

Fermions vs. Bosons, continued

Why do fermions obey Pauli Exclusion, but bosons obey “inclusion”?

We don't know why this division, but quantum mechanics distinguishes them in the symmetry under exchange of the coordinates of identical, interacting particles by the operator, $P_{1,2}$,

$$P_{1,2} \Psi_{\text{fermi}} = - \Psi_{\text{fermi}}$$

$$P_{1,2} \Psi_{\text{bose}} = + \Psi_{\text{bose}}$$

Simple example using an independent systems wave function for two particles.

$\Psi_{\text{fermi}} = A(1)B(2) - A(2)B(1)$ What happens if $A = B$, i.e., particles in same state?

Ψ_{fermi} **vanishes** if $A = B$

$\Psi_{\text{bose}} = A(1)B(2) + A(2)B(1)$ What happens if $A = B$, i.e., particles in same state?

Ψ_{bose} is **magnified** if $A = B$

True for antisymmetric and symmetric determinants for **any** number of particles

Quantum Concepts

<u>Who</u>	<u>When</u>	<u>What</u>	<u>Equation</u>
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 $+L$
<p>for FERMIONS L is half-integer (1/2, 3/2, for BOSONS L is integer (0, 1, 2</p>			
5. Heisenberg	~1925	Uncertainty Principle	$\Delta p_x \Delta x \cong h$ gives p
<p>square both sides, divide by $2m\Delta x^2$, $\Delta p_x \cong p_x$</p> <p>gives $p_x^2/2m = KE_x \cong h^2/2m\Delta x^2$ i.e., confinement to Δx creates KE_x</p>			<p>or: “why the electron does not fall into the nucleus” i.e., the concept of <u>ZERO POINT ENERGY</u></p>

Time dependent Schrödinger Equation

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

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.

We will show later in this course that ALL KINETIC RATE CONSTANTS for the rate: state 1 \rightarrow state 2 are proportional to $|H_{12}|^2$ i.e., the square of the Hamiltonian matrix element connecting states 1 and 2. (for example, the rate of electronic excitation is proportional to the electric dipole transition moment squared because the Hamiltonian = $e\mathbf{E} \cdot \mathbf{r}$, the projection of the electric field of the light on the position of an electron.

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

IF: $H\Psi = E\Psi$, where H = Hamiltonian = total energy operator

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

What is the solution?

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

$$\Psi(r,t) \propto \exp\left(-i \frac{Et}{\hbar}\right) = \exp(-i\omega t)$$

$$\Psi^*(r,t)\Psi(r,t) = \text{constant, i.e., density is stationary!}$$

ALL non-E eigenstates exhibit moving probability density!

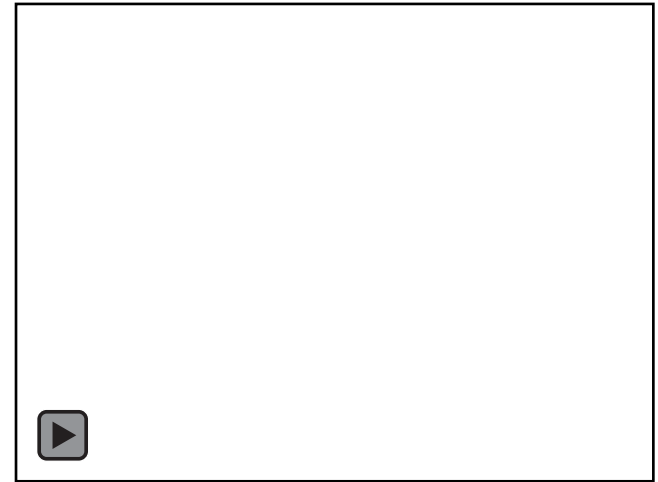
Below are videos of time dependent quantum computations of an electron moving through single and double slits.

Time dependent Schrödinger Equation Applied to a **moving SINGLE** particle (is this an energy eigenstate?)

A moving “particle” is described by a superposition of many sin and cos waves which constructively interfere to give a spherical Gaussian probability near a certain point but destructively interfere everywhere else.

The Gaussian “wave packet” moves according to the kinetic energy given by the average frequency of the sin waves. This is how Newton’s Laws emerge from quantum theory.

This demonstrates very well the uncertainty principle, and the **generation of kinetic energy during the confinement** while passing through the slit, resulting in large spreading of the wavefunction after emerging from slit.



Large single slit

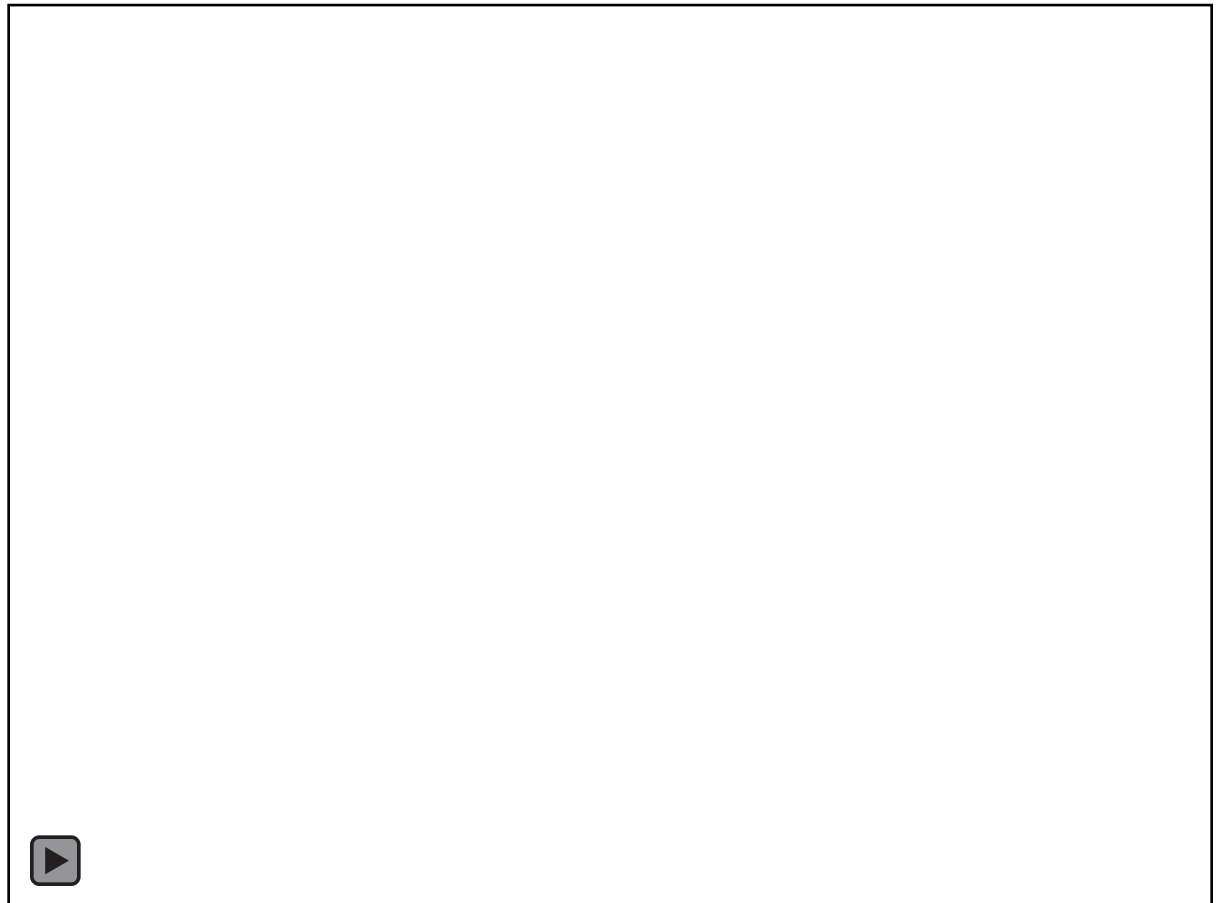


Very small single slit

A moving “particle” is described by a superposition of a great many sin and cos waves which constructively interfere to give a Gaussian probability near a certain point but destructively interfere everywhere else.

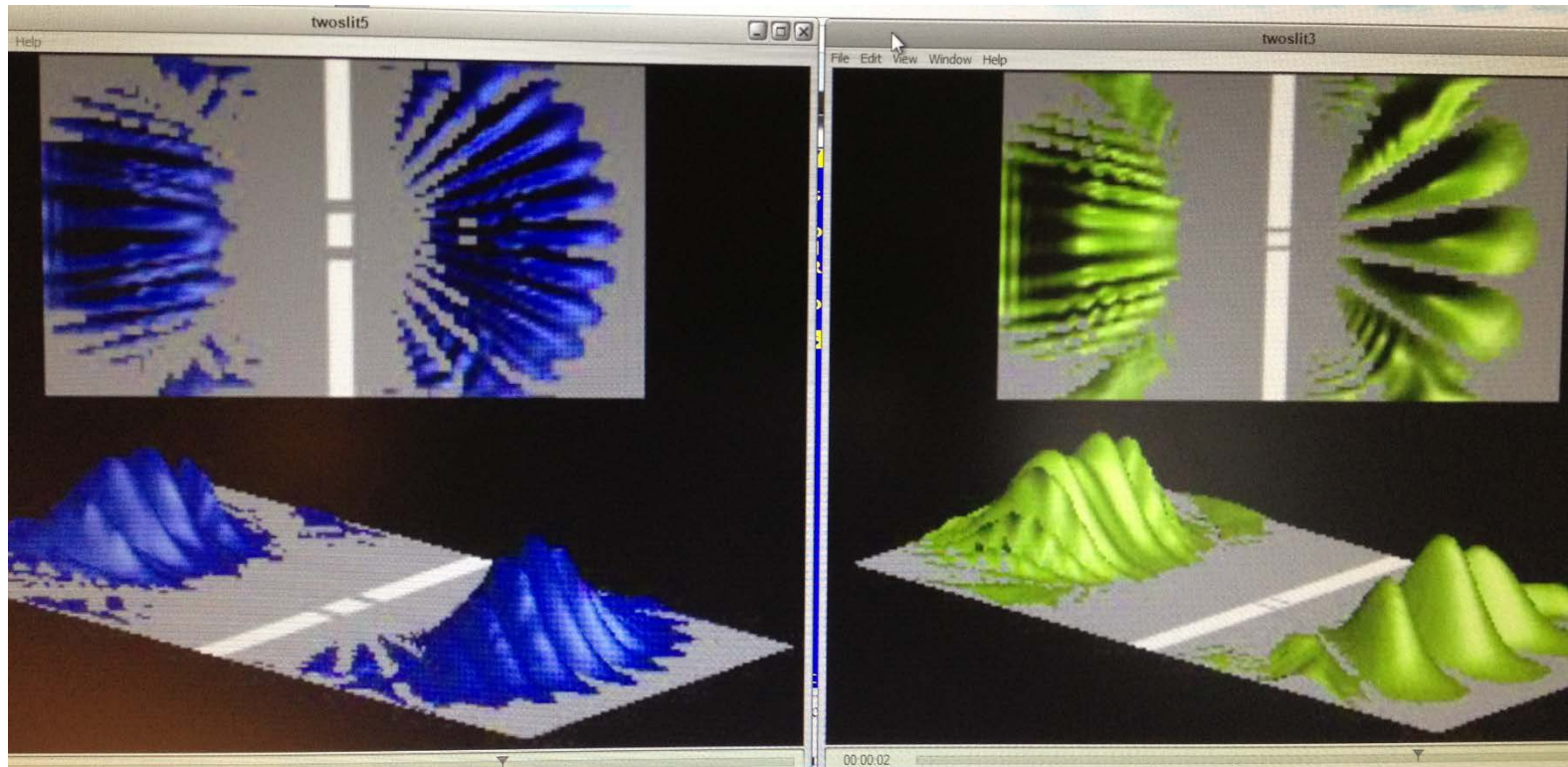
The Gaussian “wave packet” moves according to the kinetic energy given by the average frequency of the sin waves. This is how Newton’s Laws emerge from quantum theory.

Double Slits
CLOSE together



Double Slits
FAR apart





Double Slits
FAR apart

Peaks close together

Double Slits
CLOSE together

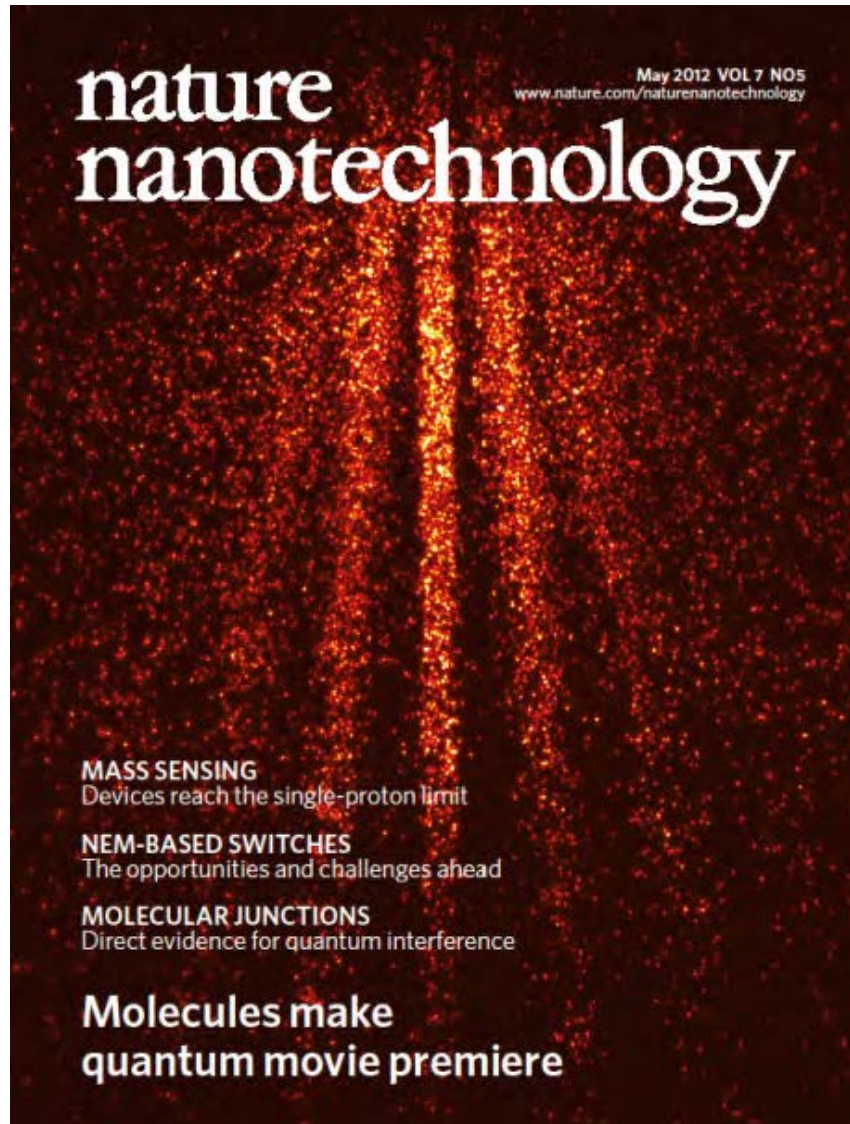
Peaks FAR apart

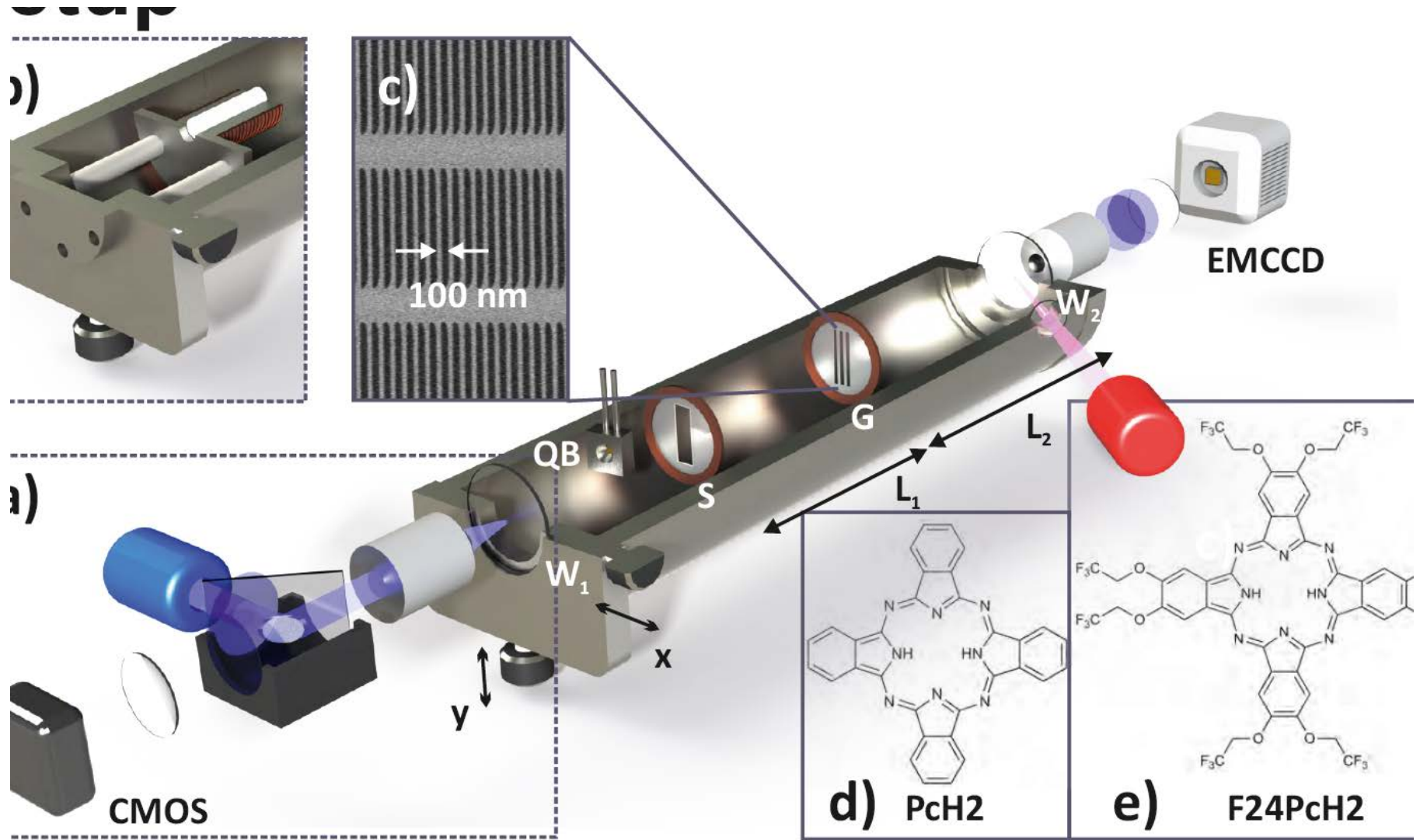
All particles may be diffracted

including massive organic molecules!!

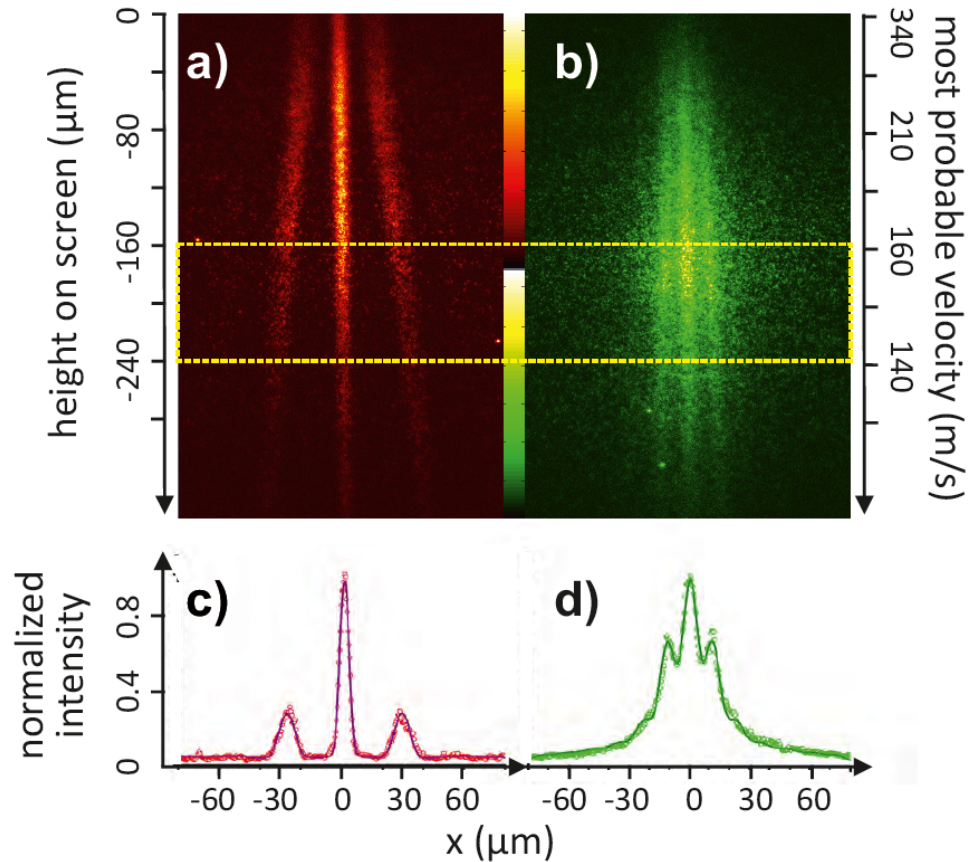
http://www-lpl.univ-paris13.fr/icap2012/docs/Juffmann_poster.pdf

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





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.

