Nonlinear Dynamics And Quantum Entanglement In Hydrogen Bonded Crystals

Neutron scattering $\left\{ \begin{array}{l} \text{Protons} \\ \text{Spins} \\ \text{Ground state} \end{array} \right.$

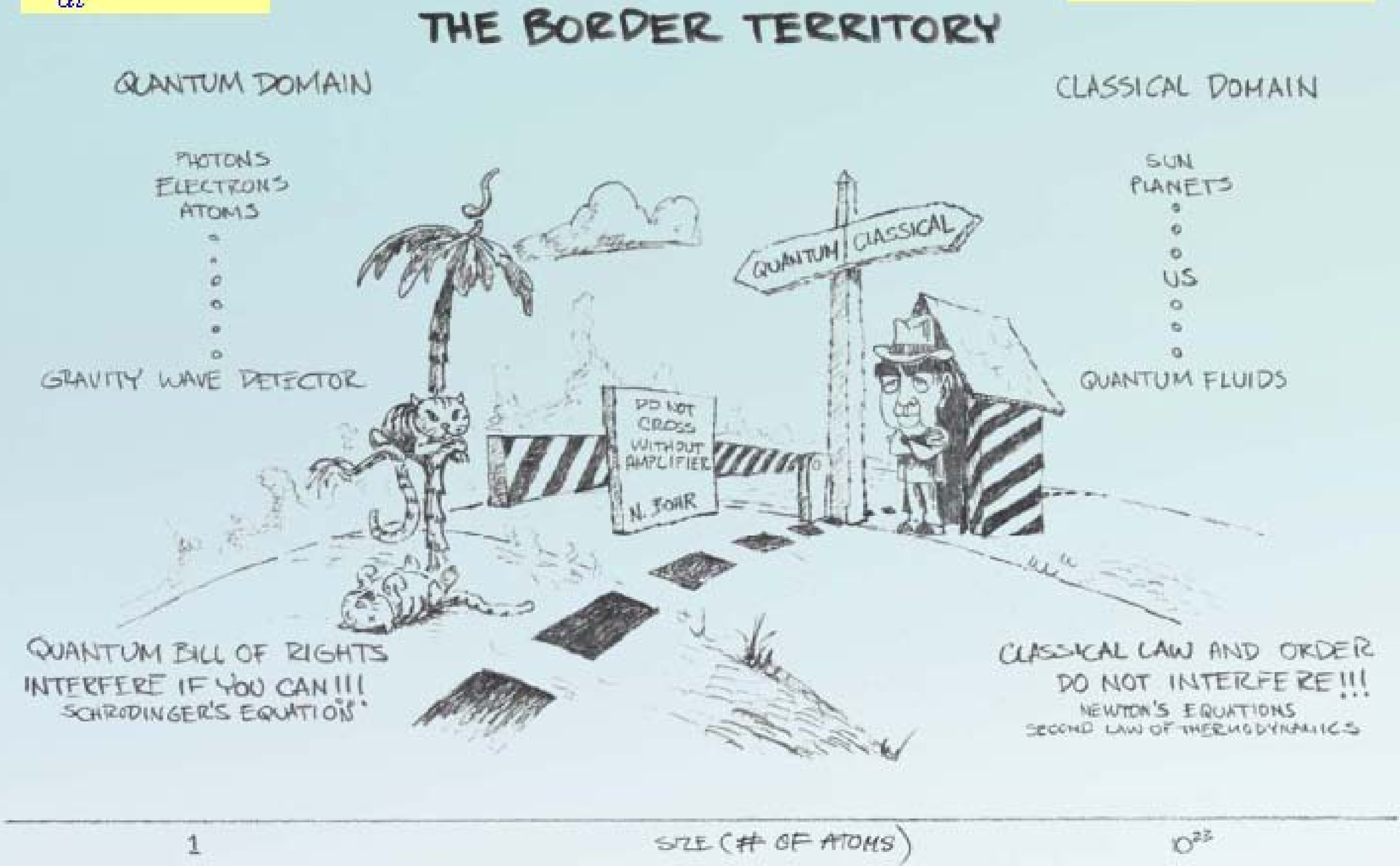
Proton oscillator mass
Normal coordinates
Proton transfer
Proton tunnelling

Quantum entanglement
EPR non-locality
Decoherence-forbidden states
Schrödinger's Cat
Quantum Measurement

F. Fillaux, Physica D **113** (1998) 172
S. Ikeda and F. Fillaux, Phys. Rev. B **59** (1999) 4134
F. Fillaux, A. Cousson and D. A. Keen, Phys. Rev. B **67**, 054301 (2003)

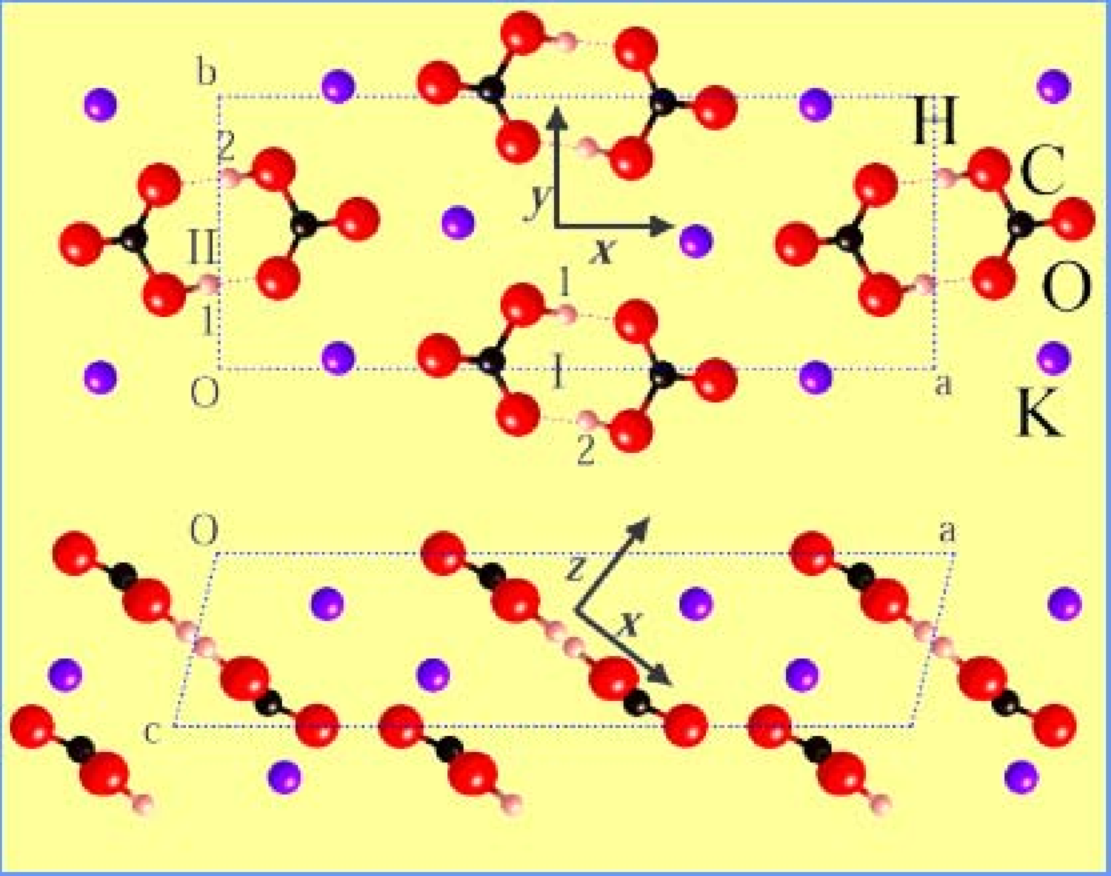
$$i\hbar \frac{d}{dt}|\Psi\rangle = H|\Psi\rangle$$

Decoherence



W. H. Zurek, Los Alamos Science, 27 (2002) 2.

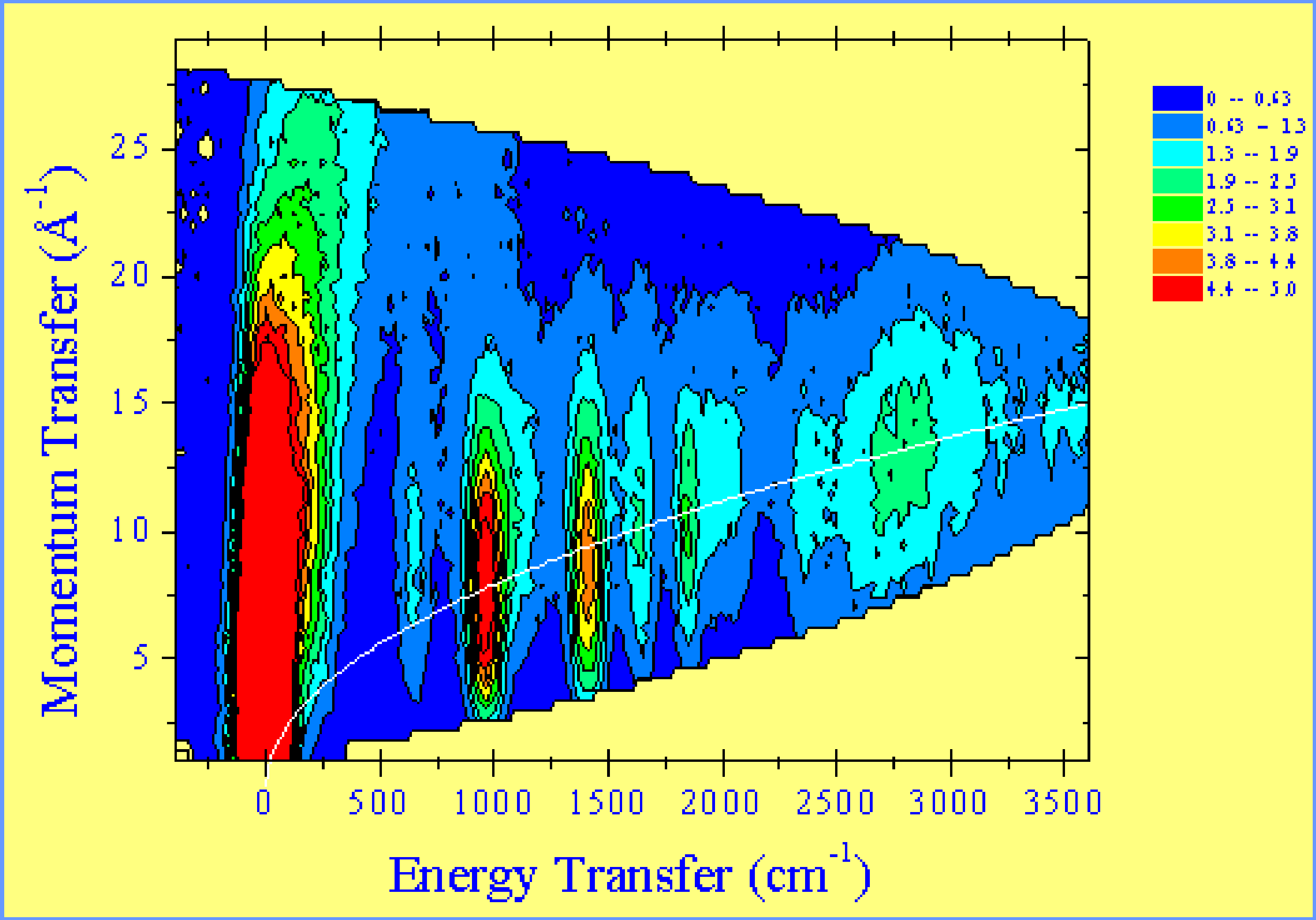
Centrosymmetric dimers in the $KHCO_3$ crystal



T =14 K

a =15.06 Å, b =5.57 Å, c =3.65 Å, β =103.97°

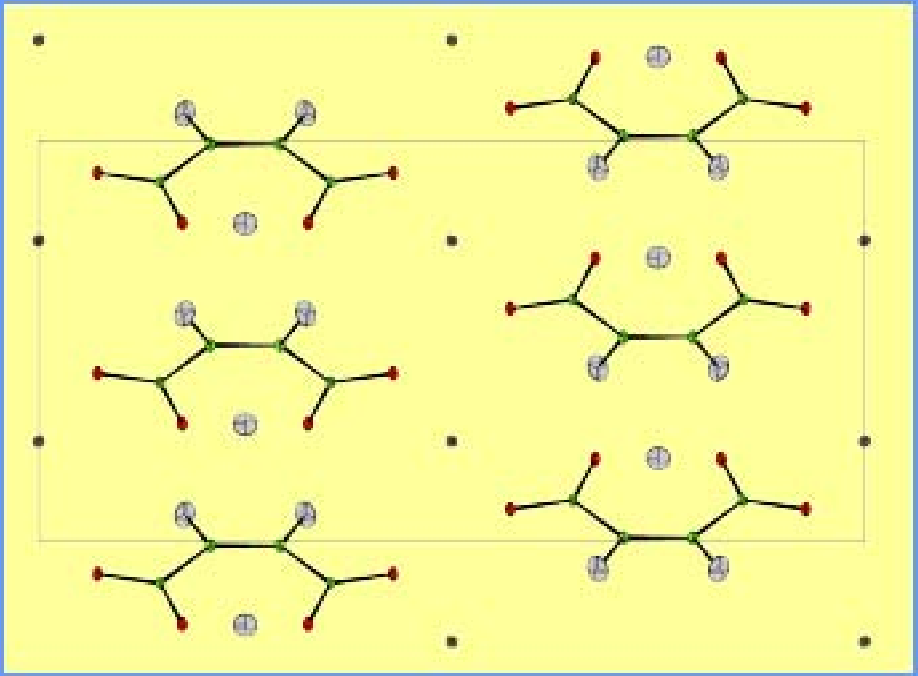
$KHCO_3$ INS

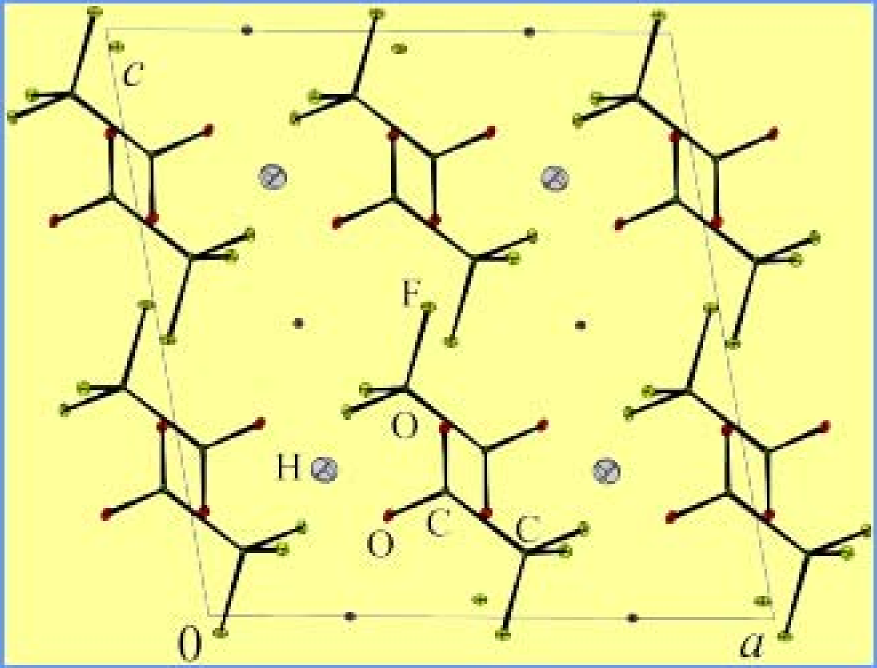


$E_i = 4000\ \mathrm{cm}^{-1}$

KHMaleate

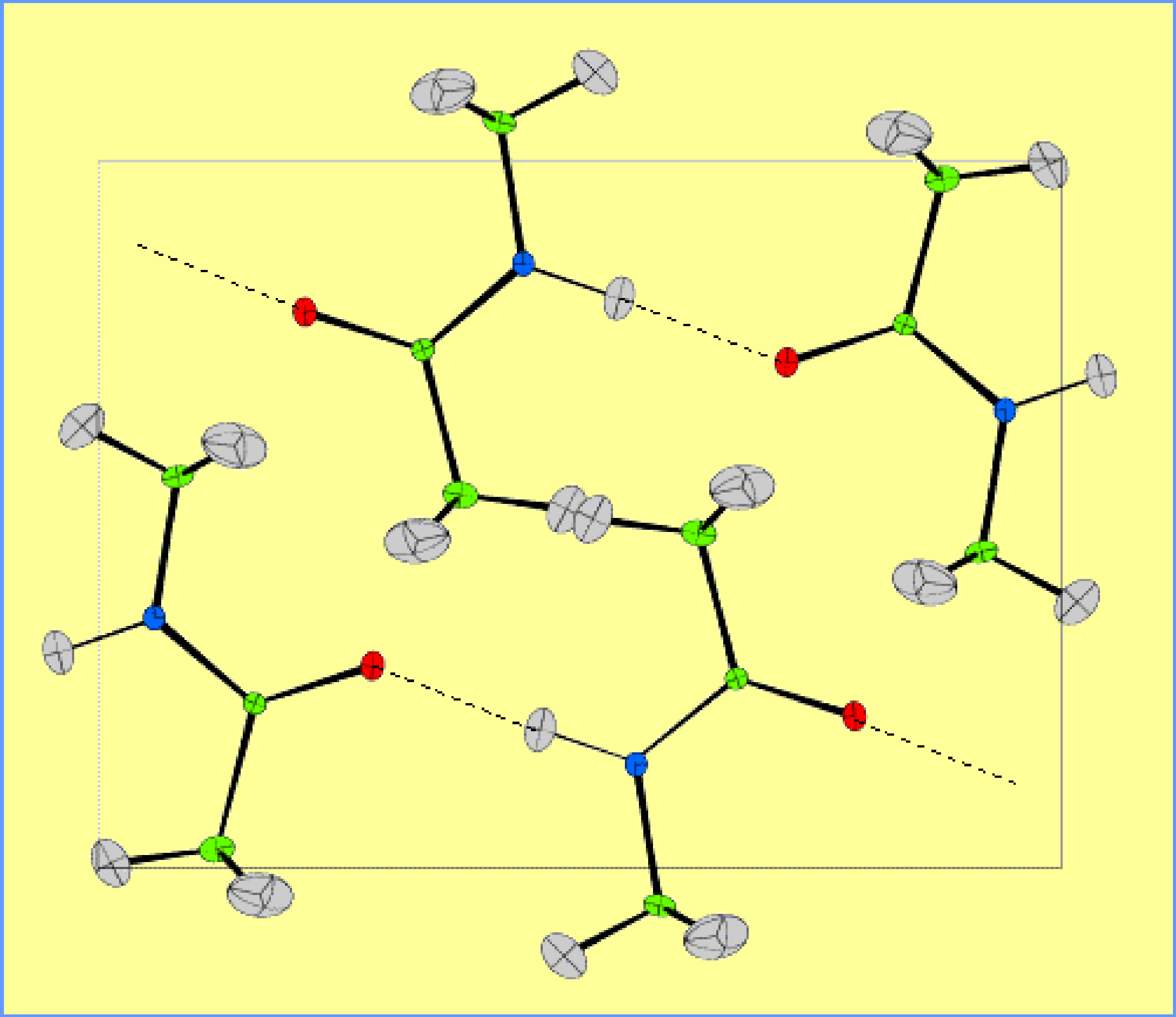
$KH(CF_3COO)_2$



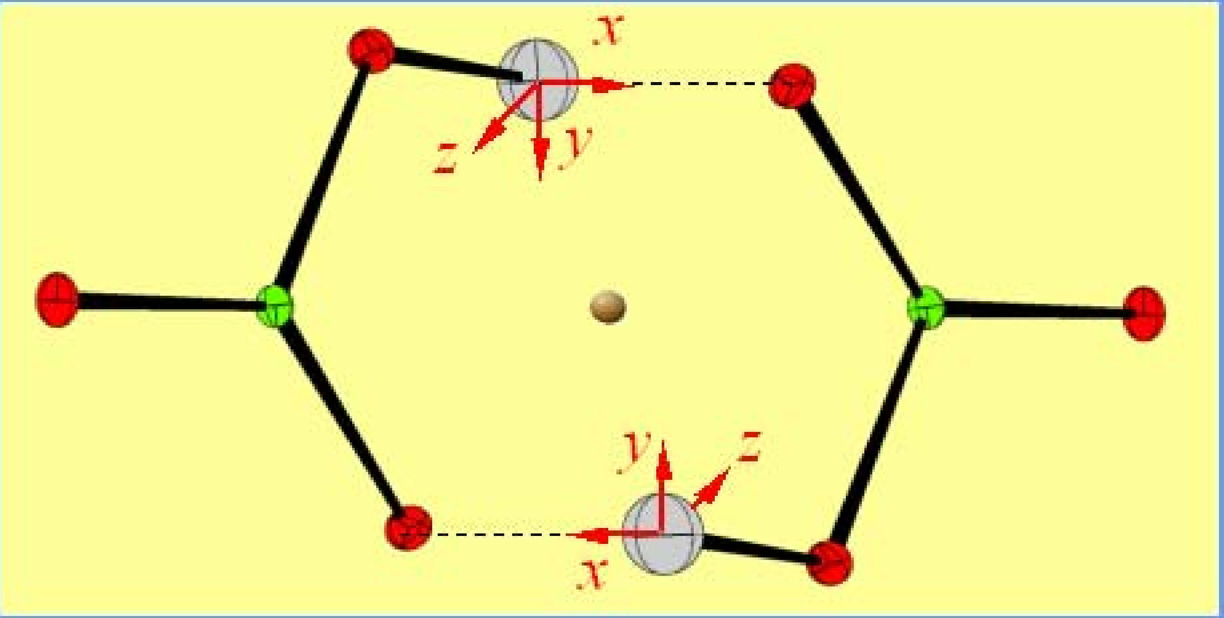


F.Fillaux *et al.*,
Chem.Phys., **244** (1999) 387.

N-methylacetamide CH_3CONH_3

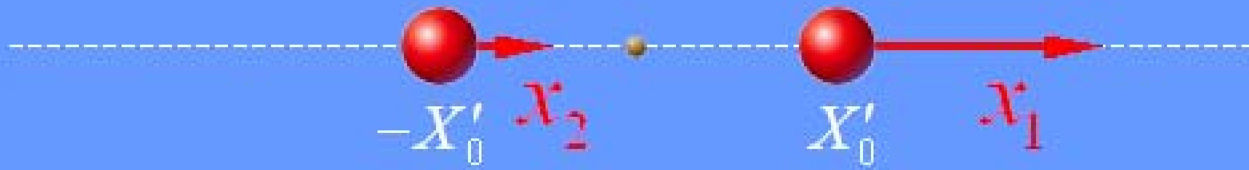


Proton dynamics in centrosymmetric dimers of $KHCO_3$



$$H = H_H + H_{at} + H_{Hat}$$

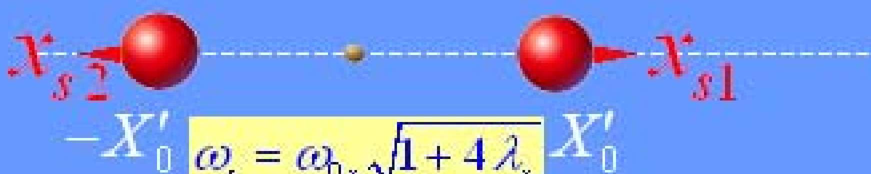
Quantum dynamics of two coupled oscillators



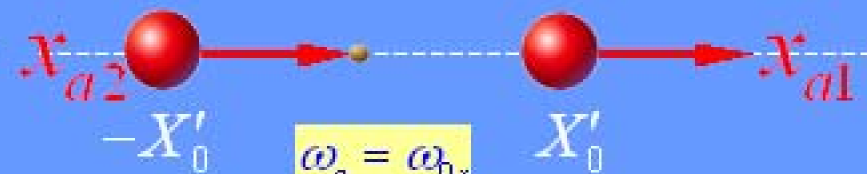
$$H=\frac{1}{2m}\left(P_1^2+P_2^2\right)+\frac{1}{2}m\omega_{0x}^2\left[\left(x_1-X_0\right)^2+\left(x_2+X_0\right)^2+2\lambda_x\left(x_1-x_2\right)^2\right]$$

$$\begin{cases} x_a=\dfrac{1}{\sqrt{2}}\left(x_1+x_2\right) \\ x_s=\dfrac{1}{\sqrt{2}}\left(x_1-x_2\right) \end{cases} \qquad \begin{cases} P_a=\dfrac{1}{\sqrt{2}}\left(P_1+P_2\right) \\ P_s=\dfrac{1}{\sqrt{2}}\left(P_1-P_2\right) \end{cases}$$

$$H=\left\{\frac{P_a^2}{2m}+\frac{1}{2}m\omega_{0x}^2x_a^2\right\}+\left\{\frac{P_s^2}{2m}+\frac{1}{2}m\omega_{0x}^2\left(1+4\lambda_x\right)\left[x_s-\sqrt{2}X_0'\right]^2\right\}$$
$$+m\omega_{0x}^2X_0'^2\frac{4\lambda_x}{1+4\lambda_x}$$



$$\omega_s=\omega_{0x}\sqrt{1+4\lambda_x}$$



$$\omega_a=\omega_{0x}$$

$$E_{an,sm}=\left(am+\frac{1}{2}\right)\hbar\omega_a+\left(sn+\frac{1}{2}\right)\hbar\omega_s$$

$$\Psi_{an,sm}=\Psi_{am}\left(x_a\right)\times\Psi_{sn}\left(x_s-\sqrt{2}X_0'\right)$$

Bosons (Deuterons)

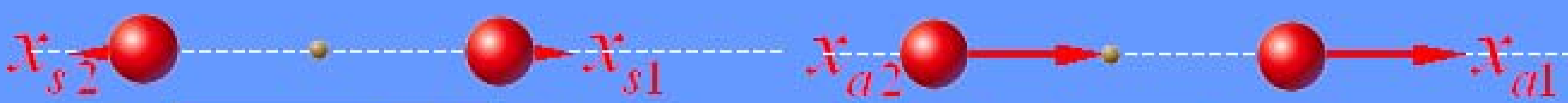
Quantum dynamics and spin correlation of two coupled oscillators

Fermions (Protons)

$\omega_a = \omega_{0x}$ and $\omega_s = \omega_{0x}\sqrt{1+4\lambda_x}$

$$E_{nm} = \left(an + \frac{1}{2}\right)\hbar\omega_a + \left(sn + \frac{1}{2}\right)\hbar\omega_s$$

Pauli Principle



$-X'_0$ $\omega_s = \omega_{0x}\sqrt{1+4\lambda_x}$ X'_0 $-X'_0$ $\omega_a = \omega_{0x}$ X'_0

$$\Theta_{0+}(x_1,x_2) = \frac{1}{\sqrt{2}}\Psi_{a0}(x_a)\times\left[\Psi_{s0}\left(x_s-\sqrt{2}X'_0\right)+\Psi_{s0}\left(x_s+\sqrt{2}X'_0\right)\right]\otimes\frac{1}{\sqrt{2}}\left[\left|\uparrow\downarrow\right\rangle-\left|\downarrow\uparrow\right\rangle\right]$$

$$\Theta_{0-}(x_1,x_2) = \frac{1}{\sqrt{2}}\Psi_{a0}(x_a)\times\left[\Psi_{s0}\left(x_s-\sqrt{2}X'_0\right)-\Psi_{s0}\left(x_s+\sqrt{2}X'_0\right)\right]\otimes\frac{1}{\sqrt{3}}\left\{\left|\uparrow\uparrow\right\rangle+\frac{1}{\sqrt{2}}\left[\left|\uparrow\uparrow\right\rangle+\left|\downarrow\downarrow\right\rangle\right]+\left|\downarrow\downarrow\right\rangle\right.$$

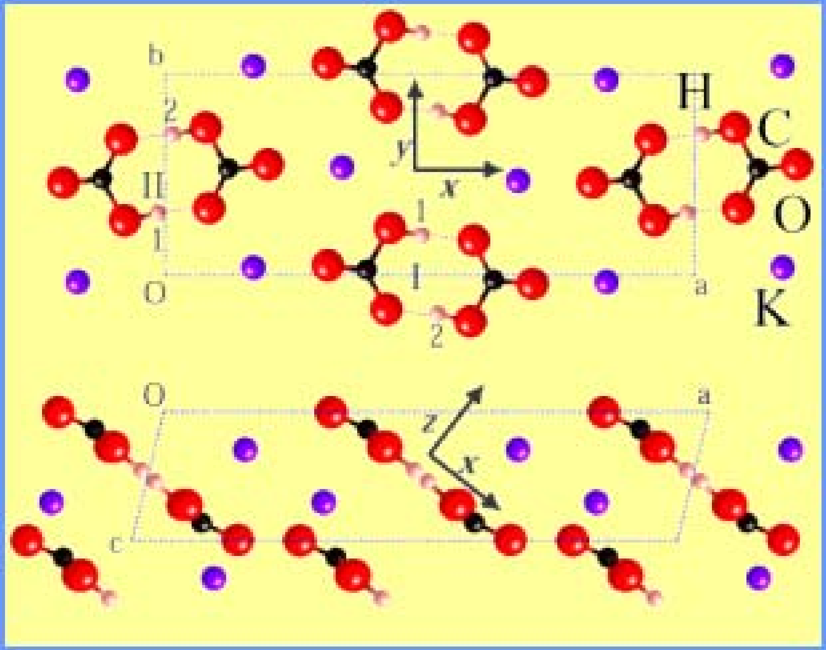
DECOHERENCE-FREE DYNAMICS

1) Entanglement is time-independent:

2) Proton dynamics decoupled from the KCO_3 sublattice

$$H = H_H + H_{at} + H_{Hat}$$

$$H_{Hat} \equiv 0$$



Crystal of protons

$$H_H = \sum_{j=j'=1}^{N_a} \sum_{k=1}^{N_b} \sum_{l=1}^{N_c} \sum_{\alpha} \left\{ H_{jkl\alpha} + H_{j'kl\alpha} \right\}, \alpha = x, y, z$$

$$\left| jkl +_{\alpha} \right\rangle = \left| \Theta_{jkl,\alpha,0+} \right\rangle \otimes \frac{1}{\sqrt{2}} \left| \uparrow\downarrow - \downarrow\uparrow \right\rangle$$

$$\left| jkl -_{\alpha} \right\rangle = \left| \Theta_{jkl,\alpha,0-} \right\rangle \otimes \frac{1}{\sqrt{3}} \left\{ \left| \uparrow\uparrow \right\rangle + \frac{1}{\sqrt{2}} \left| \uparrow\downarrow + \downarrow\uparrow \right\rangle + \left| \downarrow\downarrow \right\rangle \right\}$$

~~COLLECTIVE DYNAMICS:~~
~~Coupled pairs are Bosons~~

$$\cancel{\left|\tau\tau' s\right\rangle = \bigotimes_{j=j',k,l} \left[\left|jkl\tau\right\rangle + s\left|j'kl\tau'\right\rangle \right]}$$

Fermions (Protons): $\left|\tau\tau' s\right\rangle \equiv 0$

Macroscopic single particle states

H (fermion) sublattice
H degenerate (overlap $\equiv$ 0)
H indistinguishable

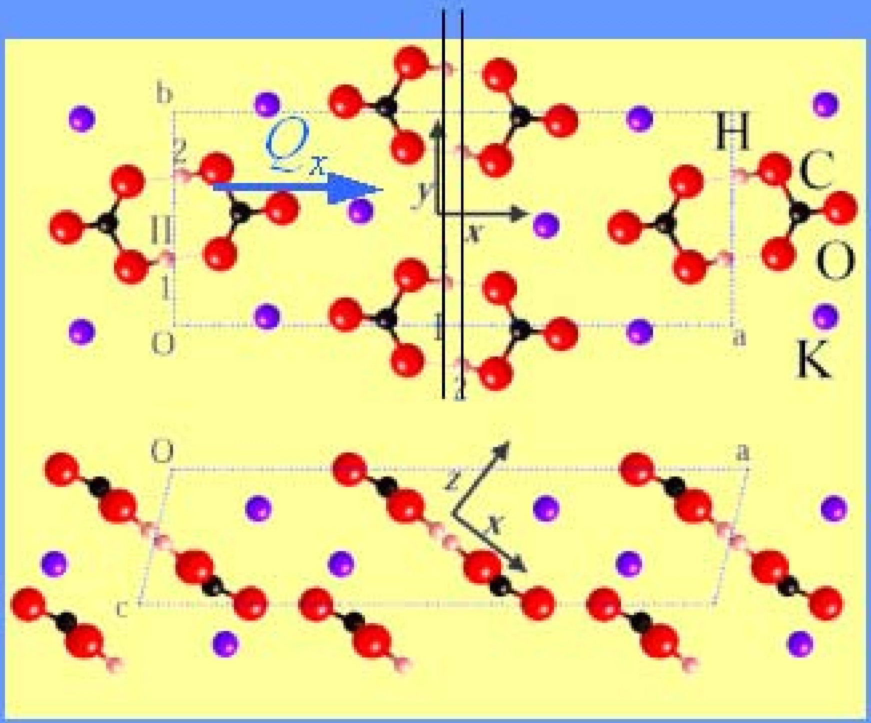
$$\left|\tau\tau's\right\rangle = \frac{1}{\sqrt{N}}\left|\sum_{l}^{N_c}\sum_{k}^{N_b}\sum_{j=j'=1}^{N_a}\left[\left|jkl\tau\right\rangle + s\left|j'kl\tau'\right\rangle\right]\right\rangle$$

$$\left|\Psi\right\rangle = \sqrt{N}\sum_{\tau,\tau',s}\left|\tau\tau's\right\rangle$$

Non locality
Macroscopic quantum entanglement
Decoherence forbidden

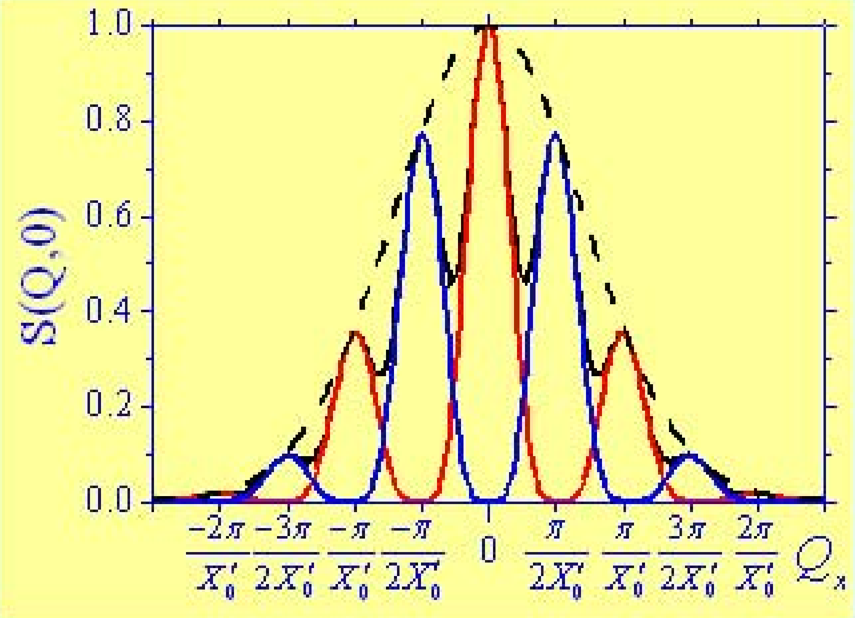
Quantum interference arising from macroscopic quantum entanglement:

1) Quantum double-slits (1D)



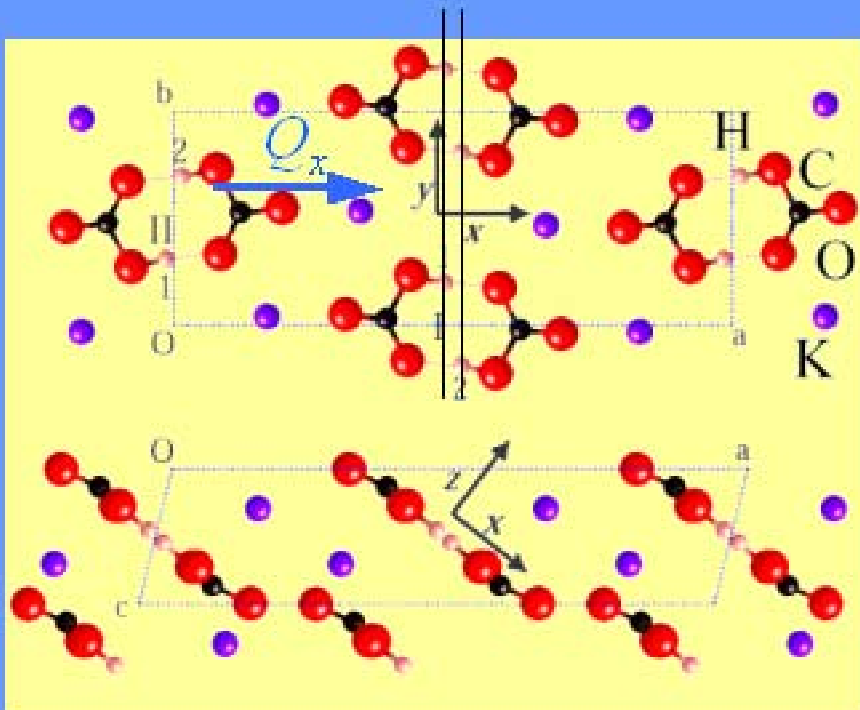
$T = 14$ K
$a = 15.06$ Å, $b = 5.57$ Å, $c = 3.65$ Å, $\beta = 103.97°$

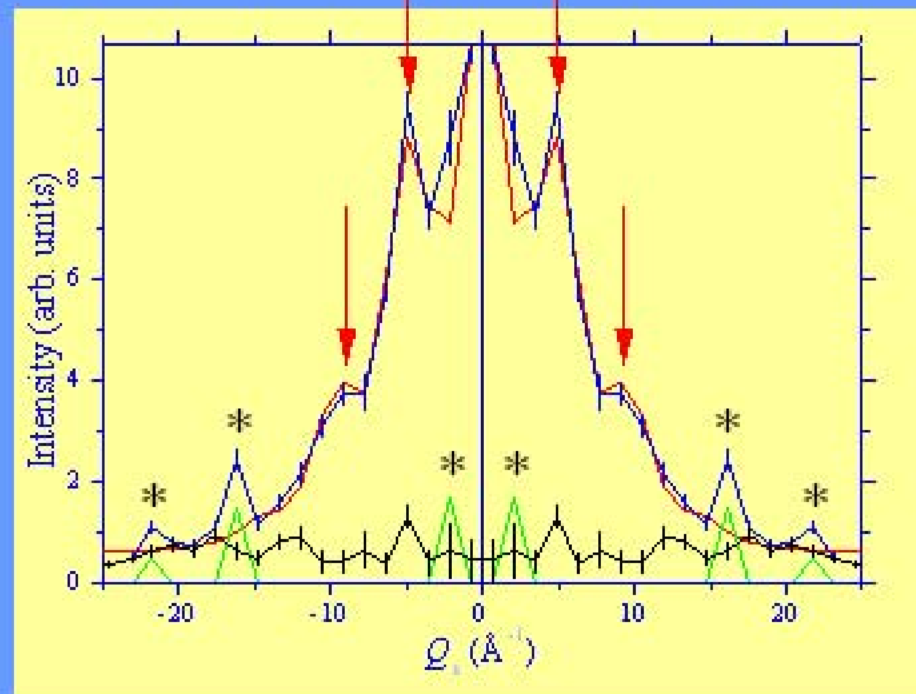
$$S(Q_x,\omega) = \left[\cos^4(Q_x X_0') + \sin^4(Q_x X_0')\right] \times \exp\left[-Q_x^2\left(\frac{u_{0x}^2}{2\sqrt{1+4\lambda_x}} + \frac{u_{0x}^2}{2}\right)\right]\delta(\omega)$$



Quantum interference arising from macroscopic quantum entanglement:

1) Quantum double-slits (1D)



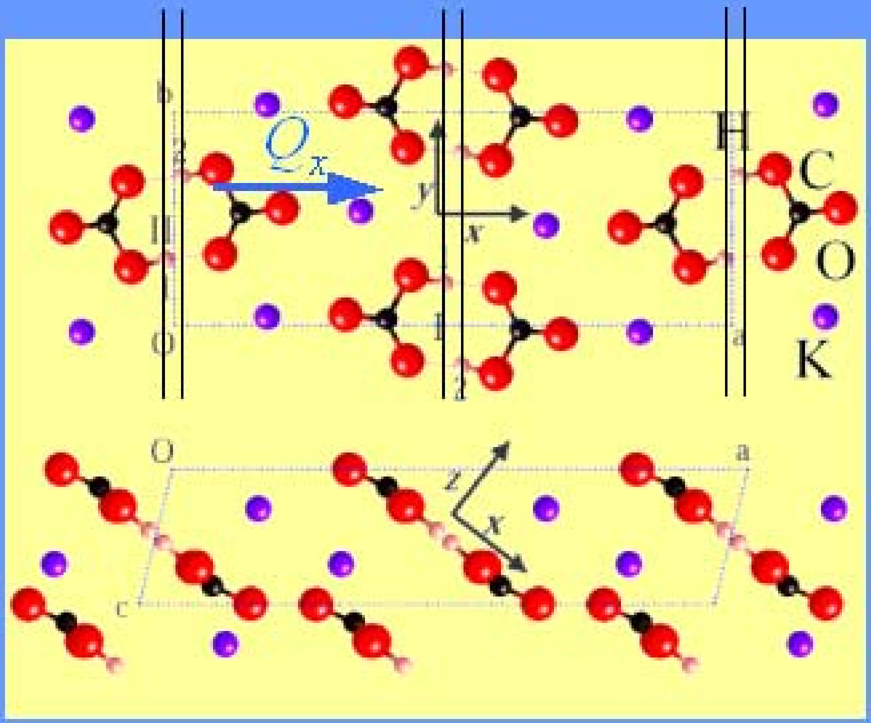


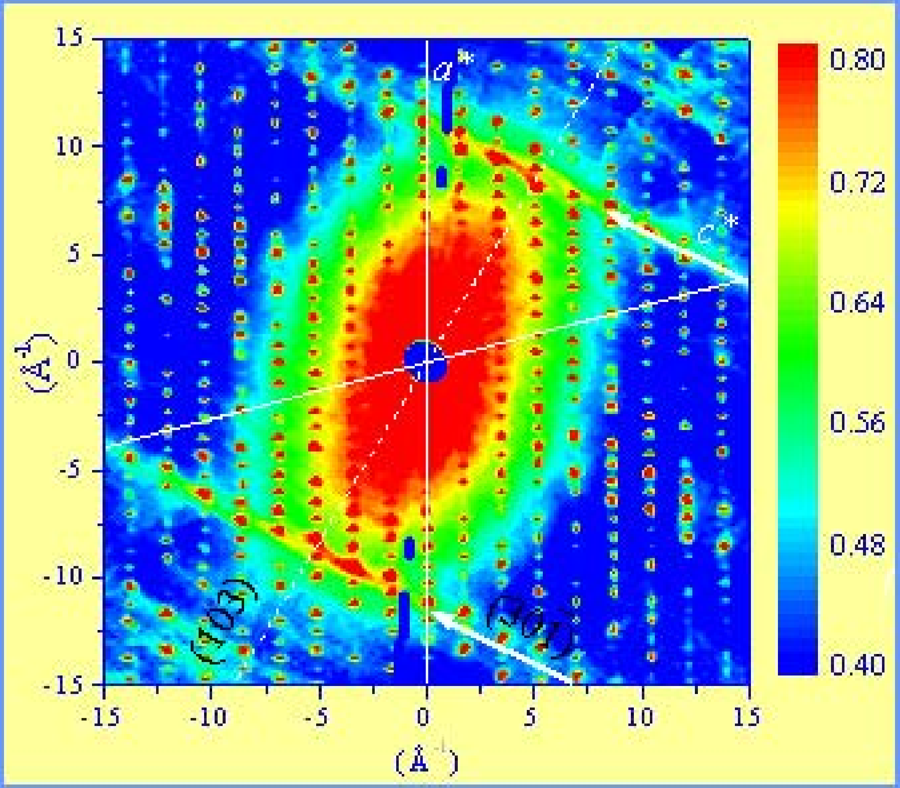
$T = 14$ K
$a = 15.06$ Å, $b = 5.57$ Å, $c = 3.65$ Å, $\beta = 103.97°$

$X_0' \approx 0.3$ Å

Quantum interference arising from macroscopic quantum entanglement:

2) Quantum grating (2D)

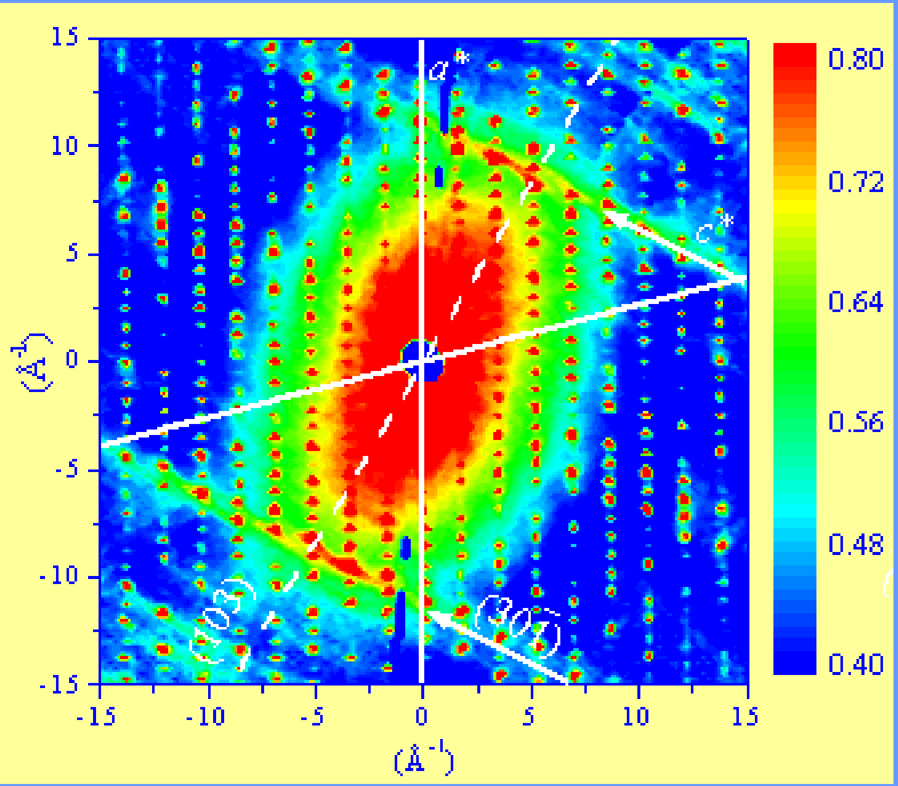




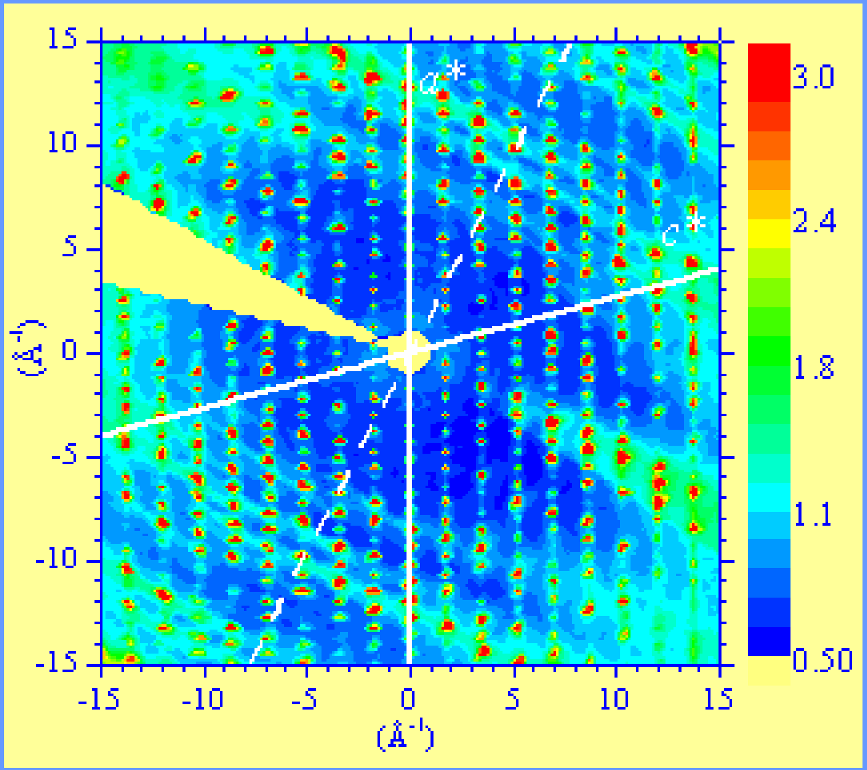
$T = 14$ K

$a = 15.06$ Å, $b = 5.57$ Å, $c = 3.65$ Å, $\beta = 103.97°$

Spatially extended and long-lived quantum coherence of H-oscillators in the $KHCO_3$ crystal

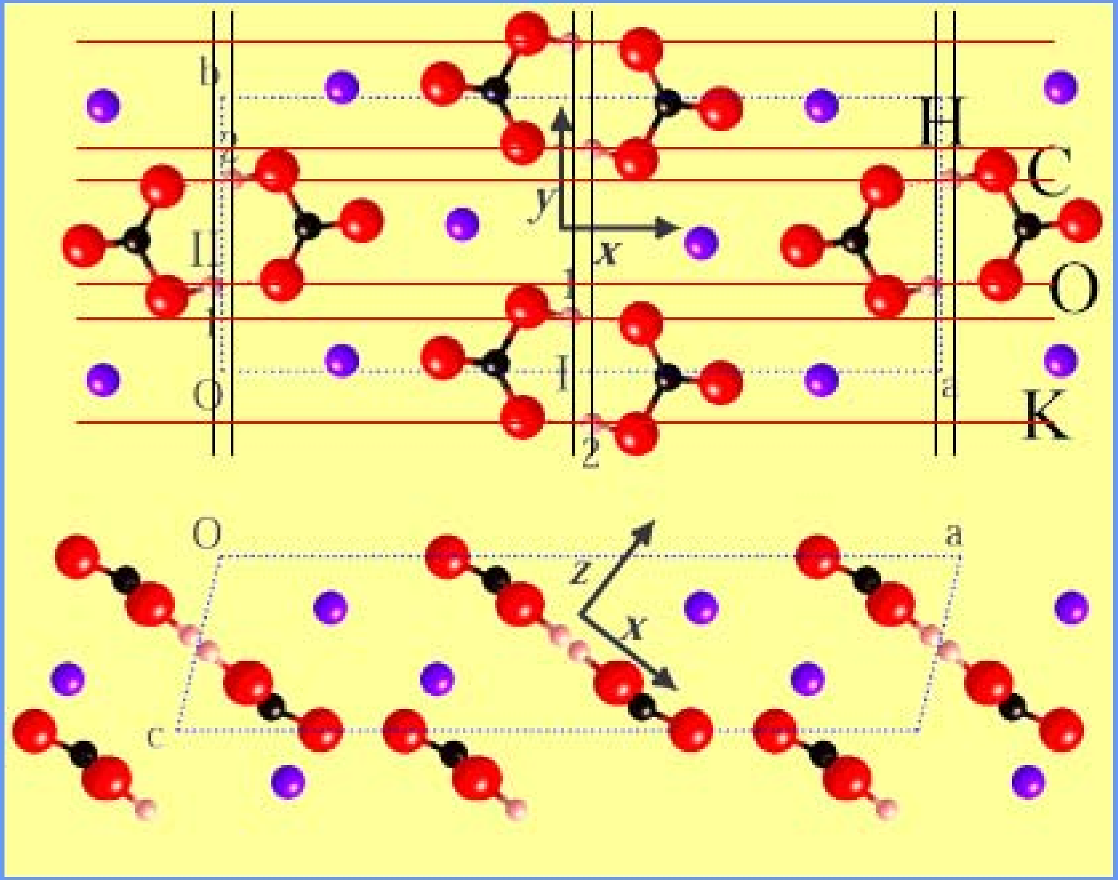


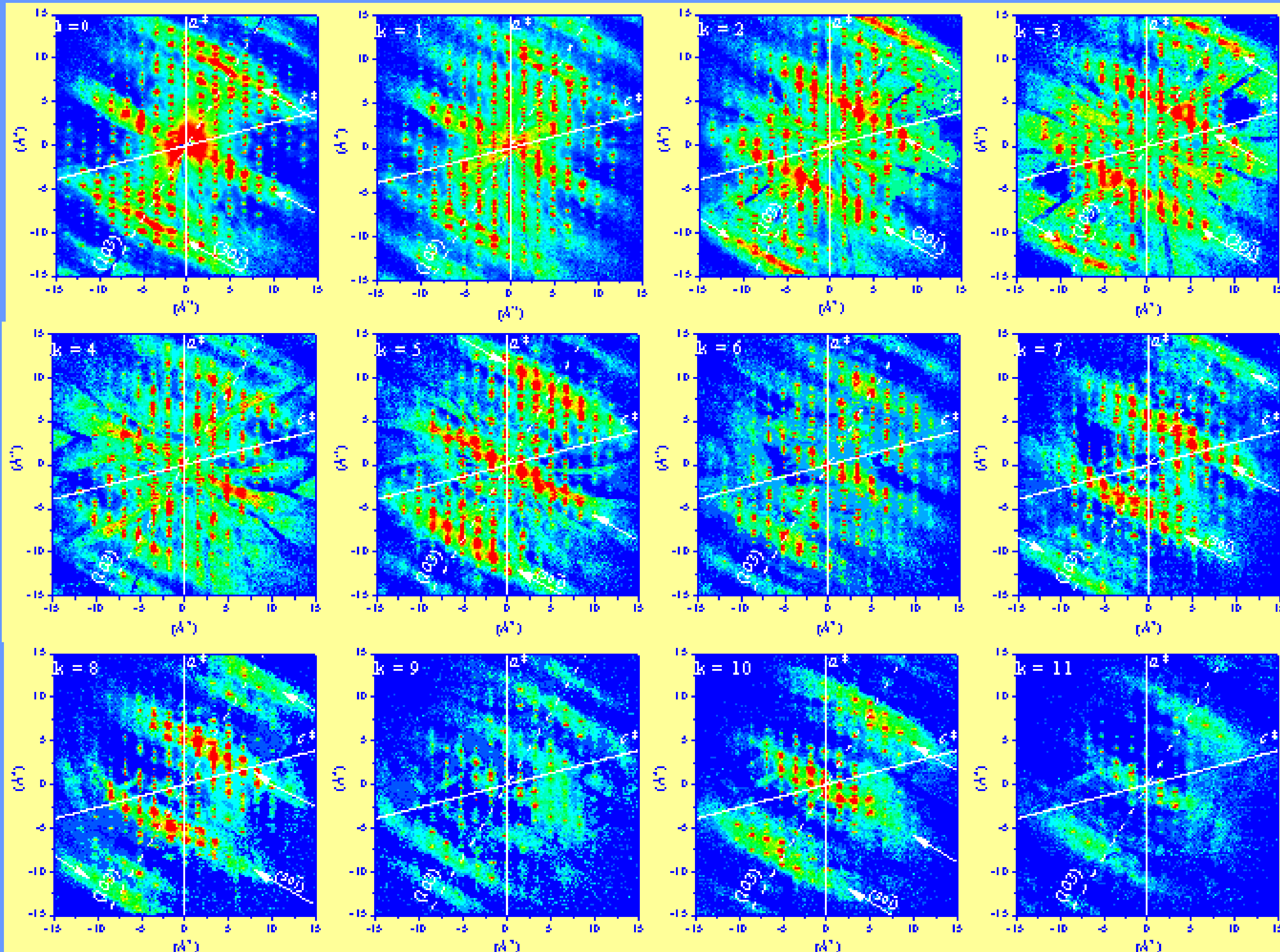
NO spatially extended and long-lived quantum coherence of D-oscillators in the $KDCO_3$ crystal



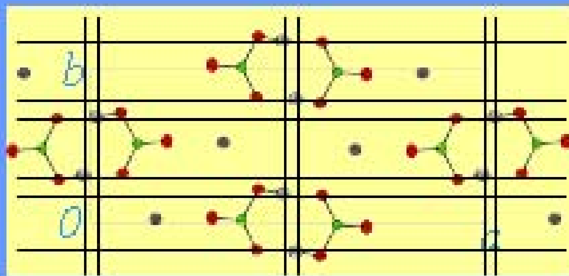
Quantum interference arising from macroscopic quantum entanglement:

2) Quantum grating (2D)

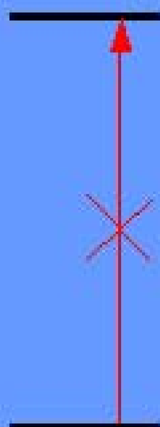



k = 0
k = 1
k = 2
k = 3
k = 4
k = 5
k = 6
k = 7
k = 8
k = 9
k = 10
k = 11
a^*
c^*
(Å^{-1})

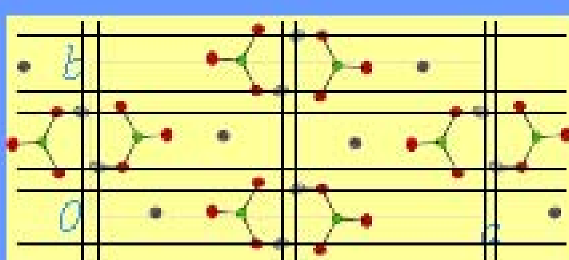
Macroscopic quantum coherence and proton transfer

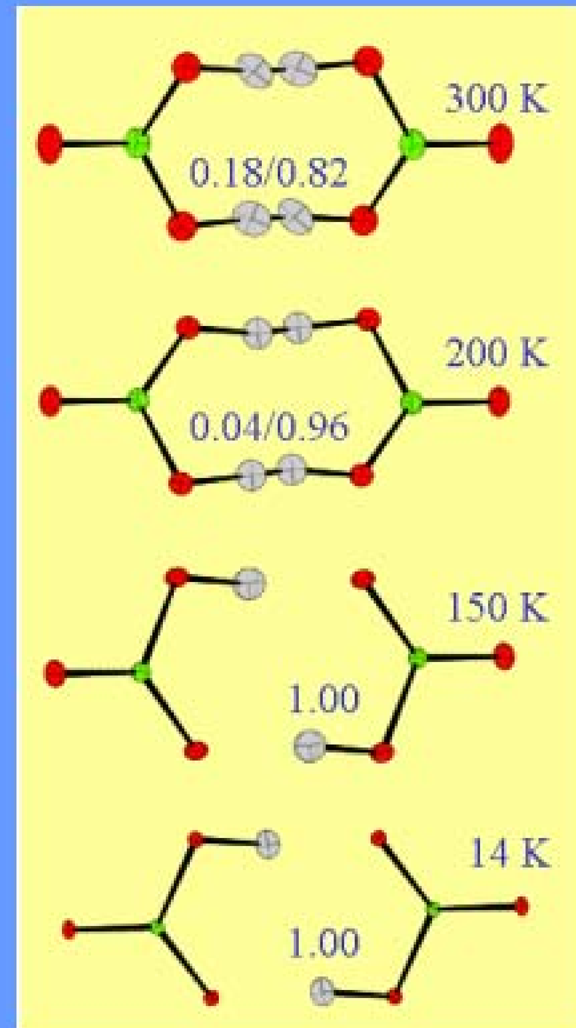


$$\overline{|1\rangle} = \sqrt{N}\sum_{\tau,\tau',s} |\tau\tau' s 1\rangle$$



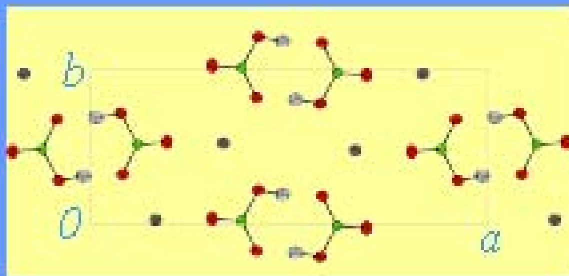
$$\overline{|0\rangle} = \sqrt{N}\sum_{\tau,\tau',s} |\tau\tau' s 0\rangle$$

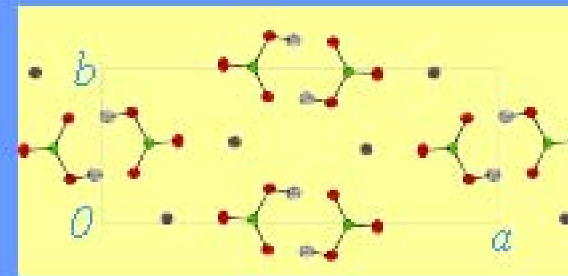




Entangled

Disentangled

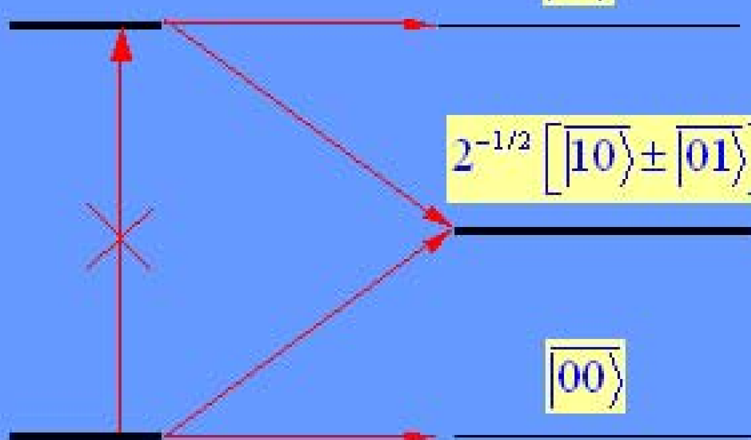


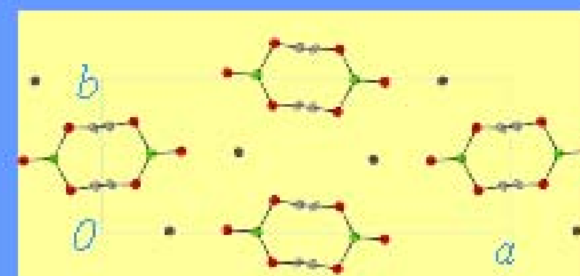


$$\overline{|1\rangle} = \sqrt{N}\sum_{\tau,\tau',s} |\tau\tau' s 1\rangle$$

$$\overline{|11\rangle}$$

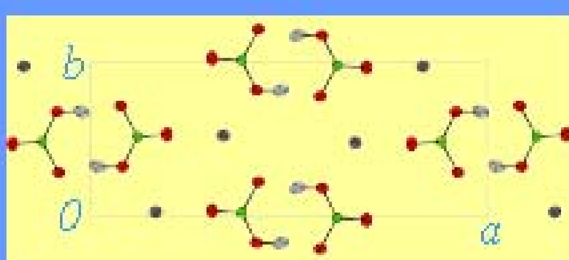
$$2^{-1/2}\left[\overline{|10\rangle} \pm \overline{|01\rangle}\right]$$

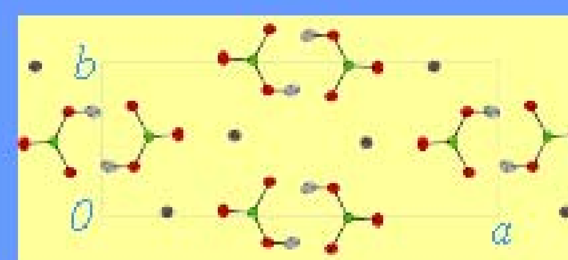




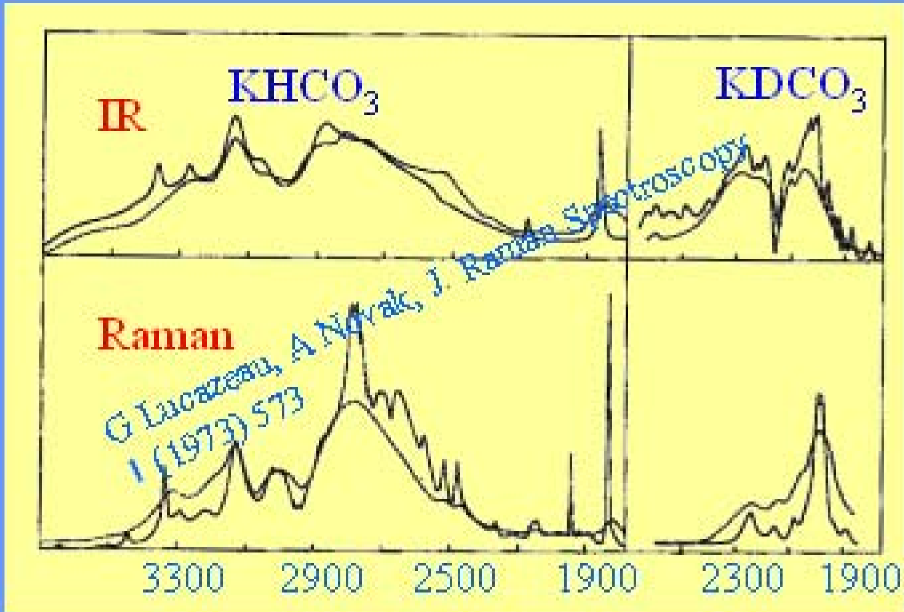
$$\overline{|00\rangle}$$

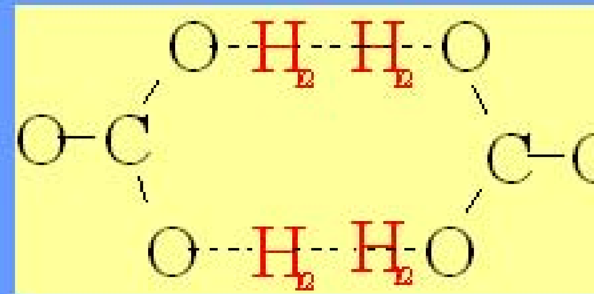
$$\overline{|0\rangle} = \sqrt{N}\sum_{\tau,\tau',s} |\tau\tau' s 0\rangle$$



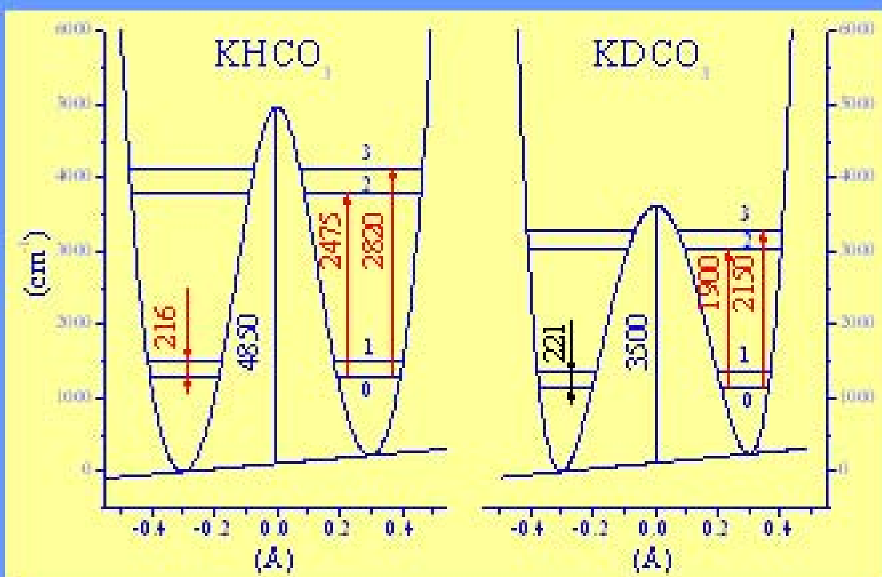


Proton Transfer

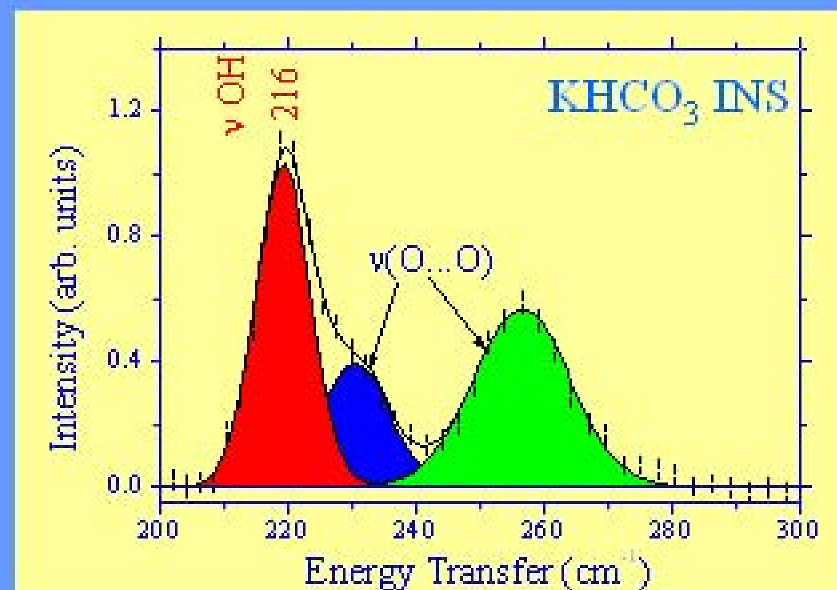




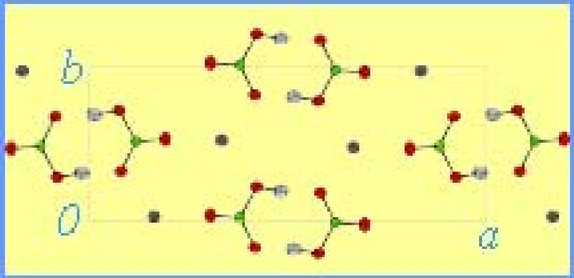
F Fillaux *et al.*, Chem. Phys. **124** (1988) 425



F Fillaux, Chem. Phys. **74** (1983) 405



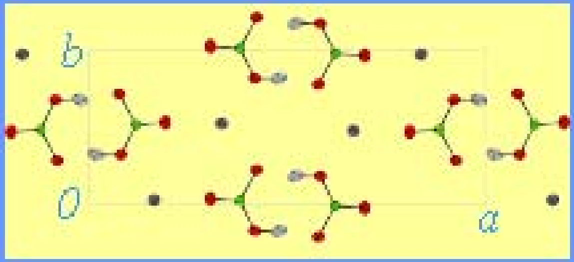
Entangled

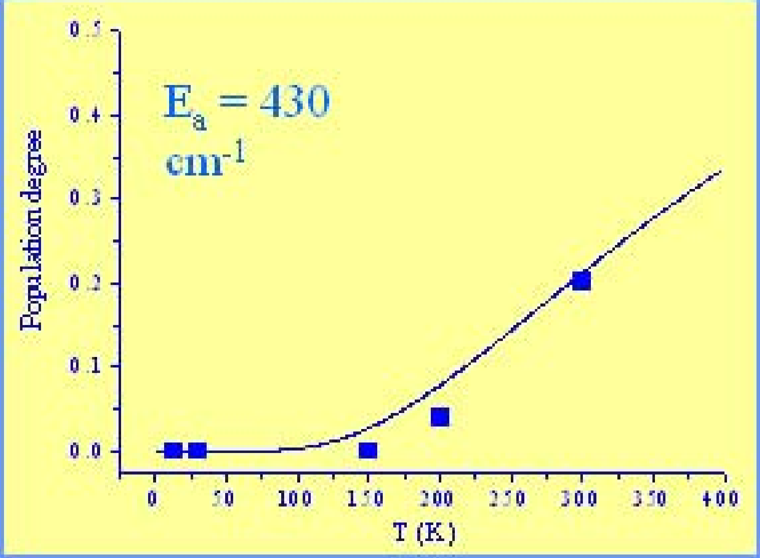


$$\overline{|1\rangle} = \sqrt{N}\sum_{\tau,\tau',s} |\tau\tau' s 1\rangle$$

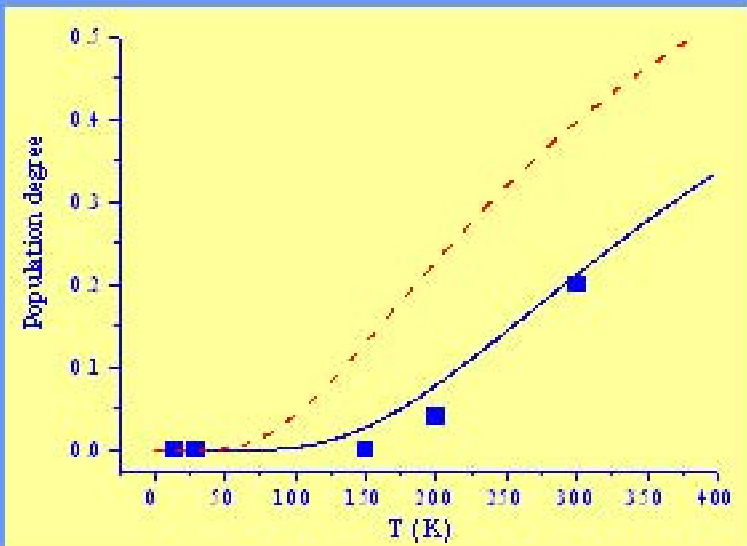
$2h\nu_{01}$

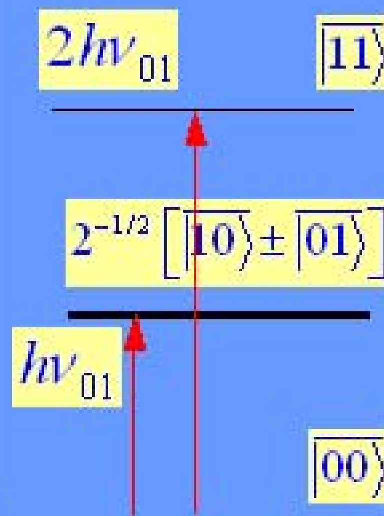
$$\overline{|0\rangle} = \sqrt{N}\sum_{\tau,\tau',s} |\tau\tau' s 0\rangle$$

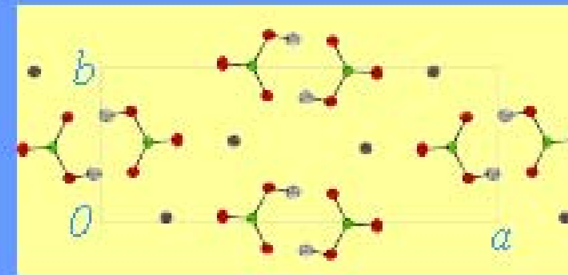


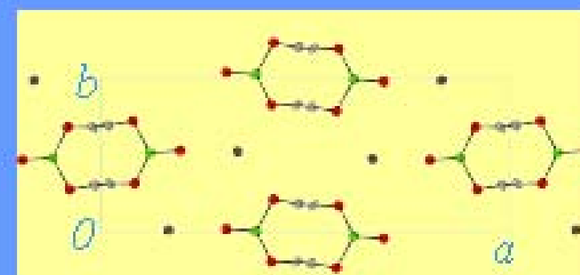


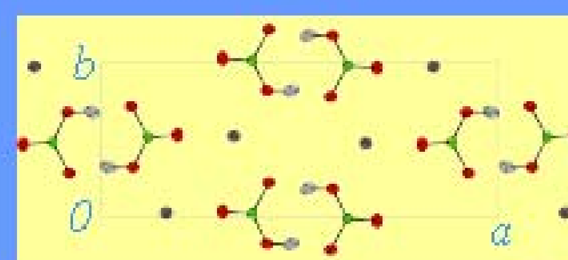
Disentangled









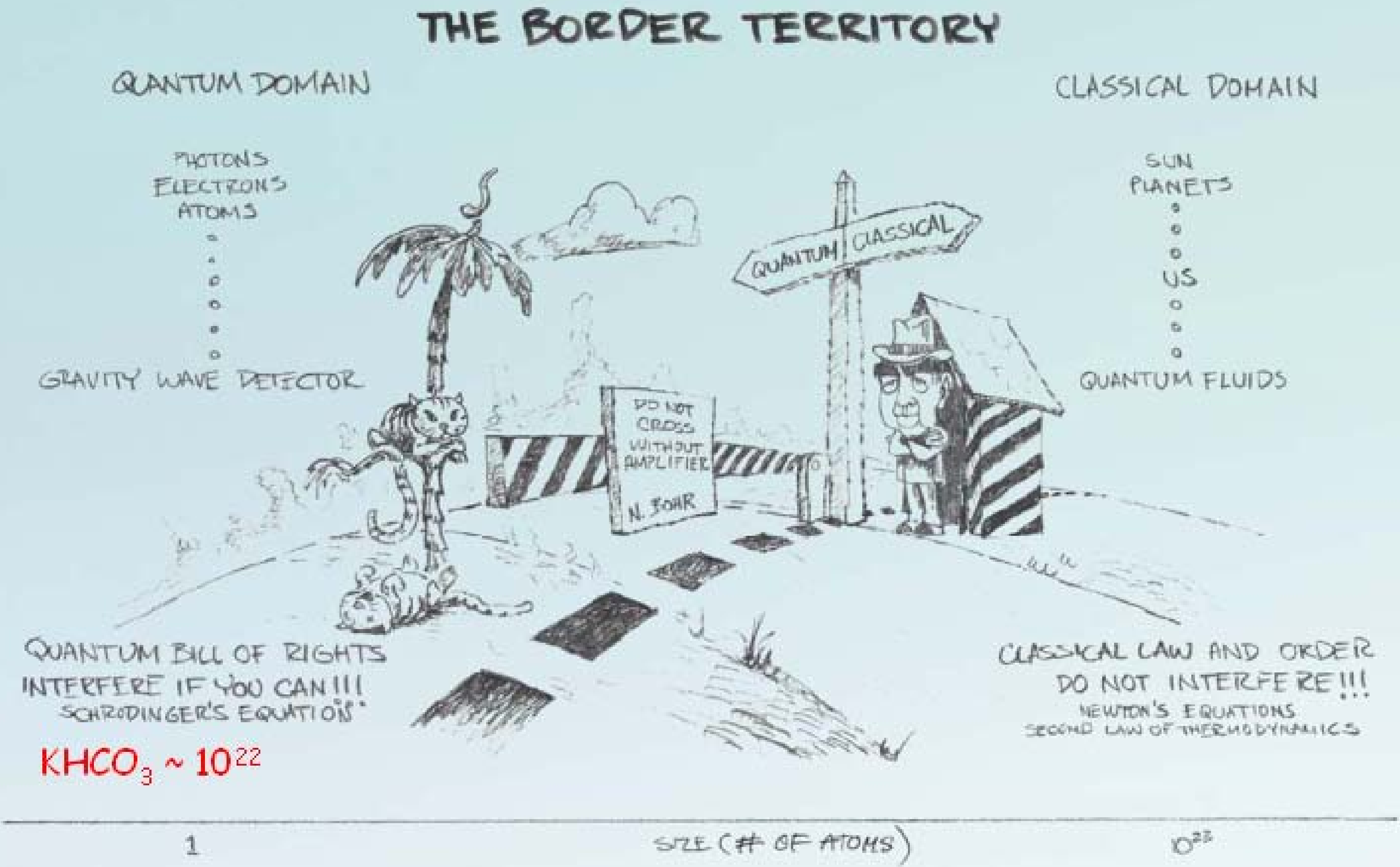


Conclusion

Normal Coordinates Give Rise to Macroscopic
Quantum Entanglement Observed for ~ 10^{22} atoms

Entanglement: No Dynamics
Disentanglement: Nonlocal Dynamics

Decoherence-forbidden states (fermions)
EPR non-locality
Schrödinger's Cat: Superposition of Macroscopically
Distinct Tunnelling States
Quantum Measurement (coherent/incoherent)



W. H. Zurek, Los Alamos Science, 27 (2002) 2.