Coulomb's Law Force

$\oplus \leftarrow 1\,\text{Å} \rightarrow \ominus$

$$\frac{(9\times10^{9})(1.6\times10^{-19})^{2}}{(1\times10^{-10}\,m)^{2}} = 2.3\times10^{-8}\,N$$

For 2 elementary charges 1Å apart.

at 0.01 Å 2.3×10^{-4} N

FOR ONE proton & ONE e^-

Equivalent to Gravitational force of EARTH ON 0.025 gram

But, Experimentally $\bar{e}$ is in the 1s orbital, even at 0 Kelvin!

Striking Example of Zero point Energy

KINETIC E = 1.3×10^{6} J/mol $u_{rms} = 2\times10^{6}\,ms^{-1}$

YET, IS ABSOLUTELY COLD (& DARK)

Quantum Behavior & Quantum Mechanics

Applies to EVERYTHING

But most evident for particles with mass equal or less than proton

Absolutely NECESSARY for electrons and light (photons),

which are neither particles or waves;
there is nothing like them in the macroscopic world !

Thus, Quantum Mechanics cannot be "understood" in the usual sense***—not even by the world's greatest minds.***

Quantum Mechanics was ***discovered***—NOT derived

Newton's Laws, however, **CAN** be derived from quantum mechanics

Quantum Mechanics has ***never failed*** to agree with experiment—yet.

Quantum Concepts

Who	When	What	Equation
1. Planck	1905	Quantization of Energy	$\Delta E = h\nu$
2. Einstein	1905	Particle Nature of Light	$p = h/\lambda$
3. DeBroglie	~1920	Wave Nature of Particles	$\lambda = h/p$
4. Bohr	~1920	Quantization of Angular Momentum	$L^2 = l(l+1)\,(h/2\pi)^2$; $L_z = m\,(h/2\pi)$ 2L+1 m values from –L to +L
5. Heisenberg	~1925	Uncertainty Principle	$\Delta p_x\,\Delta x \cong h$ or: "why the electron does not fall into the nucleus" i.e., the concept of **ZERO POINT ENERGY**

More on **zero point energy** and uncertainty principle

Zero point kinetic energy is $\cong$ **$h^2/(m\,\Delta x^2)$,** where h = Planck's constant, m = mass, and Δx is the length of the region to which the particle is confined. For example, as a nucleus pulls an electron close, the zero-point energy increases and ***the electron will not fall to the nucleus***. (It is as if the small things like electrons "refuse" to be localized.)

(Note: $h^2 = J^2\,s^2 = kg^2\,m^4 s^{-4}\,s^2$, so $h^2/(m\,\Delta x^2) = kg^2\,m^4 s^{-2}/(kgm^2) = kg\,m^2 s^{-2} = J$)

<u>Heisenberg Uncertainty</u>: $\Delta x\,\Delta p \cong h$, i.e., product of uncertainty in x and uncertainty in momentum is about = h.

ΔH of chemical reactions is equal to the **change in quantum zero point energy** at 0 Kelvin, and is only slightly different at room temperature due to heat capacity differences.

The mysterious **"DARK ENERGY"** that is apparently causing the acceleration of expansion of the Universe is most discussed as **quantum zero point energy** (of gravity, for which there is no quantum theory yet.)

THEN CAME THE Schrödinger Equation (1926)

which says all of the above

This equation was **DISCOVERED**, not derived

Schrodinger did not know what to make of Ψ when he published his equation. Everyone knew it was important because the equation gave all the correct energies for the "well behaved" solutions.

Also was immediately shown that Newton's Laws could be derived from the Schrodinger Eq.
(but not the other way around)

1926 Schrodinger's Equation:

A simple equation that was discovered (not derived)

Classical Mechanics

Kinetic Energy + Potential Energy = Total Energy

Quantum Mechanics (Schrodinger's Equation without time) translated into English:

-**h**^{2}/8pi^{2}mass x ***Curvature*** of **Wavefunction** + Potential Energy x **Wavefunction** = Energy x **Wavefunction**

curvature operation (2nd derivative

h/2π

wavefunction

$$: -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E\psi$$

mass

Kinetic energy

potential energy

Total energy

Time independent Schrodinger Equation :

$$-\frac{h^2}{8\pi^2}\times\sum_{\text{all particles j}}\left(\frac{\partial^2}{\partial x_j^2}\frac{\partial^2}{\partial y_j^2}+\frac{\partial^2}{\partial z_j^2}\right)\Psi+\text{potential E}\times\Psi=\text{total E}\times\Psi$$

$$\text{or: kinetic energy operator}\times\Psi+\text{classical potential energy}\times\Psi$$

$$=\text{total energy}\times\Psi$$

$$H\Psi=E\Psi,\ \text{where H = Hamiltonian = total energy operator}$$

$$\Psi^*\Psi=\text{probablility density for finding particle locations}$$

$$\Psi^*\ \text{is the complex conjugate. i.e., change all i -->-i}$$

$$i=\sqrt{-1}$$

Potential energy EXACTLY ***same*** as in Classical mechanics

Three things are different from Classical mechanics:

1) The wavefunction (Schrödinger *did not know* what its physical meaning was at the time he published). Later the consensus was reached that the absolute square of the wavefunction gives the ***probability density*** for finding the particle.)

2) Kinetic energy is represented by the *CURVATURE* of the *Wavefunction.* In calculus, that is the 2nd derivative (i.e., the slope of the slope of the function)

3) *h*, Planck's constant, which was empirically adjusted so that the Schrödinger Equation gives agreement with experiment.

This simple equation embodies the 5 seemingly distinct new "quantum concepts"

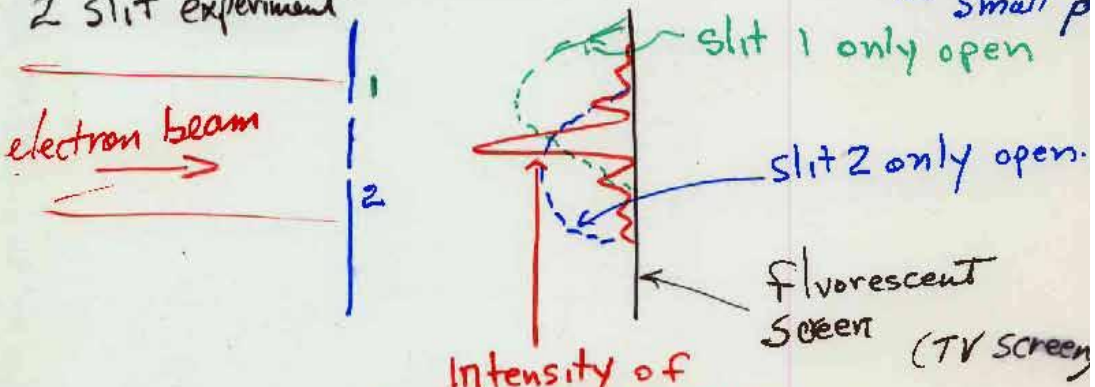
3. WAVE NATURE OF PARTICLES

de Broglie ~ 1920

$$\lambda = \frac{h}{\text{momentum}} = \frac{h}{mv} \equiv \frac{h}{p}$$

small p

2 slit experiment

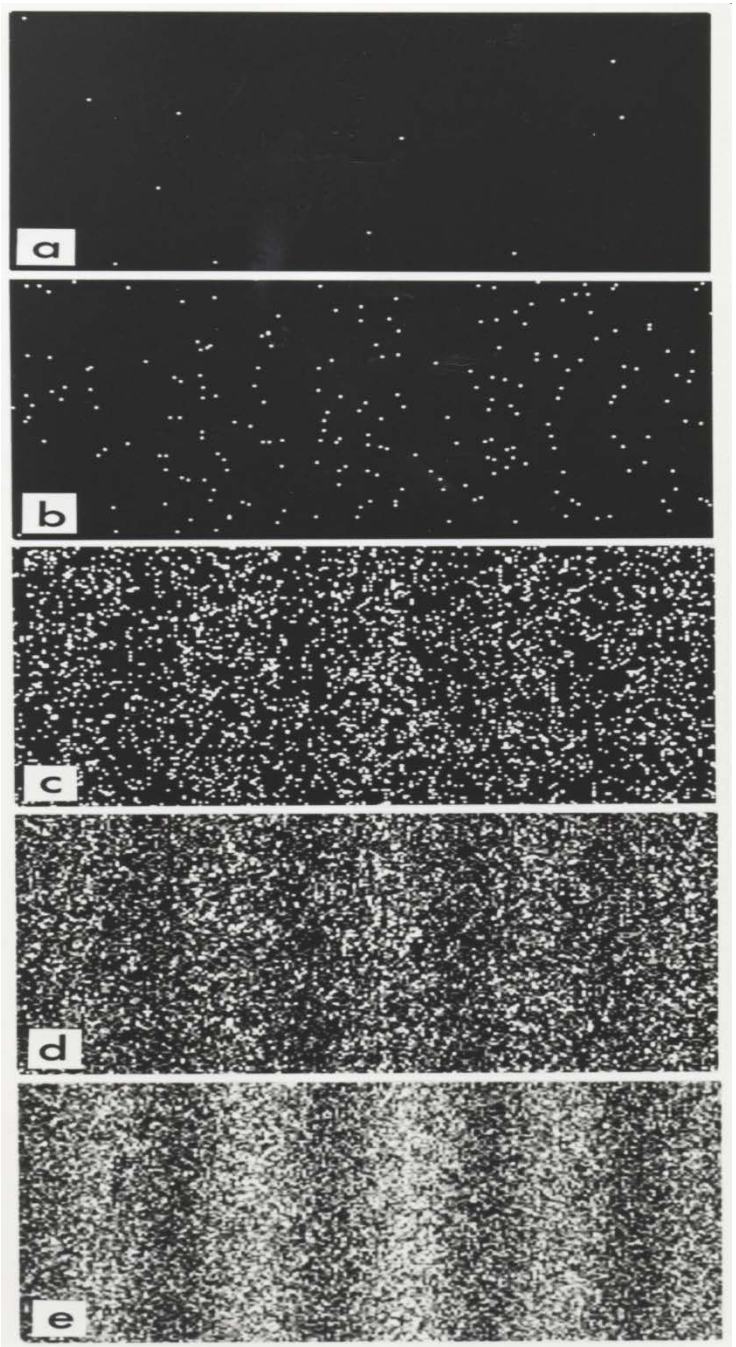


TIME EXPOSURE (1 particle per second)
GIVES EXACTLY SAME RESULT !!!

SAME FOR PHOTONS !!!

Interference is a SINGLE PARTICLE phenomenon! (one particle or photon does not interfere with another)

This phenomenon captures the essential mystery of quantum behavior



Results of a double-slit-experiment performed by Dr. A. Tonomura showing the build-up of an interference pattern of ***single electrons.*** Numbers of electrons are 10 (a), 200 (b), 6000 (c), 40000 (d), 140000 (e).
(Provided with kind permission of Dr. AkiraTonomura.)

Electron or photon interference is a **single particle phenomenon**!

Movies available at:
http://www.hitachi.com/rd/research/em/movie.html

Time dependent Schrödinger Equation

$$\frac{\partial\ \Psi(r,t)}{\partial t} = -i\frac{H}{\hbar}\Psi(r,t)$$

$$H\Psi = E\Psi, \text{ where H} = \text{Hamiltonian} = \text{total energy operator}$$

It says by inspection that the ***future*** of a quantum state is predicted, IF one knows the wavefunction at a given time.

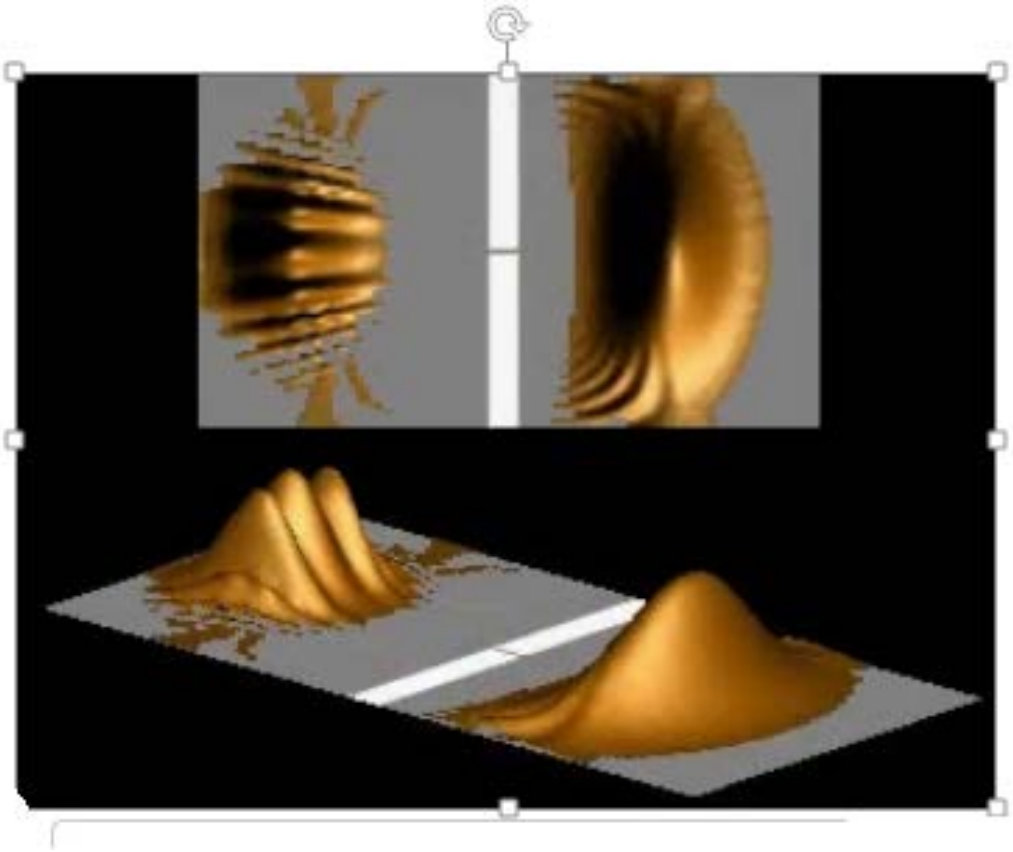
(we never do, except for very simple experiments)

All (non-relativistic) dynamics in nature are in principle described by this simple equation! Only limited by computer size and power.

Below are videos of time dependent quantum computations of an electron moving through a double slit.

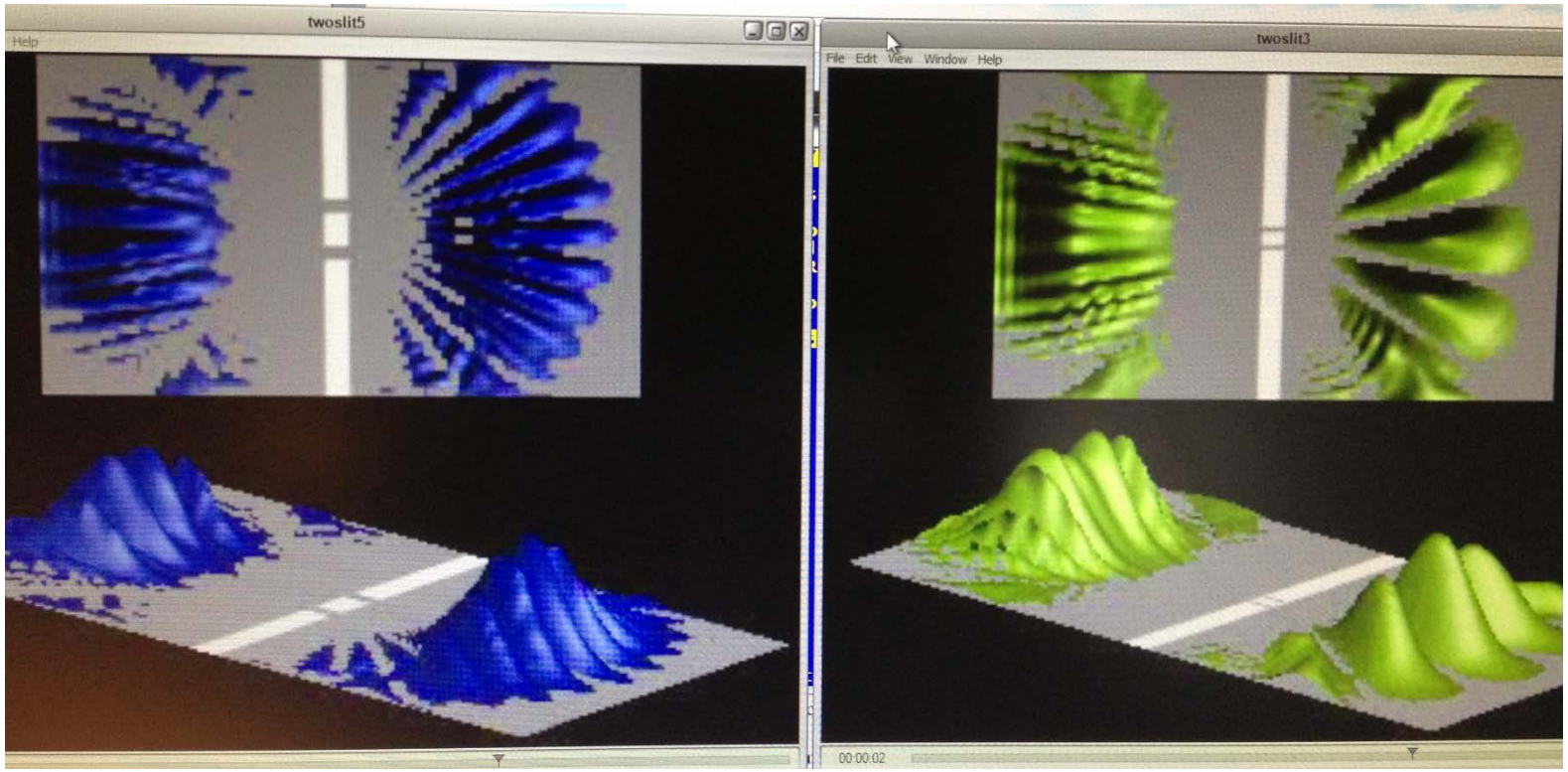
Single particle (photon or electron) diffraction from exact solutions of time dependent Schrodinger Equation.

Particle wavefunction squared moving toward a slit in a solid plate.
The particle is partially reflected backwards from plate and partially passed through the slit.

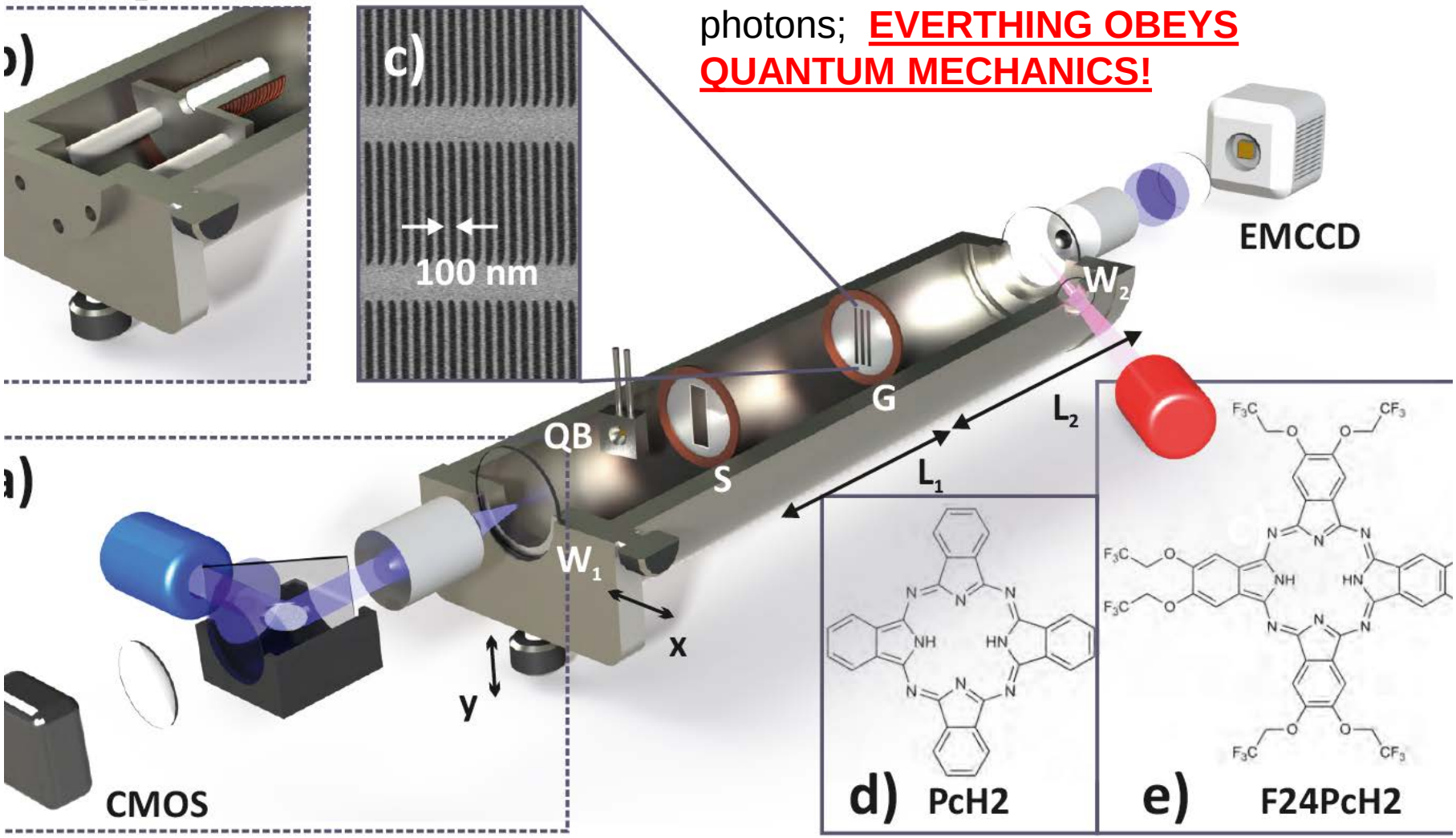


Single particle (photon or electron) diffraction from exact solutions of time dependent Schrodinger Equation.

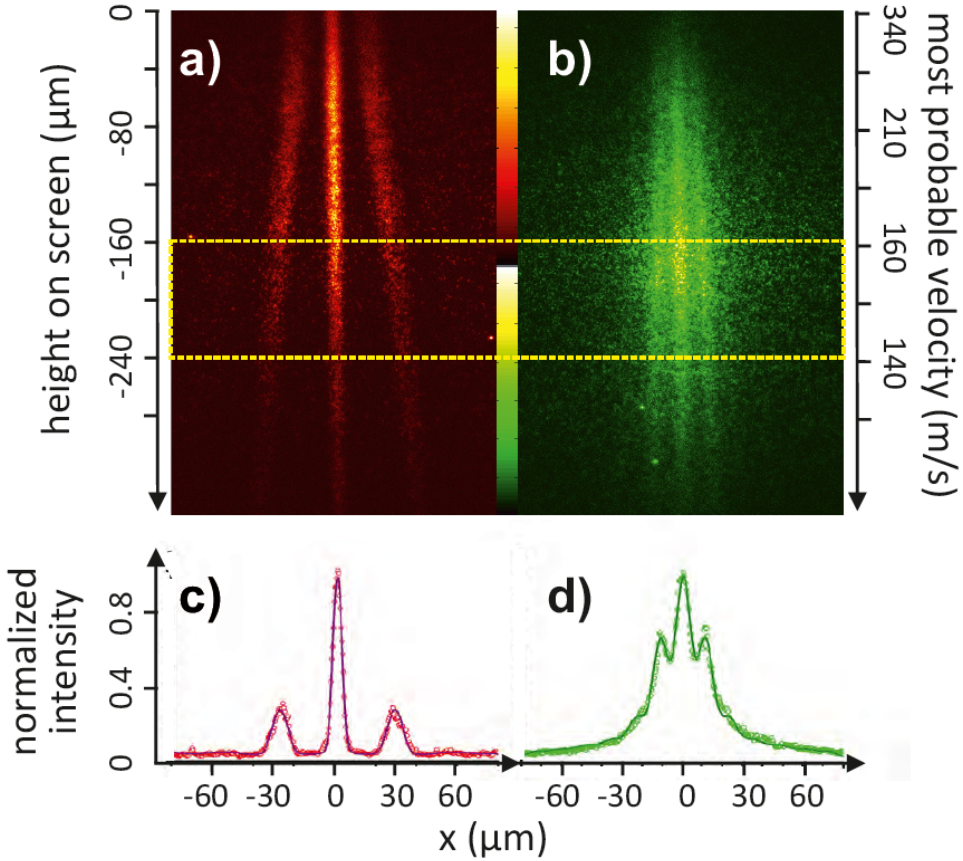
Particle wavefunction squared moving toward two slits in a solid plate. The particle is partially reflected backwards from plate and partially passed through the two slits. Peaks of the interference pattern are as predicted for Bragg's Law.



Large dye molecules also observed to diffract; not just electrons and photons; **EVERTHING OBEYS QUANTUM MECHANICS!**



Phthalocyanine derivatives



Far-field diffraction of larger molecules [2,4]

- Phthalocyanine PcH2 (red):
  Highly fluorescent dye, thermally stable

- Perfluoro-alkylated phthalocyanines (green):
  Higher masses, high volatility,
  optical properties similar to PcH2.

http://www-lpl.univ-paris13.fr/icap2012/docs/Juffmann_poster.pdf

http://www.youtube.com/watch?v=NUS6_S1KzC8