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SCHOOL AND WORKSHOP ON QUANTUM ENTANGLEMENT, DECOHERENCE, INFORMATION, AND GEOMETRICAL PHASES IN COMPLEX SYSTEMS
(1 November - 12 November 2004)

Quantum Coherence of Protrons in Condensed Matter

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These are preliminary lecture notes, intended only for distribution to participants

Trieste Workshop on "Quantum Entanglement...", Nov 2004

Quantum Coherence of Protons in Condensed Matter

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1) Background: Tunneling states of single particles

2) Exploring shorter times

3) Experiments on protons in metals

4) Scattering on two entangled particles

5) Decoherence

6) Summary

Background

A tunneling (particle) proton α is described as a

coherent quantum state

$$\psi_\pm = (1/\sqrt{2})\ \{\phi_1(\alpha) \pm \phi_2(\alpha)\}$$

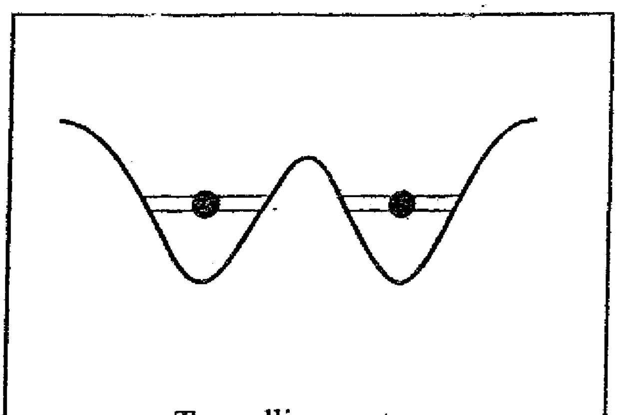
x randomly fluctuating phase factor

for two equal sites,

(1) and (2)

O- - - - - - - -O

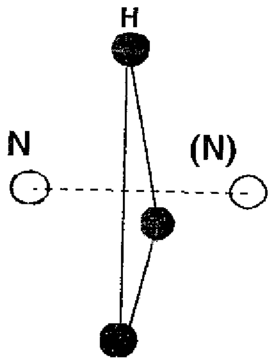
with potential



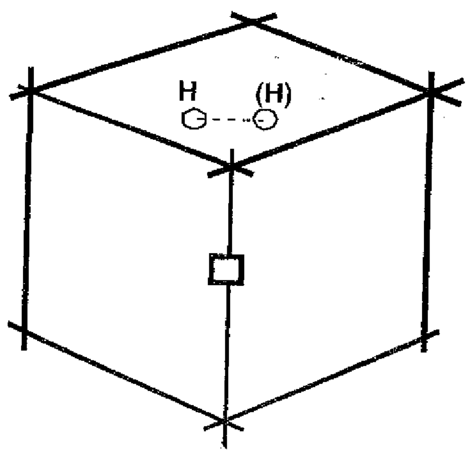
Tunnelling system

EXAMPLES

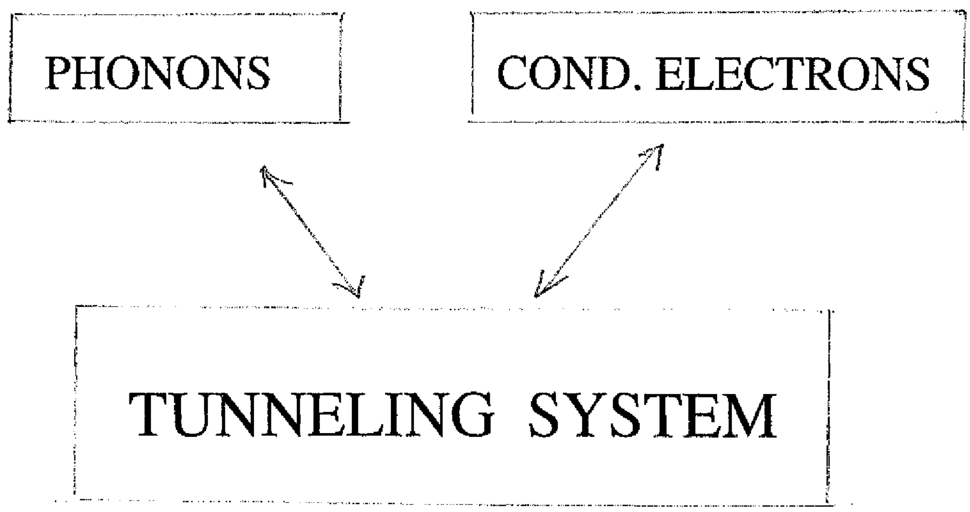
NH_3



Nb-H



<u>Interaction with environment</u> (phonons, conduction electrons,..) leads to **decoherence**, i.e. loss of phase memory between $\phi_1(\alpha)$ and $\phi_2(\alpha)$: the superposition $\psi_\pm$ collapses after a mean-life of τ_{coh} and α is later found in (1) **<u>or</u>** (2).

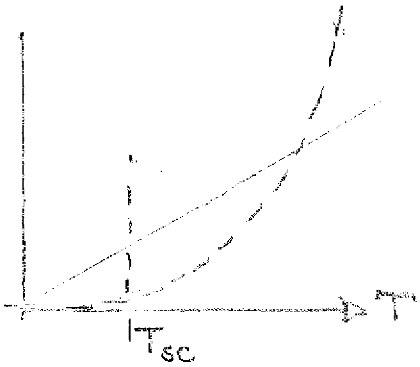


Tunneling studies have shown,

at the μ^+ time-scale (10^{-6} s), that

a) phonon-induced decoherence is small for T < 10 K, but
b) cond.- electrons would be active down to T < 10^{-4} K, but they <u>can be cut-off</u> in superconducting metals (energy-gap effect)

The decoherence rate $\lambda = [\tau_{coh}]^{-1}$: $\approx T^3$ by <u>phonons</u>



$\approx kT$ by <u>conduction electrons</u>
(in normal conductor,

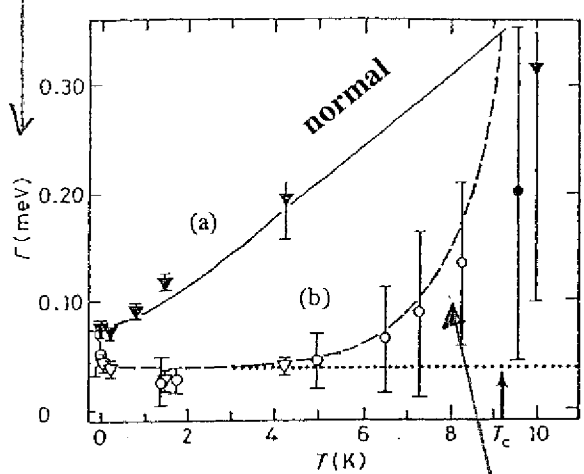
but

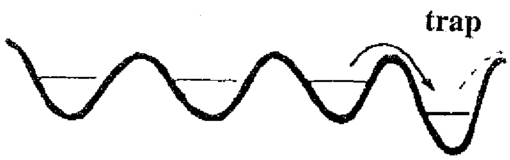
$\approx kT\exp(-\Delta_s/kT)$
in superconductor)

One way to study decoherence is to measure the width Γ ($\approx [\tau_{coh}]^{-1}$) of the energy levels in the tunneling system (by inelastic neutron scattering).

For <u>H-tunneling</u> in an Nb crystal: (Wipf et al., Europhys.Lett. 4, 1379):

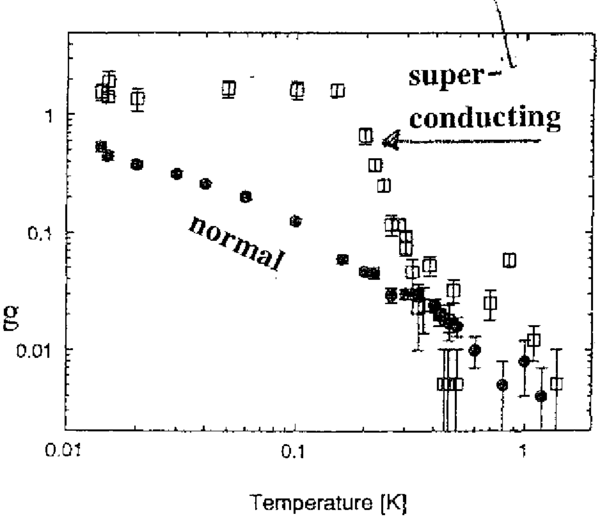
Nb-metal has $T_{SC} \approx 9$ K, but can be made normal-conducting in a magnetic field)





Another way is to study the <u>mobility</u> of positive muons (μ^+) in tunneling states

(Karlsson et al., Phys.Rev. B52, 6417)



μSR measures the <u>trapping rate</u>, as the muon reaches distant imperfections, which immobilize it (strong μ– depolarization)

Below T_{SC}=1.2 K in superconducting Al, tunneling is unperturbed and trapping rate is high.

$\tau_{coh} \approx 10^{-11}$ s -----> 10^{-7} s

normal **superconducting**

Decoherence times for delocalized single protons (or muons) at T ≈ 10 K

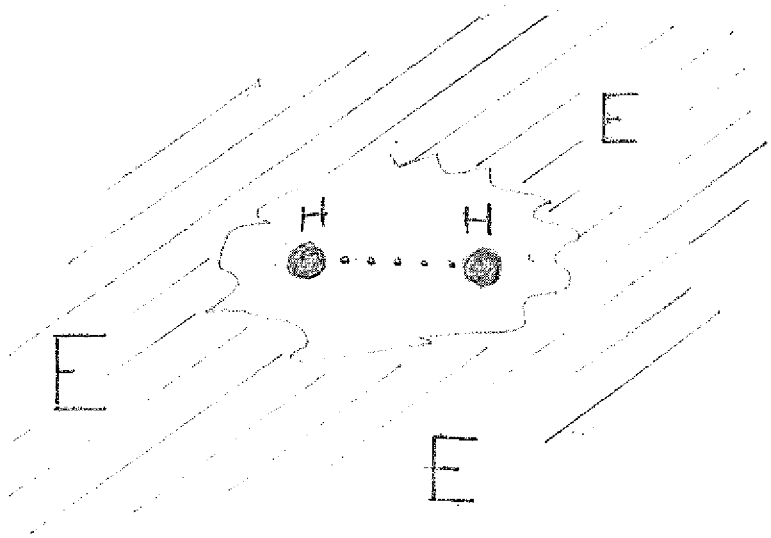
Metallic hydride — Supercond. hydride

τ_{coh}

10^{-15} s — 10^{-10} s — 10^{-5} s

EXPLORING SHORTER TIMES

What about quantum phase relations between two (or more) different protons α , β , etc ?



Some thoughts about time-scales

Electronic motion ↓ Lattice vibr. ↓ (thermalization at RT)

10^{-15} s | 10^{-12} s | 10^{-9} s

typical spin relaxation times ....

local quantum coherence in a solid ....???????

in extreme vacuum..........?

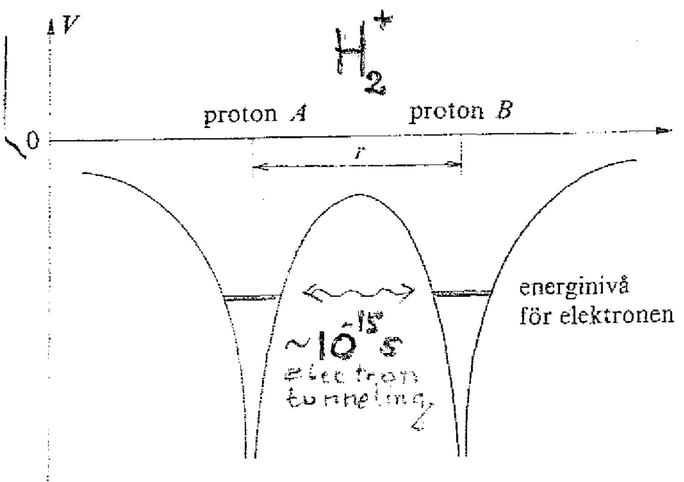
Observation times in
n-Compton scatt. n-thermal scatt.

======= H ====

=======D

======He

Time for recoil nucleus to move 0.5 Å
|-----|



An isolated two-proton state is non-separable (just because of particle identity)

$$\psi(\alpha,\beta) = (1/\sqrt{2})\underbrace{\{\phi_1(\alpha)\phi_2(\beta) + \xi\,\phi_1(\beta)\phi_2(\alpha)\}}_{\text{Orbital with } \xi = (-1)^J}\underbrace{\chi^J{}_M(\alpha,\beta)}_{\text{Spin state } J = 0,\,1}$$

(both protons α and β delocalized over sites (1) and (2)).

Protons can also be momentarily **entangled** (non-separable) by coupling to some environmental phonon or electron field $f(1,2)$

$$\psi(\alpha,\beta) =$$
$$= \{f(1\alpha,2\beta)\phi_1(\alpha)\phi_2(\beta) + f(1\beta,2\alpha)\phi_1(\beta)\phi_2(\alpha)\}\text{ x spin part}$$

Entangled states of protons are expected to be much more "brittle" than single particle coherent states:

Joos–Zeh:

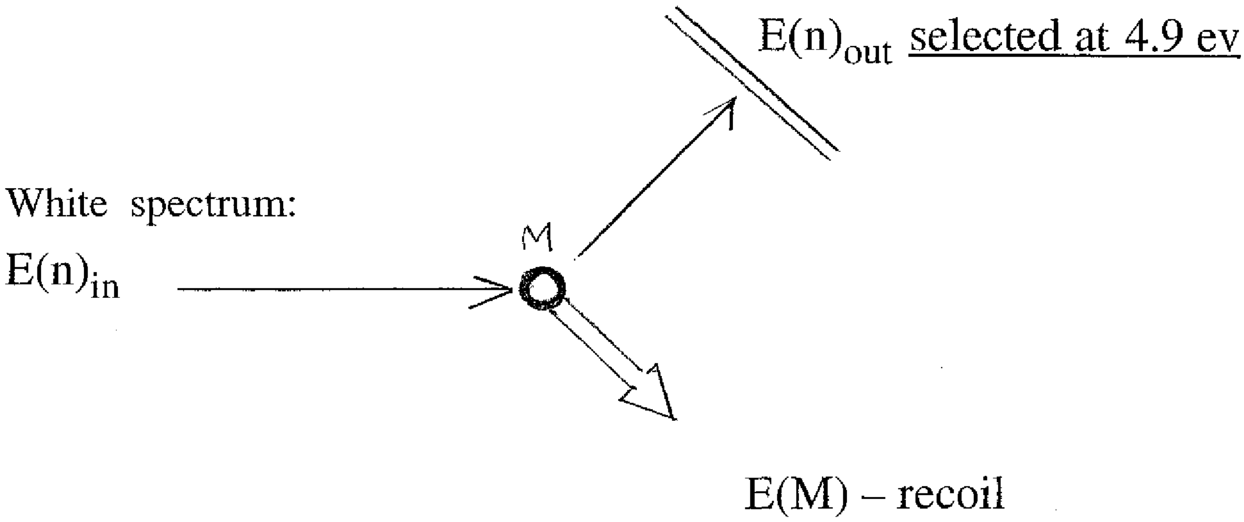
$$\mathbf{1/}\,\tau_{coh} \approx \underset{\approx k_E^2 \nu_E}{\Lambda}\,|\underset{\Delta x}{x - x'}|^2 \;\;\text{---->}\;\; \tau_{coh} < 10^{-15}\text{ s for } \Delta x = 2\text{ Å}$$

in typical condensed matter

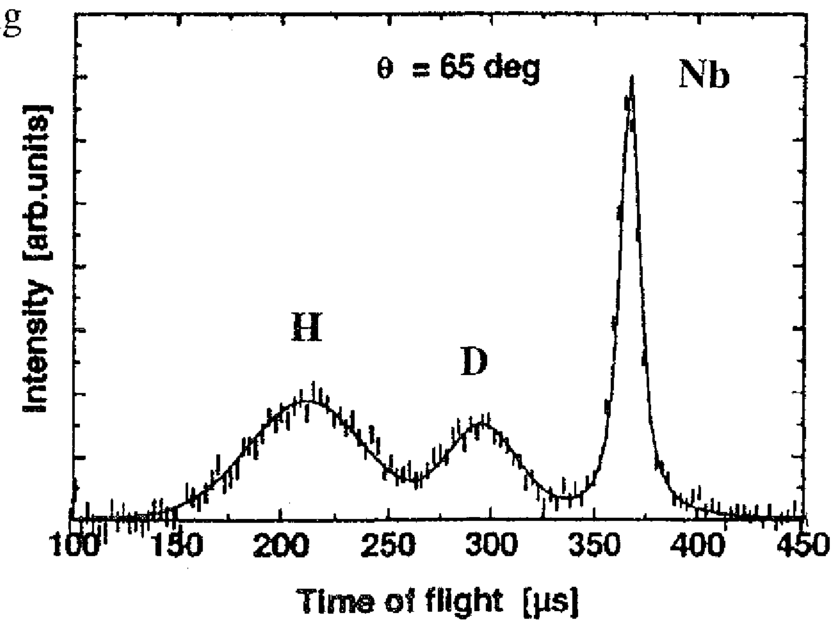
Can we take a sub-femto-second snapshot?
(which is sensitive to particle coherence)

Yes, by
<u>Neutron Compton scattering</u>

E(n) = 10 – 100 eV (i.e. 1000 x thermal)



Neutron flight time distinguishes scattering by different M



Interference in scattering

If all nuclei are quantum separable (and H/M =1):

$(\text{Area})_H / (\text{Area})_{Metal} = \sigma_H / \sigma_{Metal}$ = 81.7 / 6.3 = 13.1 for Nb

If H-H pairs are entangled:

Interferences can make $\sigma_{H\text{-}H} \neq \sigma_H + \sigma_H$! *

[known from thermal* neutron scattering on liquid H_2 at low T, where $\sigma_{H\text{-}H\,(para)} \approx 5$ barn; $\sigma_{H\text{-}H\,(ortho)} \approx 130$ b; $\neq 2 \times 81.7$ b]

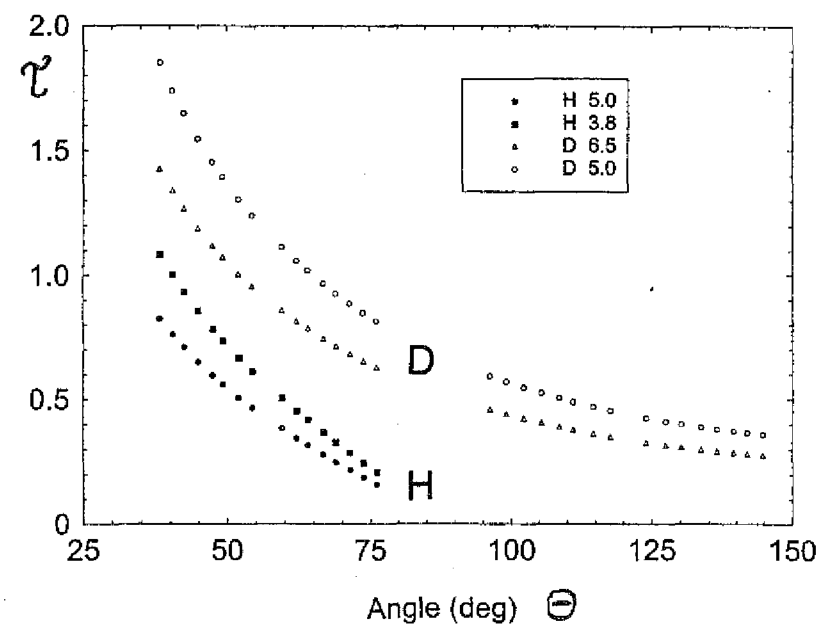
but $[\tau_{sc}]_{thermal} = 10^{-13}\text{-}10^{-12}$ s; usually $[\tau_{sc}]_{thermal} >> \tau_{coh}$!
no correlation effect

In Compton scattering

$[\tau_{sc}]_{NCS} = M / [q(\theta) \sqrt{<p^2>}]$

Scatt. angle θ (and M) determine τ_{sc}

10^{-15} s →



θ- to τ-dependence gives a glimpse of the sub-femto-second world!

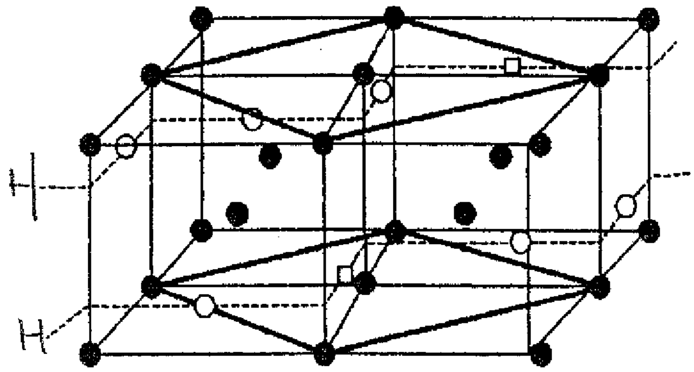
Chatzidimitriou-Dreismann et al. first found reduction of H-cross section (relative to D) in water (P.R.L 78, 2839 (97))

Here:

SOME RESULTS FOR HYDRIDES

Europhys. Lett. 46, 617 (99);
Phys. Rev. B67, 184108 (03)

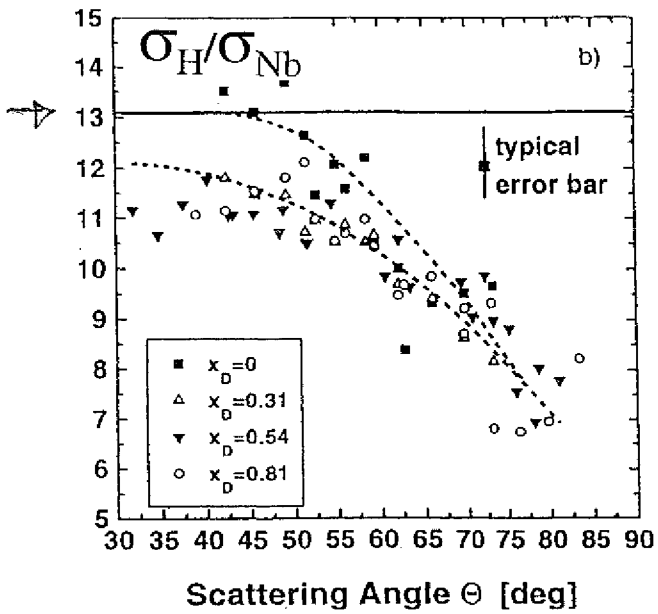
Structure of Nb-H

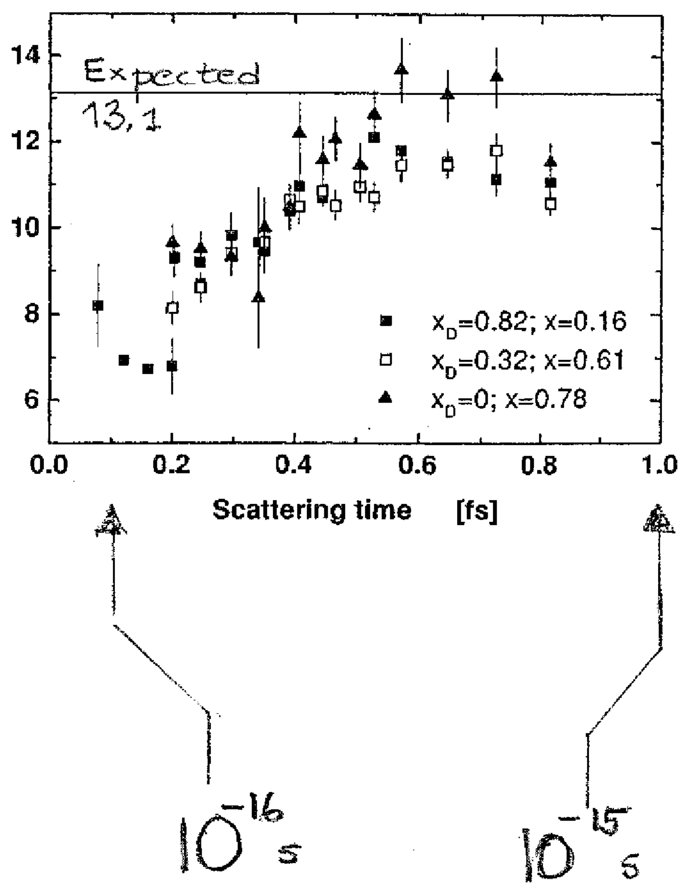


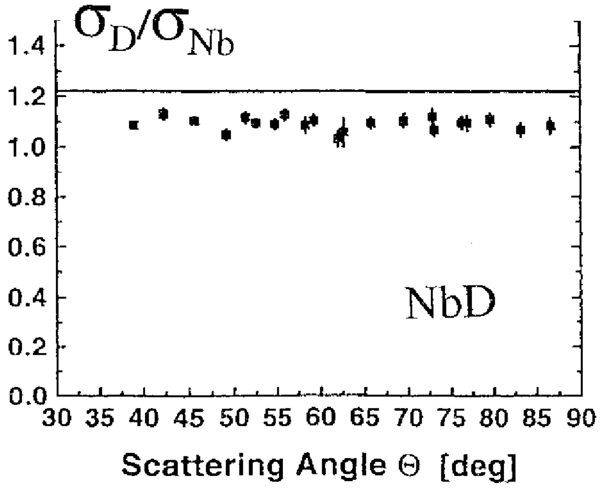
Nb-hydrides

NbH_xD_y

Time-dependence:

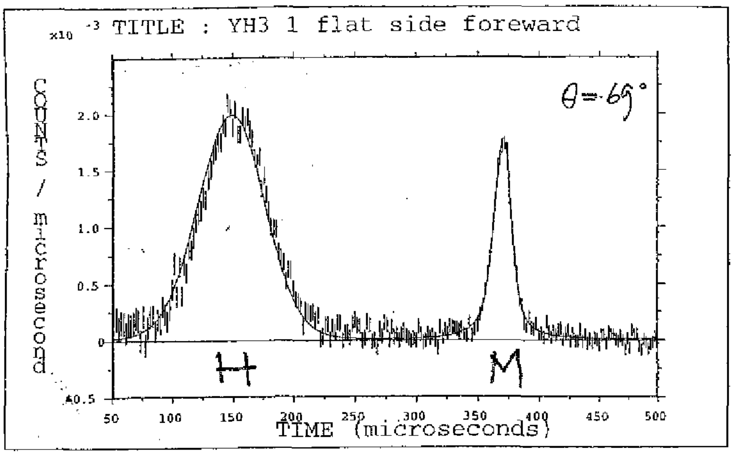




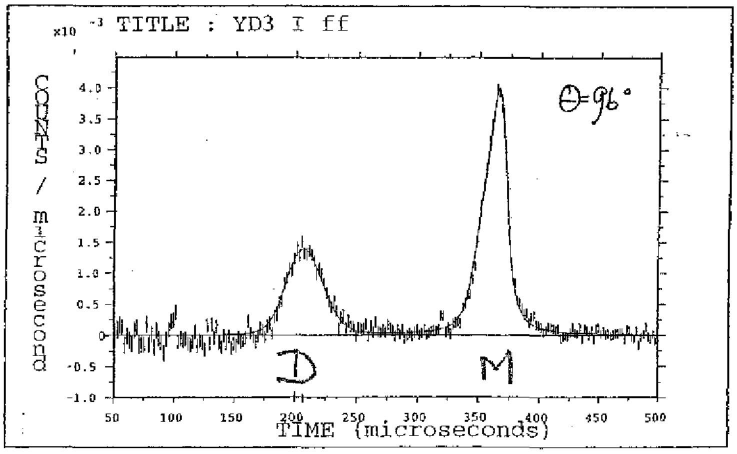


Y-hydrides

Some typical spectra



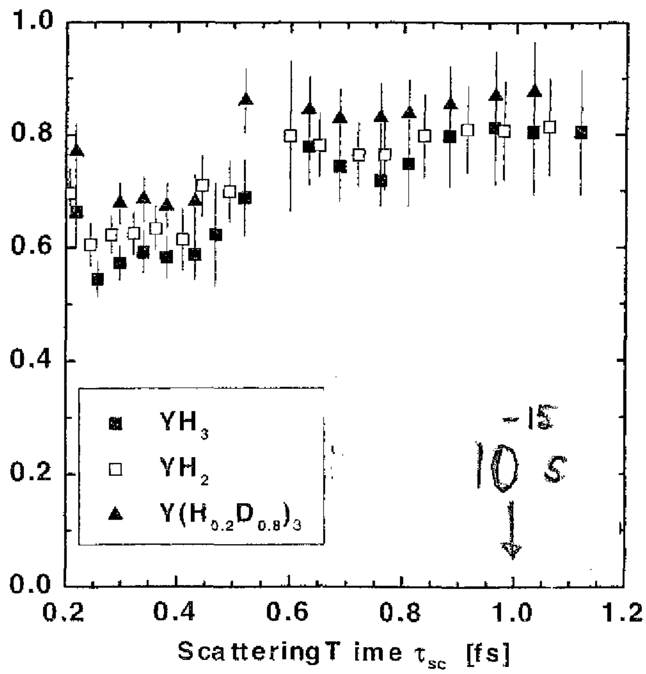
INSTRUMENT: EVS
RUN NUMBER: 8525
SPECTRUM : # 16 θ·
LOCATION: EVS_DATA:EVS08529.RAW
USER: Karlsson/Dreismann
RUN START TIME: 15-SEP-2000 09:45:
PLOT DATE: Sat 16-SEP-2000 11:45:
BINNING IN GROUPS OF 2



H/Y cross section ratios (nominal value 81.7/ 7.7 =10.6)

Time-dependence:

$$(\sigma_H/\sigma_Y)_{exp}/\underbrace{(\sigma_H/\sigma_Y)_{tab}}_{=10.6}$$



Scattering on non-separable quantum systems
(consider only 2-particles + local environment)

particle indices: α, β

site indices: **1, 2**

Environment (entangling field): Ψ

System wave-function: $\Psi(1,\alpha; 2,\beta)\phi_1(\alpha)\phi_2(\beta) + \Psi(1,\beta; 2,\alpha)\phi_1(\beta)\phi_2(\alpha)$
(not normalized)
The simplest example:
Two identical particles coupled to a common spin J

$(1/\sqrt{2})[\phi_1(\alpha)\phi_2(\beta) + \zeta\, \phi_1(\beta)\phi_2(\alpha)]\chi(\alpha,\beta)^J{}_M \qquad \zeta = (-1)^J$

Before going to Compton scattering,
take a look at

Thermal neutron scattering on H_2

Scattering matrix element $< f \mid V_\alpha + V_\beta \mid i >$

For small q: $\phi_{1,\,\mathrm{final}} \approx \phi_{1,\,\mathrm{initial}}$, etc, but J --> J' (except for q =0)

$| \mathbf{f} > = (1/\sqrt{2})\{\phi_1(\mathbf{R}_\alpha)\phi_2(\mathbf{R}_\beta) + \zeta'\, \phi_1(\mathbf{R}_\beta)\phi_2(\mathbf{R}_\alpha)\}\chi^{J'}{}_{M'}(\alpha,\beta)$

$\zeta' = (-1)^J$

In orbital part of

$< \mathbf{f} \mid V_\alpha + V_\beta \mid \mathbf{i} > = < \mathbf{f} \mid b_\alpha \exp(-i\mathbf{q}.\mathbf{R}_\alpha) + b_\beta \exp(-i\mathbf{q}.\mathbf{R}_\beta) \mid \mathbf{i} >$

eigth terms of type; $\qquad \gamma = \alpha$ or β ; i, k = 1 or 2

$\int d\mathbf{R}_\alpha\, \phi_i^*(\mathbf{R}_\alpha)\exp(-i\mathbf{q}.\mathbf{R}_\gamma)\phi_k(\mathbf{R}_\alpha) \int d\mathbf{R}_\beta\, \phi_i^*(\mathbf{R}_\beta)\, \phi_k(\mathbf{R}_\beta)$

Four of them non-zero

Two direct terms
$<\phi_1(\mathbf{R}_\alpha) \mid V_\alpha \mid \phi_1(\mathbf{R}_\alpha)>$ and $<\phi_2(\mathbf{R}_\beta) \mid V_\beta \mid \phi_2(\mathbf{R}_\beta)>$,

and two exchange terms
$\zeta\,\zeta' <\phi_1(\mathbf{R}_\alpha) \mid V_\alpha \mid \phi_1(\mathbf{R}_\alpha)>$ and $\zeta\,\zeta' <\phi_2(\mathbf{R}_\beta) \mid V_\beta \mid \phi_2(\mathbf{R}_\beta)>$

Combining and introducing the usual choice of coordinates, $\mathbf{R}_1 + \mathbf{R}_2 = 0$; $\mathbf{R}_1 - \mathbf{R}_2 = \mathbf{r}$ and $\mathbf{R}_1 = +(1/2)\mathbf{r}$; $\mathbf{R}_2 = -(1/2)\mathbf{r}$, this leads to the text-book [ ] expressions for the scattering on H_2-molecules,

		multiplying spin part:
$< \mid 2\cos[\mathbf{q}.\mathbf{r})/2 \mid >$	for $\zeta\zeta' = +1$ ($J' = J$)	A
$< \mid 2\sin[\mathbf{q}.\mathbf{r})/2 \mid >$ *	for $\zeta\zeta' = -1$ ($J' \neq J$)	B

$<\mid \ \mid>$* -----> 0 when q ----> 0, a result of interference

-----> for J = 0 (para): $\sigma = 4\pi A^2$;

for J = 1 (ortho): $\sigma = 4\pi\,[(A^2 + (1/8)B^2]$

Two observations:

1) **Both** $\mid \mathbf{i}>$ **and** $\mid \mathbf{f}>$ must be quantum superpositions (entangled) $\zeta \neq 0$, $\zeta' \neq 0$, and
2) Each neutron must "see" both sites (1) and (2)

for this specific interference to be seen.

Compton scattering

[note first that standard expression for single nucleon scattering can be obtained by putting $| f > = \exp(-i\mathbf{q} + \mathbf{p}).\mathbf{R})$]

Modify for scattering on two entangled particles

$$| \mathbf{f} >_{\text{thermal}} = (1/\sqrt{2})\{\phi_1(\mathbf{R}_\alpha)\phi_2(\mathbf{R}_\beta) + \zeta' \phi_1(\mathbf{R}_\beta)\phi_2(\mathbf{R}_\alpha)\}\chi^{J'}{}_{M'}(\alpha,\beta)$$

[in earlier notation $T_1 = (1/\sqrt{2})$; $T_2 = \zeta'(1/\sqrt{2})$]

$$| \mathbf{f} >_{\text{Compton}} =$$
$$= (1/\sqrt{2})\{\phi_1(\mathbf{R}_\alpha)\exp[-i(\mathbf{q} + \mathbf{p}).\mathbf{R}_{\beta 2}) + \zeta'\phi_2(\mathbf{R}_\alpha)\exp[-i(\mathbf{q} + \mathbf{p}).\mathbf{R}_{\beta 1}) +$$
$$+ \text{...the same for } \beta \dashrightarrow \alpha, \alpha \dashrightarrow \beta\text{...}$$

Each matrix element $< \mathbf{f} \,|\, \mathbf{V} \,|\, \mathbf{i} >_{\text{Compton}}$ will contain integrals of type

1) $\int d\mathbf{R}_\alpha \exp(i\, \mathbf{q}.\mathbf{R}_{\alpha i})\phi_k(\mathbf{R}_\alpha)$ to be neglected, and

2) $\int d\mathbf{R}_\alpha \exp[i\, \mathbf{q} - \mathbf{p}).\mathbf{R}_{\alpha i}]\phi_k(\mathbf{R}_\alpha) \int d\mathbf{R}_\beta \phi_i^*(\mathbf{R}_\beta)\phi_k(\mathbf{R}_\beta) \to \delta_{ik}$

$$\to \int d\mathbf{R}_\alpha \exp[i\, (\mathbf{p}' - \mathbf{q}).\mathbf{R}_\alpha]\phi_k(\mathbf{R}_\alpha) = \int d\mathbf{R}_\alpha \exp[i\, \mathbf{p}\, .\mathbf{R}_\alpha]\phi_k(\mathbf{R}_\alpha)$$

is the Compton integral $\mathbf{K}(\mathbf{p})$

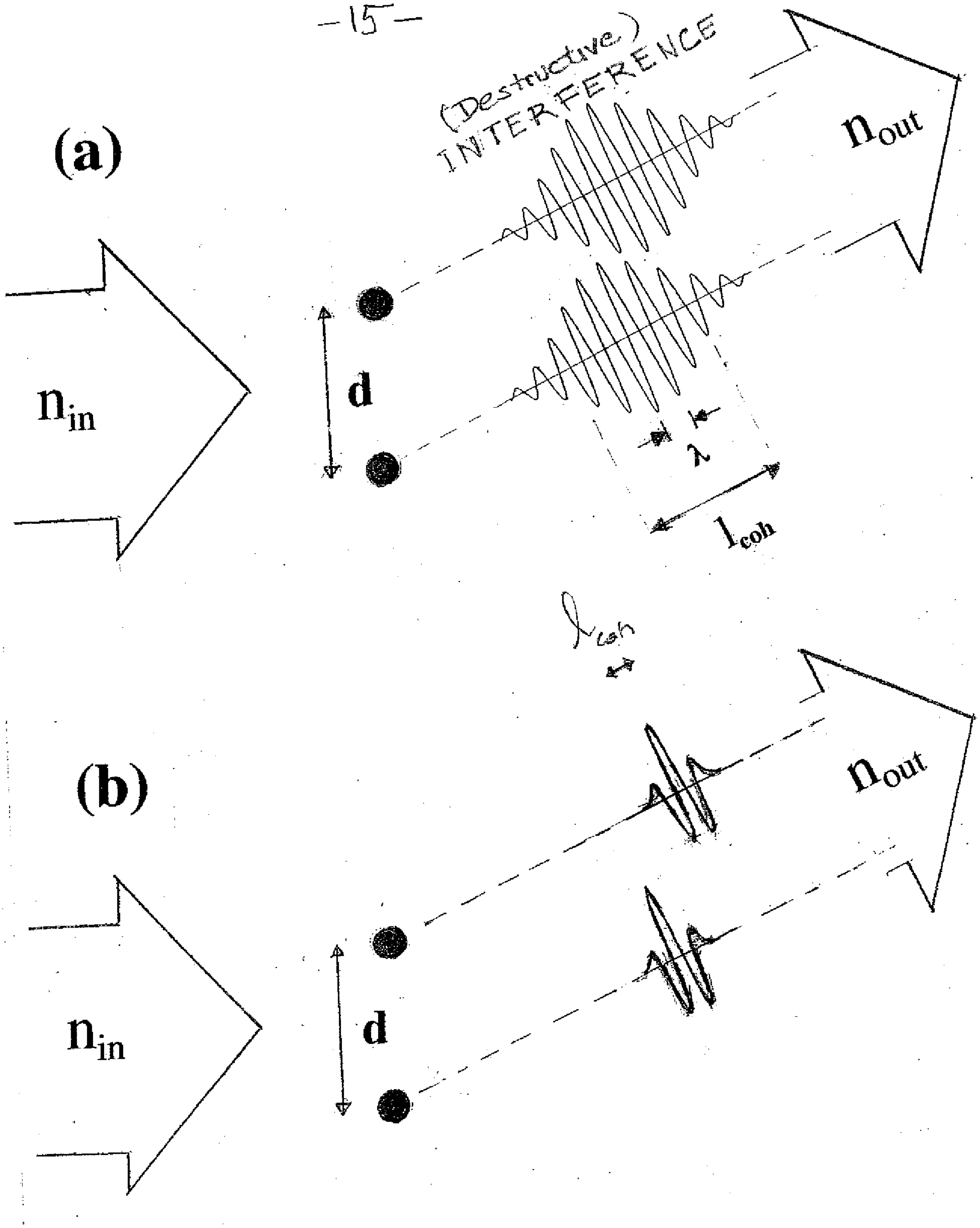
and with $\mathbf{R}_1 - \mathbf{R}_2 = \mathbf{d}$,

$$\int d\mathbf{R}_\alpha \exp[i\, \mathbf{p}\, .\mathbf{R}_{\alpha 2}]\phi_k(\mathbf{R}_\alpha) = \exp(i\mathbf{p}.\mathbf{d}) \int d\mathbf{R}_\alpha \exp[i\, \mathbf{p}\, .\mathbf{R}_{\alpha 1}]\phi_k(\mathbf{R}_\alpha) \Rightarrow$$

$$< \mathbf{f} \,|\, \mathbf{V} \,|\, \mathbf{i} >_{\text{Compton}} = (1/2)\{1 + \zeta\, \zeta' \exp(i\mathbf{p}.\mathbf{d})\}\mathbf{K}(\mathbf{p})$$

Interference reduces $< \mathbf{f} \,|\, \mathbf{V} \,|\, \mathbf{i} >$

1) when $\mathbf{J} \neq \mathbf{J}'$ (coherent and incoherent to be treated separately)
2) when $\mathbf{p}$ is not perpendicular to $\mathbf{d}$



(a) $\Delta\lambda_n \ll \lambda_n$ { selection of <u>scattered</u> neutron

(b) $\Delta\lambda_n \approx \lambda_n$ in transmission experiments

Possible generalizations:

Introduce $\zeta = \exp(-i\phi_\zeta)$; $\zeta' = \exp(-i\phi_{\zeta'})$ Then, for exchange-coupled pairs,
$\phi_\zeta , \phi_{\zeta'} = 0$ for J' even ;
$\phi_\zeta , \phi_{\zeta'} = \pi$ for J' odd,

NOTE: This treatment can be generalized to any type of orbital entanglement of two particles α and β

ζ -----> $\exp(-i\phi_{initial})$ in $|i> \approx \phi_1(\alpha)\phi_2(\beta) + \exp(-i\phi_{initial})\phi_1(\beta)\phi_2(\alpha)$
ζ' ----> $\exp(-i\phi_{final})$ ... $|f>$ ....

Decoherence

Decoherence is the loss of phase memory over time

$$\phi_{in} \;\text{------>}\; \phi(t)$$

An extended observation means
an integration over the phase factor:

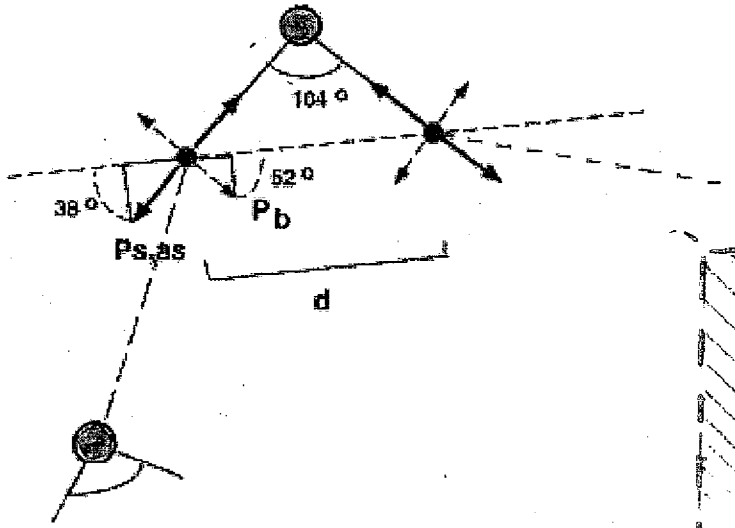
$$\int_0^{\tau_{sc}} \exp[-i\phi(t)]dt \qquad \tau_{sc} \text{ - scattering time}$$

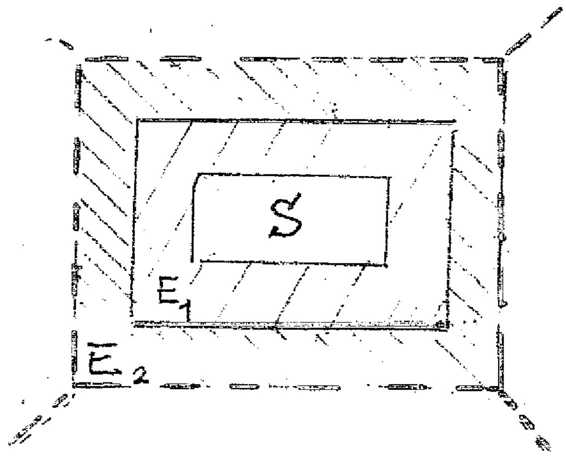
If the system is coupled to an environment E, it is

a) modulated, if E(t) has a sharp frequency
b) damped, if E(t) is randomly fluctuating: $\int dt\, P_E(t)\exp[-i\phi(t)] \text{ ---> } 0$
interferences disappear

Estimates of decoherence time

Example:
H_2O in liquid water





System **S**: H-H

System $\mathbf{E_1}$(t): OH-vibrations: ω_s, ω_b :

-------> modulation $\exp[-i(\phi_{in} + \omega_s t)]$, ...

System $\mathbf{E_2}$(t): Neighbouring H_2O-molecules (H-bonded):

-------> $\omega_{\sigma s} = \omega_s + \omega_{\sigma s}(t)$, ...

System $\mathbf{E_3}$(t):

.......................:

randomly fluctuating
(assume Gaussian spread $P_E(t) = \exp[-(\omega_{\sigma s} - \omega_s)^2/4\sigma^2]$

$$\int \exp[-(\omega_{\sigma s} - \omega_s)^2/4\sigma^2] \exp(i\omega_s t)\, d\omega_{\sigma s} = \exp[-\sigma^2 t^2] \exp(i\omega_s t)$$

σ is known from IR and Raman -------> $\tau_{coh} \approx 2.\ 10^{-14}$ s (at RT))

$$\tau_{sc,\ Compton} < \tau_{coh} < \tau_{sc,\ thermal}$$

The phase factor (with more details)

The entangled two-particle state, generalized:

$$| i> = (1/N)\{A(1,\alpha;2,\beta)\phi_1(\mathbf{R}_\alpha)\phi_2(\mathbf{R}_\beta) + A(1,\beta;2,\alpha)\phi_1(\mathbf{R}_\beta)\phi_2(\mathbf{R}_\alpha)\}$$

If $A((1,\beta;2,\alpha)$ and $A((1,\alpha;2,\beta)$ are equal except for complex amplitudes whose ratio is $\exp(i\Phi)$

$$| i> = (1/2)\{\phi_1(\mathbf{R}_\alpha)\phi_2(\mathbf{R}_\beta) + \exp(i\Phi)\phi_1(\mathbf{R}_\beta)\phi_2(\mathbf{R}_\alpha)\}$$

$\exp(i\Phi) = \zeta = \pm 1$ for exchange-correlated particles ($\Phi = \pm\pi$)

$\exp(i\Phi) = A((1,\beta;2,\alpha)/A((1,\alpha;2,\beta)$ for another (simple) entangling field

If the phase angle is perturbed by interaction with an environment E:

$$\Phi_0 \text{ ------> } \quad \Phi(t) = \Phi_0 + \omega_E t$$

$\exp(i\Phi_0)$ ---------> $\exp(i\Phi_0)\exp(i\omega_E t)$: MODULATION

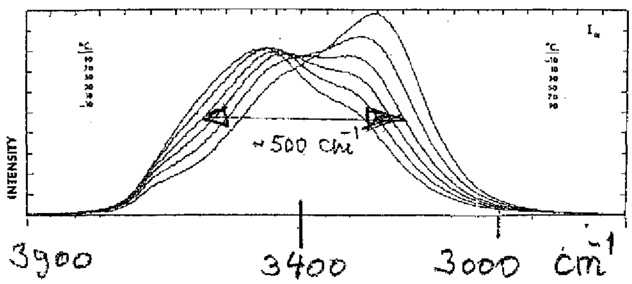
If the environment is fluctuating,

$\exp(i\Phi_0)\exp(i\omega_E t)$ ----->: $\exp(i\Phi_0)\int d\omega_E P(\omega_E)\exp(i\omega_E t)$

Raman:

If $P(\omega_E) = \exp[(\boldsymbol{\omega_E} - \boldsymbol{\omega_{E0}})^2/4\sigma_\omega]$

H_2O stretch



$\exp(i\Phi_0)$ ------> $\exp(i\Phi_0)\int d\omega_E P(\omega_E)\exp(i\omega_E t)$

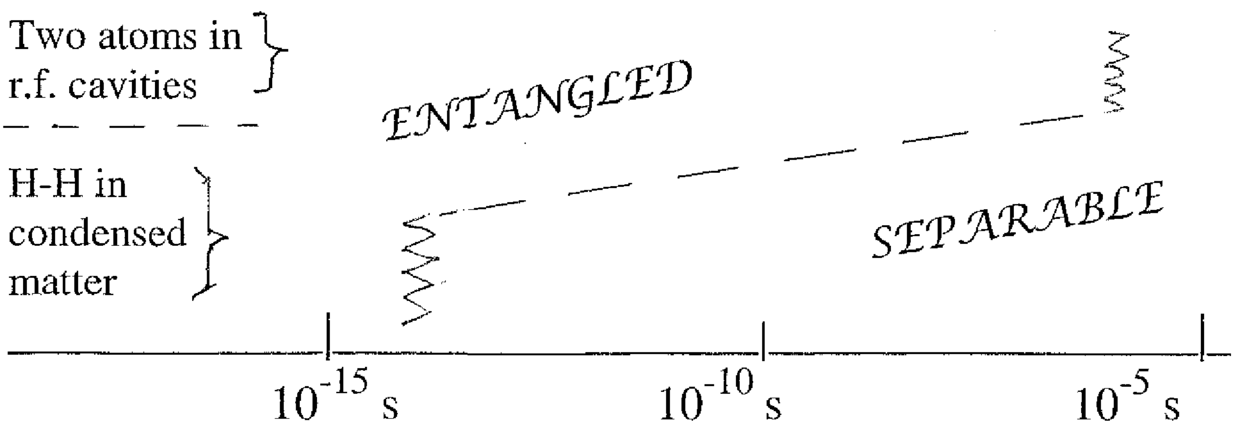
$$= \exp[-\sigma_\omega t^2]\exp(i\Phi_0)\exp(i\omega_E t)$$

----------------------> DAMPING $\tilde{\tau}_c \approx 2 \times 10^{-14}$ s

(phase memory loss)

SUMMARY

1. Existence of coherent proton states in metal hydrides
2. Existence of proton-proton coherence?
3. Exploring very short times: Methods and analysis
4. Evidence for quantum coherent proton states
5. Interferences in Compton scattering of neutrons
6. Conditions for coherence: Decoherence mechanisms
7. A comparison of two extremes:



A NEW WORLD TO EXPLORE BELOW $\approx 10^{-14}$ s !