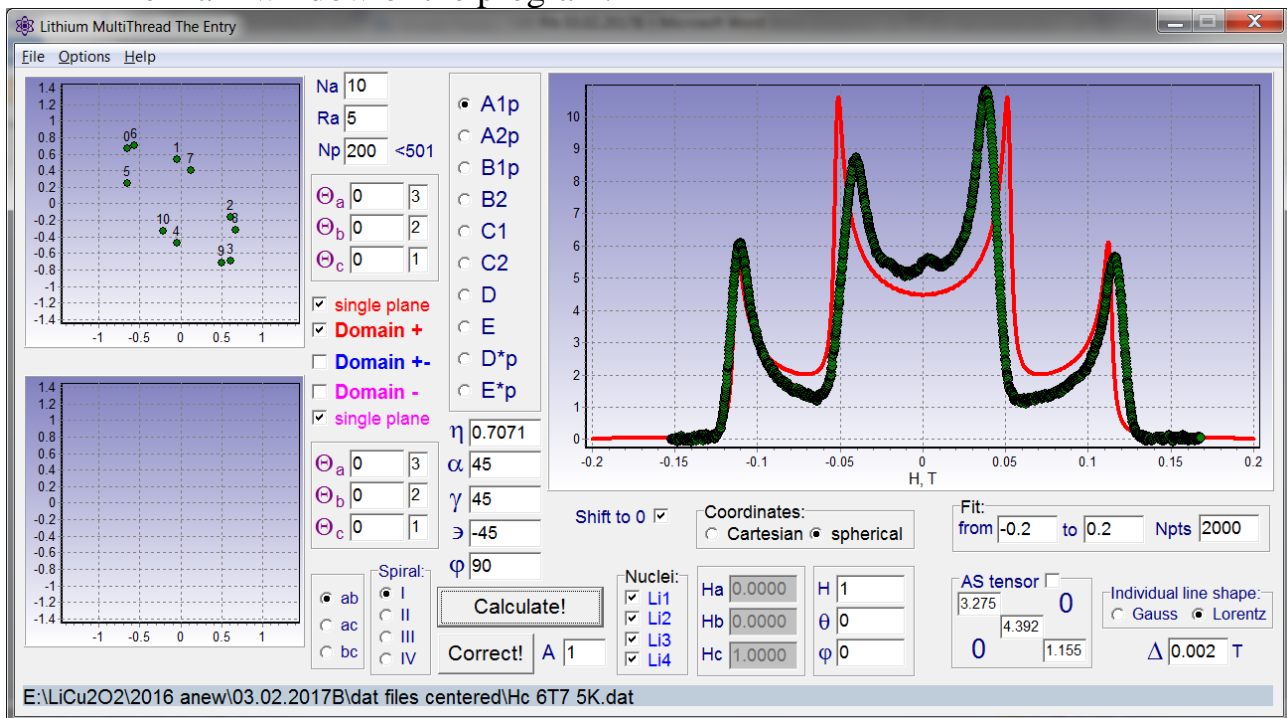


Lithium MultiThread Program Comments

The program calculates lithium NMR spectra in LiCu_2O_2 for magnetic structures discussed in the paper: A.A. Bush, N. Büttgen, A.A. Gippius, M. Horvatić, M. Jeong, W. Kraetschmer, V.I. Marchenko, Yu.A. Sakhratov, and L.E. Svistov, *Exotic magnetic structures of $J_{NN} - J_{NNN}$ frustrated antiferromagnet LiCu_2O_2* , submitted to PRB. There are two domains, **Domain +** and **Domain -**, each contains four Cu^{2+} spirals. Each spiral is calculated in a separate thread. So, it is possible to calculate eight spirals simultaneously on a quad core computer. Due to high priority set for calculation, your computer may freeze for some time during calculation.

The main window of the program:

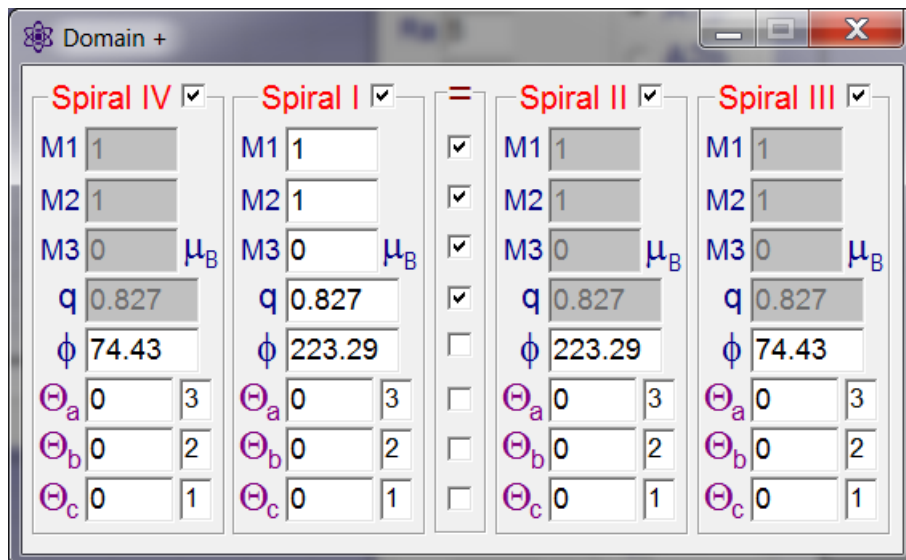


(H_a, H_b, H_c) or (H, θ, ϕ) sets a static magnetic field in Cartesian or spherical coordinates, respectively.

$A1, A2, B1, B2, C1, C2, D, E, D^*, E^*$ is the list of structures defined by Eqs. 18,19. Each of them is characterized by a fixed set of the angles $(\alpha, \gamma, \epsilon, \phi)$. These angles appear in appropriate textboxes automatically, after selecting the structure. If you modify these angles (except ϕ , $\phi = 90^\circ$) you get some structure from a set defined by Eq. 20. The order parameter η for A1, A2, B1, B2, C1, C2, D, E, D*, E* structures is chosen such that the maximum value of the magnetic moment equals to $1 \mu_B$.

$(\Theta_a, \Theta_b, \Theta_c)$ sets the spin plane orientation. The spin plane is defined by the unit vectors \mathbf{l} and \mathbf{k} . Initially vectors $\mathbf{l} \parallel \mathbf{a}$ and $\mathbf{k} \parallel \mathbf{b}$, so the spin plane coincides with ab plane of the crystal. An arbitrary orientation of the spin plane is obtained by successive rotations by the angle Θ_a around a axis, Θ_b around b axis and Θ_c around c axis. The order of rotations is set by the numbers 1, 2, 3 on the right.

The checkbox **single plane/single plane** if checked sets equal orientation of the spin planes for all four spirals, for **Domain +** and **Domain -**, respectively. Alternatively, making it unchecked allows you to set individual orientation of the spin plane for every spiral. To do this, choose menu Options, Domain+/- . A new window, **Domain +** or **Domain -**, appears which allows you to set (Θ_a , Θ_b , Θ_c) for each spiral.



This window is set 'Stay on Top', you can Minimize or Close it, it keeps all the parameters you have entered.

After pressing Calculate! button calculated NMR spectra appears on the right Chart. You can load experimental spectra for comparison, choose menu File, Open. The experimental spectrum is shown with green circles. It stays displayed until next time you load the experiment.

Two left Charts, top and bottom, correspond to **Domain +** and **Domain -**, respectively. They show projections of the magnetic moment vector endpoint on **ab**, **ac** or **bc** plane. These points are numerated as you move along the spiral. You can choose the **Spiral (I, II, III, IV)** this picture is shown for.

Correct! button allows to scale the calculated spectrum along the vertical axis by setting **A** on the right.

Na sets the range of lattice sums indexes. **Ra** defines sphere of calculation in **b** lattice constants, **Ra** < **Na**.

If some wiggles in calculated spectrum appear you can increase the value of integer valued parameter **Np** < 501. The more **Np** is the more time is needed for calculation.

Questions, suggestions and bug reports are welcomed!

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