

Simulating muon spins - QUANTUM

James Lord
ISIS

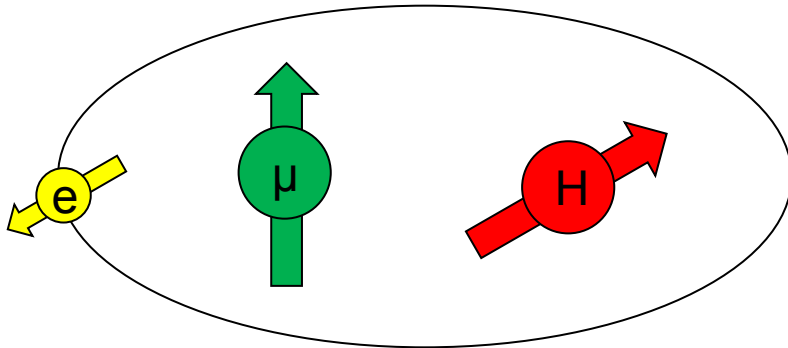


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The problem

- Muon + nearby nuclei and electrons
- Variety of interactions
 - dipolar, hyperfine, quadrupole
- Static and RF magnetic fields
- Diffusion
- How does the muon's spin evolve?



Quantum mechanics

- $H\psi = E\psi$

- $P(t) = \langle \psi | S_\mu | \psi \rangle$

- $\psi = a_1 |\uparrow\uparrow\rangle + a_2 |\uparrow\downarrow\rangle + a_3 |\downarrow\uparrow\rangle + a_4 |\downarrow\downarrow\rangle$

- $H = \begin{vmatrix} a & b & c & d \\ b^* & e & f & g \\ c^* & f^* & h & i \\ d^* & g^* & i^* & j \end{vmatrix}$

- $P(t) = p_1 \cos(\omega_1 t + \phi_1) + p_2 \cos(\omega_2 t + \phi_2) + p_3 \cos(\omega_3 t + \phi_3) \dots$



A job for a computer!

Details of muon/nucleus /electron spins

The screenshot shows the 'Enter Quantum Parameters' dialog box. Key sections are circled in red:

- Spin Parameters:** A table with columns for position (X, Y, Z), spin (I, MHz/T), easy axis (x, y, z), Electron?, and hyperfine splitting (A, D, eta). Two states are defined with spin I = 1/2 and MHz/T values of 135.5 and -2802.
- Hyperfine Coupling:** Parameters for hyperfine splitting (A, D, eta) and quadrupole (vQ, eta) are specified for each state.
- Calculation Type:** 'Plain calc' is selected. Max time for plot is 20 us with 1000 bins. Measurement is 'i - Integral asym'.
- Geometry/Averaging:** 'LF' is selected. 'Uniform' is chosen for averaging. '100% muon' is selected for the detector.
- RF Parameters:** Frequency is 10, Intensity is 0, and Phase is 0. 'Linear B1' is selected for the RF type.
- Sweep Parameters:** 'Field' is selected for the sweep type. The sweep range is from 0 to 5000 with 1001 steps.

Hyperfine coupling

RF settings

Scan fields or other parameters

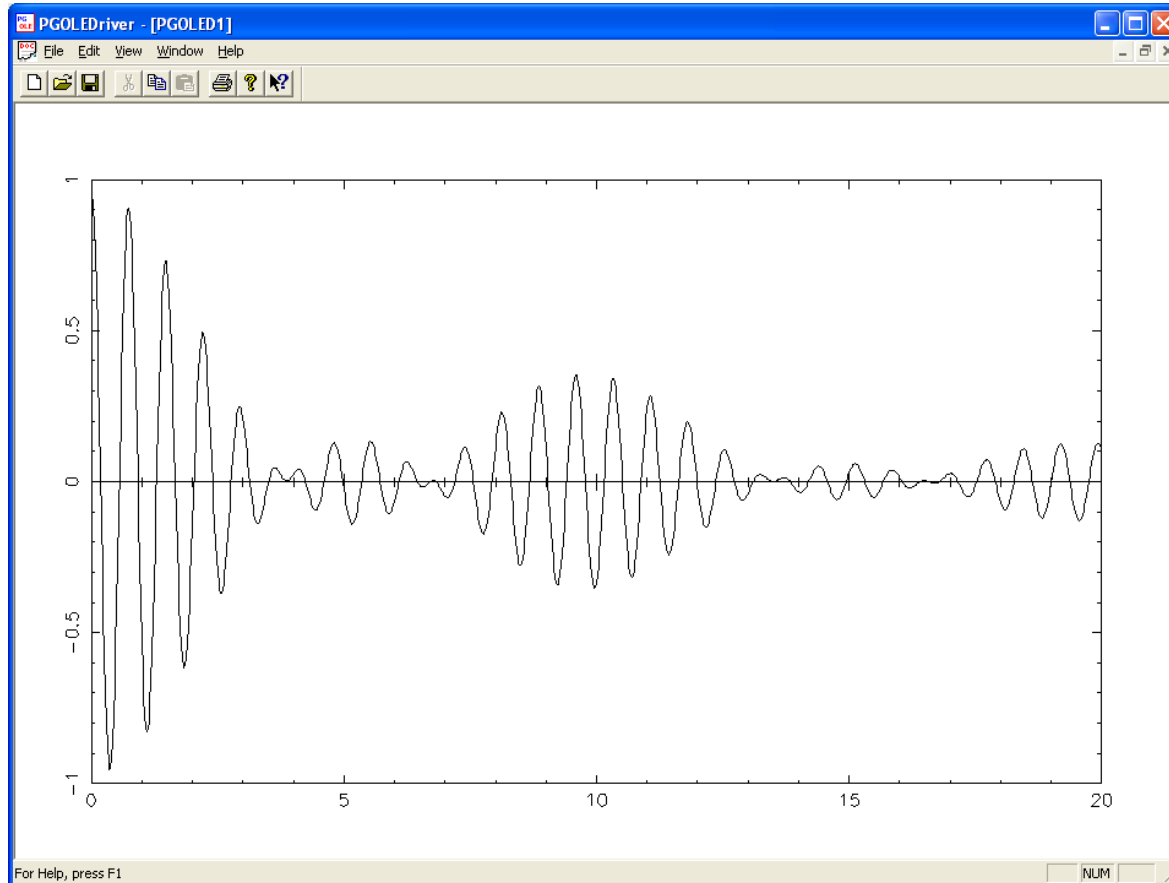
What to calculate

LF/TF and powder averaging options



Transverse field spectra

Polarisation



Time

Simulation for CdS including both Mu^+ and Mu^0 , with conversion

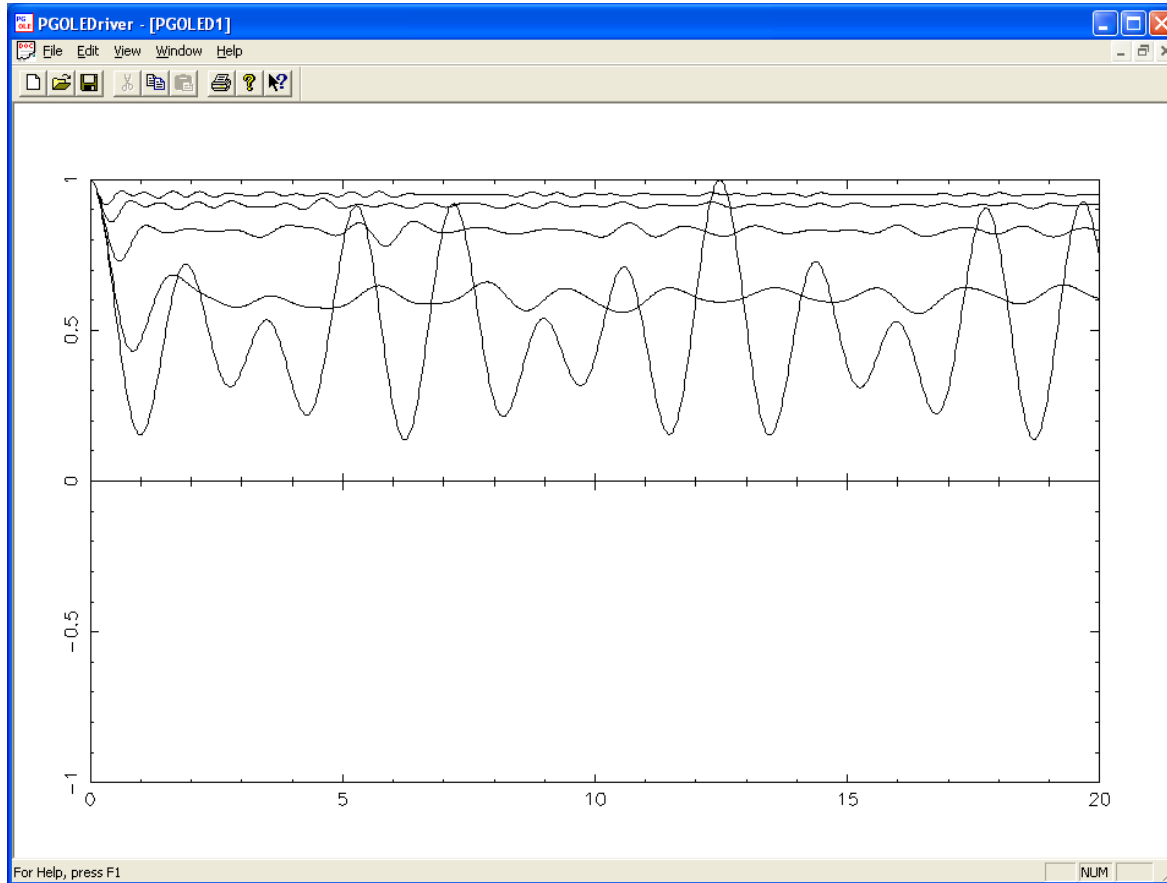


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Dipolar - $F\mu F$

Polarisation



Longitudinal
Fields
0,25,50,75,
100G

Time

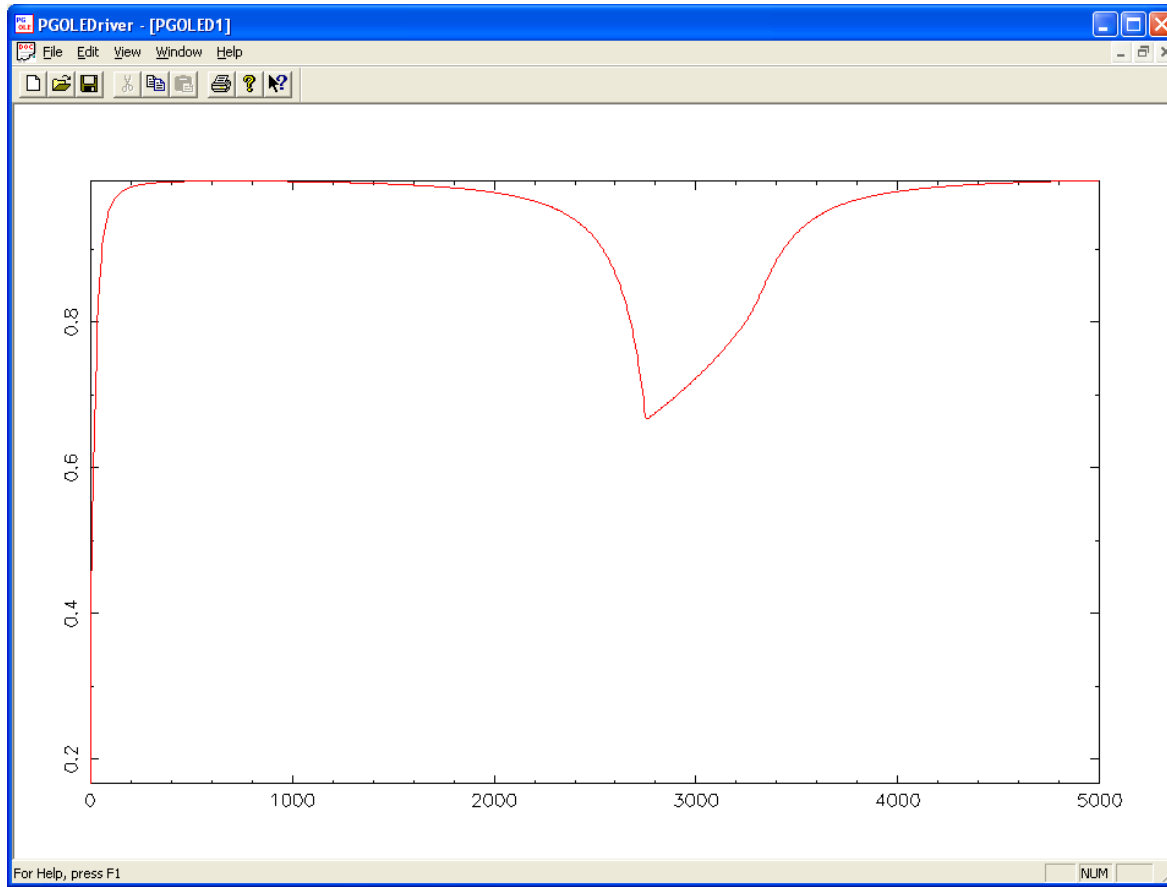


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Level crossing

Integral asymmetry



Magnetic field



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Options

Simulations giving

- Time spectrum $P(t)$
- Integral asymmetry
- Relaxation rates, frequencies
- Frequency spectrum

Scan field or other parameters

Fitting to

- Integral asymmetry, relaxation rates
- Raw data sets $P(t)$

Vary almost any parameter(s)

