



Weak values and weak measurement in elementary scattering and reflectivity – a new effect

C Aris Dreismann Institute of Chemistry, TU Berlin

dreismann@chem.tu-berlin.de

7th International Conference on New Frontiers in Physics (ICNFP 2018)

Experimental context:

non-relativistic SCATTERING: incoherent, inelastic

Here: specifically **neutrons** → **INS** (also called **IINS**)



Theoretical context:

Weak Values (WV), Weak Measurement, Post-Selection, Two-State Vector Formalism (TSVF)

Motivation:

*This theoretical frame enable us to extract **more** physical (measurable !) information about the system than just the **Born Rule** and the **Reduction Postulate** of standard QM*

Outline: *Short introductory remarks*

What is measured: Experimental setup of INS (Time-Of-Flight)

Weak values and INS experiment

New quantities being measurable

Further remarks, „educated guesses“, speculations ... technological context

For stimulation: *What we see here?*

PRL 114, 191803 (2015)

Selected for a Viewpoint in *Physics*
 PHYSICAL REVIEW LETTERS

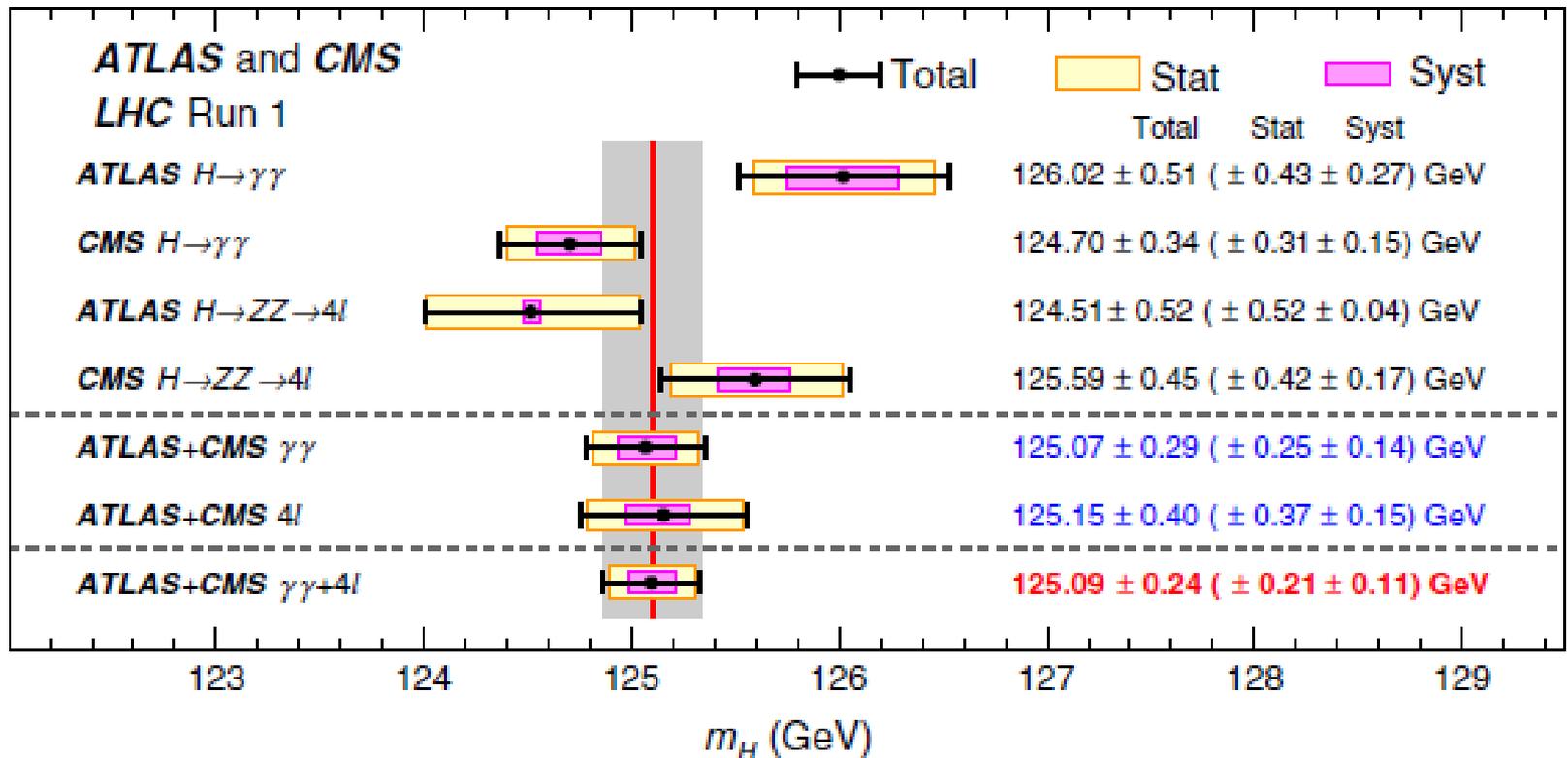
week ending
 15 MAY 2015



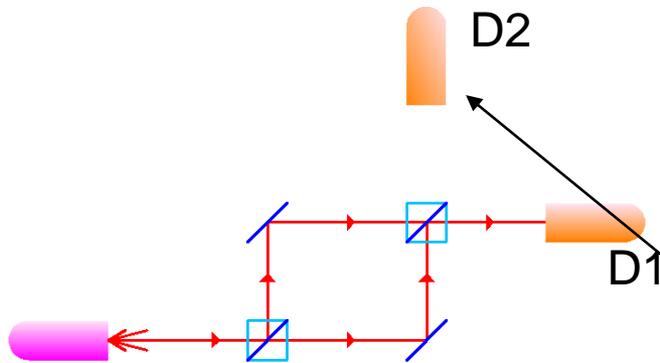
Combined Measurement of the Higgs Boson Mass in pp Collisions at $\sqrt{s} = 7$ and 8 TeV with the ATLAS and CMS Experiments

G. Aad *et al.**

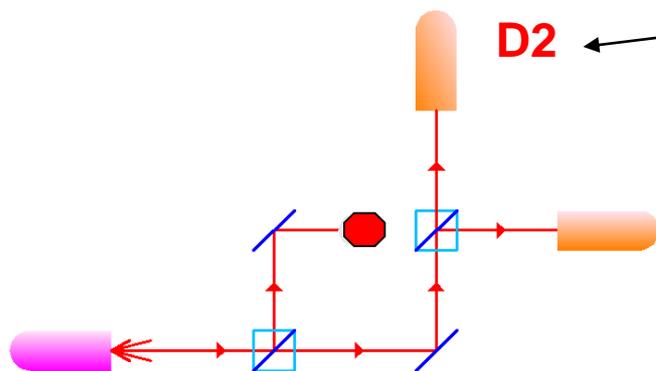
(ATLAS Collaboration)[†]
 (CMS Collaboration)[‡]



→ **Elitzur-Vaidman effect: „Bomb paradox“ (~1993)**
 (Interaction Free Measurement, IFM)



Figs. from Wikipedia.de



!!! Postselection of D2 = Photon is measured in the position of D2:
 D2 „klick“ → Bomb „measured“ with certainty but with no energy/momentum exchange!

What are the „costs“ of this information?

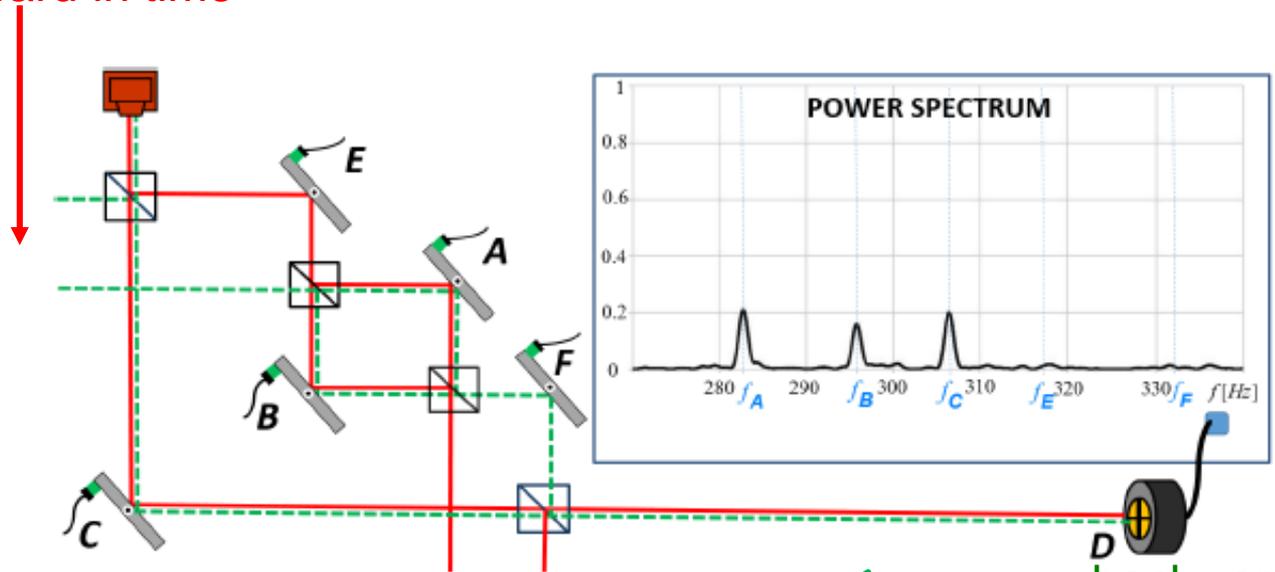
„physical meaning“ of wavefunction?

Asking Photons Where They Have Been

A. Danan, D. Farfurnik, S. Bar-Ad, and L. Vaidman

Illustration of TSVF

„forward in time“



„backward in time“

Direct measurement of the quantum wavefunction

Jeff S. Lundeen¹, Brandon Sutherland¹, Aabid Patel¹, Corey Stewart¹ & Charles Bamber¹

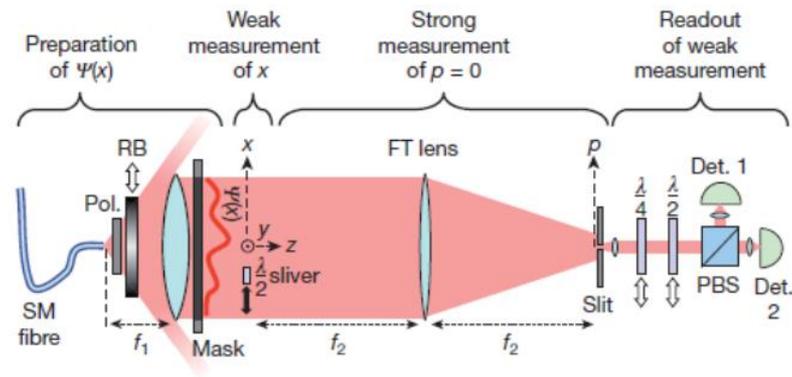


Figure 1 | Direct measurement of the photon transverse wavefunction. To begin with photons having identical wavefunctions, we transmit them through

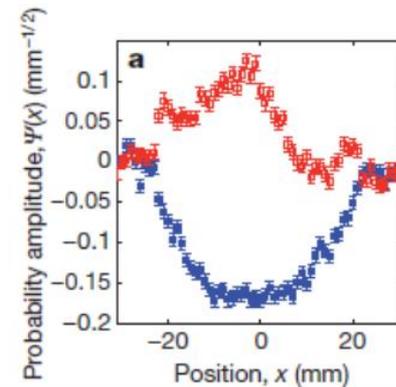


Figure 2 | The measured single-photon wavefunction, $\Psi(x)$, and its modulus squared and phase. **a**, $\text{Re}\Psi(x)$ (solid blue squares) and $\text{Im}\Psi(x)$ (open red squares) measured for the truncated Gaussian wavefunction.

Coherent vs. Incoherent Scattering

From: [The Feynman Lectures on Physics, Volume III](#)

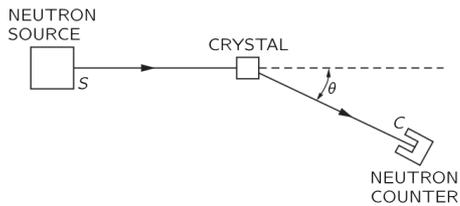


Fig. 3-5. Measuring the scattering of neutrons by a crystal.

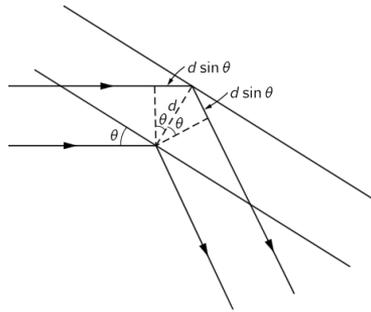
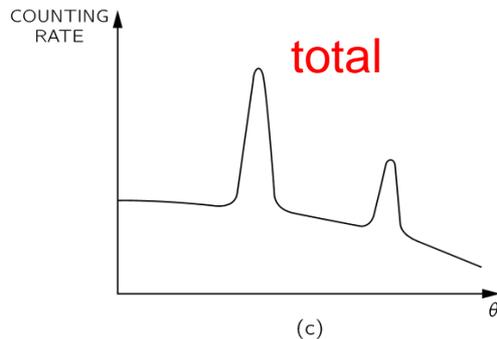
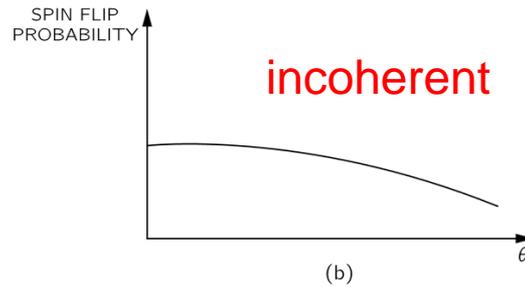
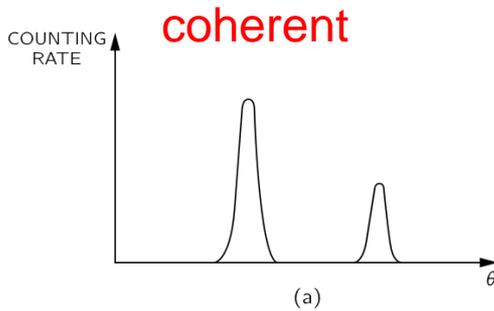


Fig. 2-4. Scattering of waves by crystal planes.

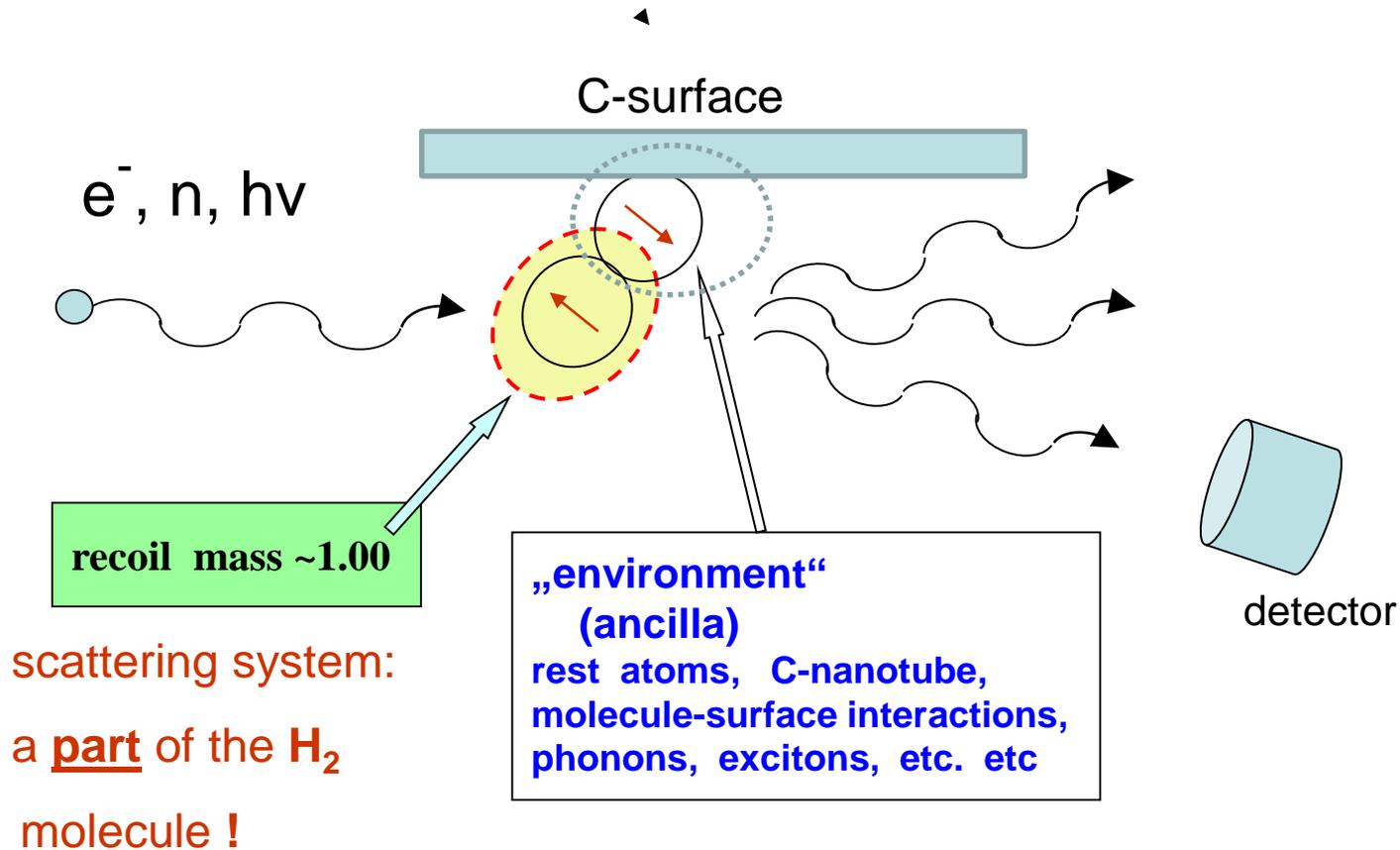
Bragg's Law
 $2d \sin \theta = n\lambda \quad (n=1,2,\dots).$

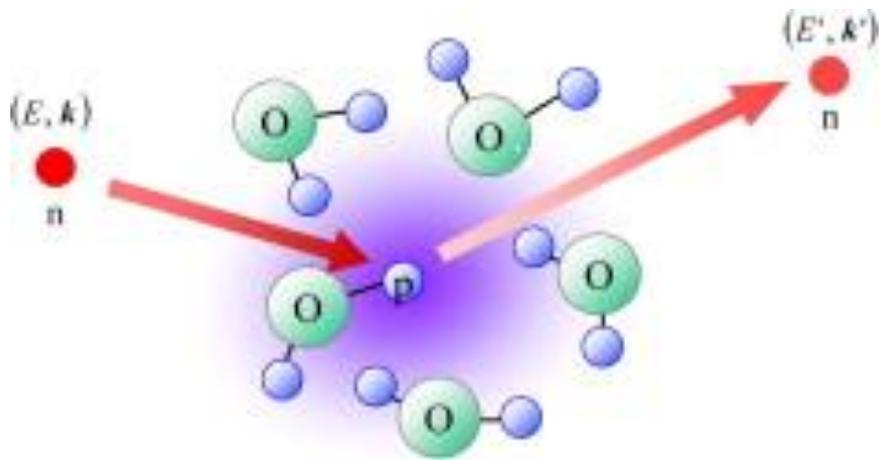


.....You may argue, "I don't care which atom is up." Perhaps you don't, but nature knows;

Compton-like (i.e. incoherent) scattering - impulsive limit

E.g. H_2 molecules in C-nanostructures





Conventional theory

Basic formula of neutron scattering theory (van Hove, 1954)

Textbook: **G L Squires**, Introduction to the Theory of Thermal Neutron Scattering (Mineola, Dover 1996)

$$\left(\frac{d^2\sigma}{d\Omega d\omega} \right)_{\mathbf{v} \rightarrow \mathbf{v}'} = \frac{k_1}{k_0} \left(\frac{m}{2\pi\hbar^2} \right)^2 \left| \langle \mathbf{v}' \mathbf{k}_1 | V(\mathbf{r}) | \mathbf{v} \mathbf{k}_0 \rangle \right|^2 \delta(E_v - E_{v'} + E_0 - E_1)$$

First-order pert. Theory,
 δ -function: E-conservation

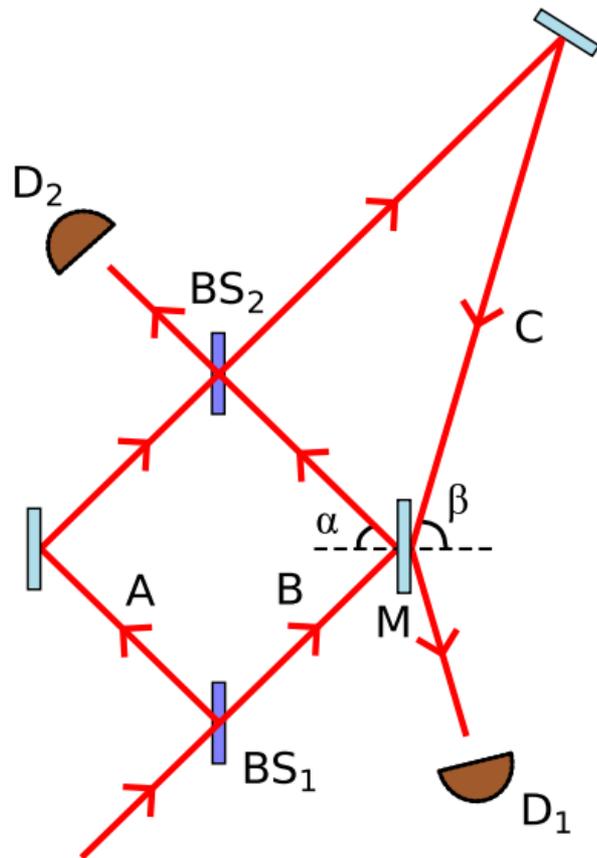
**All dynamical quantities refer to the scattering system.
The quantum degrees-of-freedom of neutron „disappeared“ here,
i.e here the neutron „is“ classical.**

Claim: post-selection and weak values yield novel effects ...

The classical limit of quantum optics: not what it seems at first sight

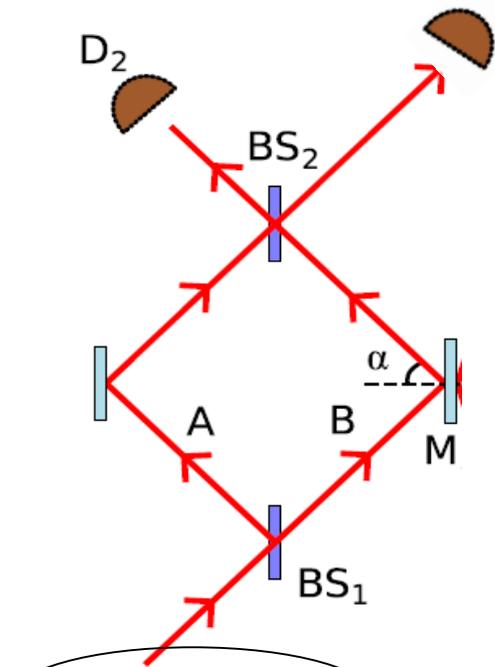
Yakir Aharonov^{1,2}, Alonso Botero³, Shmuel Nussinov¹, Sandu Popescu⁴, Jeff Tollaksen², and Lev Vaidman

New J Phys 15 (2013) 093006



.....
“An essential point to emphasize is that this whole discussion is not just restricted to interpretations. Quite the opposite. Allowing us to have a better intuition is essential for finding new and interesting quantum effects and may lead to new experiments and potential practical applications.” (p. 2)
.....

Here: postselection, WV, and „anomalous“ momentum transfer



$$|in\rangle \rightarrow ir|R\rangle + t|T\rangle$$

$$r^2 + t^2 = 1, \text{ and } \underline{r > t.}$$

Consider the photons (particles) **measured with (postselected by) detector D₂**:

M: „small“ mirror (quantum object)

What **direction** has the **momentum exchanged** with the mirror **M**?

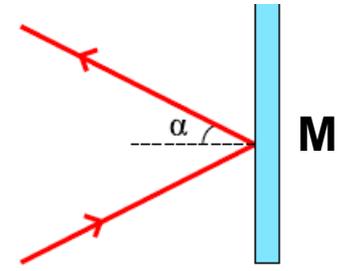
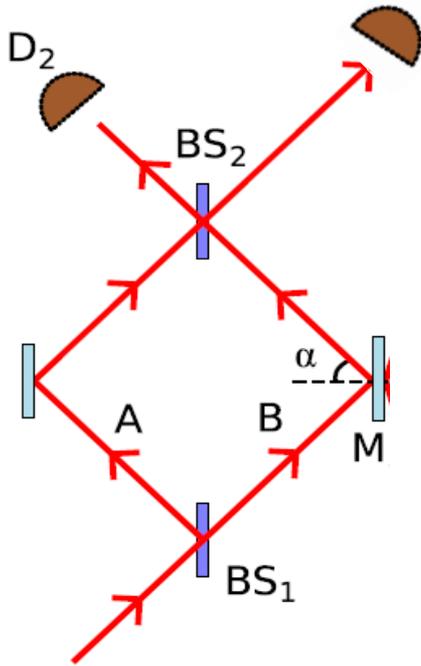


Figure 1. Light reflected on a mirror.

replace:
M → atom
?

when a single photon impinges from the left on BS₁
 the effect of the beamsplitter is to
 produce inside the interferometer the state $|\Psi\rangle = ir|A\rangle + t|B\rangle$

(... *postselection* ...)



As one can readily check, a photon in the quantum state $|\Phi_2\rangle = -ir|A\rangle + t|B\rangle$ emerges towards detector D₂.

!!!

Thus, when a single photon enters the interferometer by impinging on the left side of the beamsplitter BS₁, the probabilities to be found in the arms A and B are r^2 and t^2 respectively. The probability of emerging towards D₂ is $|\langle\Phi_2|\Psi\rangle|^2 = (r^2 - t^2)^2 = 1 - 4r^2t^2$.

if $\phi(p)$ is the initial quantum state of the mirror and by $|\Psi\rangle$ the quantum state of the photon after the input beamsplitter BS₁, but before reaching the mirror, the reflection on the mirror results in

$$|\Psi\rangle\phi(p) = (ir|A\rangle + t|B\rangle)\phi(p) \rightarrow ir|A\rangle\phi(p) + t|B\rangle\phi(p - \delta). \quad (6)$$

the kick given by the photon

$$\delta = 2\hbar\omega \cos \alpha \quad (\text{with } c=1)$$

momentum centred at ± 0

momentum centred at $+\delta$

we can approximate the state (6) of the photon and mirror just before the photon reaches the output beamsplitter by

$$\begin{aligned}
 |\Psi\rangle\phi(p) &\approx ir|A\rangle\phi(p) + t|B\rangle\left(\phi(p) - \frac{d\phi(p)}{dp}\delta\right) \\
 &= |\Psi\rangle\phi(p) - t|B\rangle\frac{d\phi(p)}{dp}\delta.
 \end{aligned}
 \tag{7}$$

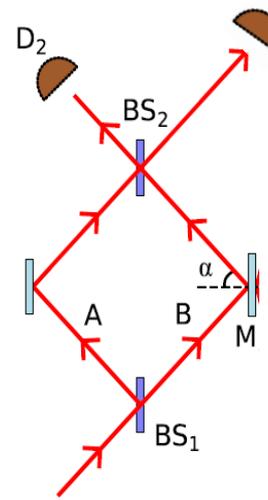
Suppose now that the photon emerges in the beam directed towards D_2 . The state of the mirror is then given (up to normalisation) by projecting the joint state onto the state of the photon corresponding to this beam,

$$\begin{aligned}
 &\langle\Phi_2|\left(|\Psi\rangle\phi(p) - t|B\rangle\frac{d\phi(p)}{dp}\delta\right) \\
 &= \langle\Phi_2|\Psi\rangle\left(\phi(p) - \frac{t\langle\Phi_2|B\rangle}{\langle\Phi_2|\Psi\rangle}\frac{d\phi(p)}{dp}\delta\right) \\
 &= \langle\Phi_2|\Psi\rangle\left(\phi(p) - \frac{\langle\Phi_2|P_B|\Psi\rangle}{\langle\Phi_2|\Psi\rangle}\frac{d\phi(p)}{dp}\delta\right) \\
 &= \langle\Phi_2|\Psi\rangle\phi(p - P_B^w\delta).
 \end{aligned}$$

with P_B^w being in this case the weak value of P_B between $|\Psi\rangle$ and $|\Phi_2\rangle$,

$$\begin{aligned}
 P_B^w &= \frac{\langle\Phi_2|P_B|\Psi\rangle}{\langle\Phi_2|\Psi\rangle} = \frac{(ir\langle A| + t\langle B|)P_B(ir|A\rangle + t|B\rangle)}{(ir\langle A| + t\langle B|)(ir|A\rangle + t|B\rangle)} \\
 &= -\frac{t^2}{r^2 - t^2}.
 \end{aligned}
 \tag{12}$$

Negative for $r > t$!!!



Hence the momentum kick received by the mirror due to a photon emerging towards D_2 is

$$\delta p_M = P_B^w\delta = -\frac{t^2}{r^2 - t^2}2\hbar\omega \cos\alpha.
 \tag{13}$$

Astonishingly, although the photons

collide with the mirror only from the inside of the interferometer, they do not push the mirror outwards; rather they somehow succeed to pull it in! This is realized by a superposition of giving the mirror zero momentum and positive momentum - the superposition results in the mirror gaining negative momentum.

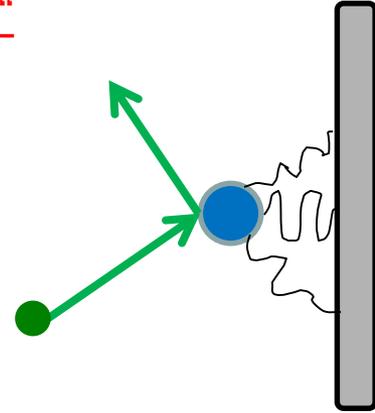
**This is a novel effect
predicted by WM and WV
!**

WM, Short Remarks – „two-body collision“

von Neumann
(strong, impulsive)
measurement
(1932)

$$\hat{H}_{\text{VN}} = -g(t) \hat{q} \otimes \hat{A}.$$

meas. device (n) | system



the device-momentum is shifted by a measured \hat{A} -eigenvalue \mathbf{a}_i :

$$\langle \hat{p} \rangle_f - \langle \hat{p} \rangle_i = +g \mathbf{a}_i \quad \text{where} \quad g = \int g(t) dt$$

Aharonov et al. (1988): „Weak Measurement“:

Device (apparatus) measures:

$$\langle \hat{p} \rangle_f - \langle \hat{p} \rangle_i = +g \text{Re}[A_w] \quad \text{where} \quad \hat{A}_w \equiv \frac{\langle \psi_f | \hat{A} | \psi_i \rangle}{\langle \psi_f | \psi_i \rangle}$$

is the „weak value“ of A defined for the selected initial and final states ψ_i and ψ_f

original publication
Aharonov Y, Albert DZ, Vaidman L. How the result of a measurement of a component of the spin of a spin- $\frac{1}{2}$ particle can turn out to be 100. *Physical Review Letters* 1988; **60**(14): 1351–1354. doi:10.1103/PhysRevLett.60.1351

interaction (von Neumann-type) Hamiltonian

$$\hat{H}_{\text{int}}(t) = +\lambda \delta(t) \hat{q} \otimes (\hat{P} - \hbar K \hat{I}_A)$$

Represents a WV-correction to the conventional momentum-transfer operator

Assuming momentum conservation in the two-body collision, it holds

$$-\hbar K_n = \hbar K_A \equiv \hbar K, \tag{40}$$

where $\hbar K_A$ is the momentum transfer *on the atom* due to the collision. (We choose K_A with positive sign, following

The scattering atom is assumed at rest in its initial state before collision, $\langle \hat{P} \rangle_i = 0$. After the collision, one conventionally expects that

$$\hbar K_A = +\hbar K = \langle \hat{P} \rangle_f = \langle \hat{P} \rangle_f - \langle \hat{P} \rangle_i \tag{41}$$

and correspondingly for the neutron momentum

$$\hbar K_n = -\hbar K = \langle \hat{p} \rangle_f - \langle \hat{p} \rangle_i. \tag{42}$$

weak value of atomic operator

$$(\hat{P} - \hbar K \hat{I}_A)_w = P_w - \hbar K$$

Represents a WV-correction to the conventional momentum transfer

a Special Case:

Initial and final states have the same width in momentum space.

initial atomic wave function $\Xi(P)_i$ can often be approximated by a Gaussian G_A centered at zero momentum,

$$\Xi(P)_i \approx G_A(P).$$

The atomic final state is centered at the transferred momentum:

$$\Xi(P)_f = \Xi(P - \hbar K_A)_i$$

The weak value of the atomic momentum operator is now as follows:

$$\begin{aligned} P_w &= \frac{\langle \Xi_f | \hat{P} | \Xi_i \rangle}{\langle \Xi_f | \Xi_i \rangle} \\ &= \frac{\int dP \Xi(P - \hbar K_A)_i P \Xi(P)_i}{\int dP \Xi(P - \hbar K_A)_i \Xi(P)_i} \\ &= +\frac{\hbar K_A}{2} = +\frac{\hbar K}{2}. \end{aligned} \tag{57}$$

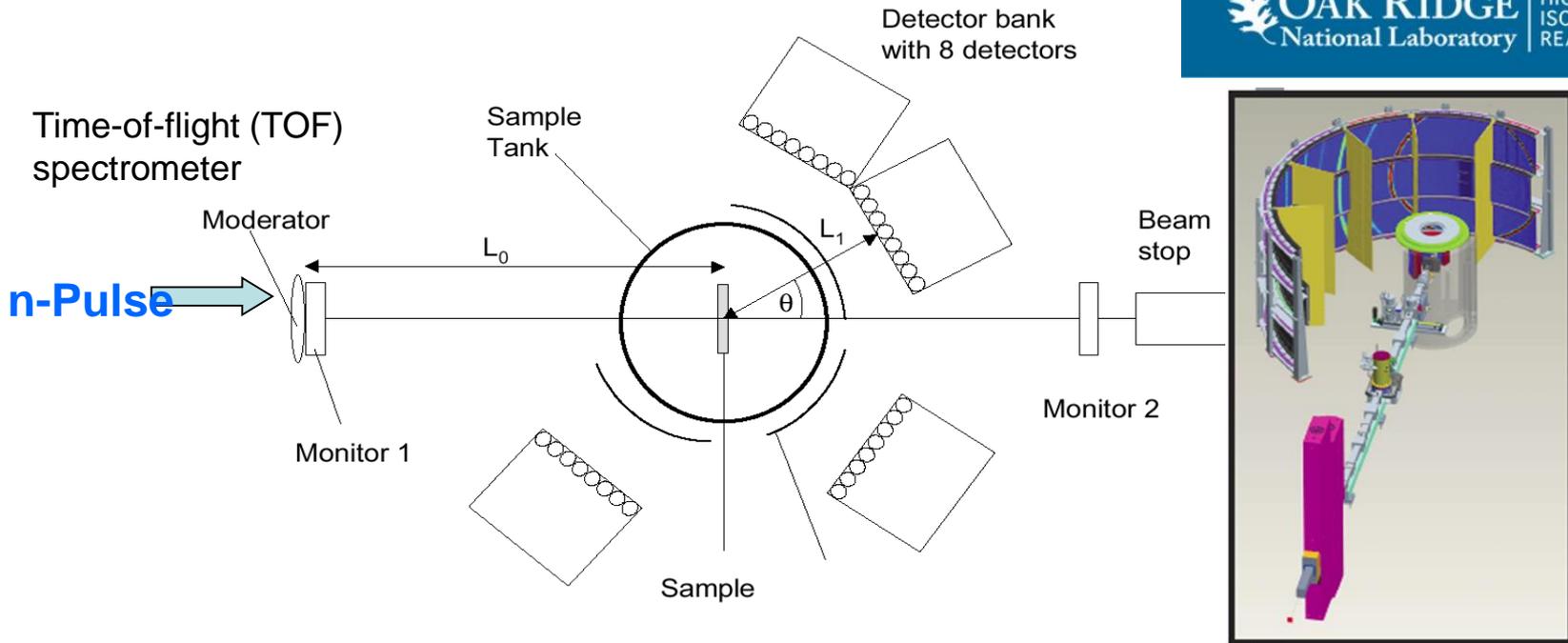
applying the above formulas yields:

$$\langle \hat{p} \rangle_f - \langle \hat{p} \rangle_i = -\lambda (\hat{P} - \hbar K \hat{I}_A)_w = +\lambda \frac{\hbar K}{2}.$$

i.e., the apparatus measures only half of the conventionally expected momentum transfer !

EXPERIMENT: Inelastic incoherence Neutron Scattering (INS)

Schematic:



TOF (time of flight):

$$t = \frac{L_0}{v_0} + \frac{L_1}{v_1} + t_0$$

Time-of-Flight (TOF) spectrometer

Sample-Detectors: **3.0 – 3.4m**

Detectors (pixels) **~110.000**

CALIBRATION parameters: L_0 , L_1 , **scatt. angle θ** , t_0 , v_0

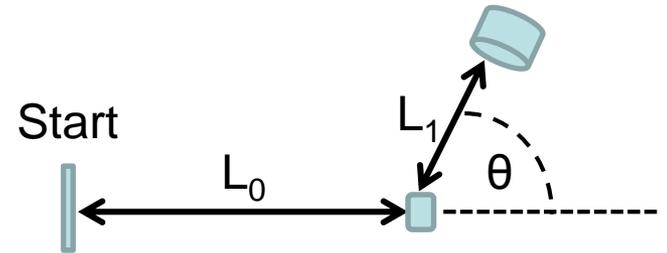
TOF-Measurement:

V_0 is **FIXED** (in case under consideration)

$E_0 = mv_0^2/2 = (\hbar k_0)^2/2m$: Kinetic energy

$mv_0 = \hbar k_0$: Momentum

TOF (time of flight): $t = \frac{L_0}{v_0} + \frac{L_1}{v_1} + t_0$



TOF measured, then one calculates:

→ **energy transfer** $E_0 - E_1 = E = \hbar\omega = \frac{(\hbar k_0)^2}{2m} - \frac{(\hbar k_1)^2}{2m}$

→ **momentum transfer** $\hbar q = \hbar k_0 - \hbar k_1$

$$q = \sqrt{k_0^2 + k_1^2 - 2k_0k_1 \cos \theta}$$

important:

each measured TOF-point → only one E- and only one q-value !

Detector „sees“ (selects) one **trajectory** (line) in the two-dim. **q-E** plane

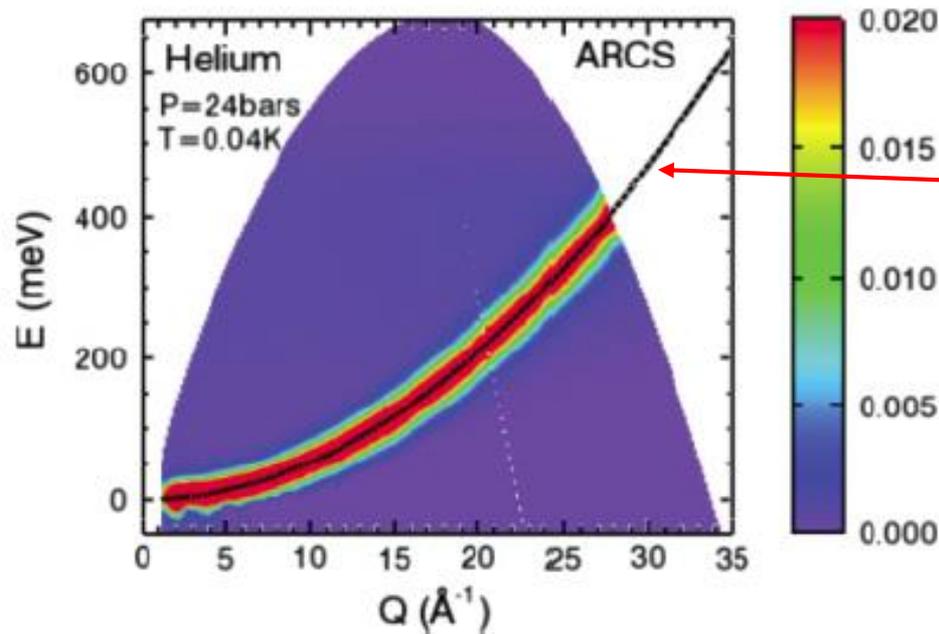
Elastic Scattering, crystallography: **energy transfer = 0** and **|k₀| = |k₁|**

Incoherent Inelastic NEUTRON Scattering (INS)

Example: PHYSICAL REVIEW B 85, 140505(R) (2012)

Bose-Einstein condensation in liquid ^4He near the liquid-solid transition line

DIALLO, AZUAH, ABERNATHY, ROTA, BORONAT, AND GLYDE



$$E_r = \hbar^2 Q^2 / 2m$$

Measured effective mass
 $m = 4.00$ amu,
as conventionally expected

FIG. 1. (Color online) Observed scattering intensity $S(Q, \omega)$ as a function of energy transfer $E = \hbar\omega$ and momentum transfer $\hbar Q$ from liquid ^4He at $p = 24$ bars and $T = 40$ mK. The signal from the empty Al container has been subtracted. The black dashed line is the calculated ^4He recoil line $E_r = \hbar^2 Q^2 / 2m$, shown as a guide to the eye.



ELSEVIER

Available at www.sciencedirect.com

SciVerse ScienceDirect

journal homepage: www.elsevier.com/locate/carbon

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Ab



Quantum excitation spectrum of hydrogen adsorbed in nanoporous carbons observed by inelastic neutron scattering

Raina J. Olsen ^{a,b,*}, Matthew Beckner ^a, Matthew B. Stone ^c, Peter Pfeifer ^a, Carlos Wexler ^a, Haskell Taub ^a

^a Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA

^b Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

^c Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Inelastic neutron scattering spectra have been collected over a wide range of momentum transfer from H₂ adsorbed in several high-porosity carbon substrates.



FIGURE 2. Sample with oriented adsorption planes used for INS experiment.

pores: ~ 5-30 Å

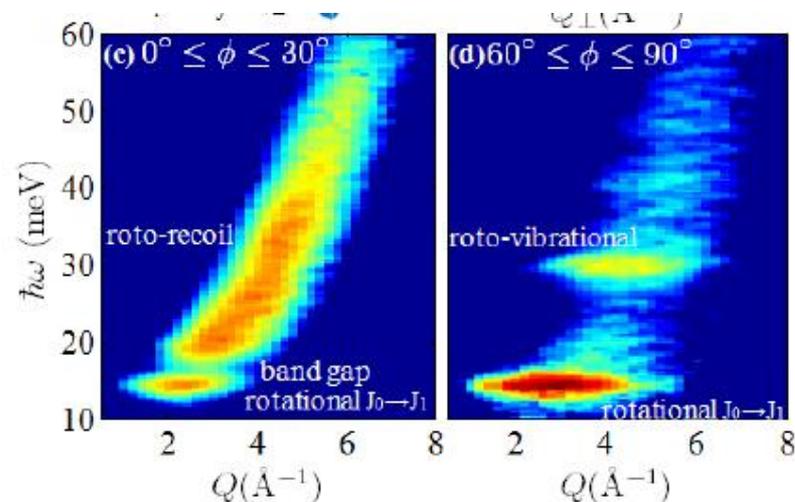


FIGURE 3. (a) Experimental geometry for IINS measurements of an oriented carbon sample, with energy transfer ($\hbar\omega$) and momentum transfer relative to the adsorption plane (Q) defined. (b) Spectrum of the main rotational peak as a function of $Q_{||}$ and Q_{\perp} . (c) Spectrum with the momentum transfer tending to be parallel or (d) perpendicular to the adsorption plane. Intensity is plotted on a log scale, temperature is 15 K, and the sample contains hydrogen at 25% coverage.

Copyright: CARBON

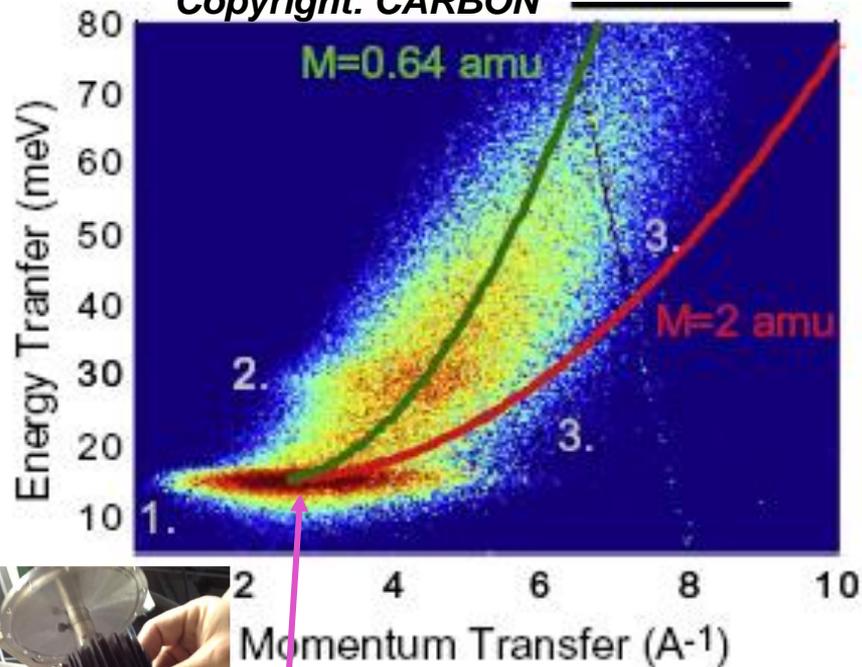


FIGURE 2. Sample with oriented adsorption planes used for INS experiment.

Neutron- H_2 collision
excites molecular **rotation**,
and scattering particle has
mass $M \approx 1$ amu,
as **conventionally** expected

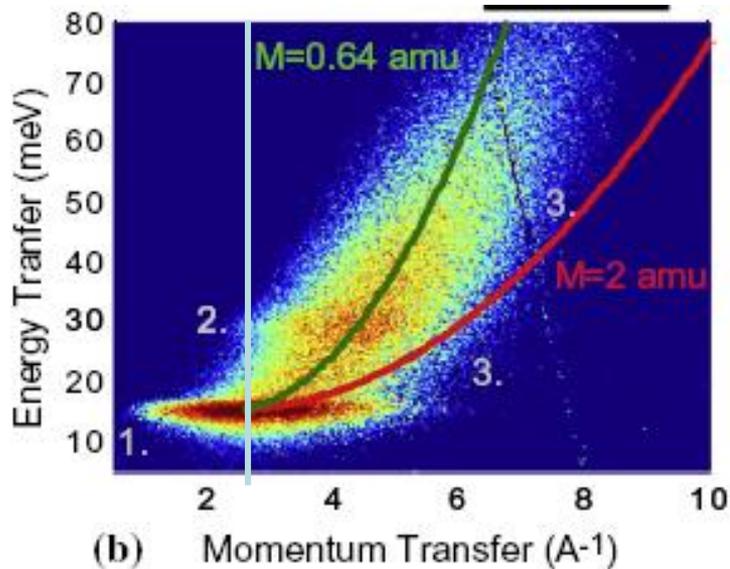
→ Neutron collides with a „particle“ (H_2)
which **recoils (= translation)**
as having mass

$$M_{trans} = 0.64 \text{ amu} !!!$$

**This effect has NO conventional
interpretation**

Remark:

H_2 , n, C-surface are quantum objects



At any fixed E_{trans} -transfer:
 this measurement determines width of final-state
 wavefunction.

*width of $\Xi(P)_f$ is „somewhat smaller“
 than that of $\Xi(P)_i$*

In conv. theory: Final state is a **plane wave**
 i.e. it has $\Delta p_f = 0$!

For more details, see:

Weak Measurement and Two-State-Vector Formalism: Deficit of Momentum Transfer in Scattering Processes

Chariton Aris Chatzidimitriou-Dreismann

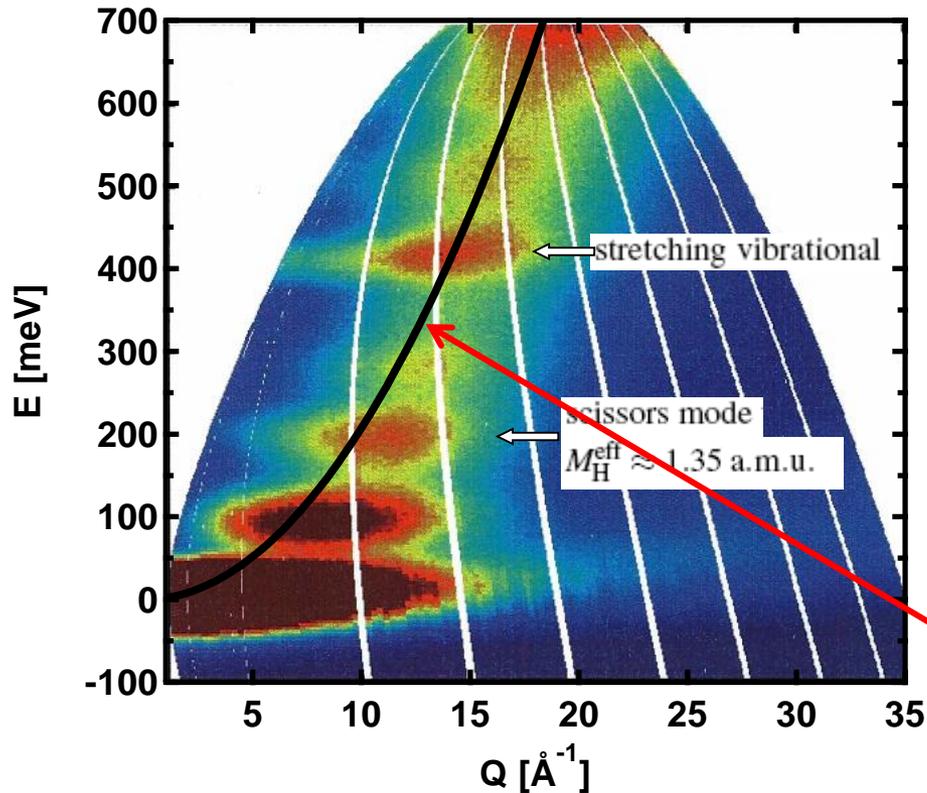
Institute of Chemistry (C2), Faculty II, Technical University of Berlin, D-10623 Berlin, Germany
 E-mail: dreismann@chem.tu-berlin.de

Editors: Eliahu Cohen & Tomer Shushi

Article history: Submitted on July 31, 2015; Accepted on October 20, 2016; Published on October 28, 2016.

WATER molecule, INS off protons

Example: *H₂O-ice in Al-cell, 20K, E₀=750 meV, MARI-spectrometer*



INS from protons (hydrogen atoms; with mass M_H) of a molecule. Due to the similarity of neutron and proton masses, one may put $m_n = M_H$, and then the kinetic equations (8) and (9) yield the simple result $k_0^2 - k_1^2 = Q^2$. Thus one obtains for the neutron energy transfer (6) for n-H scattering:

$$E = E_0 - E_1 = \frac{\hbar^2 Q^2}{2m_n} \tag{12}$$

.....
 Rutherford Appleton Laboratory, UK) [32]. The inserted black (parabola) line is the calculated recoil line of a free hydrogen atom (being at rest before collision)

$$E_r^{\text{free}} = \frac{\hbar^2 Q^2}{2M_H}, \tag{13}$$

(M_H : hydrogen atom mass) shown as a guide to the eye.

Z. Naturforsch. **69a**, 287–296 (2014)

increased effective mass: conventional effect --- no surprise

SEQUOIA | BL-17

Water molecules in nanotubes

A. I. Kolesnikov, L. M. Anovitz, E. Mamontov, A. Podlesnyak, G. Ehlers, *J. Phys. Chem. B* **2014**, *118*, 13414.

Scattering from single H – stretching vibrational mode

$$M_{\text{H}}^{\text{eff}} \approx 0.55 \pm 0.1 \text{ a.m.u.}$$

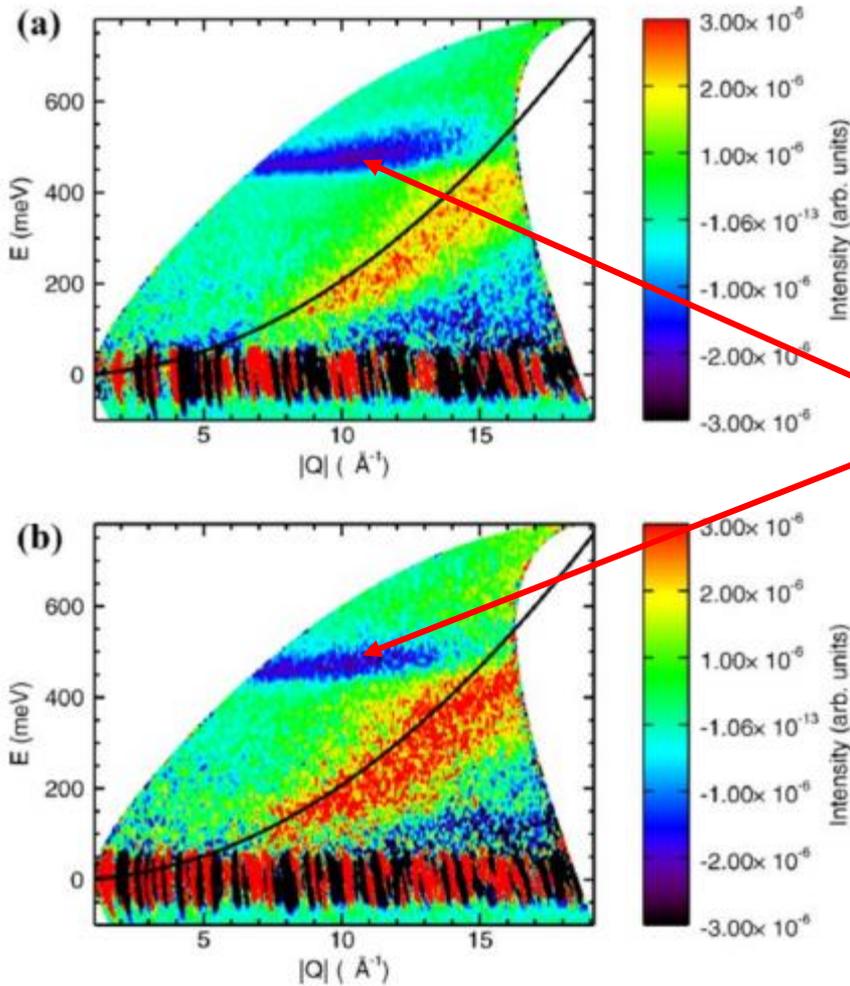
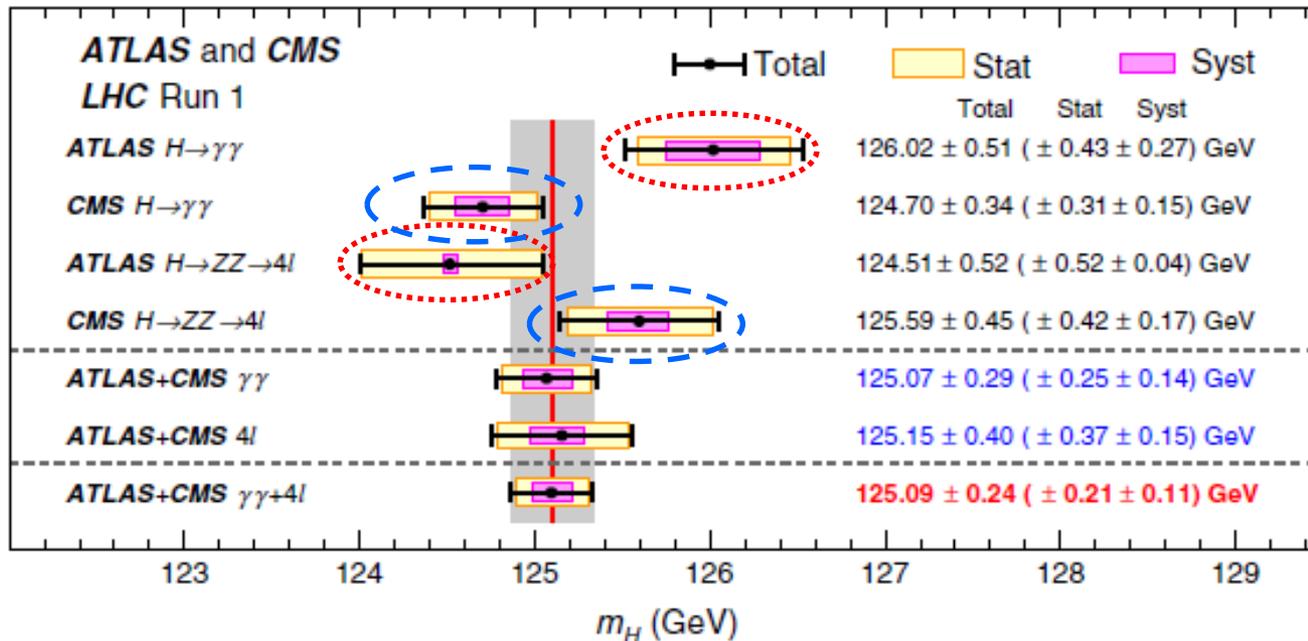


Figure 7. Difference of the measured $S(Q, E)$ intensity maps of oriented single H_2O molecules in sub-nano-channels of (a) beryl and (b) cordierite, at $T = 6 \text{ K}$ with $E_0 = 800 \text{ meV}$, for Q -perpendicular-to- c and Q -parallel-to- c orientations (see the text), recorded on SEQUOIA (SNS, Oak Ridge).^[86] The black line (parabola) shows the calculated recoil trajectory of a free proton. Reprinted with permission from Ref. [86]; copyright 2014 American Chemical Society.

A speculative consideration:



Combined Measurement of the Higgs Boson Mass in pp Collisions at $\sqrt{s} = 7$ and 8 TeV with the ATLAS and CMS Experiments



Do the two detectors ATLAS and CMS „make“ different post-selections?
 What is precisely, directly measured?
 What (and how) is it „deduced“?

Summary of main new results:

1. New effect of INS
2. Neutron **must** be treated as a quantum object (contrary to textbook wisdom)
3. Experimental determination of (minimal) **number of qubits** „affected“ in scatt. experiments (neutron, electron X-rays, ...)
4. Experimental determination of **width** of **final-state** wavefunction of a scattering particle (atom, molecule, nucleus, ...)
5. Indicated applicability to „broader“ scientific & technological fields (e.g., H-mobility in fuel cells, H storage materials, ionic mobility in batteries...)

Concluding remarks:

The theoretical formalisms of

weak values, weak measurement and two-state-vector formalism (Aharonov et al.) not only shed new light on interpretational issues concerning fundamental quantum theory but they also offer a new guide for our intuition to predict, plan, and also to carry out new experiments and reveal novel quantum effects.

Thank you !

