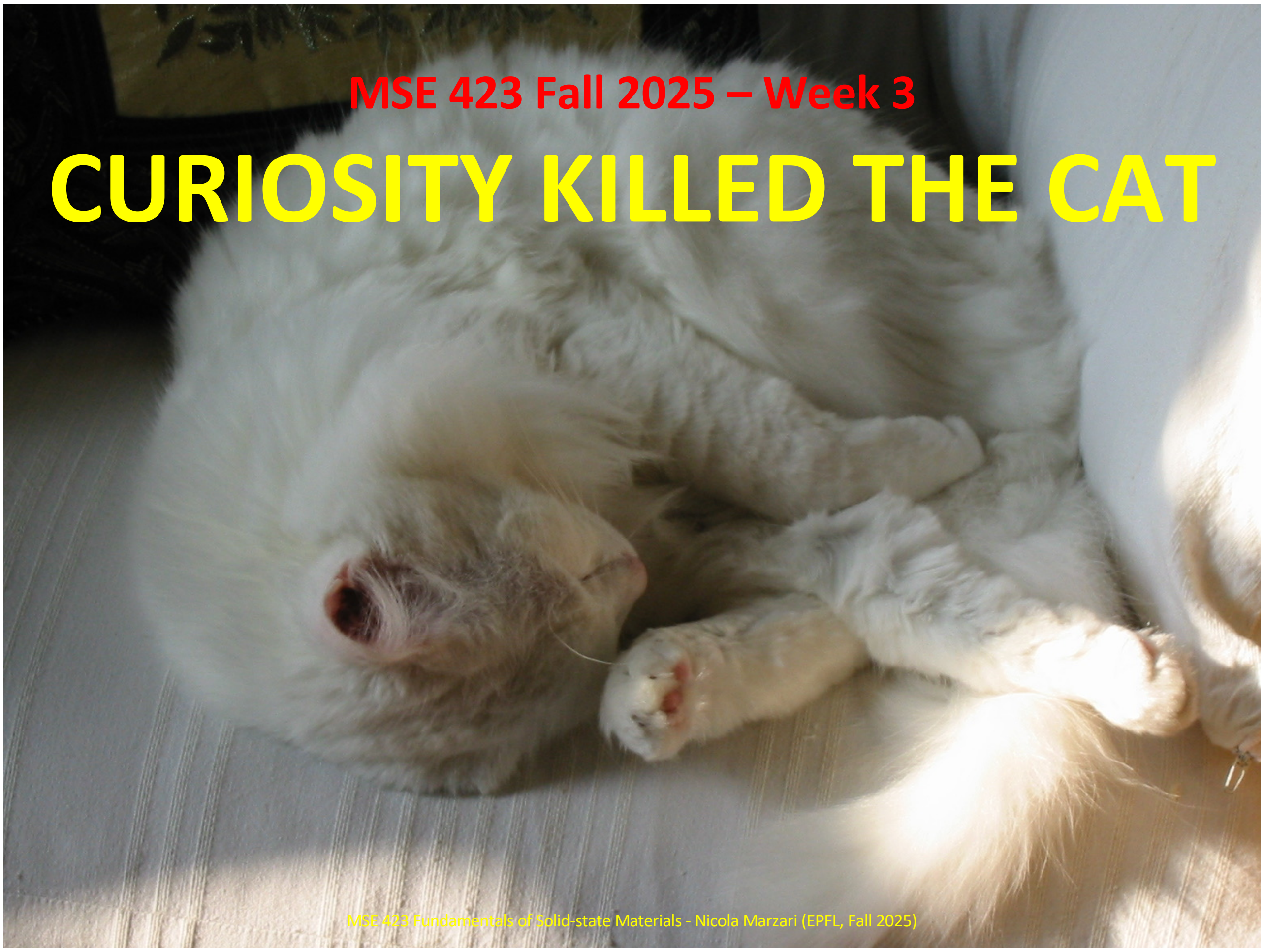
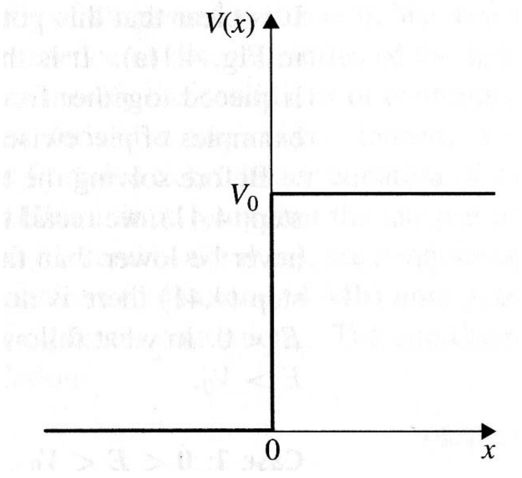


Last week: First steps

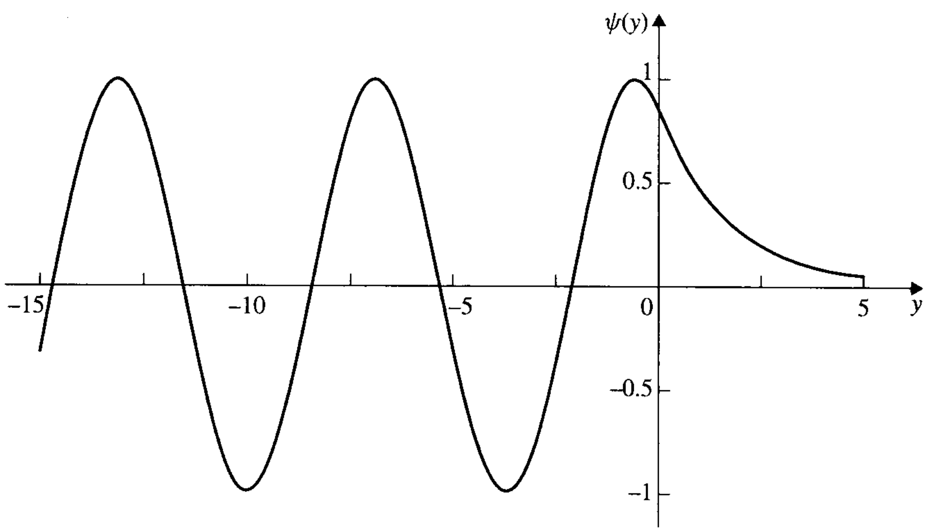
1. From one time-dependent Schroedinger eq. to two eqs.: stationary Schr. Eq. for $\varphi(\vec{r})$, and one for *f(t)*
2. Recovering the free particle, plane wave solution
3. Particle in a 1D, 2D, 3D box.
4. Potential step/metal surfaces
5. Quantum applets on osscar.org

Metal Surfaces (I)

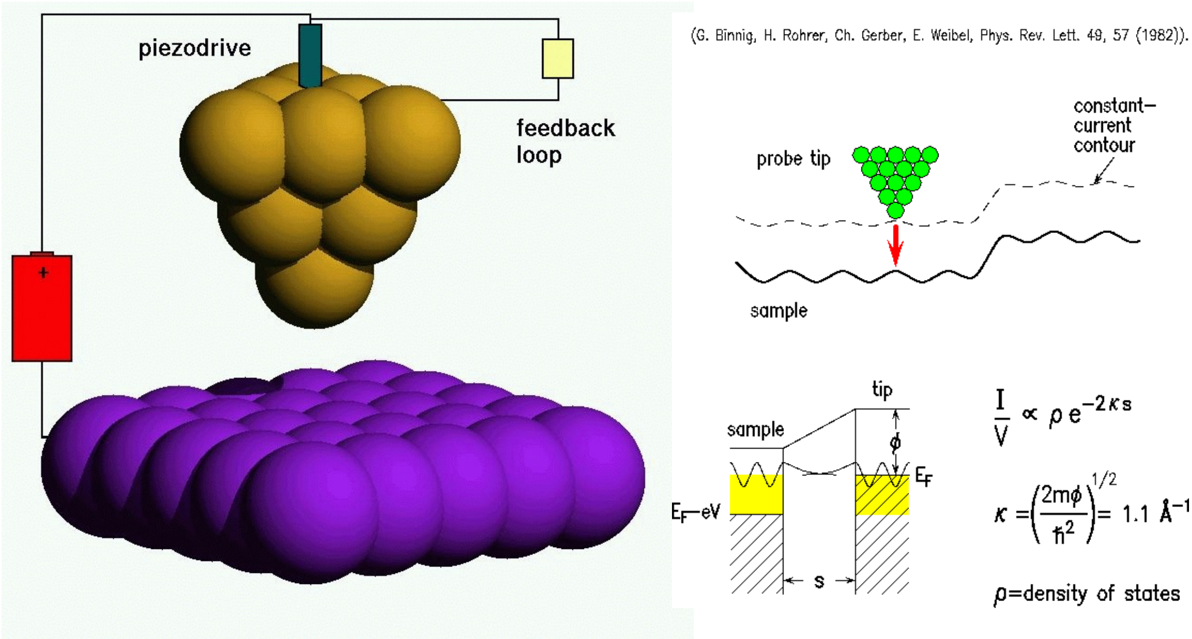
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\varphi(x)=E\varphi(x)$$



Metal Surfaces (II)



Scanning Tunnelling Microscopy



Eigenvalue equation and expectations

Schrödinger equation: operator, eigenvalues

E can be obtained as an "expectation value"

Dirac notation

Dirac's <bra|kets> (elements of vector space)

Scalar product (induces a metric → Hilbert space)

Eigenvalue equation and expectations

Schrödinger equation: operator, eigenvalues

E can be obtained as an "expectation value"

4 concepts

- Operators
- Eigenvalues
- Eigenfunctions
- Expectation values

Operators: Linear, Hermitian

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

Hermitian Operators

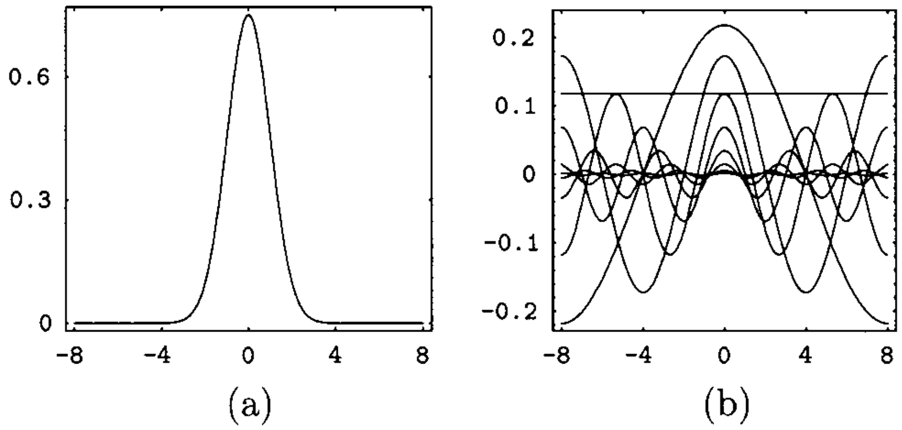
1. The eigenvalues of a Hermitian operator are real

2. Two eigenfunctions corresponding to different eigenvalues are orthogonal

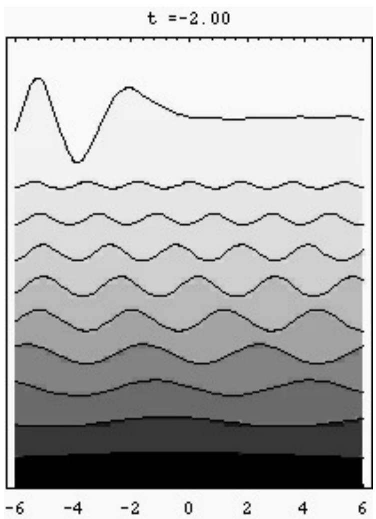
3. The set of eigenfunctions of a Hermitian operator is complete

4. Commuting Hermitian operators have a set of common eigenfunctions

The set of eigenfunctions of a Hermitian operator is complete



The set of eigenfunctions of a Hermitian operator is complete



Product of operators, and commutators

Commuting Hermitian operators have a set of common eigenfunctions

First postulate: wavefunctions

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

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

Second postulate: operators

- For every physical observable there is a corresponding Hermitian operator

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

From classical mechanics to operators

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

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

The total energy of the system

- Kinetic energy K

- Potential energy V

Third postulate: measurements

- 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.

Position and probability

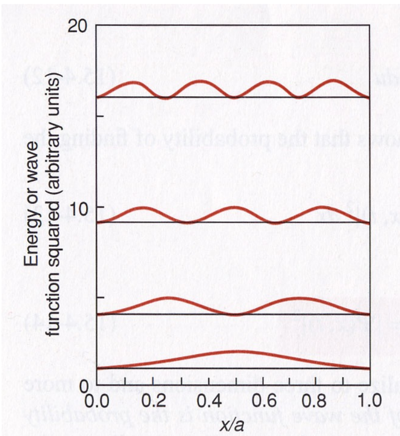


Figure 15.2. The Probability Density for Positions of a Particle in a One-Dimensional Hard Box. This diagram shows the squares of the energy eigenfunctions (probability densities) for the first four states of a particle in a one-dimensional hard box.

MSE 423 Fundamentals of Solid-state Materials - Nicola Marzari (EPFL, Fall 2025)

Fourth postulate: expectation values and probabilities

If a series of measurements is made of the dynamical variable A on an ensemble described by Ψ, the average ("expectation") value is

$$\langle A \rangle = \frac{\langle \Psi | \hat{A} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

i.e. the probability of obtaining an eigenvalue a_n is

$$P(a_n) = (p_n)^2 = \left| \langle \varphi_n | \Psi \rangle \right|^2$$

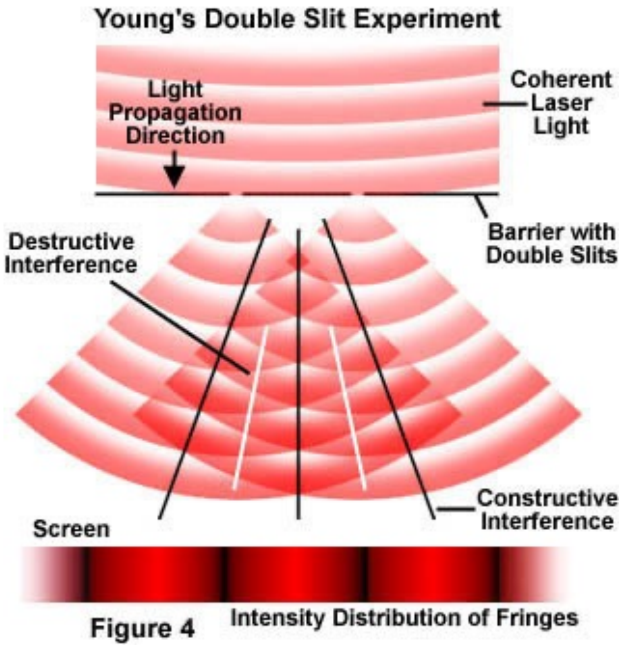
MSE 423 Fundamentals of Solid-state Materials - Nicola Marzari (EPFL, Fall 2025)

Deterministic vs. stochastic

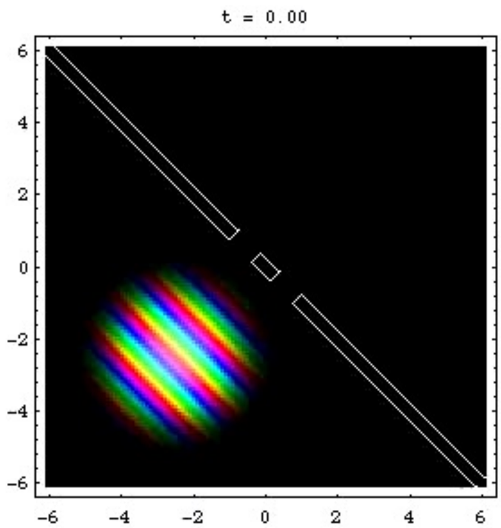
- Classical, macroscopic objects: we have well-defined values for all dynamical variables at every instant (position, momentum, kinetic energy…)

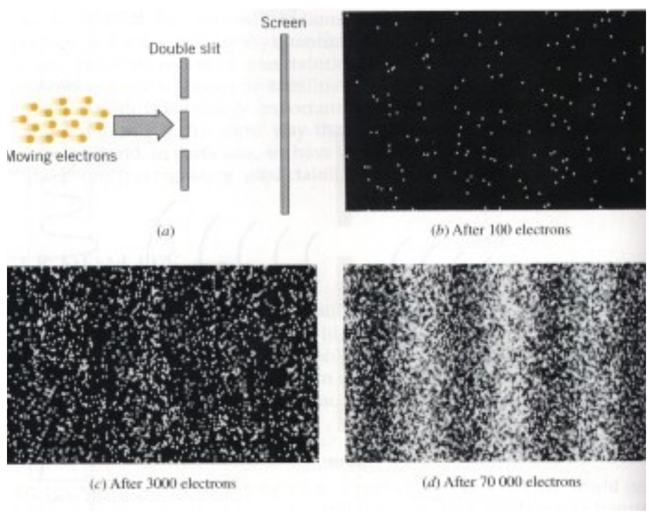
- Quantum objects: we have well-defined probabilities of measuring a certain value for a dynamical variable, when a large number of identical, independent, identically prepared physical systems are subject to a measurement.

Quantum double-slit

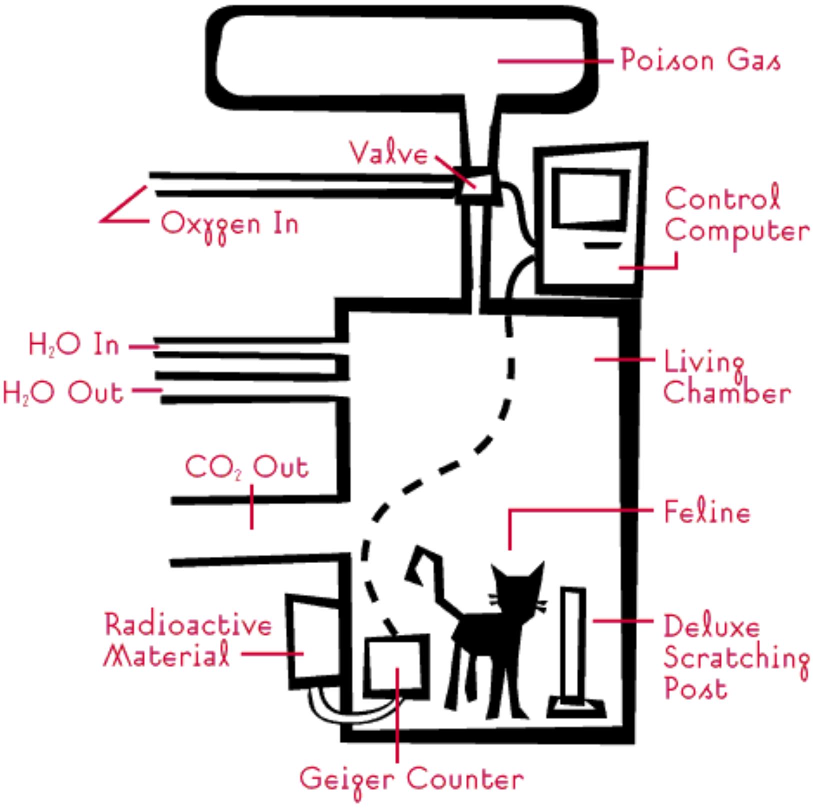


Quantum double-slit





When scientists turn bad…



Cat wavefunction

$$\left|\Psi_{cat}(t)\right\rangle = \left|\Psi_{alive}\right\rangle \left(\exp\left(-\frac{t}{\tau}\right)\right)^{\frac{1}{2}} + \left|\Psi_{dead}\right\rangle \left(1-\exp\left(-\frac{t}{\tau}\right)\right)^{\frac{1}{2}}$$

- There is not a value of the observable until it's measured (a conceptually different "statistics" from thermodynamics)

MENU nature International journal of science

Search E-alert Submit Login

News & Comment Research

News Opinion Research Analysis Careers Books & Culture

NEWS · 18 SEPTEMBER 2018

Reimagining of Schrödinger's cat breaks quantum mechanics — and stumps physicists

In a multi-'cat' experiment, the textbook interpretation of quantum theory seems to lead to contradictory pictures of reality, physicists claim.

Davide Castelvecchi

Fifth postulate: collapse

- 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 $|\varphi_n\rangle$

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!"*