Entrevista con el grupo de investigación Sistemas Carentes de Orden de Largo Alcance

Convocatoria JAE intro 2019
Ref: JAEFINT19_EX_0477

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Título: Simulación multiescala de procesos físico químicos de interés nano-tecnológico

Instituto de Estructura de la Materia (IEM)

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Dispersión de Neutrones

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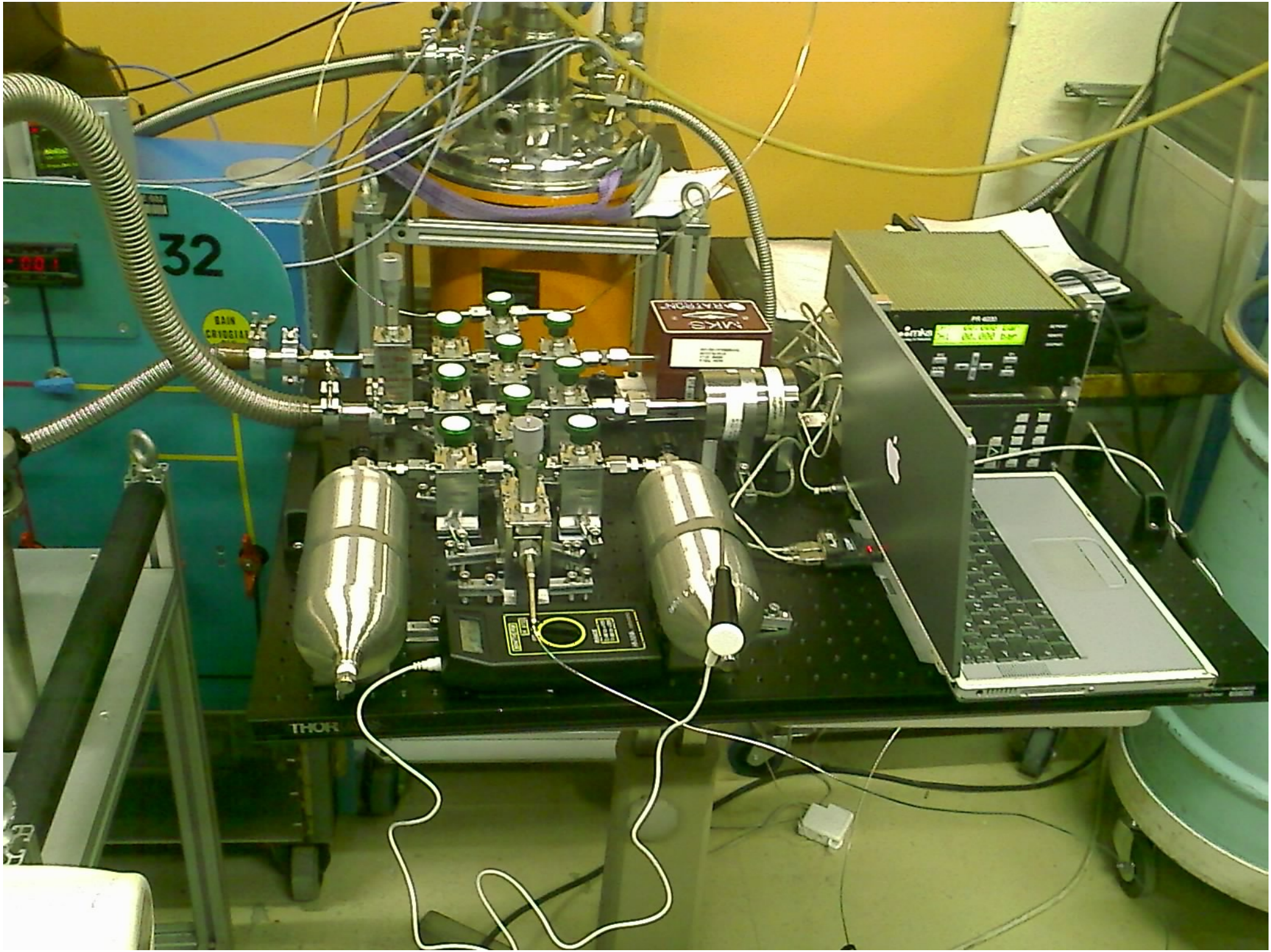
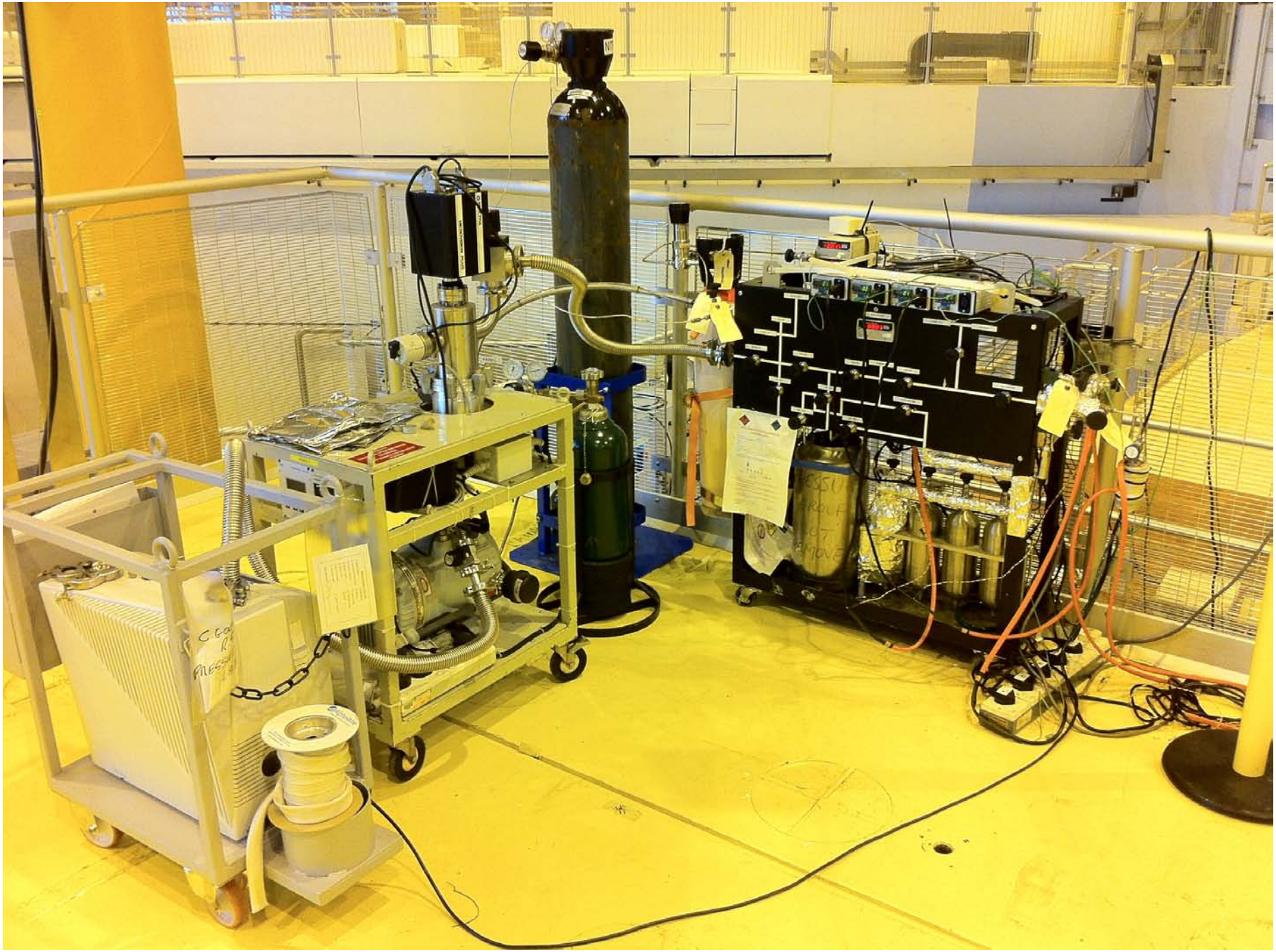
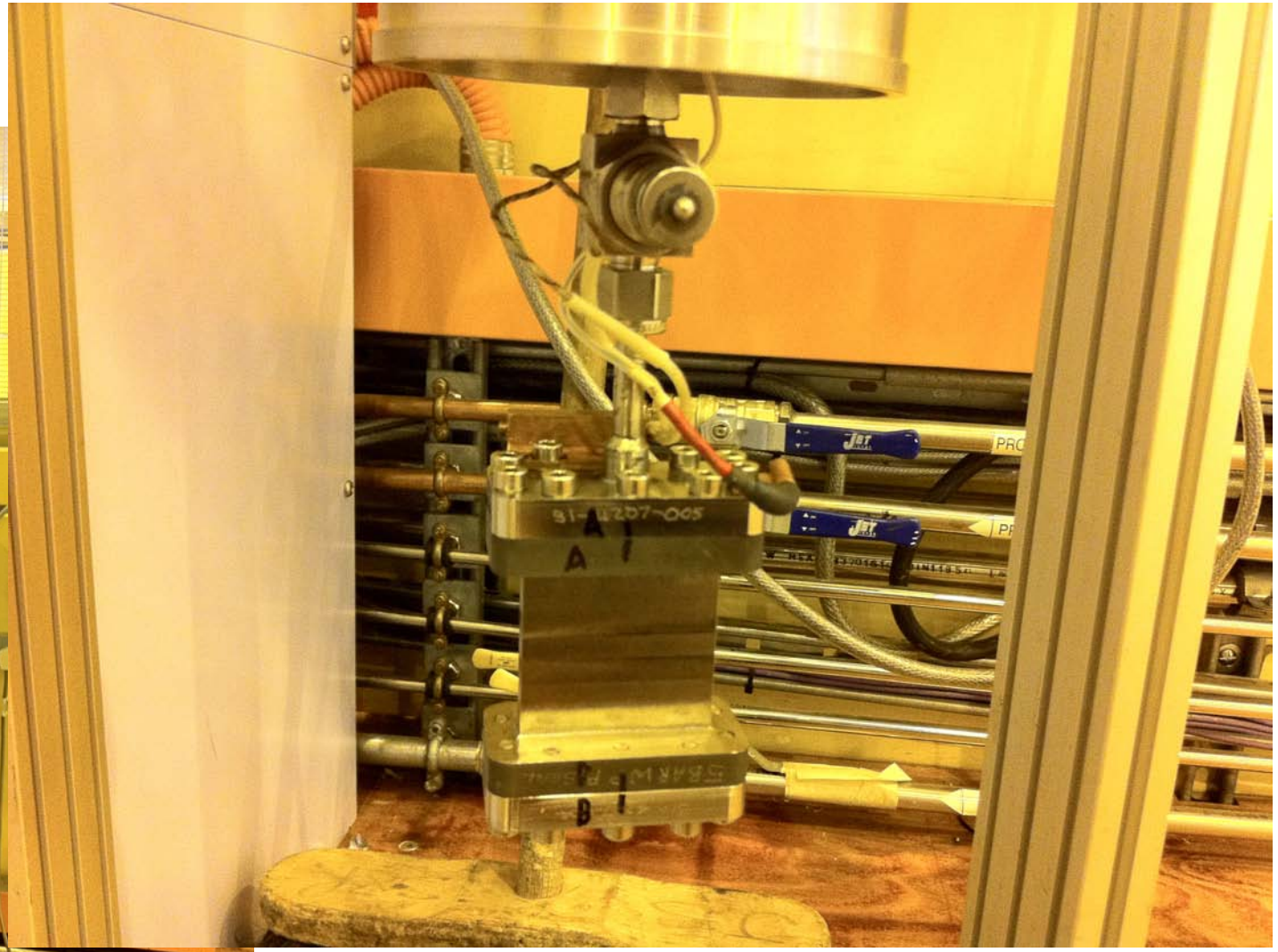

32
THOR

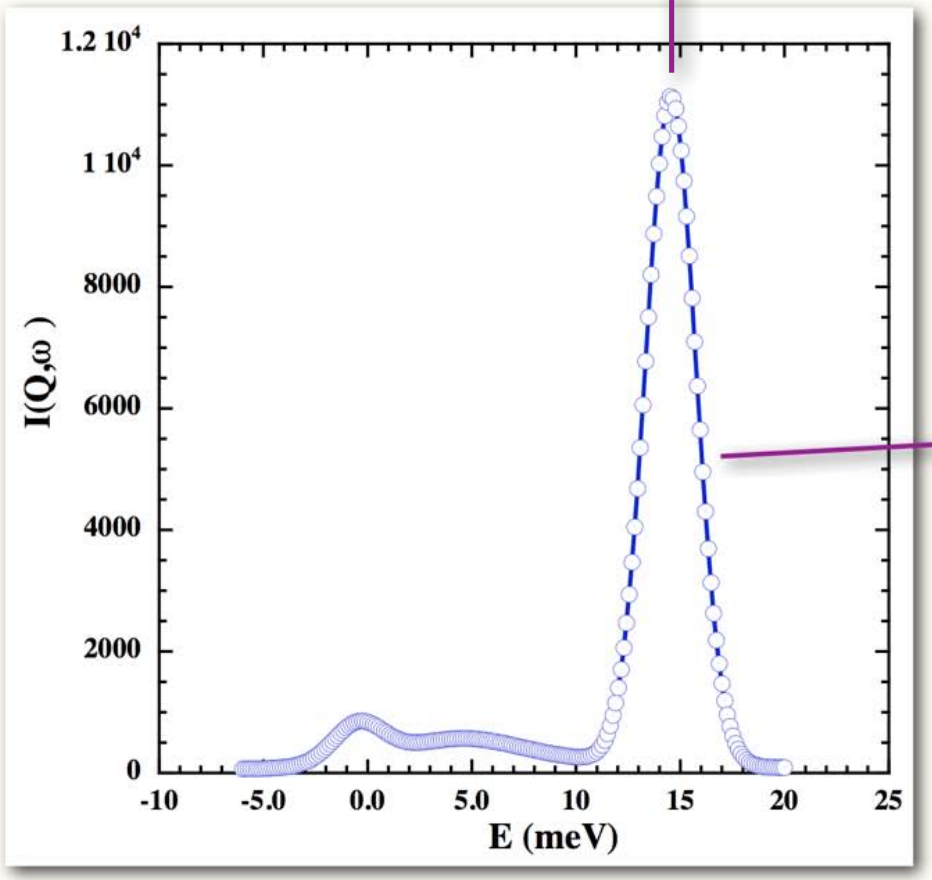


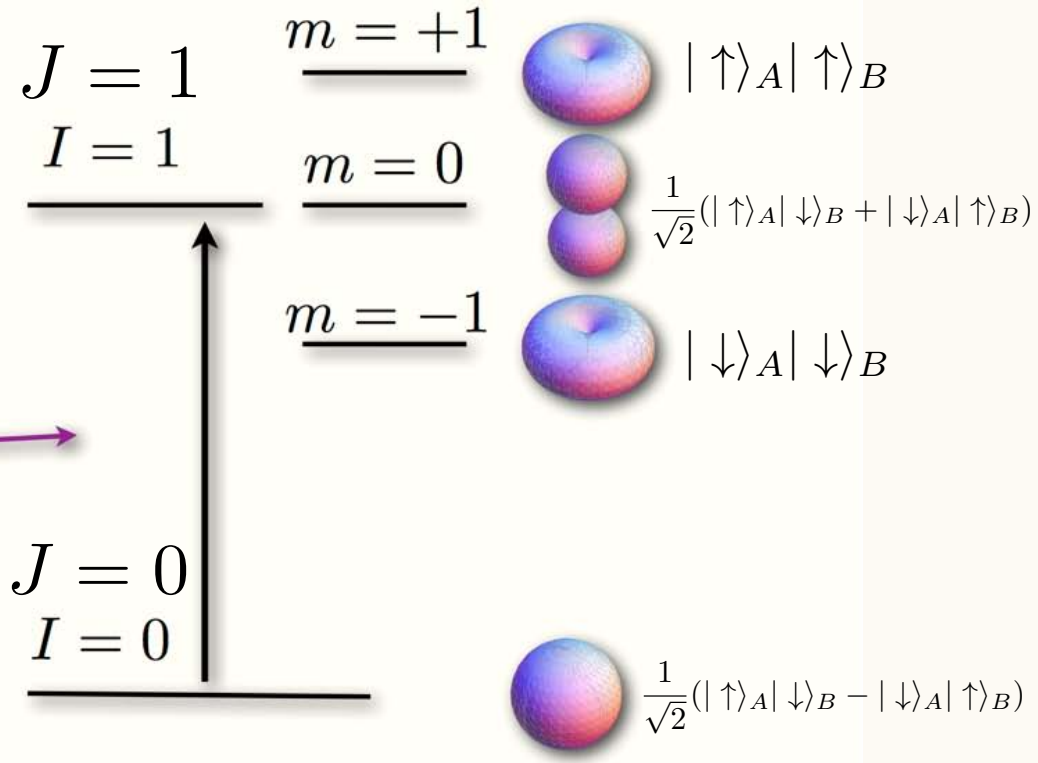


H_2 quantum aspects

Rotational degrees of freedom

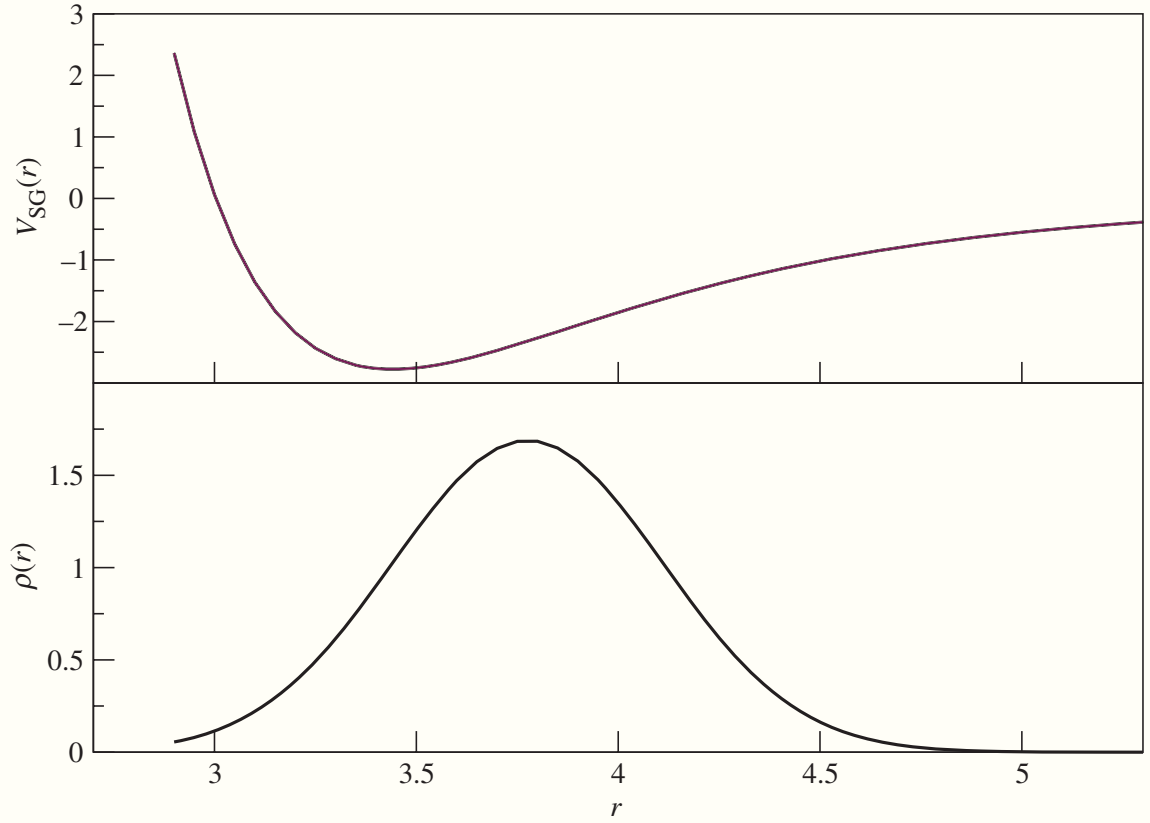
$$E_{01} \simeq 14.6 \text{ meV} \rightarrow \ T \simeq 169 \text{ K}$$





Molecules in the *J = 0* (fundamental level) are very well approximated by structureless entities
Interaction very well approximated by an isotropic (T independent) potential (Silvera-Goldman)
I. F. Silvera and V. V. Goldman, *J. Chem. Phys.* **69**, 4209 (1978)

Translational degrees of freedom (crystal)



Anharmonic crystal even at low temperatures.
Breakdown of the harmonic approximation around equilibrium position

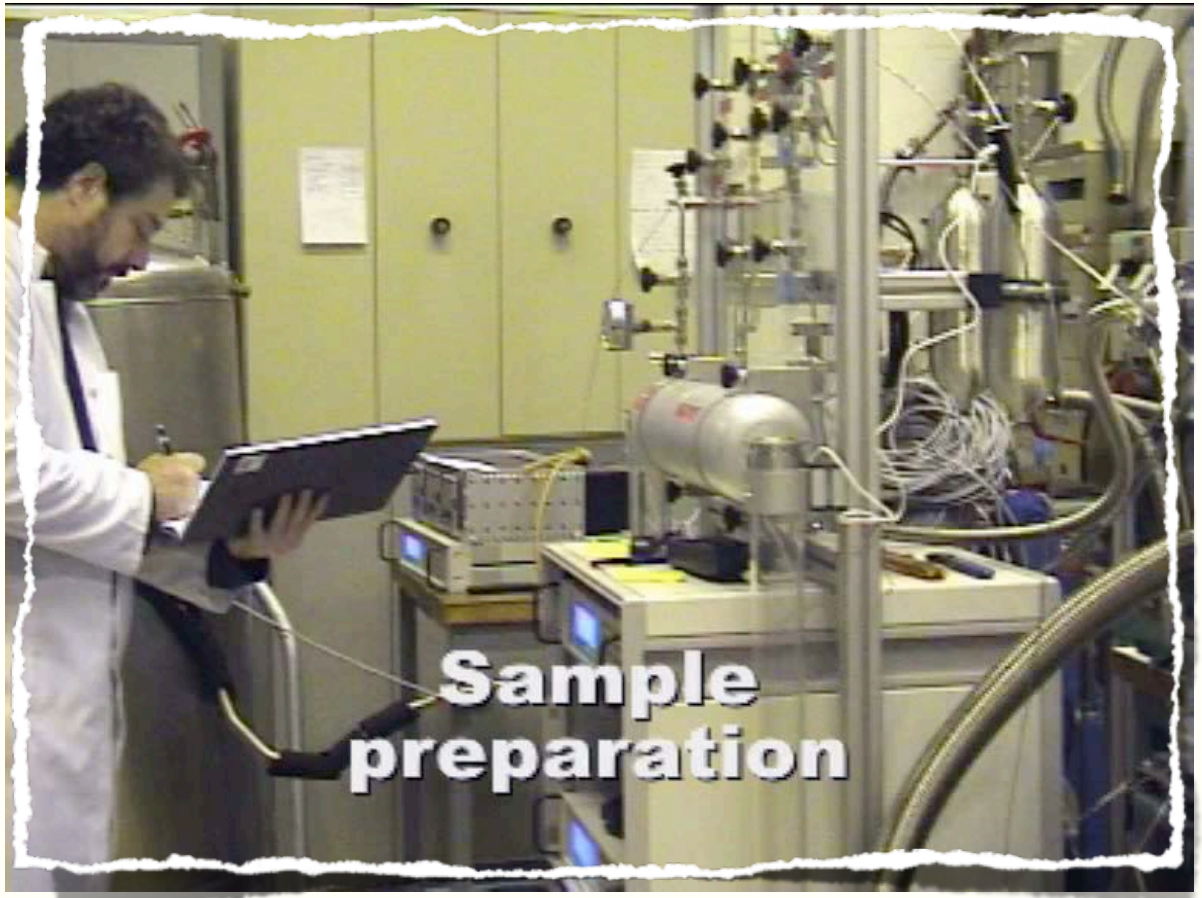
Thermal expansion ~ 0 below a threshold temperature

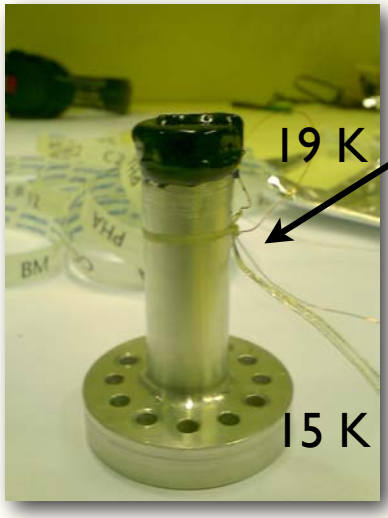
para-H_2: experimental T_{tp} = 13.8 K (*hcp*)

Quasiclassical T_m well above T_{tp} (25 K, ie., ~ 1.8 T_{tp})

$$\sqrt{\langle u^2 \rangle_{qc}} = 0.75 \text{ Å}$$

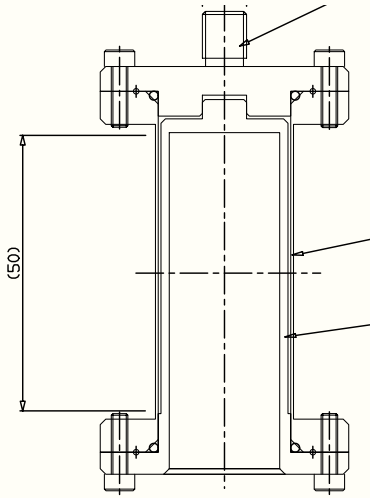
Experiment



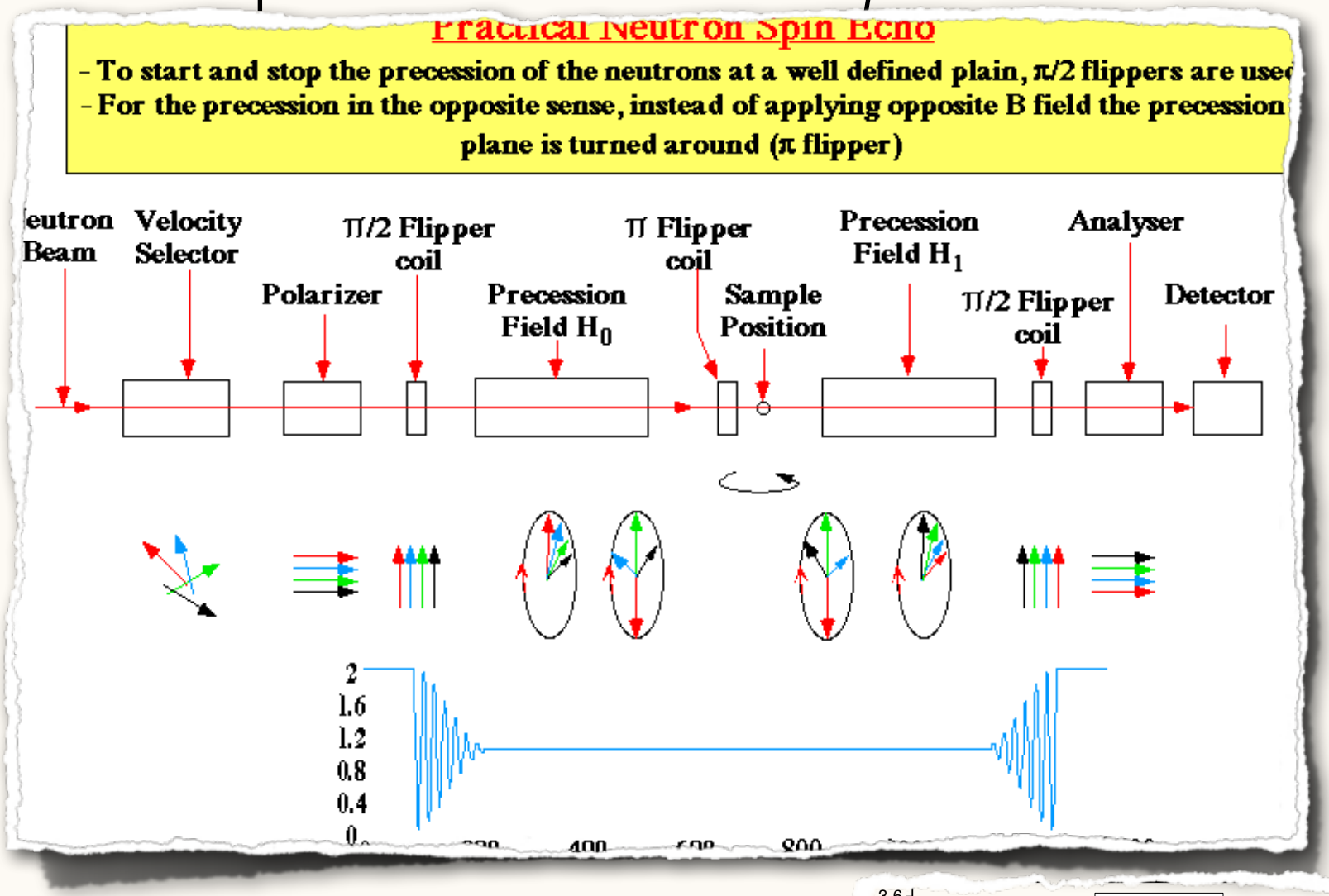


Half filled with
6 g of Oxisorb (CrO_3)

Liquid H_2 were left in
this catalytic cylinder
during 5 days before
loading to the sample can
while cooling to 13 K



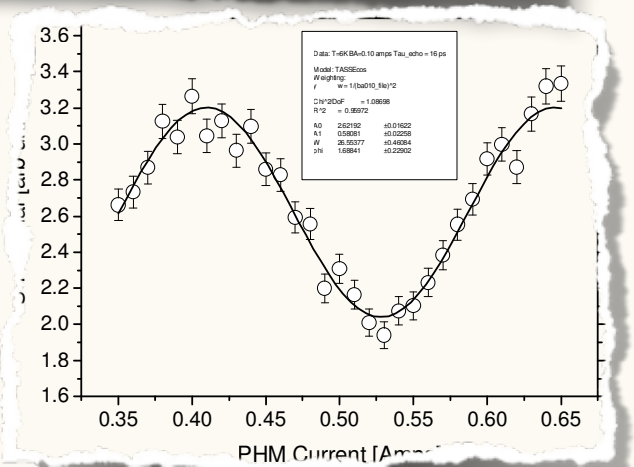
Experimental: *Inelastic TAS Spin Echo*



$$k_f = 2.66 \text{ Å}^{-1}$$

$$(Q, \omega) = (2.5 \text{ Å}^{-1}, 14.7 \text{ meV})$$

Incoherent SE = 1/3 Coherent SE

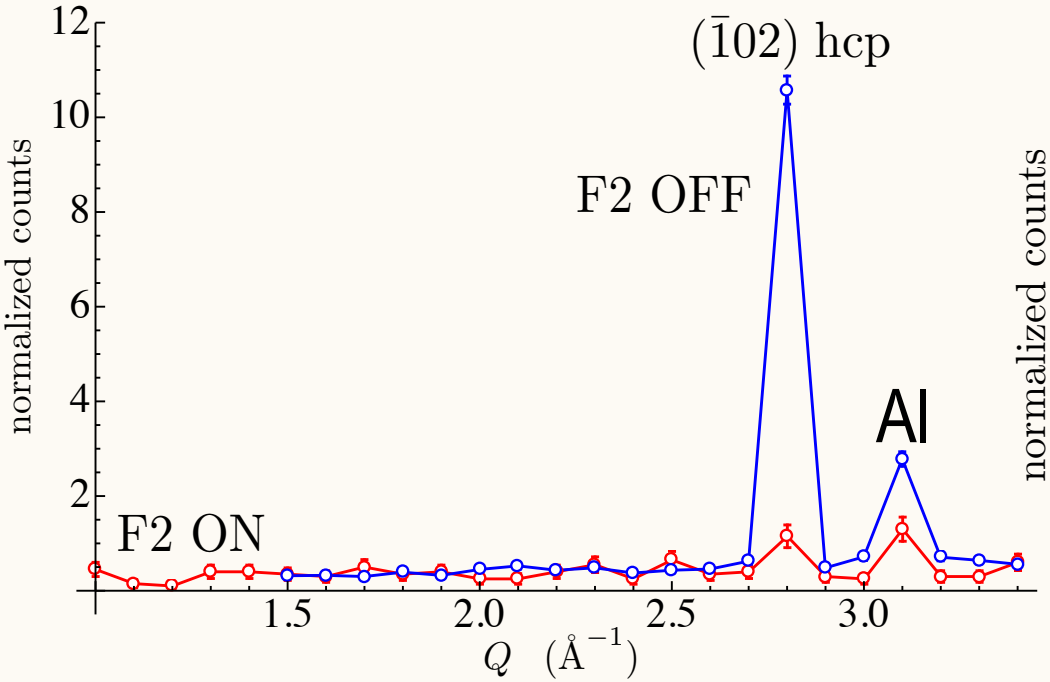


Results

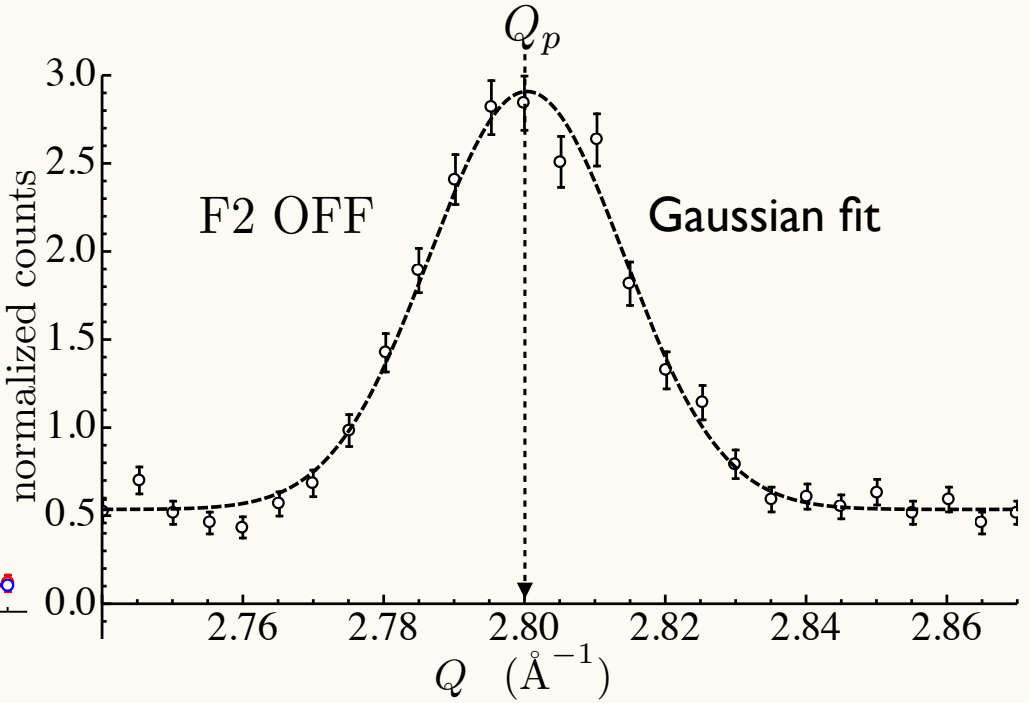
Bragg scattering

F1 OFF, $E = 0$ meV, $T = 13.2$ K

Rough scans



Fine scans around 2.8



- Monocrystalline sample
- High-purity *para*-H_2

$c_0 = 0.001 \pm 0.002$

$Q_p = 2.8004 \pm 0.0008$ Å^{-1}, $T = 13.17$ K, i.e., $0.95\,T_{tp}$

$Q_p = 2.8023 \pm 0.0006$ Å^{-1}, $T = 3.1$ K, i.e., $0.22\,T_{tp}$

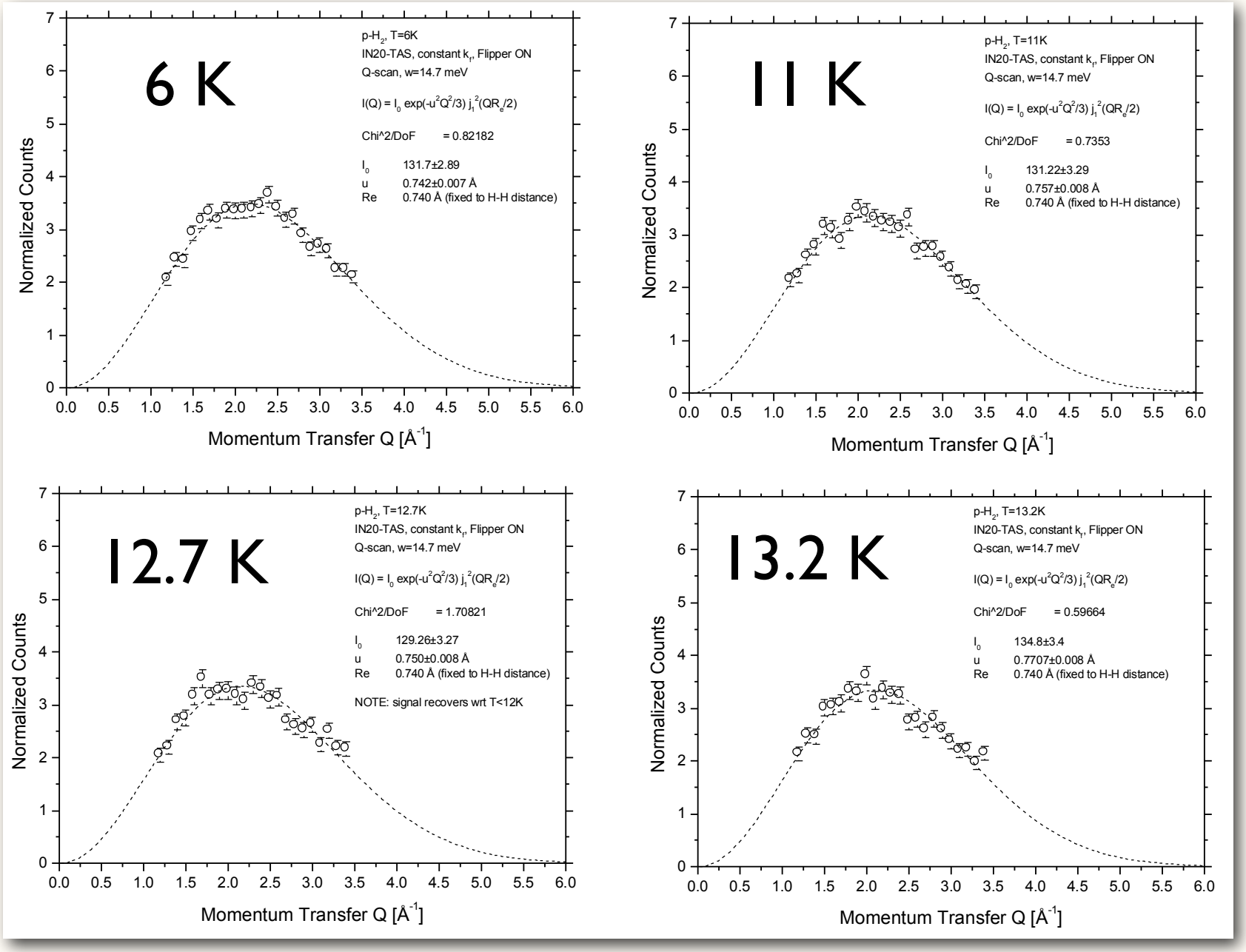
$Q_p(13.7)/Q_p(3.1) = 1.0007$

hcp with $R_{NN} = 3.78$ Å

Results

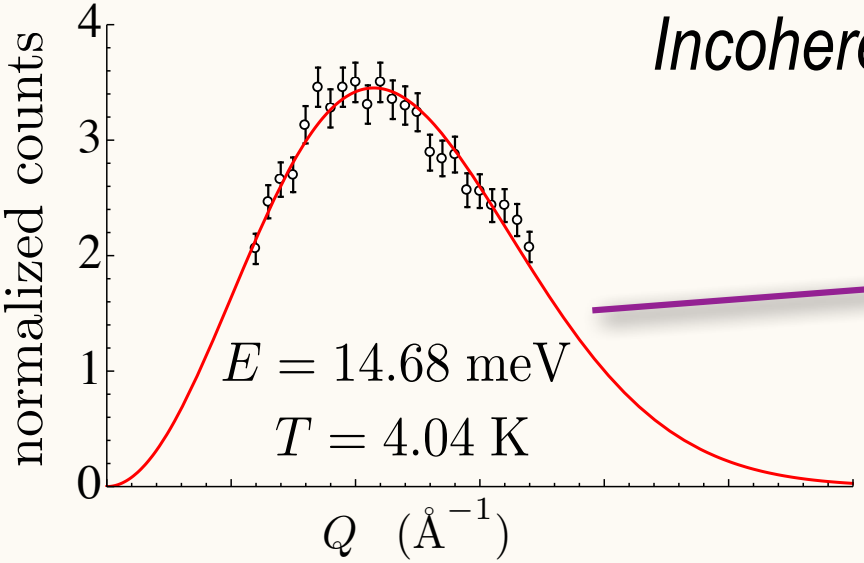
Incoherent Q-scans

F2 ON, $E \simeq 14.7$ meV



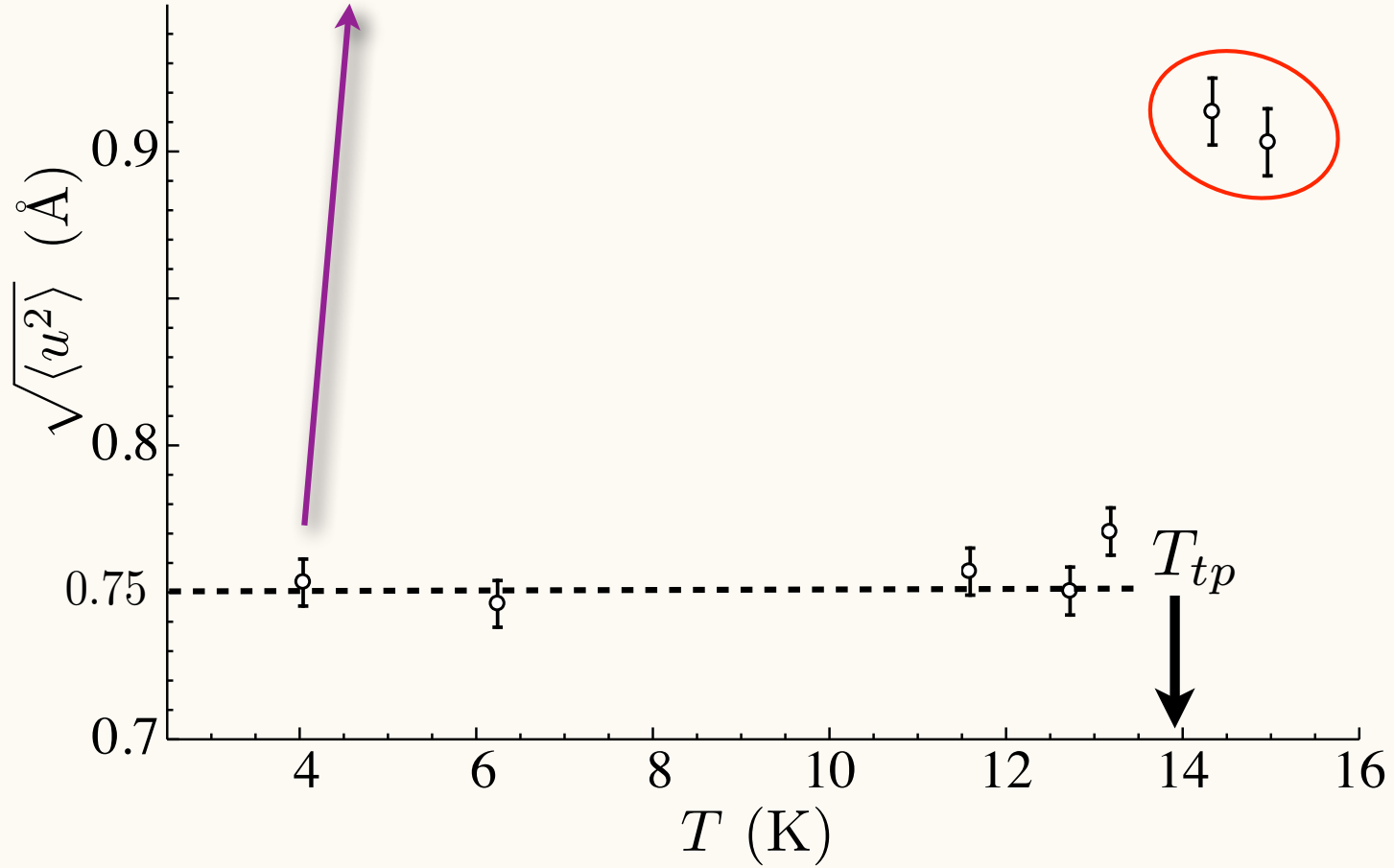
Results

Incoherent Q-scans



$$I(Q) = j_1(Q\,d/2)\exp\left(-\frac{\langle u^2\rangle}{3}Q^2\right)$$

$d = 0.74$ Å

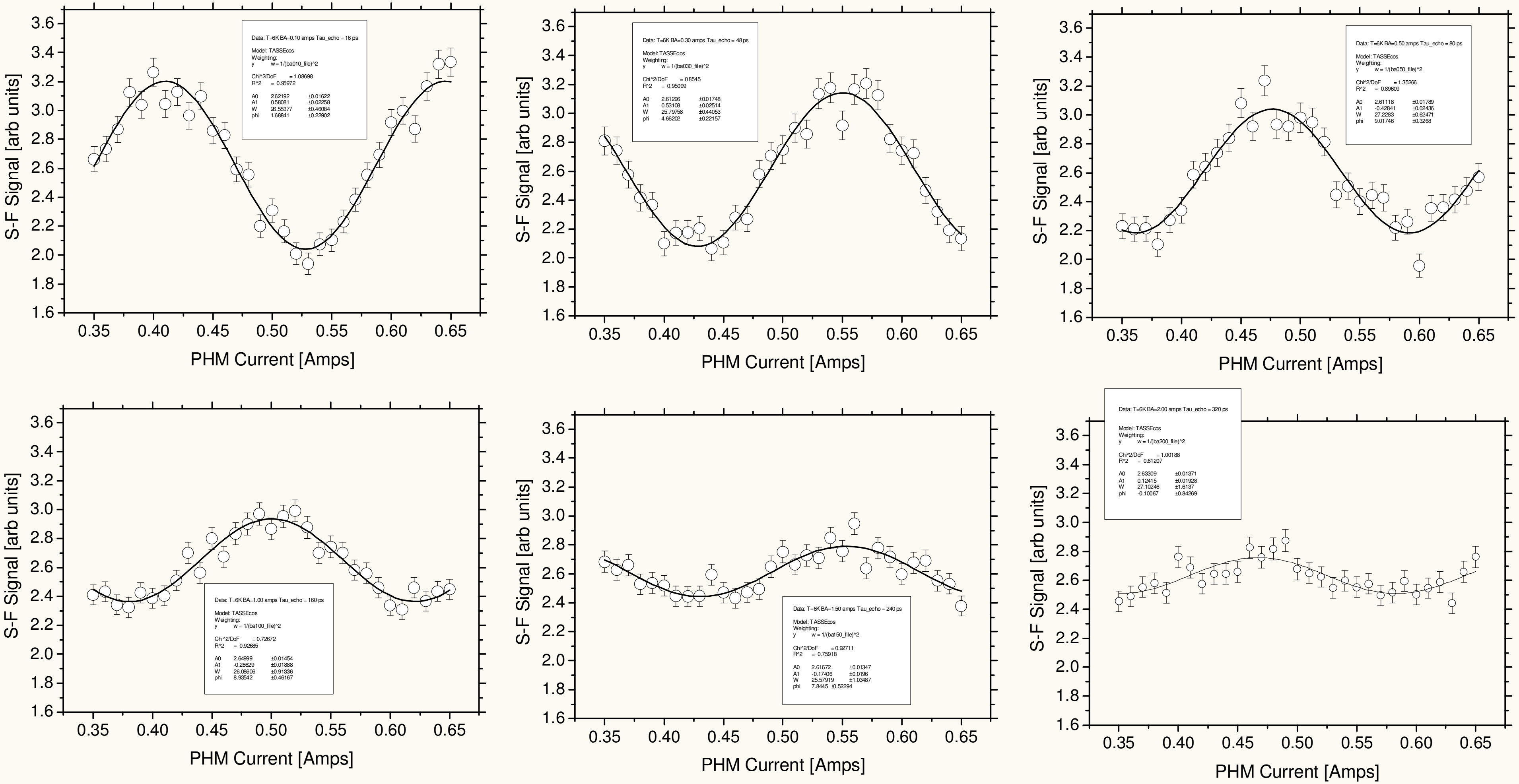


Liquid

Results

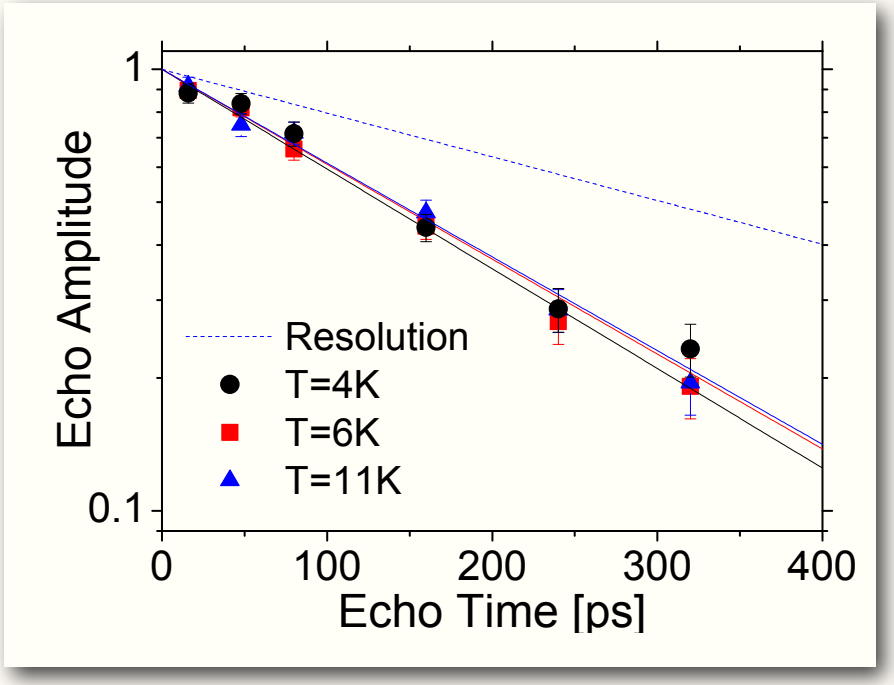
Spin echo scans

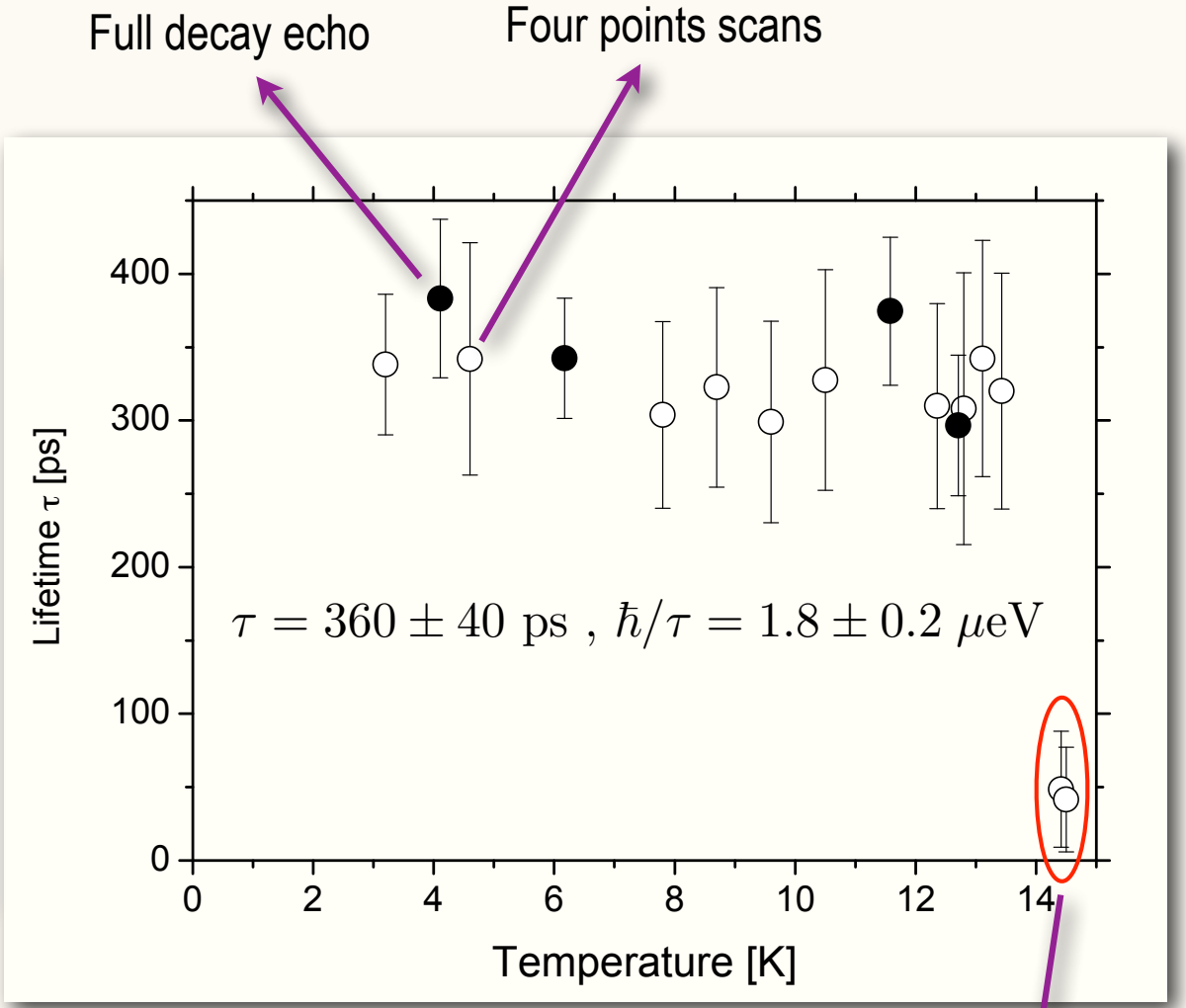
$$E \simeq 14.7\ \mathrm{meV},\ Q = 2.5\ \text{Å}^{-1},\ T = 6\ \mathrm{K}$$

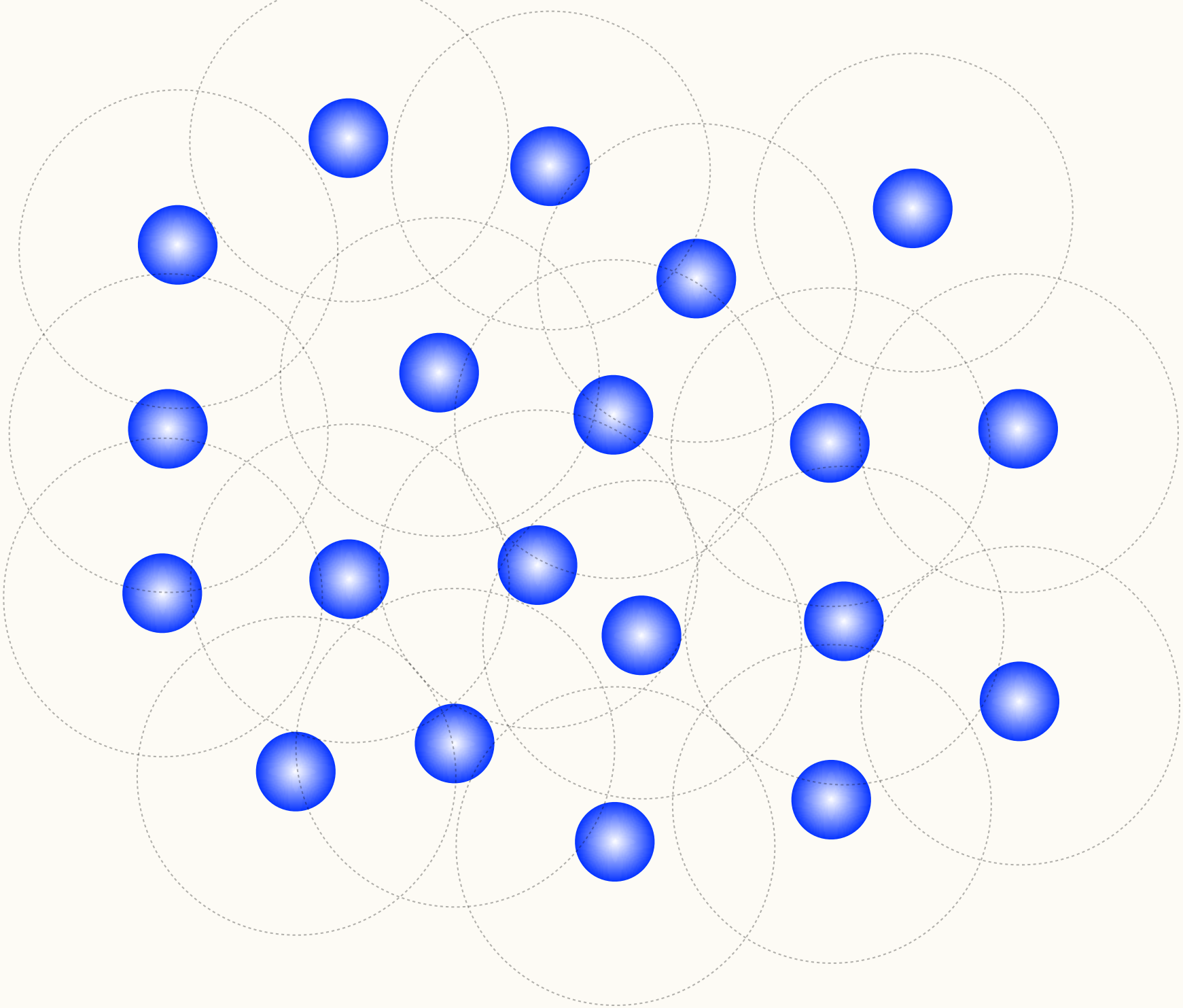


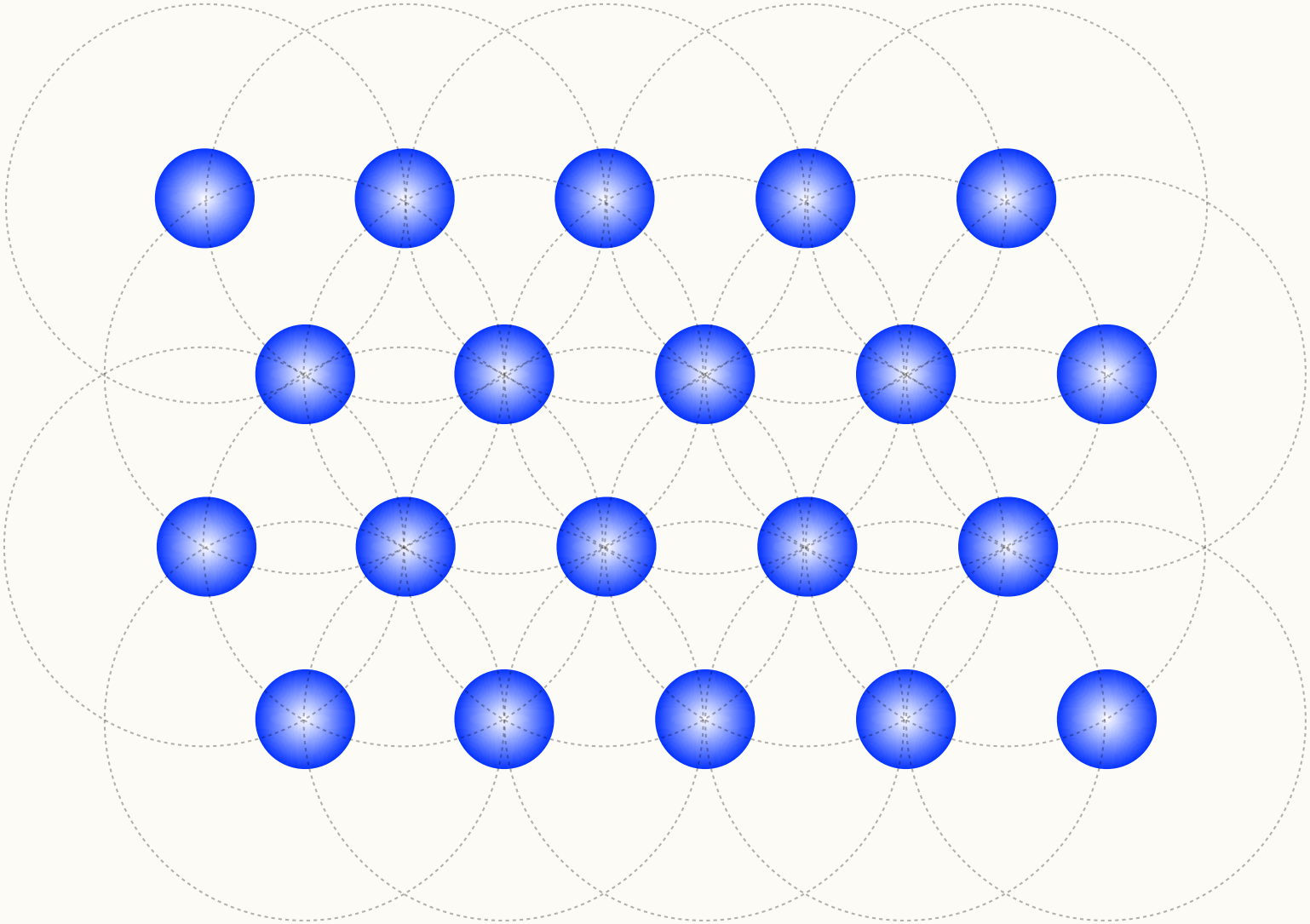
Results

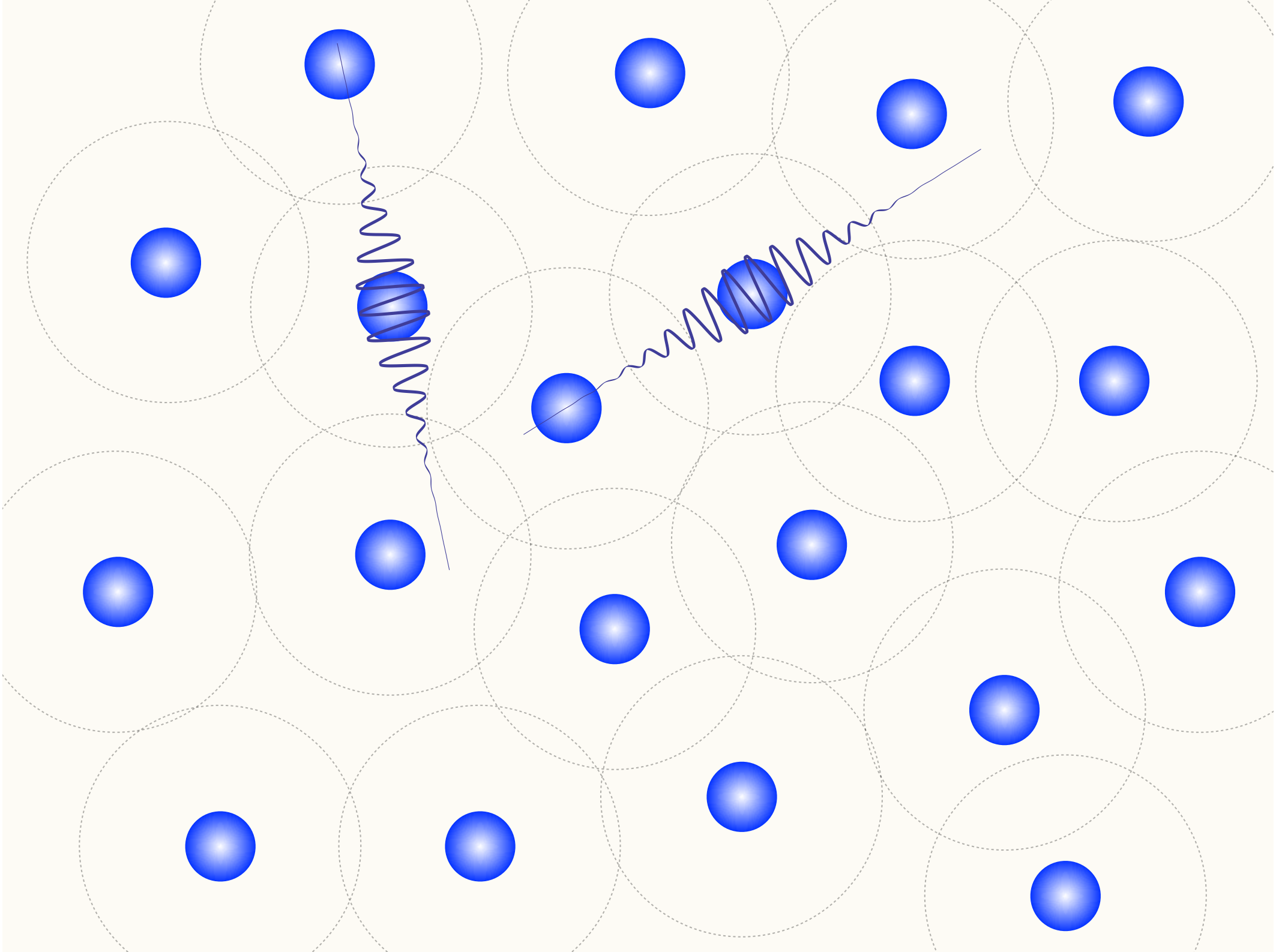
Inelastic Spin Echo

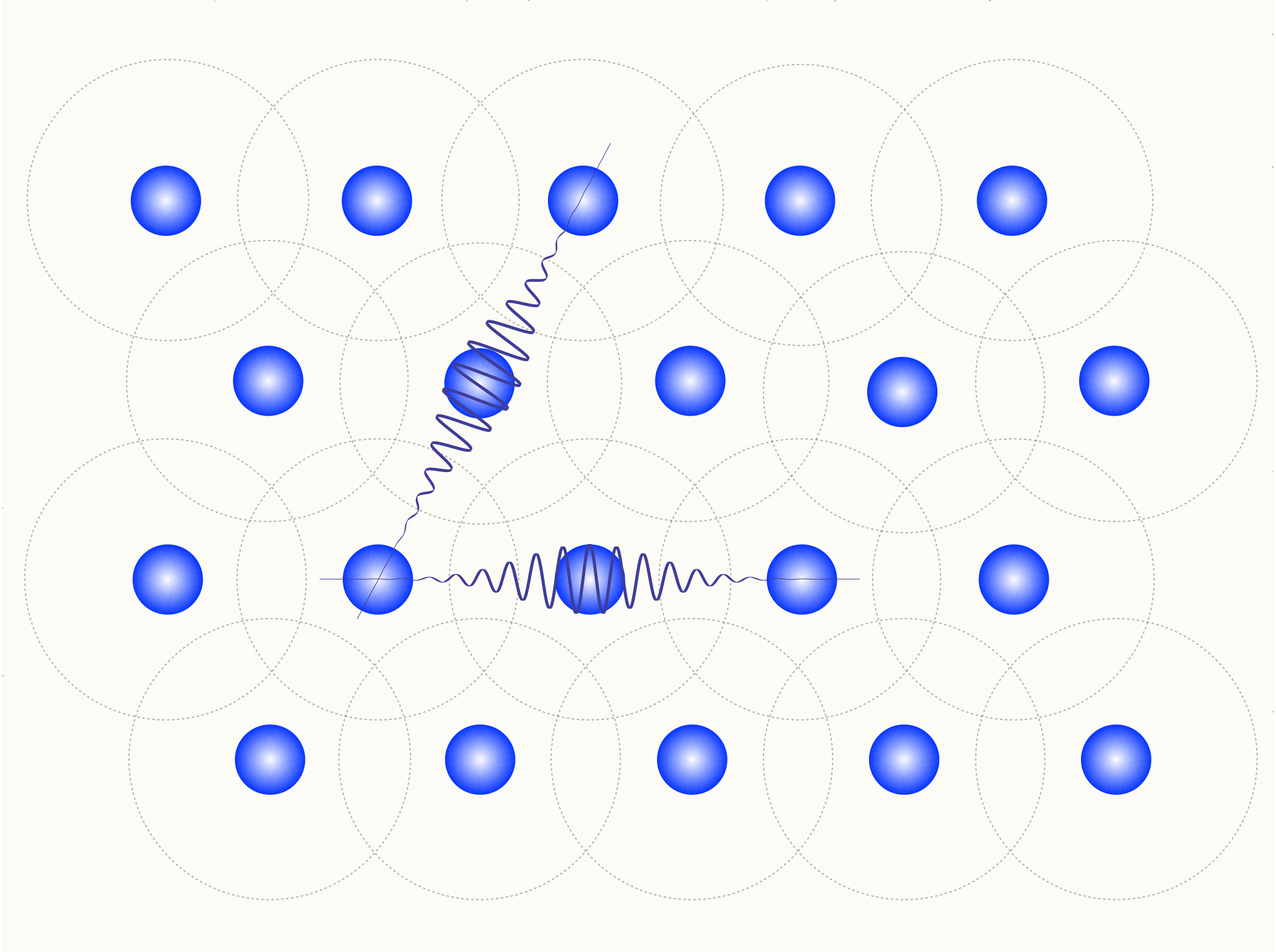












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