# Some Examples of the use of Quantum

# 1) Repolarisation of tetrahedral muonium in silicon

 $Mu_T$  in silicon is an isotropic muonium species which is mobile between cage-centred sites in the Si lattice. At 100K, its hyperfine parameter A=2010MHz, and there is no dipolar part (D=0). A repolarisation curve for this species can be generated in Quantum using the input parameters shown in Fig. 1. The repolarisation curve is generated by calculating the average asymmetry for each of a number of field values, and is shown in Fig. 2.

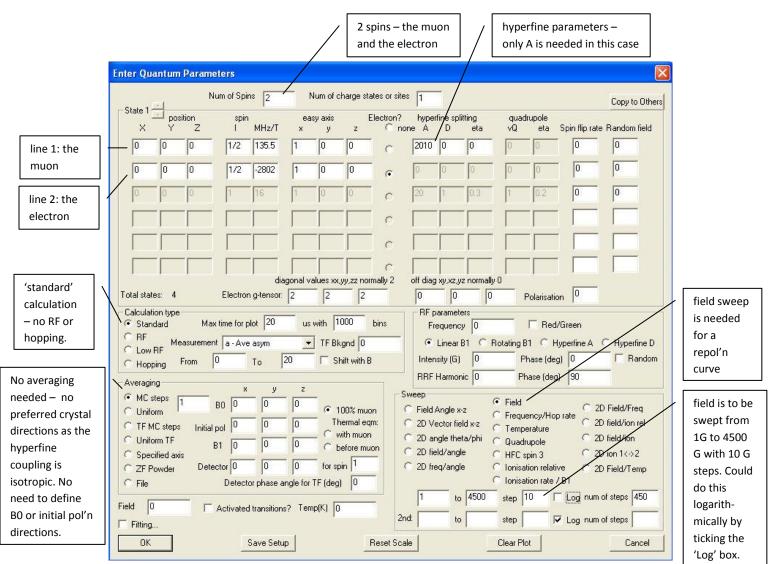


Fig 1: Quantum inputs for isotropic muonium in silicon.

With the parameters as above, click 'OK'. If you just want the repolarisation curve, you can click 'no' or 'cancel' to all the various options for saving files, etc. At the end of the calculation, you'll get a plot in the 'PGOLEDriver' screen like the one in Fig. 2. Note the repolarisation starts at 0.5 at low field and finishes close to 1 at full field.

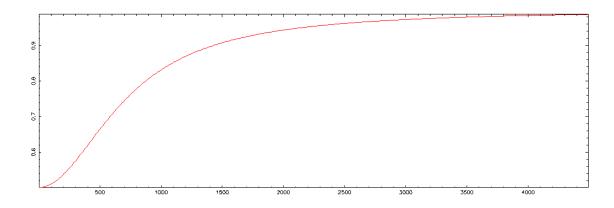


Fig. 2. Repolarisation curve for isotropic muonium in Si at around 100K.

#### 2. Repolarisation of bond centred muonium in Si

In this case the muonium species,  $Mu_{BC}$ , has axial symmetry, along a [111] bond direction. The hyperfine parameter is expressed in terms of the isotropic (A) and dipolar (D) parts; Quantum defines these as:

A=1/3(A<sub> $\perp$ </sub> + 2A<sub> $\parallel$ </sub>); D=2/3(A<sub> $\perp$ </sub> - A<sub> $\parallel$ </sub>), where A<sub> $\perp$ </sub> and A<sub> $\parallel$ </sub> are the perpendicular and parallel components of the hyperfine interaction.

For  $Mu_{BC}$  in Si at low temperatures, A=-67.33MHz, D=50.52 MHz.

In this case, it is necessary to define axes for both the muonium species, the applied field and the initial muon polarisation direction.

# Case 2a: [100] crystal

In this case, we will assume that the field direction and initial muon polarisation direction area along [100]. This means that there are four equivalent [111] muonium species. The Quantum input parameters are given in Fig. 3; the resulting repolarisation curve is given in Fig. 4.

	the 'easy axis' for the muonium species has to be defined – [111] in this case
line 1: the	Num of Spins 2 Num of charge states or sites 1 Copy to Others   State 1 position spin easy axis Electron? hyperfine splitting quadrupole   X Y Z 1 MHz/T x y z none A D eta Spin flip rate Random field   0 0 1/2 135.5 1 1 1 c 67.33 50.52 0 0 0
line 2: the electron	0   0   0   1/2   2802   1   0
Applied field B0 is along [100]	diagonal values xx,yy,zz normally 2 off diag xy,xz,yz normally 0   Total states: 4   Electron g-tensor: 2   2 2   0 0   Polarisation   0
Initial muon polarisation is along [100]	• Standard     • Max time for plot     20     us with     1000     bins     Frequency     10     □     Red/Green     • Linear B1     C     Rotating B1     C     Hyperfine A     C     Hyperfine     Averaging     Averaging
Detectors along [100]	x   y   z     C   MC steps   1   0   0   0   100% muon     C   Dinform   B0   1   0   0   0   100% muon     C   Thermal eqm:   C   Field Angle x-z   Frequency/Hop rate   C 2D Field/Freq     C   Uniform T   B1   1   0   0   C with muon   C 2D angle theta/phi   C Quadrupole   C 2D field/ion     C   Specified axis   C   Direction (C 2D field/angle   C HEC spin 3   C 2D ion 1<>2
'specified axis' must be ticked to allow the B field to be defined	C ZF Powder   Detector 11   0   0   for spin 1     C File   Detector phase angle for TF (deg)   0   0   File   Image: Constant on relative   C 2D Field/Temp     Field   0   Image: Constant on relative   C 2D Field/Temp   Image: Constant on relative   C 2D Field/Temp     Field   0   Image: Constant on relative   C 2D Field/Temp   Image: Constant on relative   C 2D Field/Temp     Field   0   Image: Constant on relative   C 2D Field/Temp   Image: Constant on relative   C 2D Field/Temp     Field   0   Image: Constant on relative   C 2D Field/Temp   Image: Constant on relative   C 2D Field/Temp     Field   0   Image: Constant on relative   Constant on relative   C 2D Field/Temp     OK   Save Setup   Reset Scale   Clear Plot   Cancel

Fig. 3. Quantum inputs for  $Mu_{BC}$  in Si, field along [100]

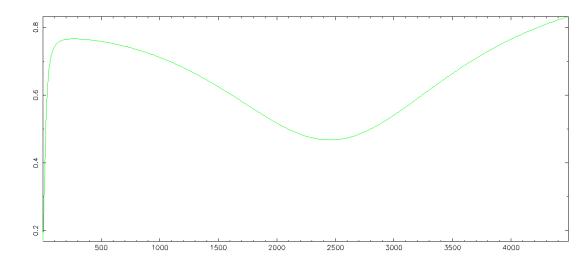


Fig. 4. Repolarisation curve for bond-centred muonium in Si, [100] crystal.

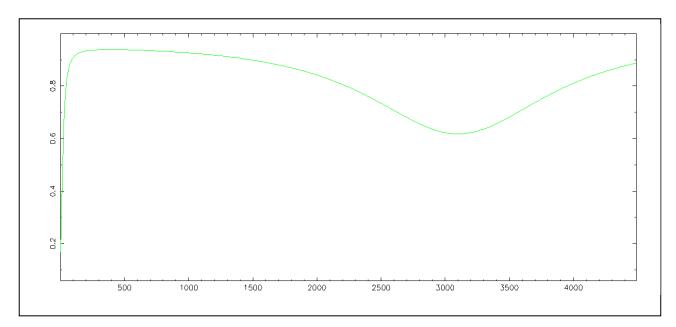
# Case 2b: [111] crystal

In this case, we assume that the field and initial muon polarisation area along [111]. This means that there are is one muonium species which lies within bonds that are parallel to the field (species, or 'state', 1), and three species lying within bond which are not parallel to the field direction (species, or state, 2). This requires a slightly more complicated Quantum input scheme, as the two different muonium species need to be created. This is done by:

- changing the 'Num of charge states or sites' at the top of the input screen to 2.
- entering the correct parameters for Mu<sub>BC</sub> species 1 in Quantum's 'State 1'
- press 'copy to others', which duplicates State 1 to State 2
- entering the correct parameters for Mu<sub>BC</sub> species 2 in Quantum's 'State 2' (just change the muonium state axis)
- running Quantum at which point it will ask for the relative state abundances.

Quantum then does its calculations twice, once for each muonium species, and combines these according to the abundances given.

(NB – for multiple states, as here, Quantum runs through the calculations for each state separately when in 'standard' and 'RF' modes – when in 'hopping' mode, all the states are combined into one big calculation.)



See Fig. 6 for the Quantum input screens. The resulting repolarisation plot is given in Fig. 5.

Fig. 5. Repolarisation curve for bond-centred muonium in Si, [111] crystal.

still 2 spins in each state this screen shows State 1: Mu <sub>BC</sub> parallel to the field (25% of Mu <sub>BC</sub> species)	Enter Quantum Parameters     Num of charge states or sites   2   Copy to Others     State 1   position   spin   2   Num of charge states or sites   2   Copy to Others     X   Y   Z   I   MHz/T   x   y   z   Electron?   hyperfine splitting   quadrupole   vQ   eta   Spin flip rate Random field     0   0   0   1/2   135.5   1   1   1   67.33   50.52   0	number of states is now 2 Mu <sub>BC</sub> axis is [111] for State 1.
Applied field B0 is along [111], as is the initial polarisation and detector Specified axis still ticked.	Index stels.   Image: Clear Definition of the clear Biology of the cle	
this screen shows State 2: Mu <sub>BC</sub> not parallel to the field (75% of MuBC species)	Enter Quantum Parameters     Num of Spins   Copy to Others     State 2	The only difference from the State 1 screen is that the Mu <sub>BC</sub> axis is now along one of the [111] crystal directions that is not parallel to the applied field.

Fig. 6a. Quantum input screens for repolarisation of  $Mu_{BC}$  in Si for a [111] crystal.

			Change fr	om this		
	1	2	3	4	5	6
1	.25					
	🗐 Flip	Flip	Flip	Flip	Flip	Flip
2		.75	-			
)	Flip	Flip	Flip	Flip	Flip	Flip
3					-	
	Flip	Flip	Flip	Flip	Flip	Flip
4					-	
	Flip	└ Flip	Flip	Flip	Fip	Flip
5		-		-		
	Flip	Flip	Flip	Flip	Flip	Flip
6				-	-	
	Flip	Flip	Flip	Flip	Fip	Flip.
	Diagonal ent	tries = fractiona	al occupation o	of each state		

*Fig. 6b. When Quantum begins to run with 2 states, it asks for the relative state fractions. For the case of the input screens given in Fig. 6a. state 1 needs to be given 0.25 and state 2 0.75.* 

# 3. $Mu_{BC}$ level crossing resonance with <sup>29</sup>Si in silicon

As explored by Kiefl et al (Phys Rev Lett 60 (1988) 224), it is possible to observe the level crossing resonance between  $Mu_{BC}$  and the spin-1/2 <sup>29</sup>Si nuclei – a careful experiment as <sup>29</sup>Si is only 4.7% abundant. The resonance, shown in the Kiefl paper fig. 3 as its differential, can be modelled in Quantum by assuming that one of the Si nuclei neighbouring the  $Mu_{BC}$  centre is a spin-1/2 <sup>29</sup>Si. Here we use the nuclear hyperfine parameters from the Kiefl paper to reproduce the resonance. Fig. 7 shows the Quantum input screen; Fig. 8 the resulting resonance.

(NB: The position and shape of the resonance are correct here, but the relative abundance of <sup>29</sup>Si has not been included so the amplitude of the resonance would be smaller in reality – the curve would need to be multiplied by about 0.09 to represent the probability that a  $Mu_{BC}$  was next to a <sup>29</sup>Si nucleus.)

3 spins now needed.	2 <sup>9</sup> Si hyperfine parameters (from Kiefl paper)
	Enter Quantum Parameters
	Num of Spins 3 Num of charge states or sites 1 Copy to Others
	State 1 position spin easy axis Electron? hyperfine splitting quadrupole
muon	X     Y     Z     I     MHz/T     x     y     z     C none     A     D     eta     vQ/     eta     Spin flip rate     Random field       0     0     0     1/2     135.5     1     1     1     -67.33     50.52     2     0     0     0
electron	
<sup>29</sup> Si nucleus.	
(gyro-	
magnetic	
ratios are available	
from	diagonal values xx,yy,zz normally 2 off diag xy,xz,yz normally 0
webelements	Total states: 8 Electron g-tensor: 2 2 0 0 Polarisation 0
.com)	Calculation type       Calculation type     RF parameters       Standard     Max time for plot     20     us with     1000     bins     Frequency     10     Red/Green
.com)	
	C Low RF
specified axis	
for B0, muon	Averaging x y z RRF Harmonic 0 Phase (deg) 90
polarisation	C MC steps 10 50 1 1 0 C 100% muon
and detector	C Uniform 1 0 1 1 0 Thermal eqn: C 2D Vector field Angle x-z C Frequency/Hop rate 2D Field/Freq C TF MC steps Initial pol 1 1 0 Thermal eqn: C 2D Vector field x-z C Temperature 2D field/ion rel
is [1-10] to	C Uniform TF and F In C with muon C 2D angle theta/phi C Quadrupole C 2D field/ion
be at 90° to	C Specified axis C 2D field/angle C HFC spin 3 C 2D ion 1<→2
the Mu <sub>BC</sub>	C ZF Powder Detector 1 1 0 for spin 1 C 2D freq/angle C Ionisation relative C 2D Field/Temp
[111] axis as	C File Detector phase angle for TF (deg) 0 6300 to 6700 step 0.4 Log num of steps 1001
per fig. 3 of	Field 0 Activated transitions? Temp[K] 0 appropriate
Kiefl paper.	Fitting
	DK     Save Setup     Reset Scale     Clear Plot     Cancel     Chosen

Fig. 7. Quantum input screens for the level crossing resonance of  $Mu_{BC}$  with <sup>29</sup>Si in silicon.

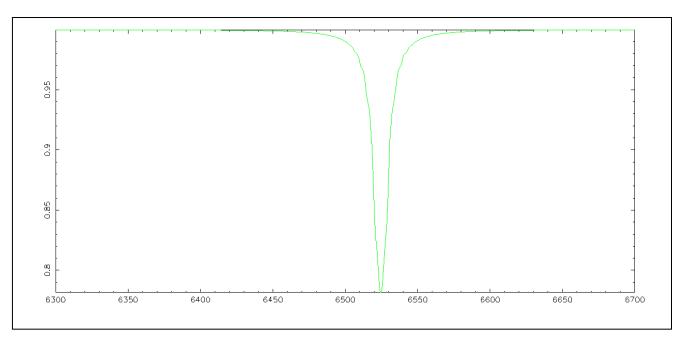


Fig. 8. Level crossing resonance for  $Mu_{BC}$  with <sup>29</sup>Si in silicon, applied field at 90° to the [111]  $Mu_{BC}$  axis.

# 4. RF resonance of triplet muonium in quartz

Quantum allows RF resonance lines to be simulated. In this example, the triplet isotropic muonium resonance in quartz is reproduced. Integral asymmetry is used, together with 'red-green' mode, i.e. Quantum will plot the difference between 'RF on' (red) and 'RF off' (green) states. Fig. 9 shows the Quantum input screen, and Fig. 10 the resulting RF resonance plot.

(NB: note that Quantum's definition for linearly polarised fields is the peak B1; sometimes B1 in the rotating frame is quoted which will have half this value. Integral counting start=0 corresponds to a continuous beam instrument in integral mode; start times greater than 0 will usually apply to time domain data that has been averaged afterwards.)

	Enter Quantum Parameters	hyperfine
	Num of Spins     2     Num of charge states or sites     1     Copy to Others       State 1     position     spin     easy axis     Electron?     hyperfine splitting     ouerfruingle	coupling for isotropic
back to 2 spins again	position spin easy axis Electron? hyperfine splitting quadruppole   Y Z I MHz/T x y z C none A D eta vQ eta Spin flip rate Random field   0 0 0 1/2 135.5 1 1 1 c 4500 0 0 0 0 0	, muonium in quartz
	0   0   0   1/2   -2802   1   0 </td <td></td>	
choosing integral asymmetry		100 MHz RF frequency
asymmetry	diagonal values xx,yy,zz normally 2 off diag xy,xz,yz normally 0	Red/Green
now an RF calculation	Total states: A Electron g-tensor: 2 2 2 0 0 Patarisation   Calculation type RF parameters	mode selected
need to enter the muon lifetime	• RF     Measurement     i - Integral asym     TF Bkgnd     0     C Low RF     Lifetime     2.197     Start     0     Shift with B     Averaging     X     V     Z     X     V     Z     X     V     Z     X     V     Z     X     V     Z     X     V     Z     X     V     Z     X     V     Z     X     V     Z     X     V     Z     X     X     V     Z     X     X     X	B1 field of 1G seems reasonable
need to	C Uniform B0 1 0 0 0 100% muon C Field Angle x-z Field C 2D Field/Freq	
enter a start time	C TF MC steps   Initial pol   I   0   0   Thermal eqm:   C 2D Vector field x-z   C Temperature   C 2D field/ion rel     C Uniform TF   B1   0   I   0   0   C before muon   C 2D field/angle   C 2D field/ion     C Specified axis   0   1   0   0   C interval   C 2D field/angle   C 2D field/ion	suitable field range
Assume applied field B0, muon polarisation and detector are along	ZF Powder   Detector   1   0   for spin   1   C 2D freq/angle   C Ionisation relative   C 2D Field/Temp     File   Detector phase angle for TF (deg)   0   0   60   to 90   step   0.1   Log num of steps   301     Field   0   Activated transitions?   Temp(K)   0   2nd:   to   step   Ice Log num of steps   301     DK   Save Setup   Reset Scale   Clear Plot   Cancel	chosen
[100]	RF field B1 must be at 90° to B0, i.e. B1 along [010] here	

*Fig.9. Quantum input screen for reproducing the RF triplet resonance for isotropic muonium in quartz.* 

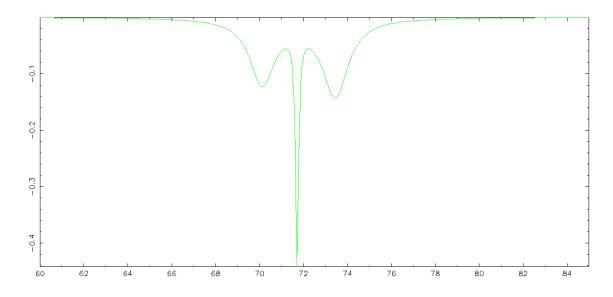


Fig.10. RF resonance for isotropic muonium in quartz.

# 5. Quadrupolar level crossing resonance in copper

Level crossing resonances can occur when the Zeeman energy for muons in field matches the combined Zeeman and quadrupolar levels for the spin 3/2 Cu nuclei in copper. See, for example, R. Kadono et al, 'Quantum diffusion of positive muons in copper' Phys Rev B **39** 23-41 (1989) – fig. 13 in particular.

Cu can be simulated most easily if we approximate to only one Cu nucleus instead of 6 nearest neighbours (so the sigma comes out at about 1/sqrt(6) of the experimental value). Put the muon at (0,0,0) and Cu at (0,0,1.9) (O-site, 5% dilation), Cu I=3/2, gyromagnetic ratio 11.2979 (63Cu), easy axis (0,0,1), quadrupole splitting 1.05 MHz. Average over orientations (100), "uniform" mode. Easy axis along (001) chosen as this gives the best uniformity.

Fig. 11 shows the output level crossing resonance; fig. 12 the Quantum input screen.

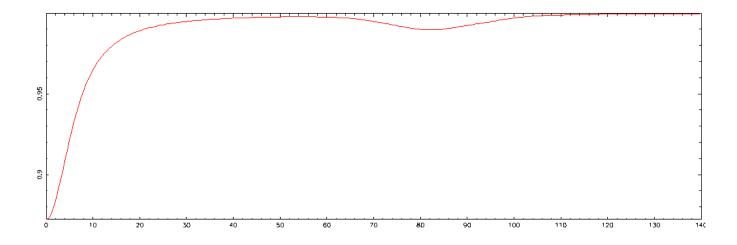


Fig. 11. Quadrupolar resonance in copper.

	no electrons involved this time
	Enter Quantum Parameters
	Num of Spins     2     Num of charge states or sites     1     Copy to Others       State 1
muon	X Y Z I MHz/T x y z • none A D eta vQ eta Spin flip rate Random field 0 0 0 1/2 135.5 1 0 0 0 0 0 0 0
Cu	
Integral	
asymmetry used	
	diagonal values xx,yy,zz normally 2 off diag xy,xz,yz normally 0   Total states: Electron g-tensor: 2 2 0 0 Polarisation 0
	Calculation type
muon	C RF Measurement i Integral asym TF Bkgnd 0 C Linear B1 C Rotating B1 C Hyperfine A C Hyperfine D
lifetime and	C Hopping Lifetime 2.197 Start t 0 T Shift with B Intensity (G) 0 Phase (deg) 0 Random
start time	Averaging X Y Z RBF Harmonic 0 Phase (deg) 90
needed	C MC steps 200 B0 0 0 0 C 100% mum Sweep C Field Ande x 2
	C TF MC steps Initial pol 0 0 Thermal eqm: C 2D Vector field x-z C Temperature C 2D field/ion rel
uniform	C Uniform TF B1 0 0 0 C before much C 2D angle theta/phi C Quadrupole C 2D field/ion
averaging	C Specified axis C ZF Powder Detector 0 0 0 for spin 1 C 2D freq/angle C HFC spin 3 C 2D ion 1<→2 C 2F Powder Detector 0 0 0 for spin 1 C 2D freq/angle C Ionisation relative C 2D Field/Temp
	C File Detector phase angle for TF (deg) 0 C Ionisation rate / B1
	Field 0 to 140 step 0.5 □ Log num of steps 281
	Fitting 2nd: to step IV Log num of steps
	OK Save Setup Reset Scale Clear Plot Cancel

# *Fig.9. Quantum input screen for reproducing the quadrupolar level crossing resonance in copper.*

NB: In uniform and Monte Carlo modes the field direction is calculated from angles theta (with respect to the z-axis) and phi (in the x-y plane). Any distribution which is uniform over cos(theta)=-1 to +1 and uniform over phi=0 to 2pi will map to a spherical average. (For TF and RF there's a third angle, the direction psi of the initial polarisation, or RF B1, around B0 starting at a fixed point perpendicular to x for example). So for N points in Uniform mode it takes N equally spaced values for cos(theta). Phi increments by 2pi/e per point to give a uniform scatter of points over the sphere. (Psi increments by 2pi\*e to hopefully remain uncorrelated with phi).