

Simulating muon spins - QUANTUM

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ISIS

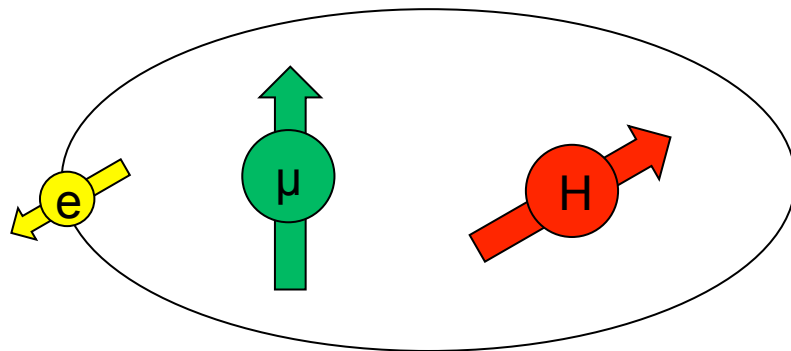


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The problem

- 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

What to calculate

LF/TF and
powder
averaging
options

The screenshot shows the 'Enter Quantum Parameters' dialog box with several sections highlighted by red circles:

- Top section:** Contains 'Num of Spins' (2) and 'Num of charge states or sites' (1).
- State 1 table:** A table with columns for position (X, Y, Z), spin (I, MHz/T), easy axis (x, y, z), Electron?, hyperfine splitting (none, A, D, eta), quadrupole (vQ, eta), Spin flip rate, and Random field. The first two rows are populated with values like 1/2, 135.5, 0, 0, 1, 80, 10, 0, 0, 0, 0.
- Calculation type section:** Includes 'Calculation type' (Plain calc), 'Max time for plot' (20 us with 1000 bins), 'Measurement' (Integral asym), 'TF Bkgnd' (0), 'Lifetime' (2.197), 'Start t' (0), and 'Shift with B'.
- Geometry/Averaging section:** Includes radio buttons for LF, RF, RRF, Specified axes, ZF Powder, and Orientations from File. It also has fields for B0, B1, Initial pol, and Detector phase angle for TF (deg).
- RF parameters section:** Includes 'Frequency' (10), 'Intensity (G)' (0), 'Phase (deg)' (0), 'RRF Harmonic' (0), and 'Phase (deg)' (90).
- Sweep section:** Includes radio buttons for Field, Field Angle x-z, 2D Vector field x-z, 2D angle theta/phi, 2D field/angle, 2D freq/angle, and 2D Field/Freq. It also has fields for 'to', 'step', and 'Log num of steps'.

Hyperfine
coupling

RF settings

Scan fields
or other
parameters

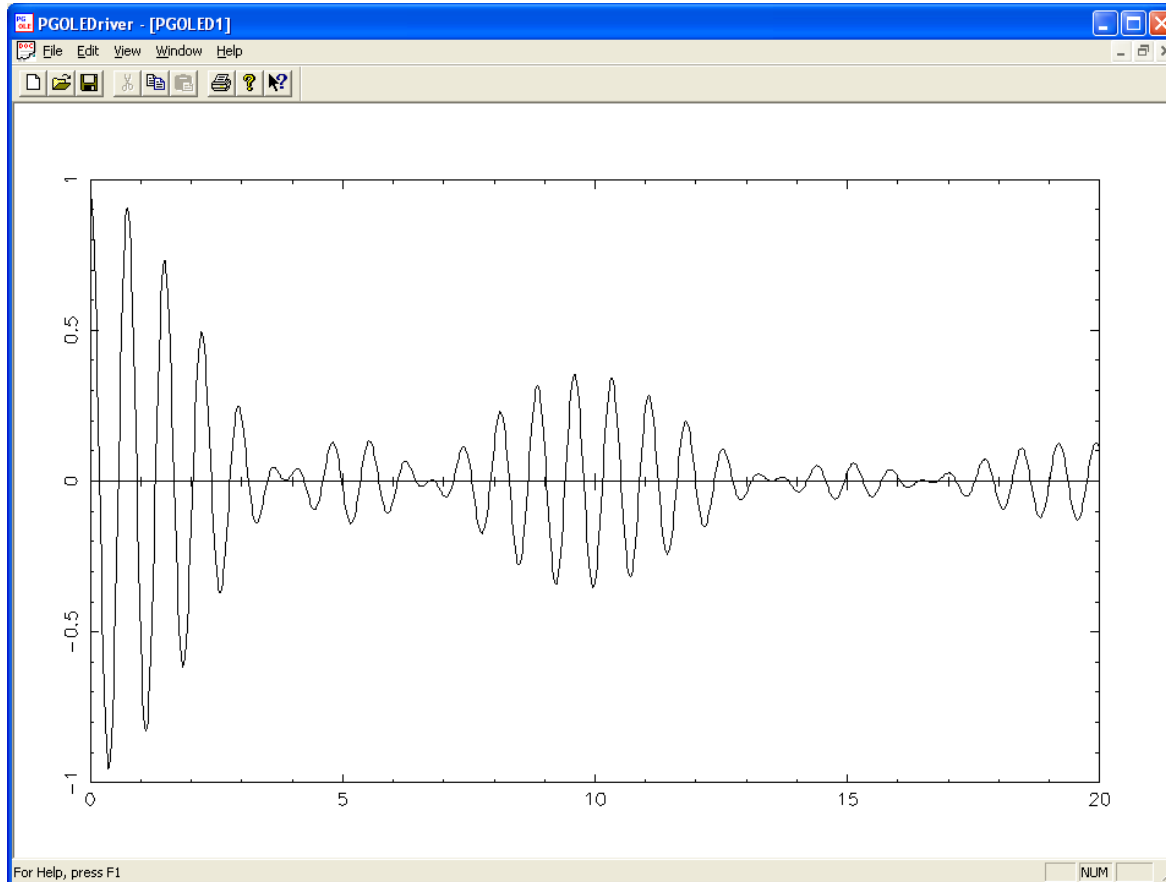


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Transverse field spectra

Polarisation



Time

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

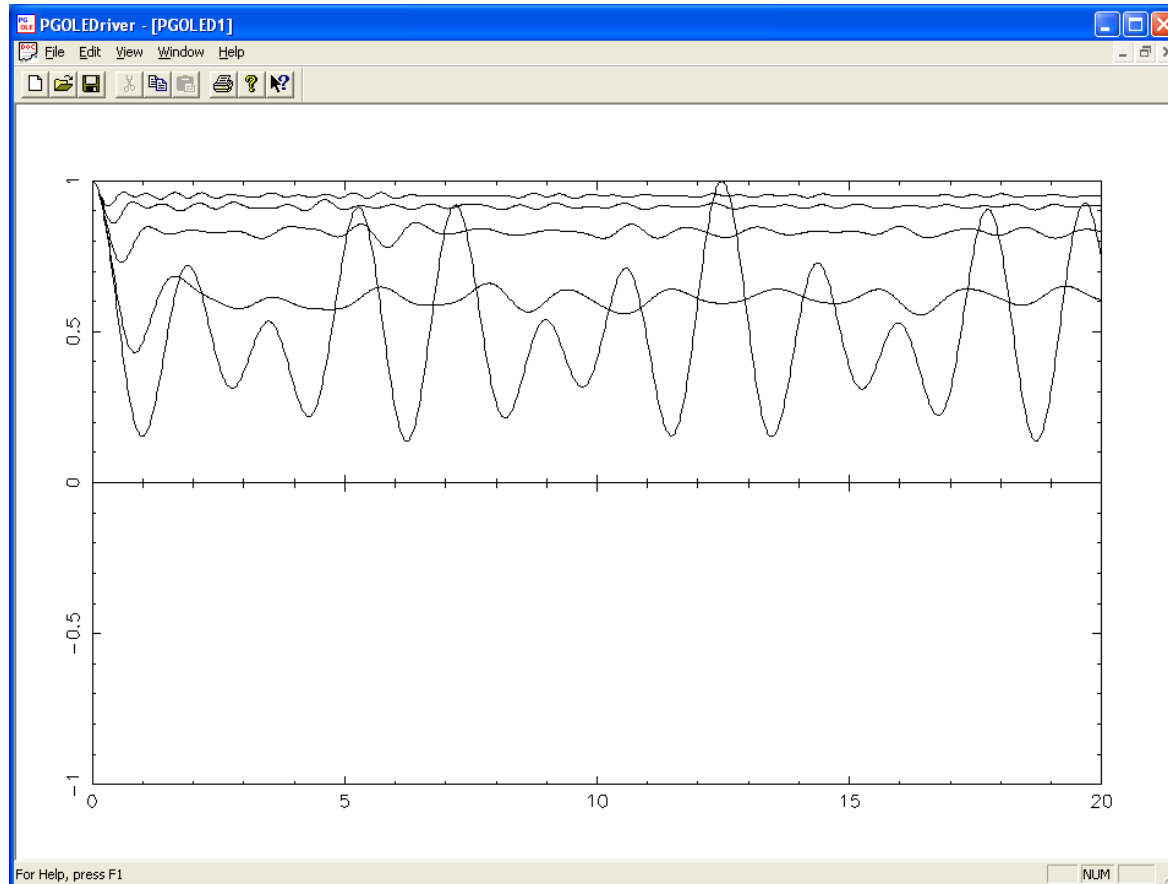


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Dipolar - $F\mu F$

Polarisation



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

Time



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Level crossing

