Simulating muon spins - QUANTUM

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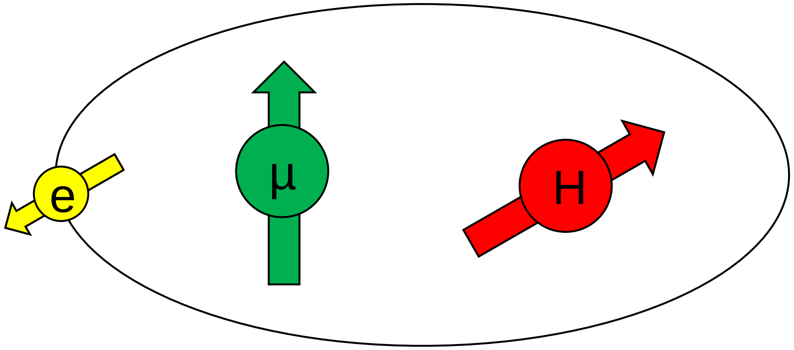
ISIS

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?



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Quantum mechanics

- $H\psi = E\psi$
- $P(t) = <\psi|\sigma_\mu|\psi>$

- $\psi = a_1|\uparrow\uparrow> + a_2|\uparrow\downarrow> + a_3|\downarrow\uparrow> + a_4|\downarrow\downarrow>$
- $$H = \begin{vmatrix} a & b & c & d \\ b^* & e & f & g \\ c^* & f^* & h & i \\ d^* & g^* & i^* & j \end{vmatrix}$$

Can solve analytically but much easier to do numerically

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Density Matrix

- $P_\mu^\alpha(t) = \mathrm{Tr}(\sigma_\mu^\alpha \, \rho(t))$

  $= \mathrm{Tr}(\sigma_\mu^\alpha \, U(t) \, \rho(0) \, U^+(t))$

  $= \Sigma \, a_{mn} \exp(i\omega_{mn} \, t)$

- Evaluate P(t) for time bins 0-20μs
  - Can then fit a model function
- Or calculate the integral asymmetry directly $I = \int P(t) \exp(-t/\tau_\mu) \, dt$
- Or plot frequency spectrum directly

Resonance

- "Integrate" the evolution operator U over a whole cycle of the RF waveform
- Then solve for longer times
- Works best for high RF frequencies where the applied frequency is not resolved in the measured signal (e.g. integral asymmetry)

Relaxation and site changes

- Elements of ρ evolve as a series of coupled differential equations
- Multiple sites: two or more copies of ρ each evolving with its own U(t)
- Assemble into larger set of equations (matrix)
- Site changes: $d/dt\ \rho_{mn}^{b} = -d/dt\ \rho_{mn}^{a} = K_{ab}\ \rho_{mn}^{a}$
- Relaxation: $d/dt\ \rho_{mn} = -d/dt\ \rho_{m'n'} = \lambda_i(\rho_{m'n'} - \rho_{mn})$

  where (m,n) and (m',n') differ by spin i
- Solve to get a series of damped oscillating terms

Pulsed experiments

- Before step change: Hamiltonian H_1, evolution matrix $U_1(t)$
- Change at $t=t_1$ to H_2
- Evaluate $\rho(t<=t_1) = U_1(t_1)\ \rho(0)\ U_1^{+}(t_1)$
- Then use new evolution matrix U_2
- Evaluate $\rho(t>t_1) = U_2(t-t_1)\ \rho(t=t_1)\ U_2^{+}(t-t_1)$

  Take care about different eigenstates!

Orientation

- Zero field: $P = 1/3(P_x+P_y+P_z)$
- General: Integrate over θ,φ (Monte Carlo or uniform)
  - Double integral for TF or RF
- Single crystals: average over equivalent axes

Scans and Loops

- Vary some parameter of H
  - e.g. magnetic field, hyperfine coupling, distances for dipolar interaction
- Re-evaluate P(t) or Integral asymmetry
- Collect results
  - Set of time spectra
  - Repolarisation or ALC spectrum

Fitting data

- Use Quantum as a fit function in Mantid
- Specify which model parameters are to be fit parameters
- E.g. F-mu distance, hyperfine constants, relaxation rates, TF field magnitude

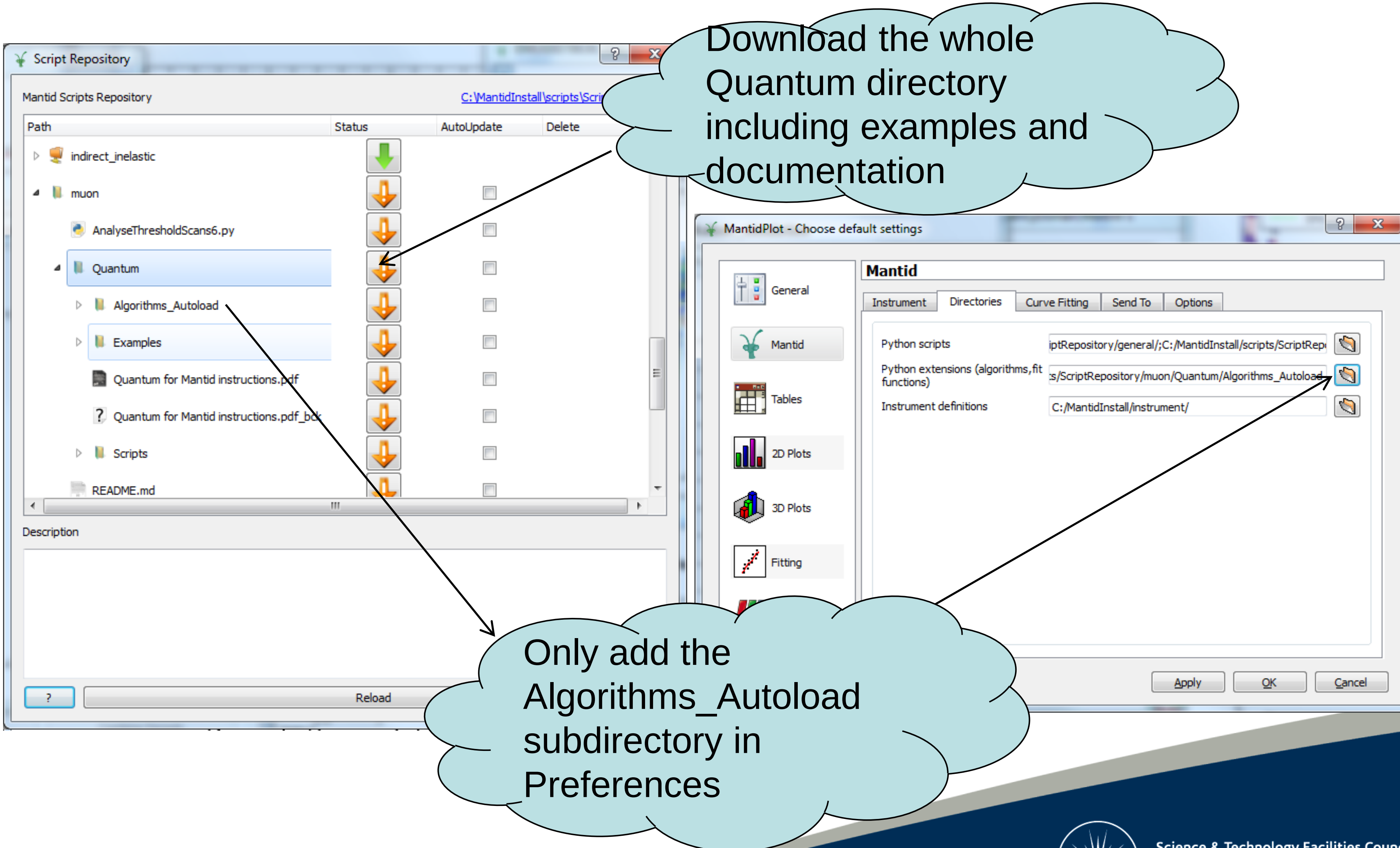
Fitting raw data

- Fit to one or more spectra (global parameters)
  - Different magnetic fields
  - Different detectors (x,y) in TF
  - Different "periods" (RF on or off)
- P(t) evaluated at experimental time bins

Fitting integral data

- Evaluate <P(t,B)> at the applied field values
- Usually add an empirical background function (instrumental correction)

Installing in Mantid



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Using Quantum

Table-1

	Code[Y]	Value[Y]
1	spins	Mu,e
2	a(Mu)	80,10,1,1,1
3	lfuniform	10
4	measure	integral
5	loop0par	bmag
6	loop0range	0.1,0.5,201
7		
8		
9		
10		

- Create a Table workspace
  - Helper algorithm for this
- Fill it with instructions

Using Quantum

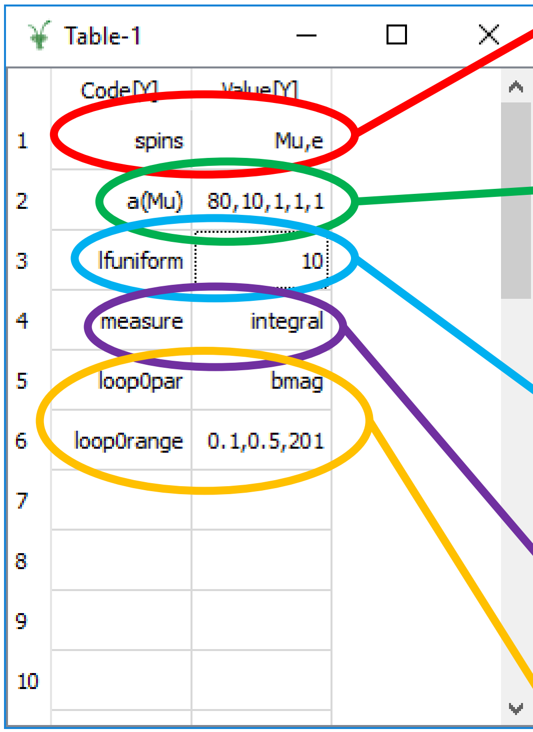


Table-1

	Code[Y]	Value[Y]
1	spins	Mu,e
2	a(Mu)	80,10,1,1,1
3	lfuniform	10
4	measure	integral
5	loop0par	bmag
6	loop0range	0.1,0.5,201
7		
8		
9		
10		

Always a "spins" line saying what the muon is interacting with

Hyperfine coupling between the muon and the electron (implied). Axial symmetry along (1,1,1)

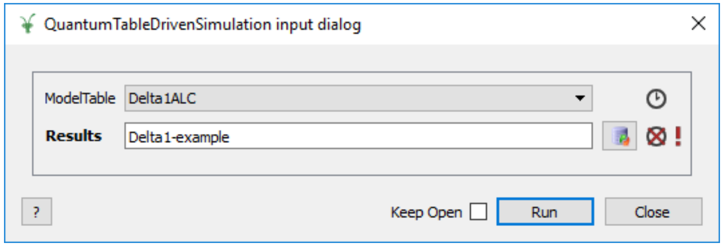
Average over orientations of the "sample" with respect to the muon polarisation and field, e.g. powder. Here it's LF

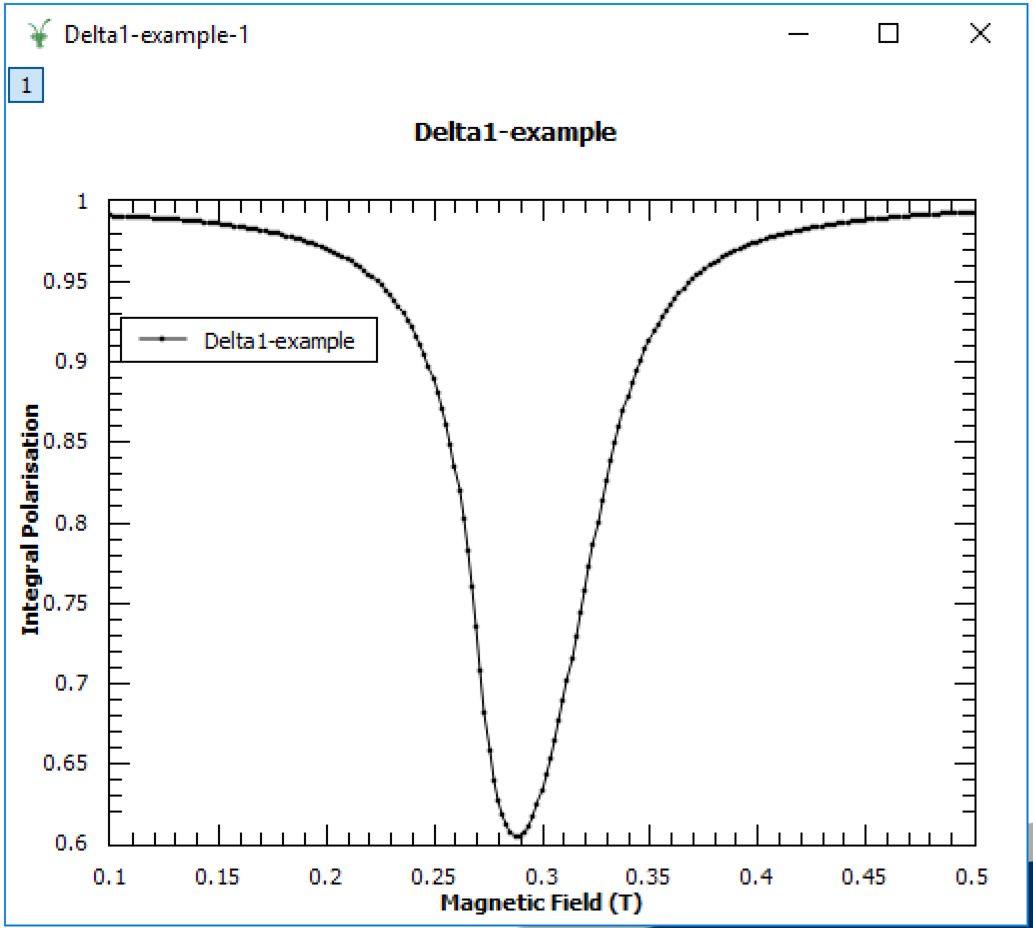
What quantity to plot

Scan the magnetic field from 0.1 to 0.5 Tesla with 201 steps. Zeeman interactions implied.

Using Quantum

Run Quantum





Output:

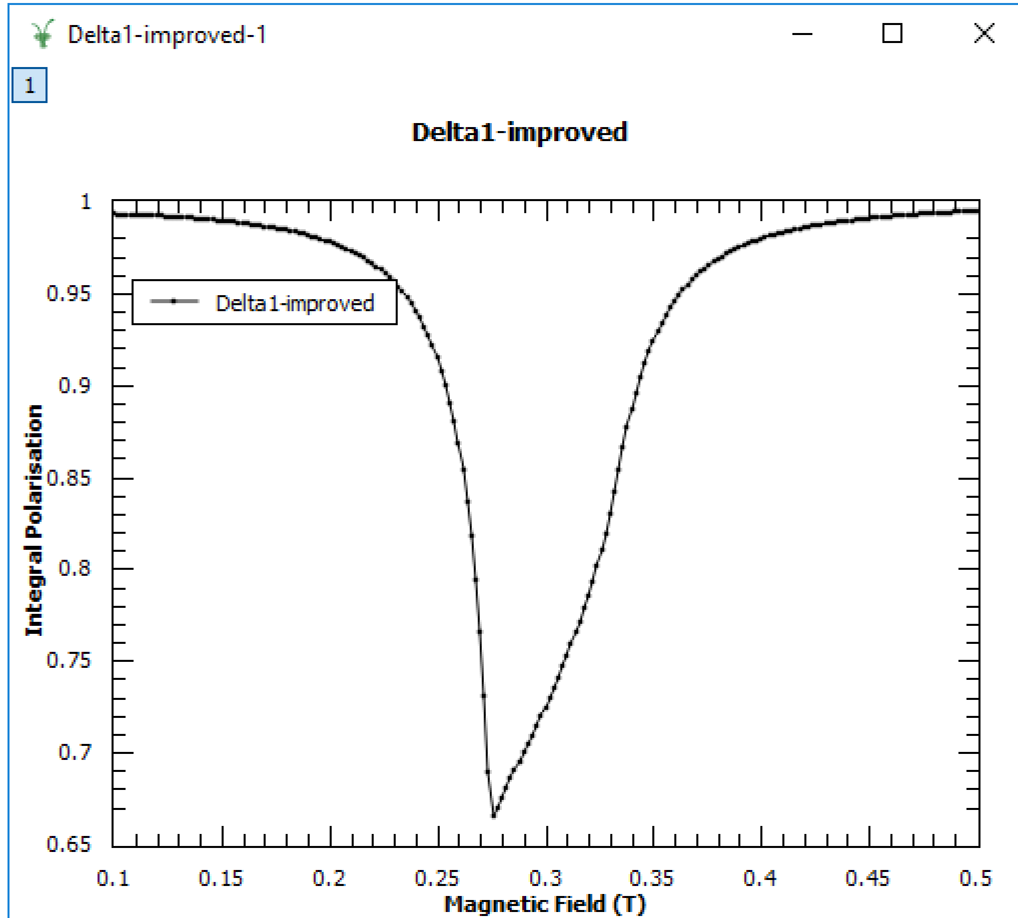
(not a very good powder pattern)

Improving the output

- Increase the averaging of orientations

Table-1

	Code[Y]	Value[Y]
1	spins	Mu,e
2	a(Mu)	80,10,1,1,1
3	lfuniform	200
4	measure	integral
5	loop0par	bmag
6	loop0range	0.1,0.5,201
7		
8		
9		
10		

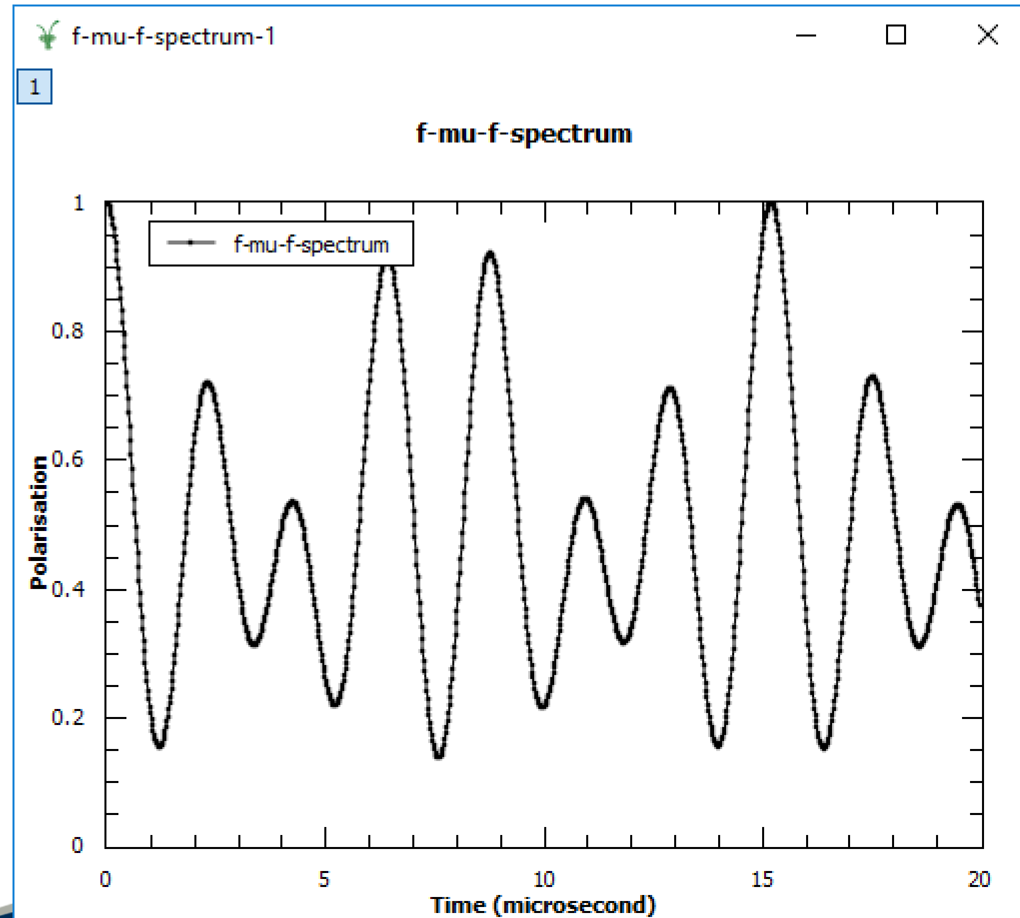


More options

- Specify location of spins – calculates dipolar coupling

Table-3

	Code[Y]	Value[Y]
1	spins	Mu,F1,F2
2	r(Mu)	0,0,0
3	r(F1)	0,0,-1.23
4	r(F2)	0,0,1.23
5	measure	timespectra
6	lfaxes	1,0,0
7		

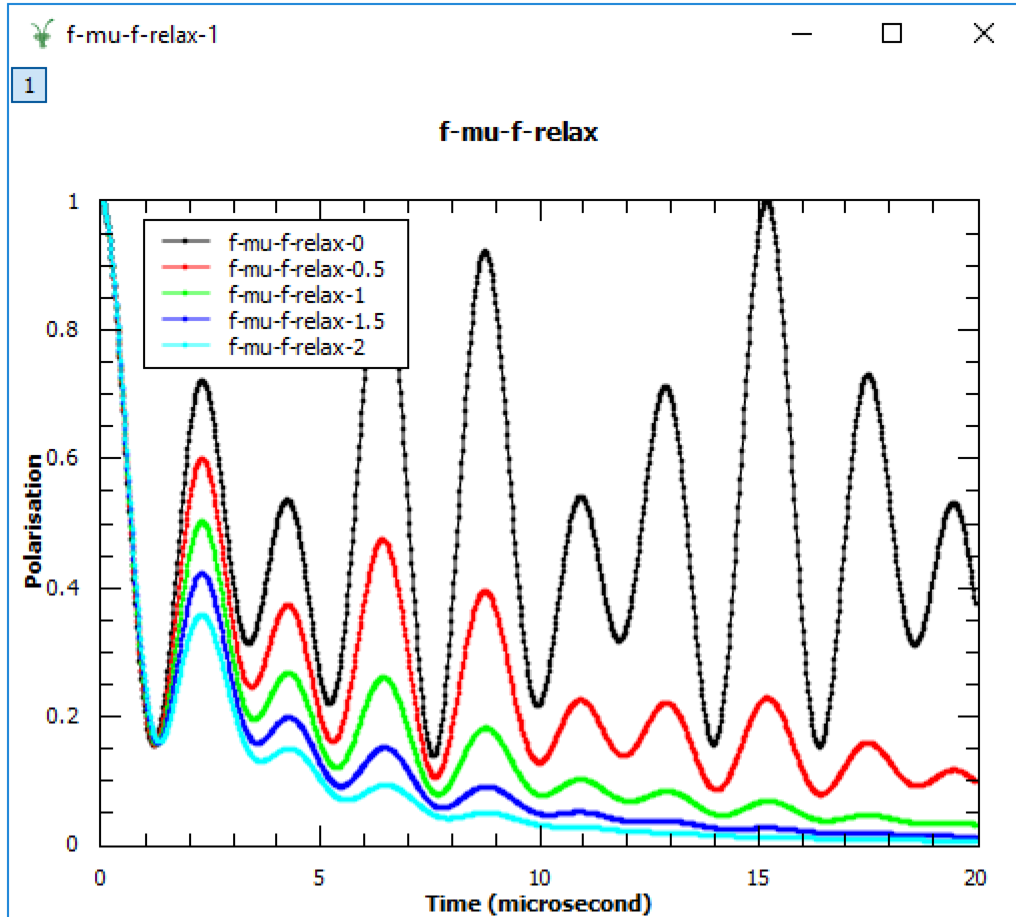


More options

- Add relaxation

Table-3

	Code[Y]	Value[Y]
1	spins	Mu,F1,F2
2	r(Mu)	0,0,0
3	r(F1)	0,0,-1.23
4	r(F2)	0,0,1.23
5	measure	timespectra
6	lfaxes	1,0,0
7	dynamic	1
8	relax(F1)	0.1
9	relax(F2)	0.1
10	loop0par	relax(F1);relax(F2)
11	loop0range	0,0.5,0,0.5,6
12		



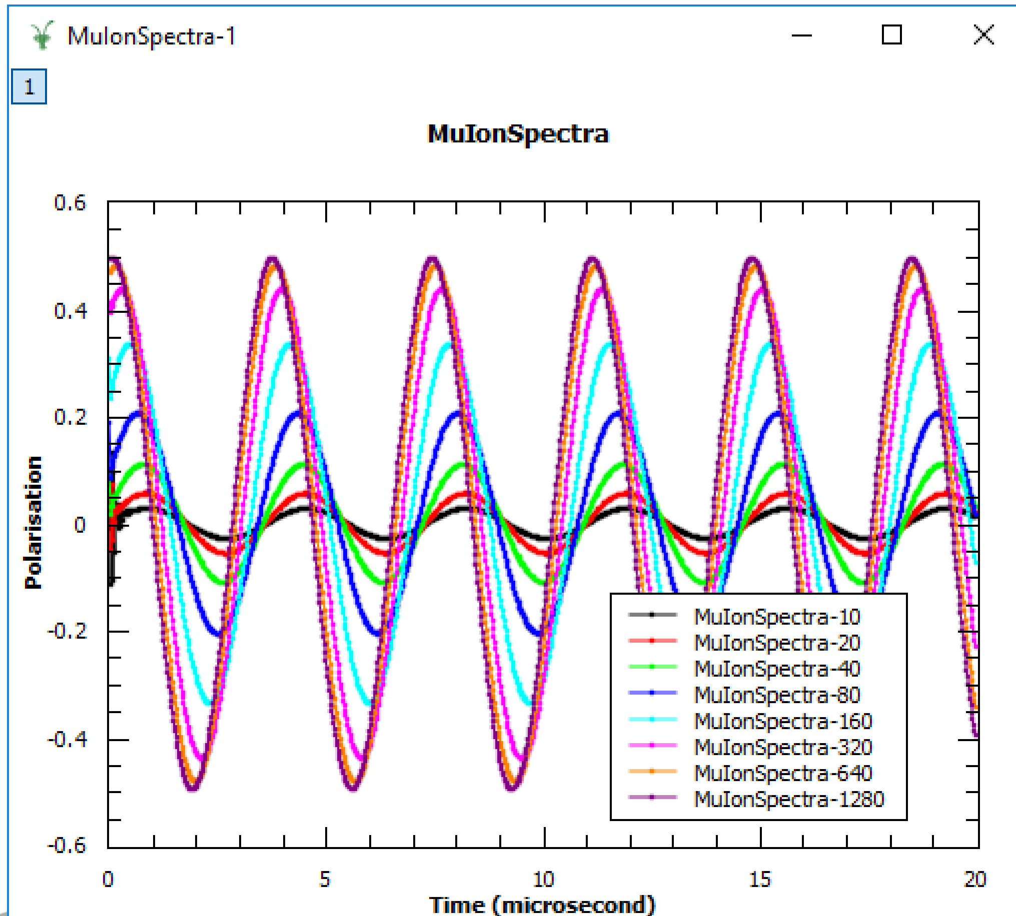
More options

- Muonium converting to diamagnetic, measure TF precession

Table-4

	Code[Y]	Value[Y]
1	spins	Mu,e
2	dynamic	2
3	pop(0)	1
4	pop(1)	0
5	a(@0,Mu)	4400
6	convert(0,1)	100
7	measure	timespectra
8	tfuniform	1
9	bmag	0.002
10	loop0par	convert(0,1)
11	loop0range	10,1280,-8
12		

Negative steps for log scale



Fitting the simulated results within Quantum

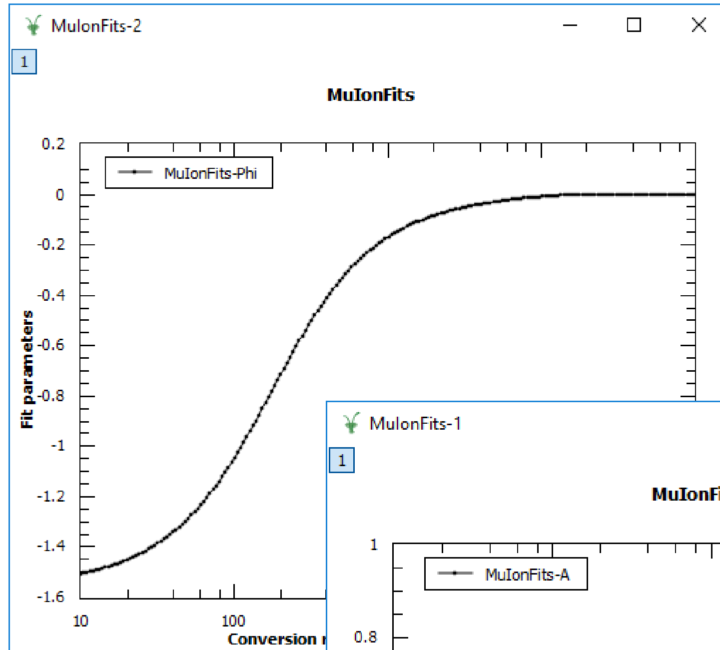
Table-4

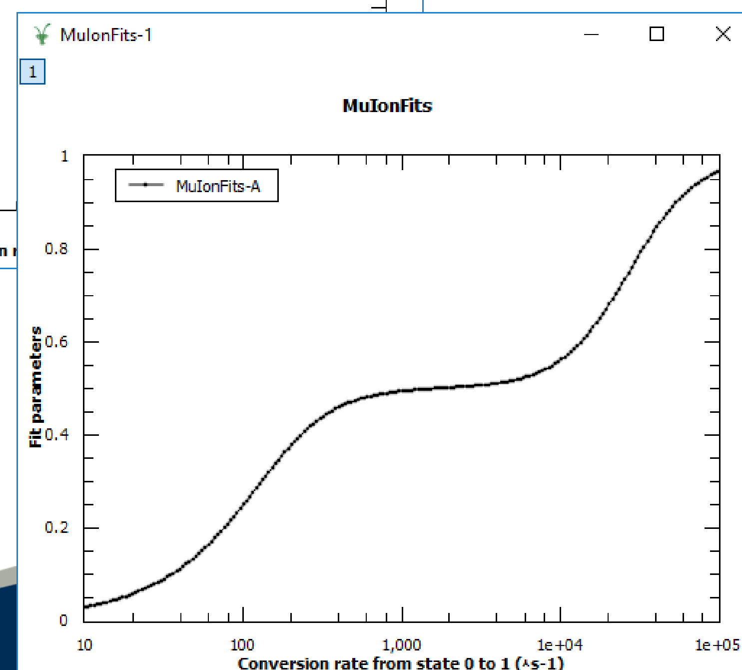
	Code[Y]	Value[Y]
1	spins	Mu,e
2	dynamic	2
3	pop(0)	1
4	pop(1)	0
5	a(@0,Mu)	4400
6	convert(0,1)	100
7	measure	fit
8	tfuniform	1
9	bmag	0.002
10	loop0par	convert(0,1)
11	loop0range	10,100000,-200
12	fitfunction	name=ExpDecayOsc,A=0.5,Frequency=0.271,Phi=-0.5

MuIonFits

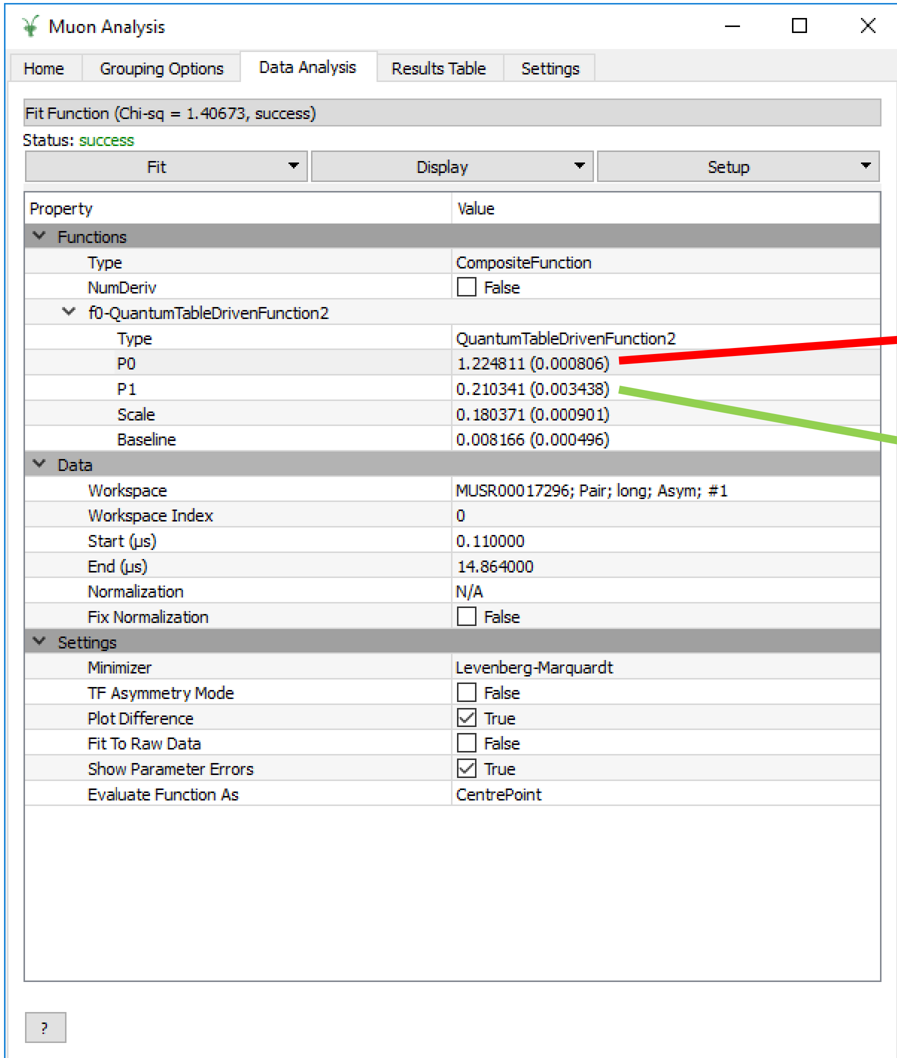
Y values | X values | Errors

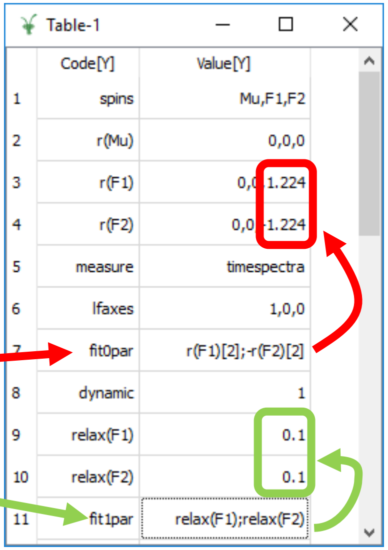
	0 10^s-1	1 10.473
A	0.0282173	0.0295496
Lambda	1.70715e-05	1.76169e-
Frequency	0.271011	0.271011
Phi	-1.5096	-1.50694
Cost function value	0.0404696	0.037281

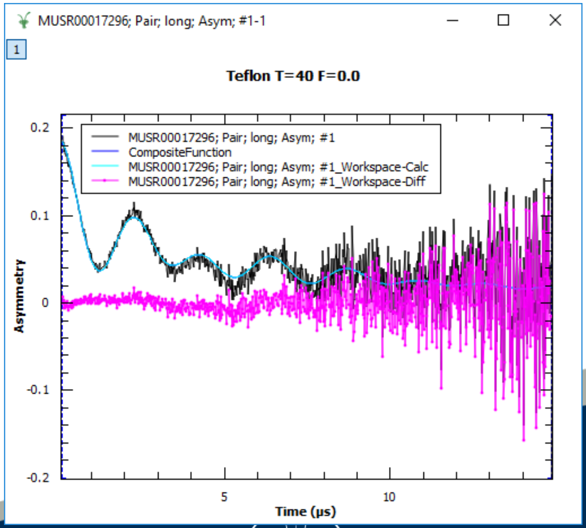




Using Quantum to fit data







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More…

- Quadrupole splitting
- RF resonance (pulsed or CW) and rotating reference frames
- Rare earth ions and crystal fields
- TF Frequency spectra
- Lower level code
  - Flexible, faster, but harder to set up
- Have a go yourself in the tutorials!