Slide 1

Quantum Mechanics, and Shakespeare

Slide 2


the
Reduced Shakespeare Company
US Tour
2001-02
West End &
UK Tour
"Reducing expectations for over 20 years!"

Slide 3

Calculation and Design of Material Properties From First Principles

- The STANDARD MODEL of matter:
  look at your hands – everything, from your biopolymers to the minerals of your bones is made of atomic nuclei bonded together by electrons.
- If you understand electron bonding, you are done (sort of).

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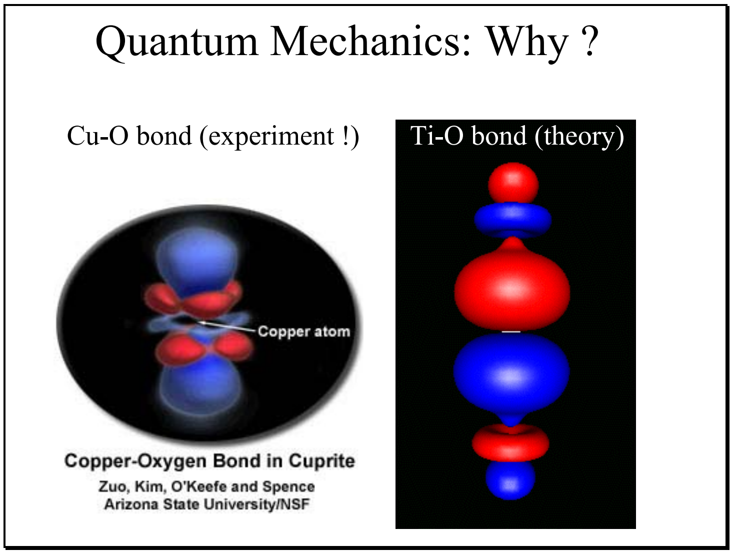
STANDARD MODEL

- Atoms are made by MASSIVE, POINT-LIKE NUCLEI
- Surrounded by tightly bound, rigid shells of CORE ELECTRONS
- Bound together by a glue (GAS) of VALENCE ELECTRONS

Slide 5



Jian-Min Zuo, Miyoung Kim, Michael O'Keefe and John Spence, Arizona State University.
http://clasdean.la.asu.edu/news/images/cuprite/

Slide 6

Why Is It Important ?

- It provides us microscopic understanding
- It has predictive power (remember, it is “first-principles”)
- It allows controlled “gedanken” experiments
- Challenges:
  - **Length scales**
  - **Time scales**
  - **Accuracy**

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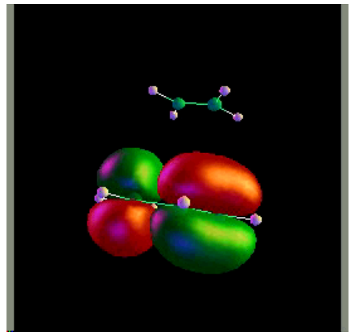
Diels-Alder Reaction



http://www.wag.caltech.edu/home-pages/jim/

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So, What Is It ? A Misnomer…

It’s the mechanics of WAVES, instead of CLASSICAL particles

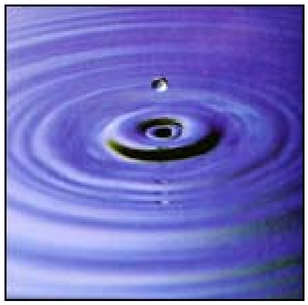
Slide 9

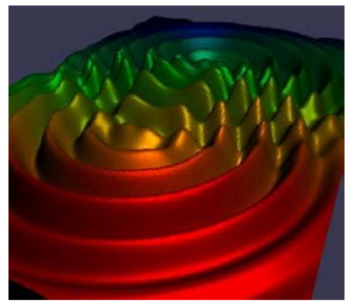
Wave-particle Duality

- Waves have particle-like properties:
  - Photoelectric effect: quanta (photons) are exchanged discretely
  - Energy spectrum of an incandescent body looks like a gas of very hot particles
- Particles have wave-like properties:
  - Electrons in an atom are like standing waves (harmonics) in an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes

Slide 10

If you are a wave, you interfere





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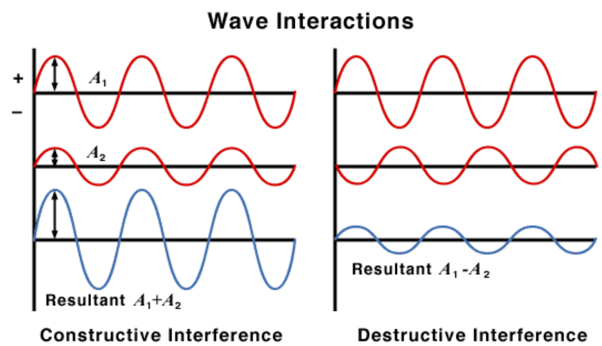
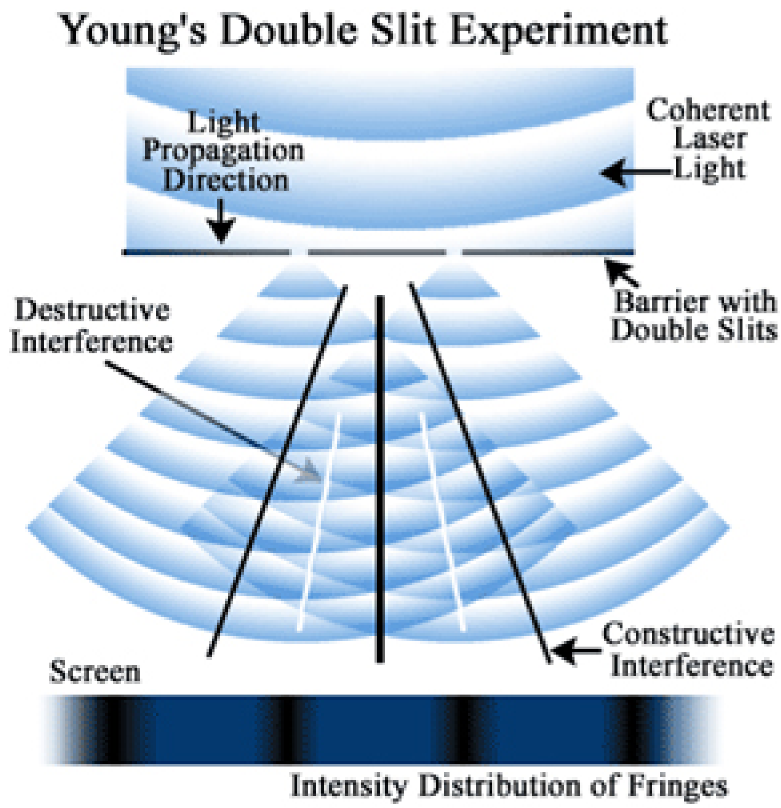
Interference patterns



Interference out of slits



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When is a particle like a wave?

Wavelength * momentum = Planck

See http://www.kfunigraz.ac.at/imawww/vqm/

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The electron has gone through both slits

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Remember the standard model

- The atomic nuclei are massive, point-like particles
- The electrons are waves, gluing together the nuclei.
- Inner electrons (CORE) are tightly bound around their own nucleus. They do not bind, but they screen the nucleus
- Outer electrons (VALENCE) are ready to interfere and bind and glue everything together

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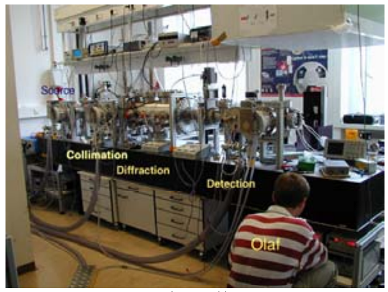
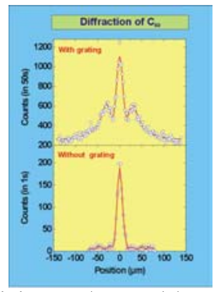
Soccer Balls Diffract





http://www.quantum.univie.ac.at/research/c60/

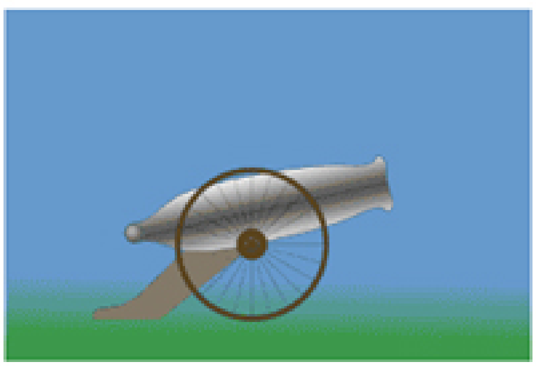
Prof. Markus Arndt Institute of Experimental Physics Vienna University, Austria

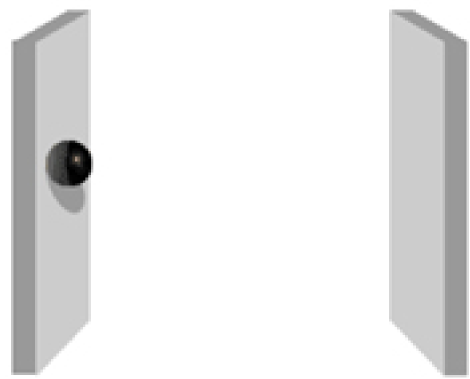
http://www.quantum.univie.ac.at/research/c60/

Mechanics of a Particle

$$m\frac{d^2\vec{r}}{dt^2} = F(\vec{r}) \quad \rightarrow \quad \begin{matrix}\vec{r}(t)\\ \vec{v}(t)\end{matrix}$$

The sum of the kinetic and potential energy is conserved





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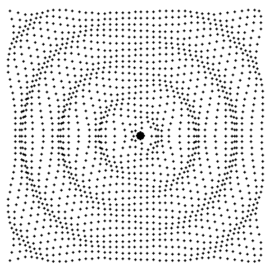
Description of a Wave



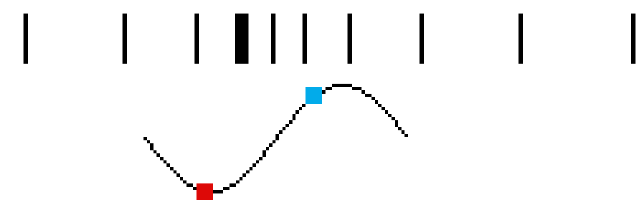
The wave is an excitation (a vibration): We need to know the amplitude of the excitation at every point and at every instant

$$\Psi = \Psi(\vec{r}, t)$$

Mechanics of a Quantum Wave

Free particle, with an assigned momentum

$$\Psi(\vec{r},t) = A\exp[i(\vec{k}\bullet\vec{r}-\omega t)]$$



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Time-dependent Schroedinger's equation

Exercise: our free particle satisfies this wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} \quad \text{provided} \quad E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

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

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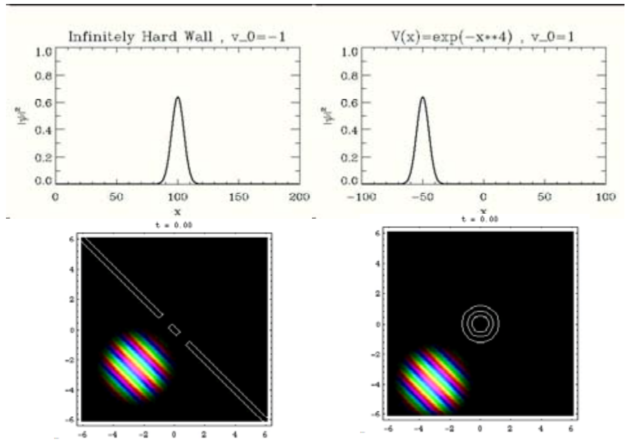
How Does It Look ?



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Time-independent Schroedinger's equation

$$\Psi(\vec{r},t) = \psi(\vec{r})\,f(t)$$

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

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Interpretation of the Quantum Wavefunction

$$\left\| \Psi(\vec{r}, t) \right\|^2$$ is the probability of finding an electron in *r* and *t*

Remember the free particle, and the principle of indetermination:if the momentum is perfectly known, the position is perfectly unknown

Slide 24

Solutions in a Coulomb Potential: the Periodic Table

http://www.orbitals.com/orb/orbtable.htm