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.

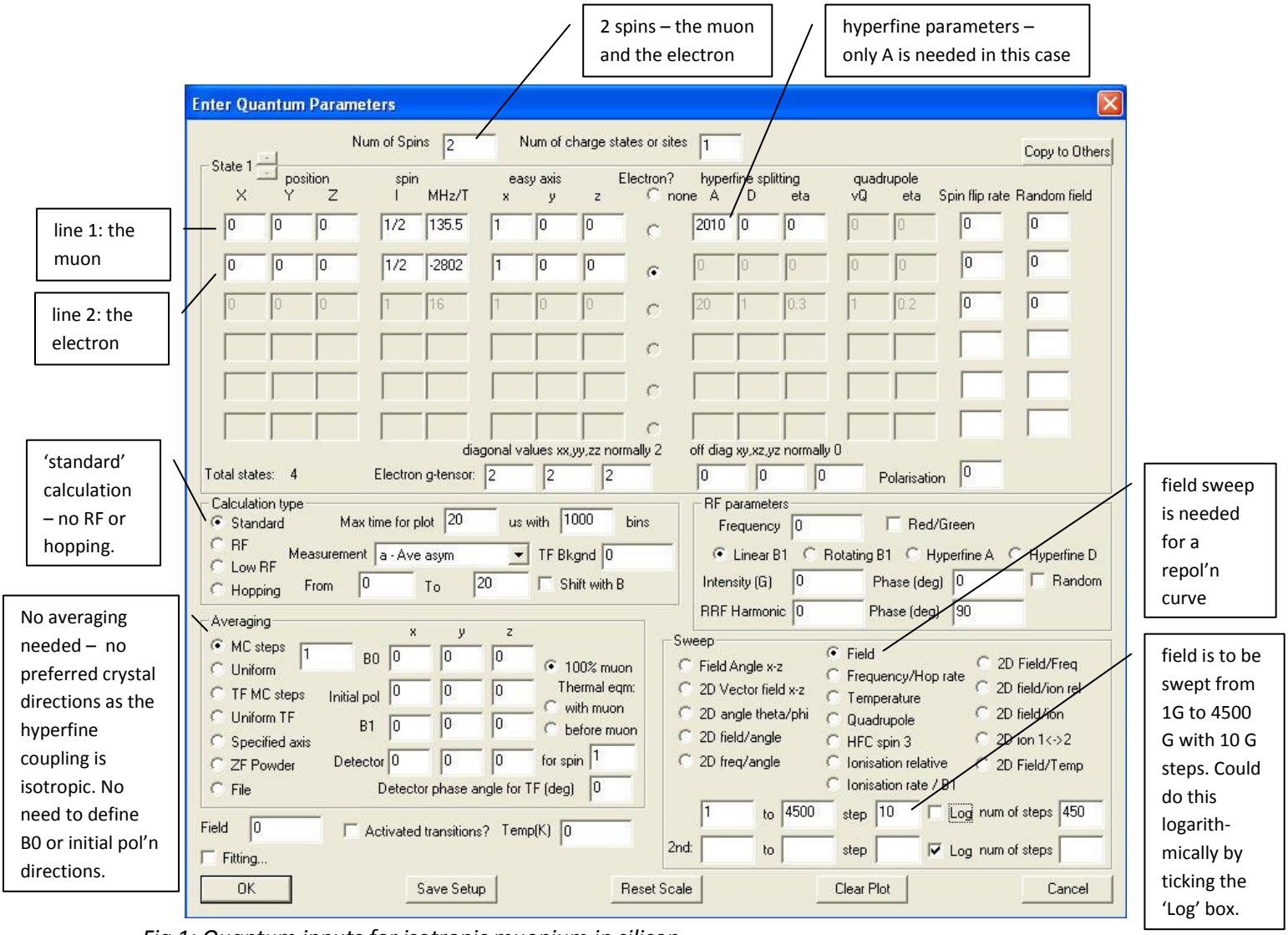


Fig 1: Quantum inputs for isotropic muonium in silicon.

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.

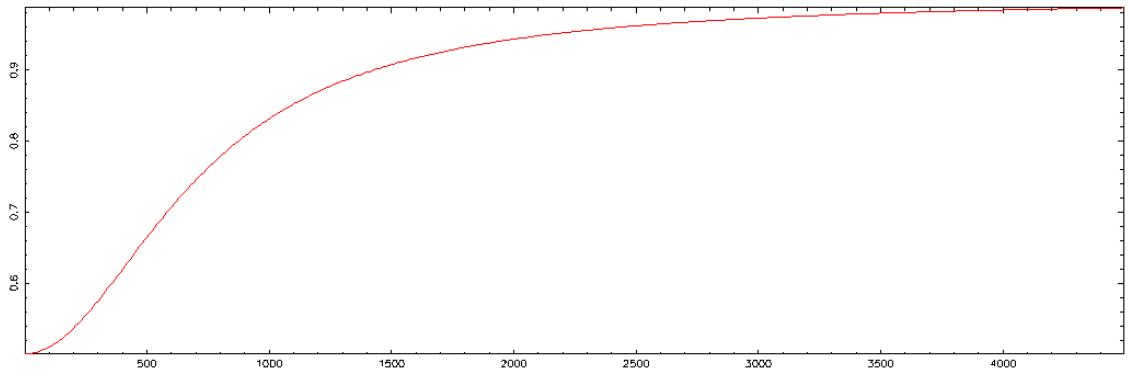


Fig. 2. Repolarisation curve for isotropic muonium in Si at around 100K.

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:
$A=1/3(A_{\perp} + 2A_{\parallel})$; $D=2/3(A_{\perp} - A_{\parallel})$, where $A_{\perp}$ and $A_{\parallel}$ 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.

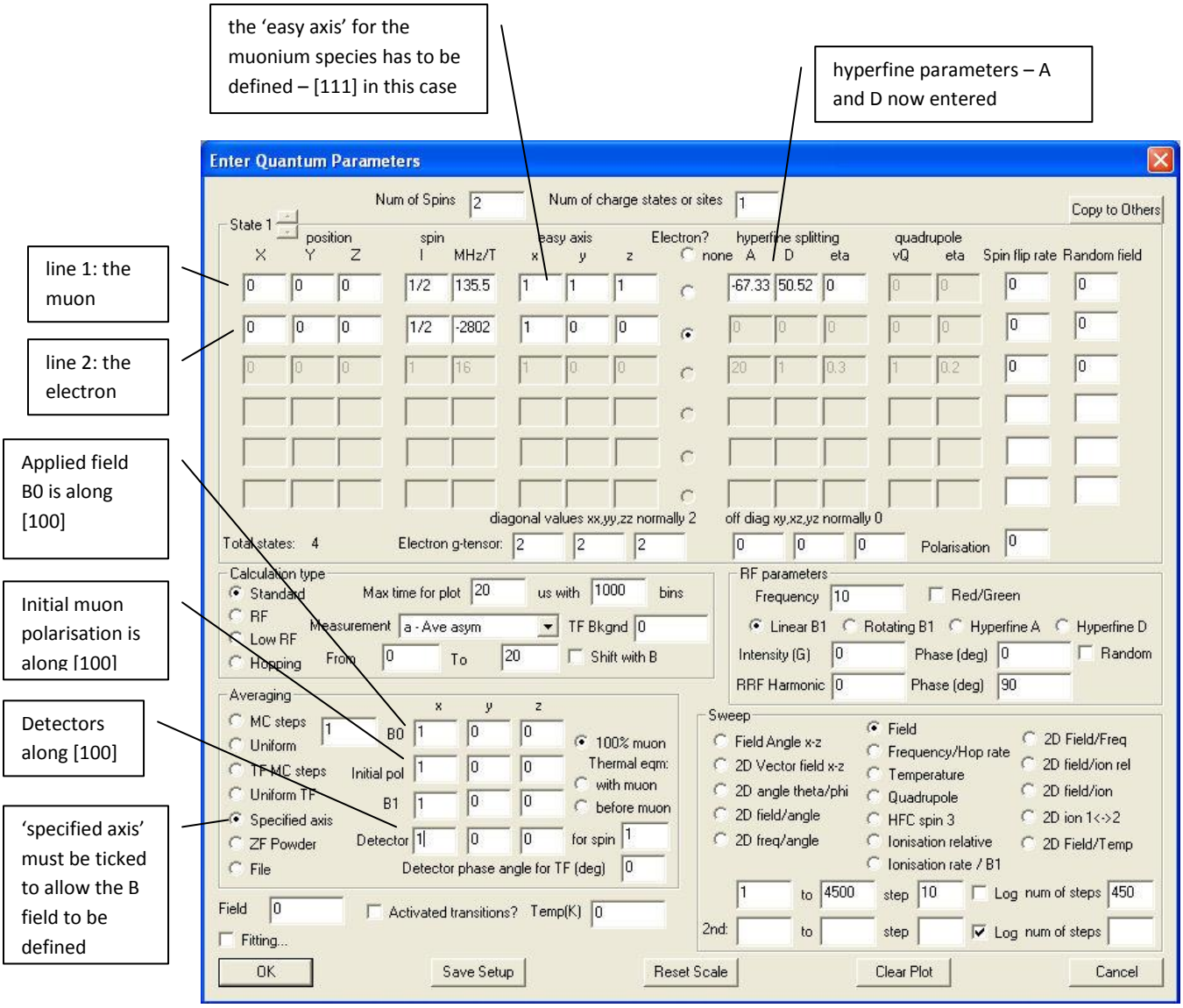


Fig. 3. Quantum inputs for Mu_{BC} in Si, field along [100]

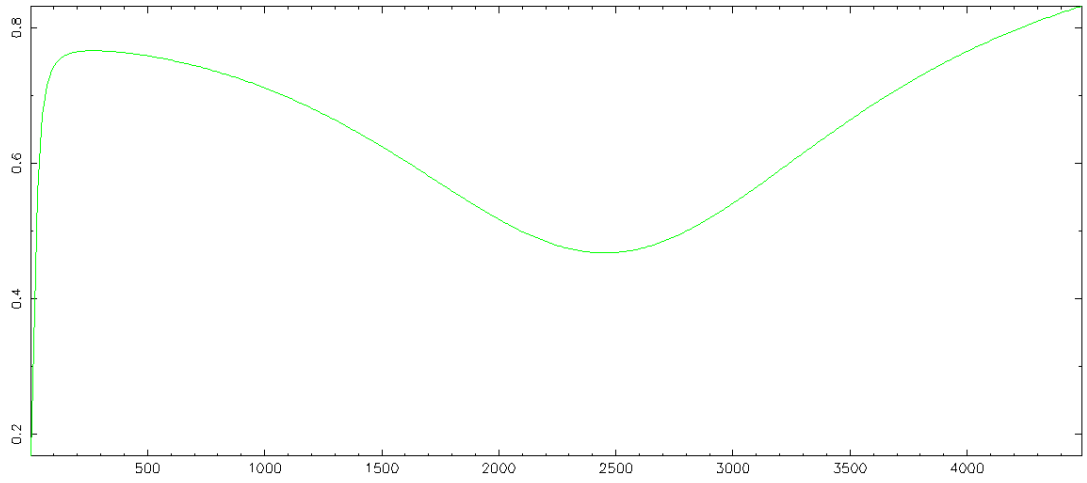


Fig. 4. Repolarisation curve for bond-centred muonium in Si, [100] crystal.

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_{BC} species 1 in Quantum's 'State 1'
- press 'copy to others', which duplicates State 1 to State 2
- entering the correct parameters for Mu_{BC} 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.

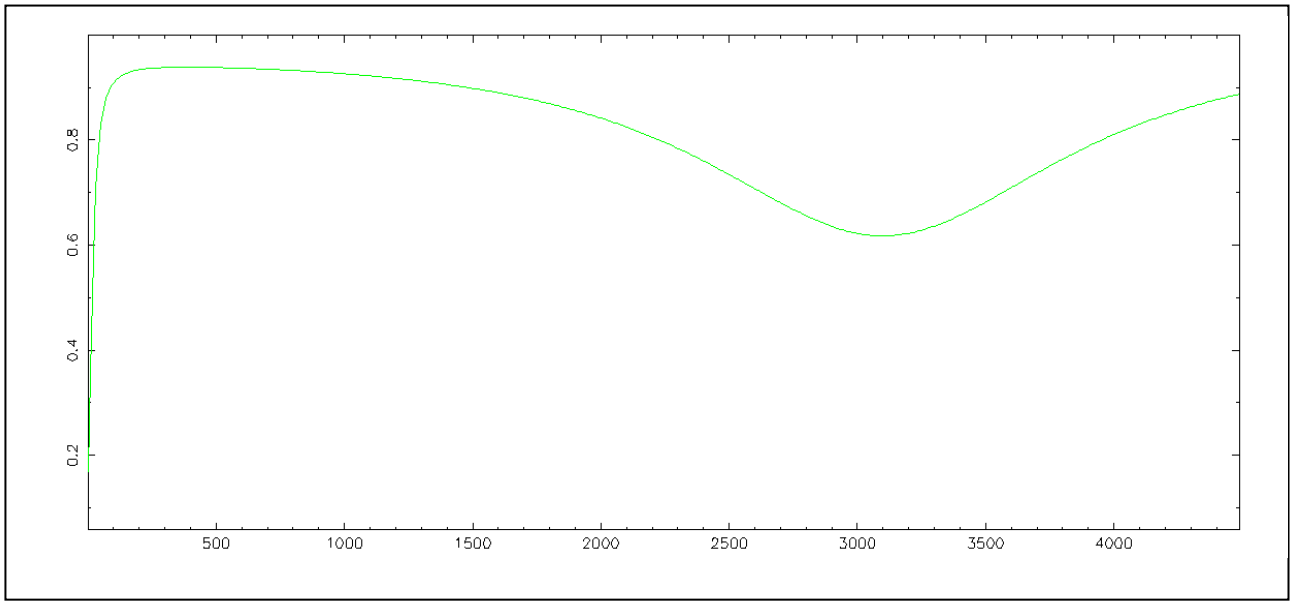


Fig. 5. Repolarisation curve for bond-centred muonium in Si, [111] crystal.

still 2 spins in each state

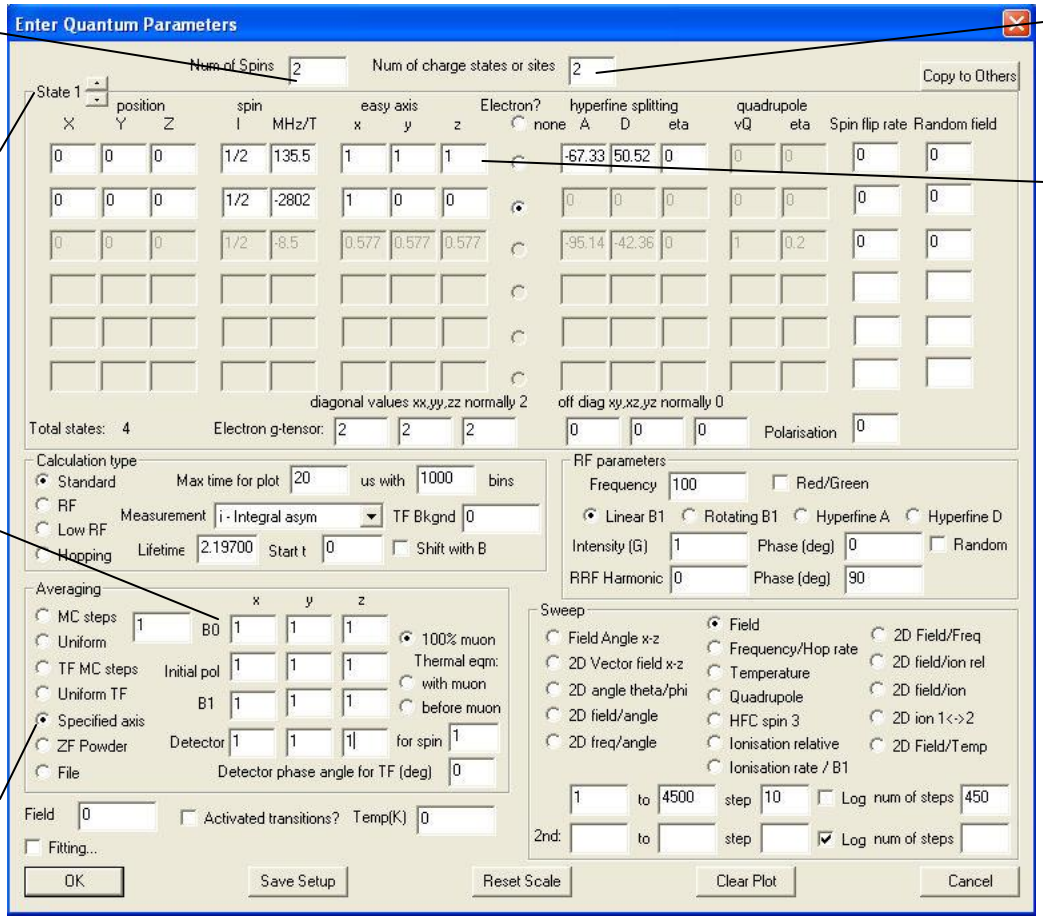
this screen shows State 1: Mu_{BC} parallel to the field (25% of Mu_{BC} species)

Applied field B0 is along [111], as is the initial polarisation and detector

Specified axis still ticked.

number of states is now 2

Mu_{BC} axis is [111] for State 1.



this screen shows State 2: Mu_{BC} not parallel to the field (75% of MuBC species)

The only difference from the State 1 screen is that the Mu_{BC} axis is now along one of the [111] crystal directions that is not parallel to the applied field.

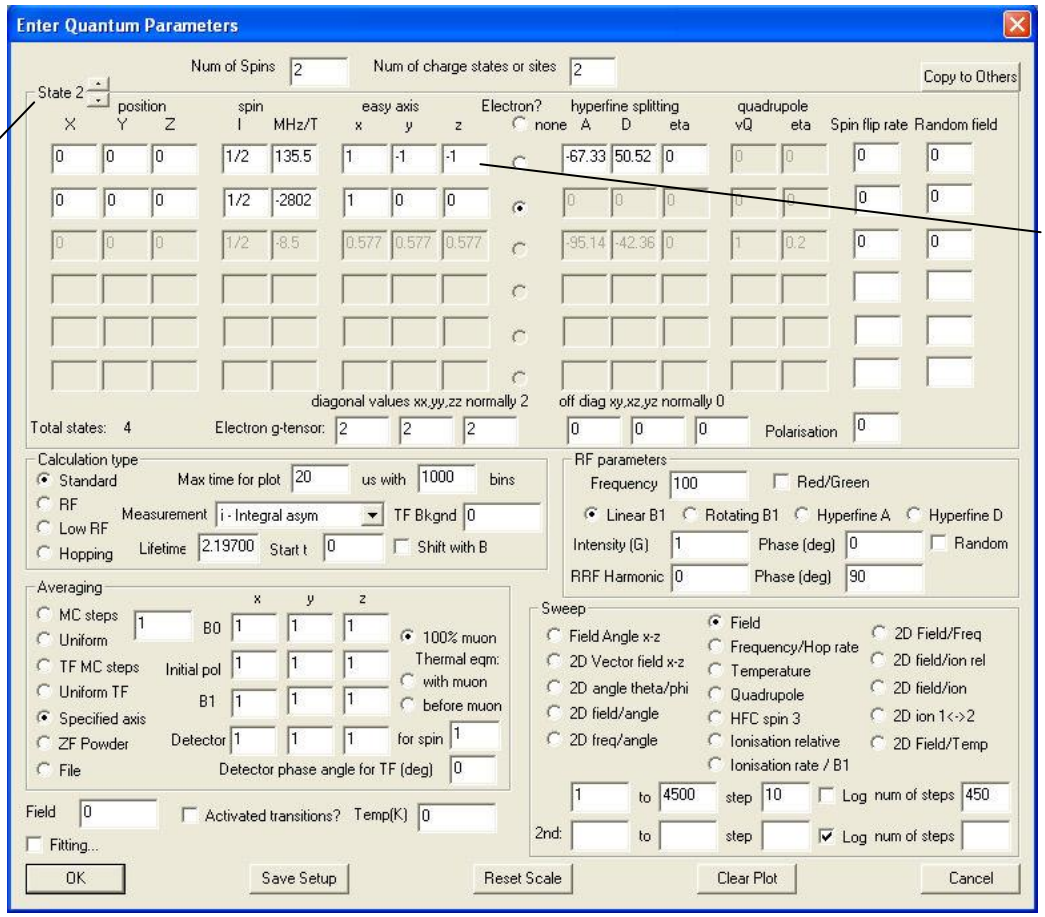


Fig. 6a. Quantum input screens for repolarisation of Mu_{BC} in Si for a [111] crystal.

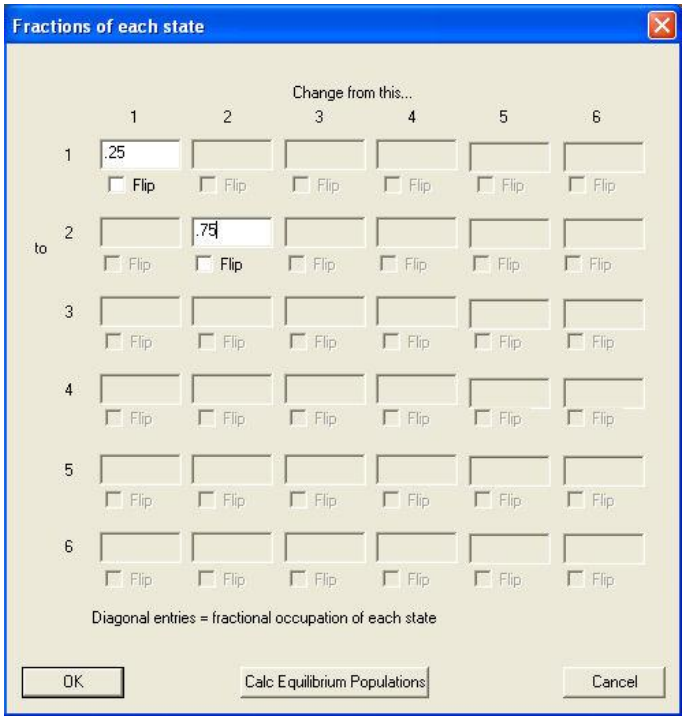


Fig. 6b. When Quantum begins to run with 2 states, it asks for the relative state fractions. For the case of the input screens given in Fig. 6a. state 1 needs to be given 0.25 and state 2 0.75.

3. Mu_{BC} level crossing resonance with ^{29}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 ^{29}Si nuclei – a careful experiment as ^{29}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 ^{29}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 ^{29}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 ^{29}Si nucleus.)

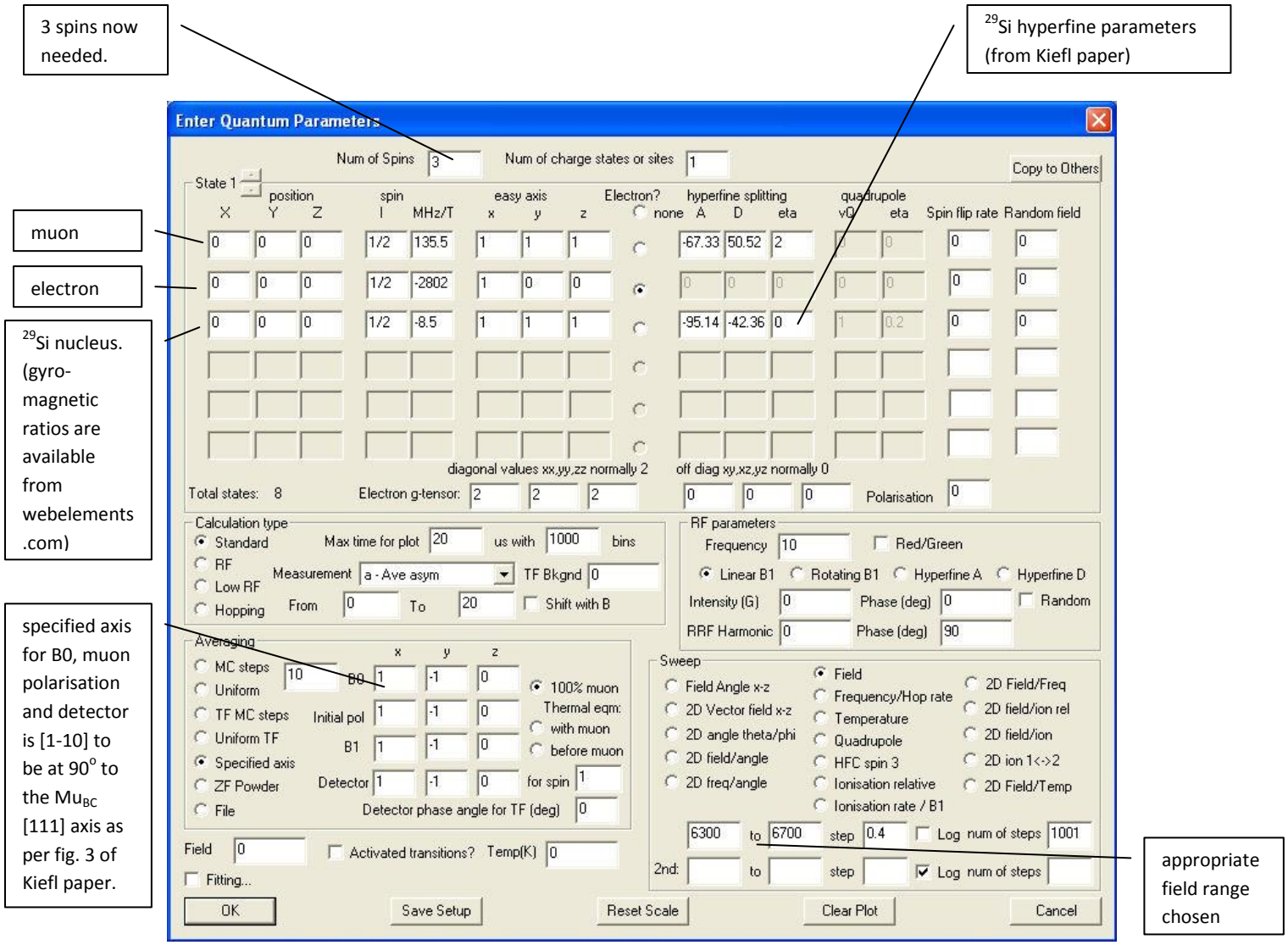


Fig. 7. Quantum input screens for the level crossing resonance of Mu_{BC} with ^{29}Si in silicon.

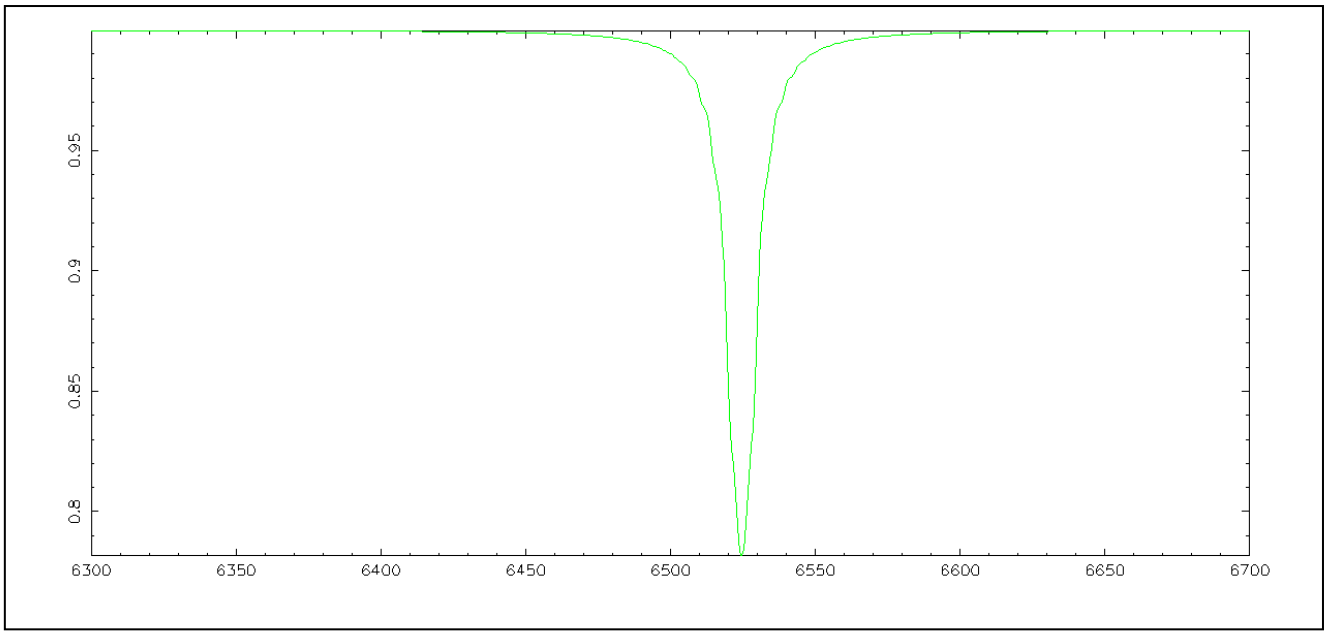


Fig. 8. Level crossing resonance for Mu_{BC} with ^{29}Si in silicon, applied field at 90° to the [111] Mu_{BC} axis.

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.)

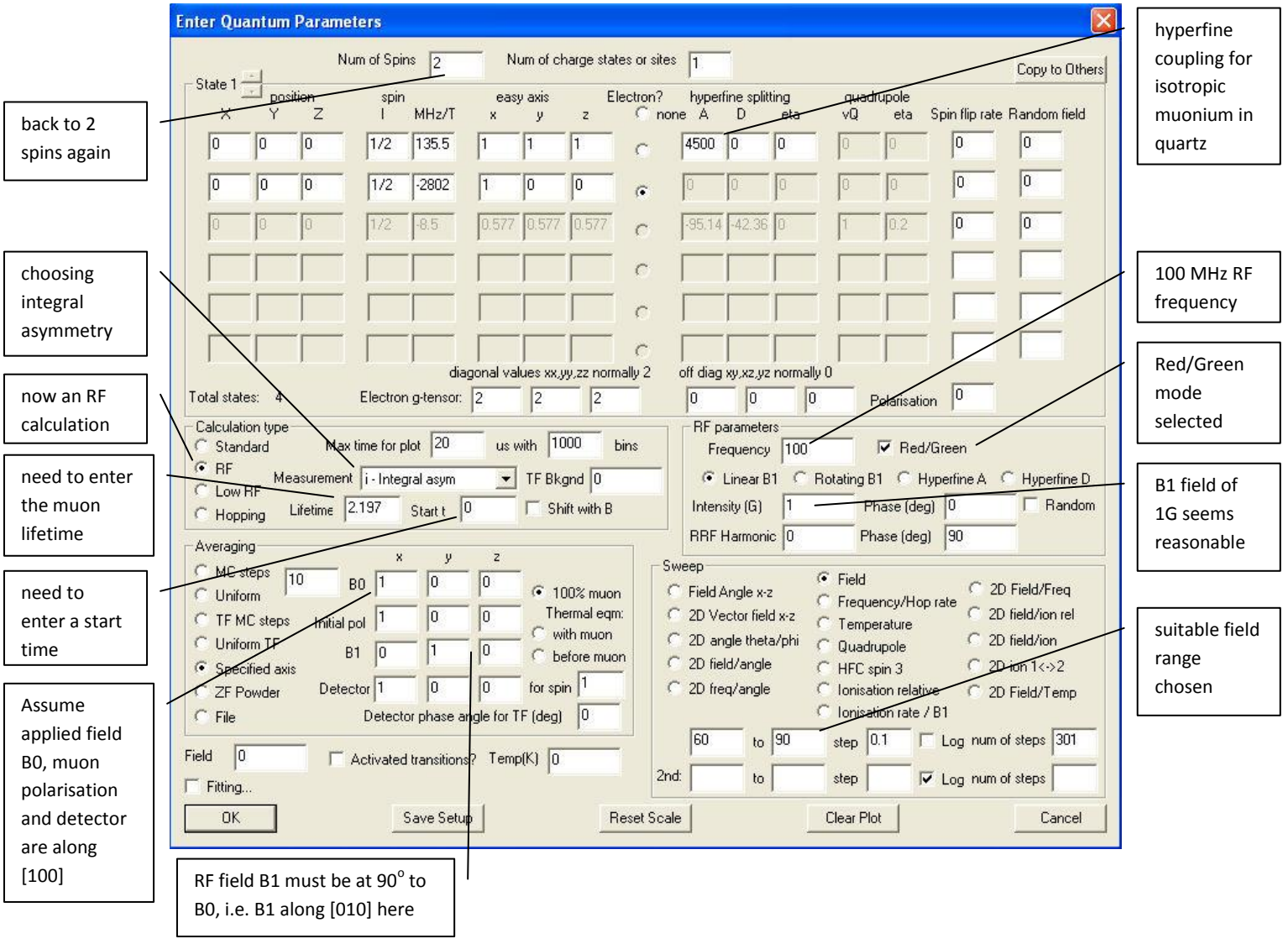


Fig.9. Quantum input screen for reproducing the RF triplet resonance for isotropic muonium in quartz.

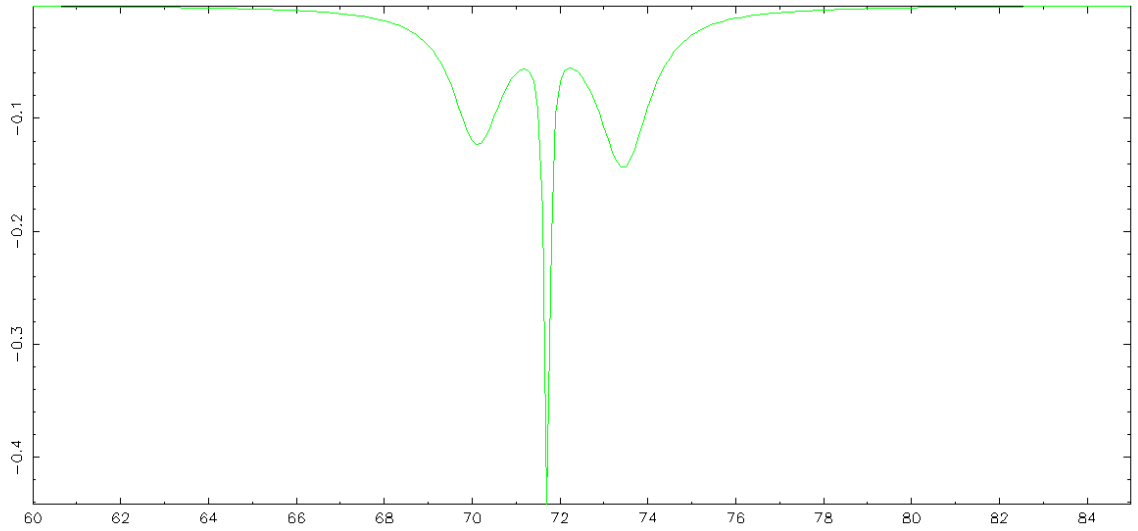


Fig.10. RF resonance for isotropic muonium in quartz.

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.

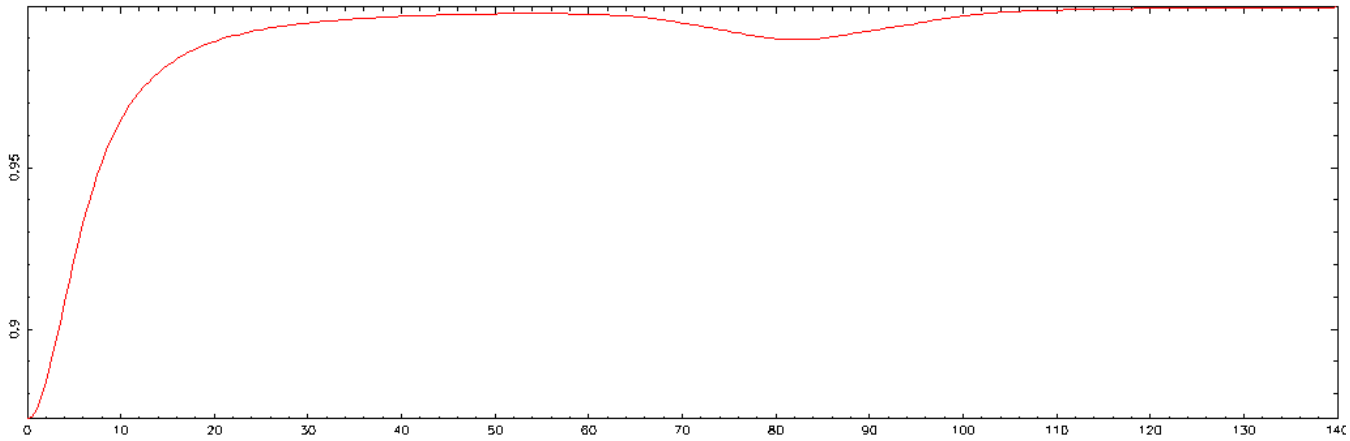


Fig. 11. Quadrupolar resonance in copper.

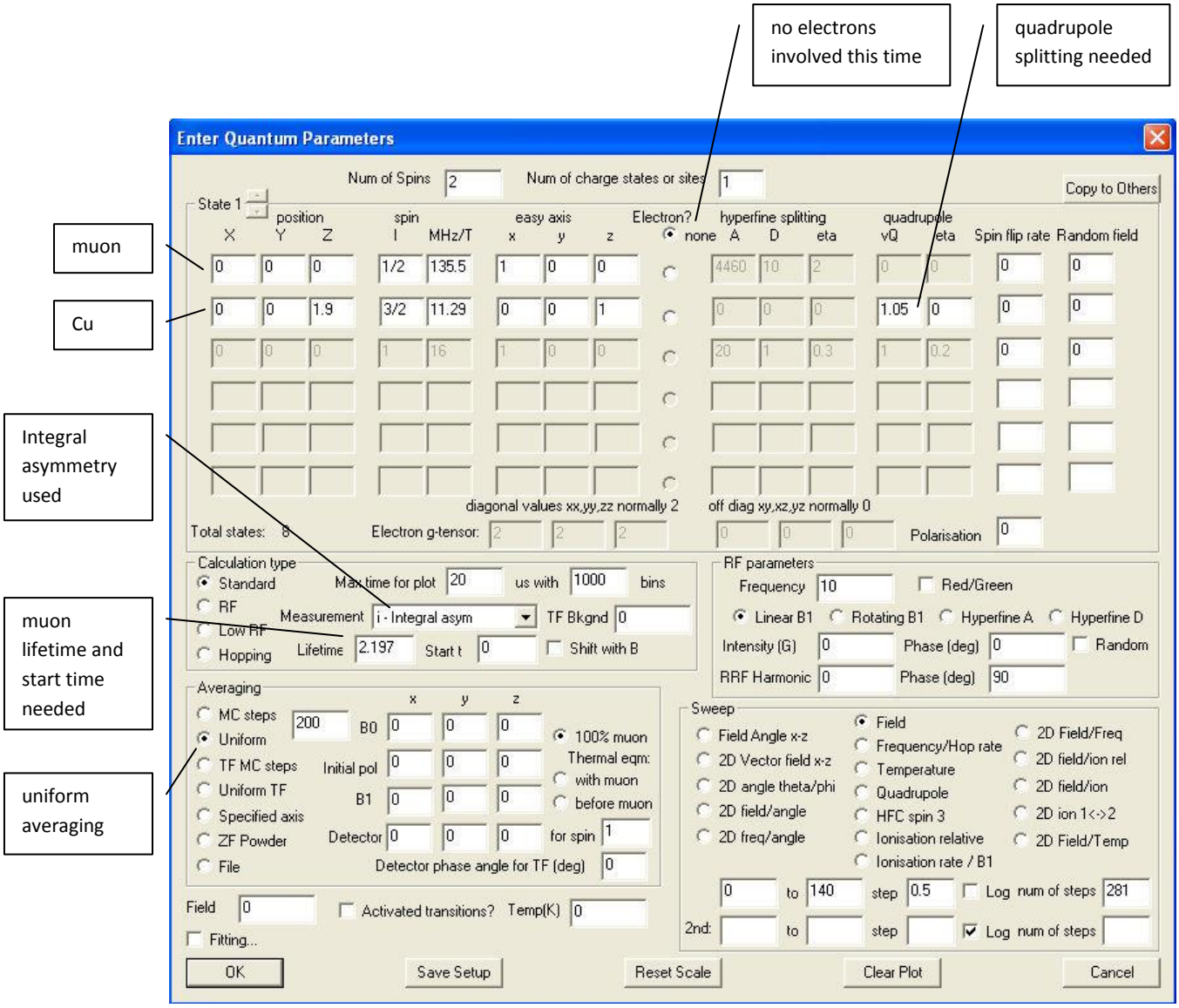


Fig.9. Quantum input screen for reproducing the quadrupolar level crossing resonance in copper.

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).