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Development of Single-Magnon Cross-Section/ Spin Wave Dispersion Software

Breakdown

TASK

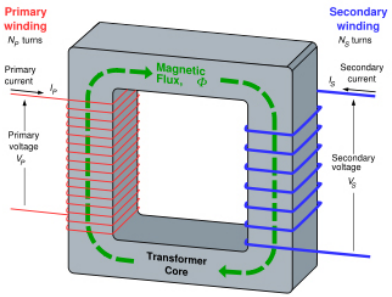
- Understand properties of magnetic solids
  - Simulate interactions with magnetic lattices
    - Simple systems – very tedious
    - Complex systems – often impossible to do by hand
  - Analyze experimental data
    - Fitting

GOAL

- SOFTWARE
  - Improve current features of software in development
  - Expand this software to allow more functionality

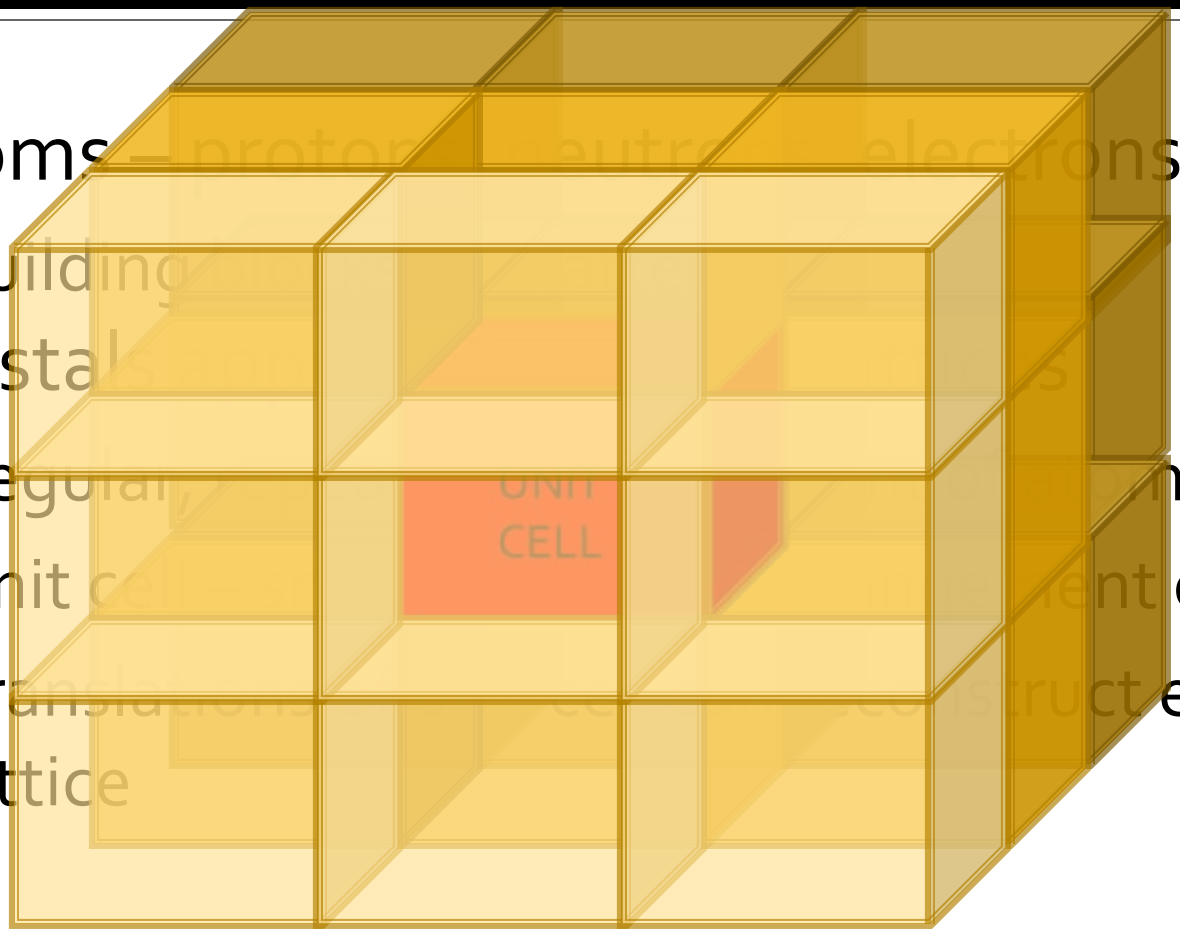
Magnetism

- Used often in everyday life
  - Hard drives, credit cards, VHS
  - Transformers, generators
  - Electric Motors
  - Speakers, microphones



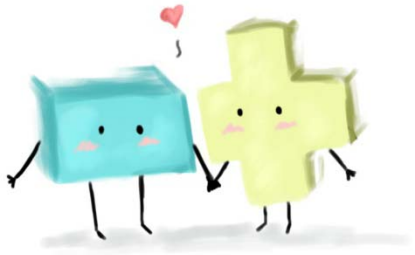
Atoms and Crystals

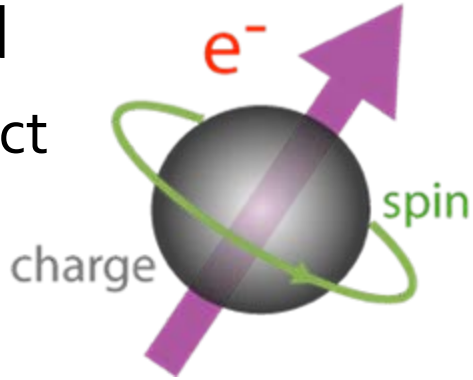
- Atoms – protons, neutrons, electrons
  - Building blocks
- Crystals
  - Regular arrangements
  - Unit cell – smallest component of atoms
  - Translations reconstruct entire lattice



Spin

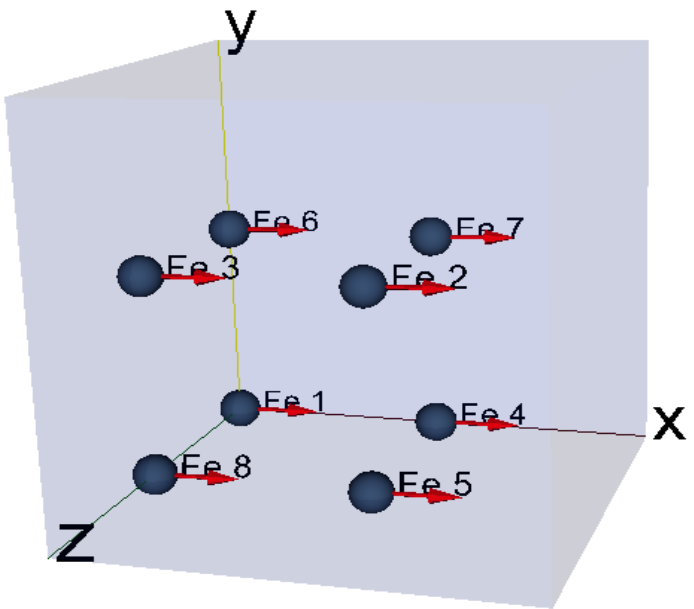
- Electrons throughout lattice interact
  - Like charges repel
    - Coulomb Repulsion
  - Intrinsic quantized angular momentum - SPIN
    - Spin vector (Sx,Sy,Sz) points in direction of spin
    - Pauli Exclusion Principle
  - Moving electrons create magnetic field
    - Magnetic fields of multiple electrons interact



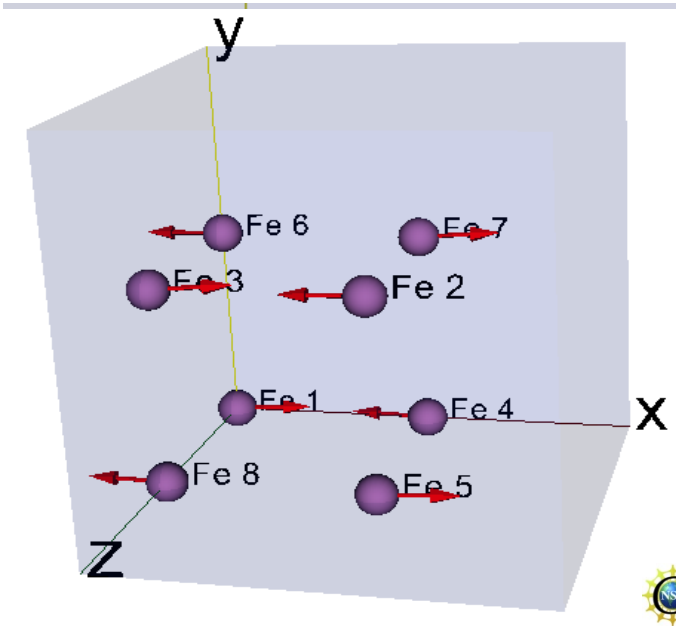


Ground states

- Depending on interactions, different patterns of spins on the lattice can develop
- Ground state is spin configuration with least energy
- Example:
  - Ferromagnetic



Antiferromagnetic



Heisenberg Hamiltonian

- Approximate interactions by pair-wise spin interactions

$$H = -\sum_{i\,j} \vec{S}_i \, J_{ij} \, \vec{S}_j - \sum_i \sum_\alpha D_i^\alpha (S_i^\alpha)^2$$

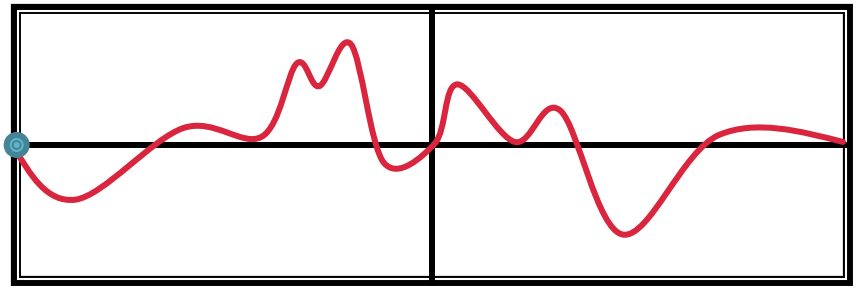
- 1st term – Interactions between two spins
- 2nd term – Anisotropy
  - Point spins preferentially along a particular direction in space

Simulated Annealing

- Monte Carlo Simulation
  - Time Independent
  - Minimize energy
  - Global minimum of Hamiltonian → ground state
  - Results not perfect
  - Implemented in C

Local optimization

- Simulated annealing puts us in the ball park of the global minima
  - Local optimization can then focus on the correct region of space to obtain more accurate result
- Rewrite energy as a matrix product
- Use sparse matrices to save memory
- Implemented in python and very fast!

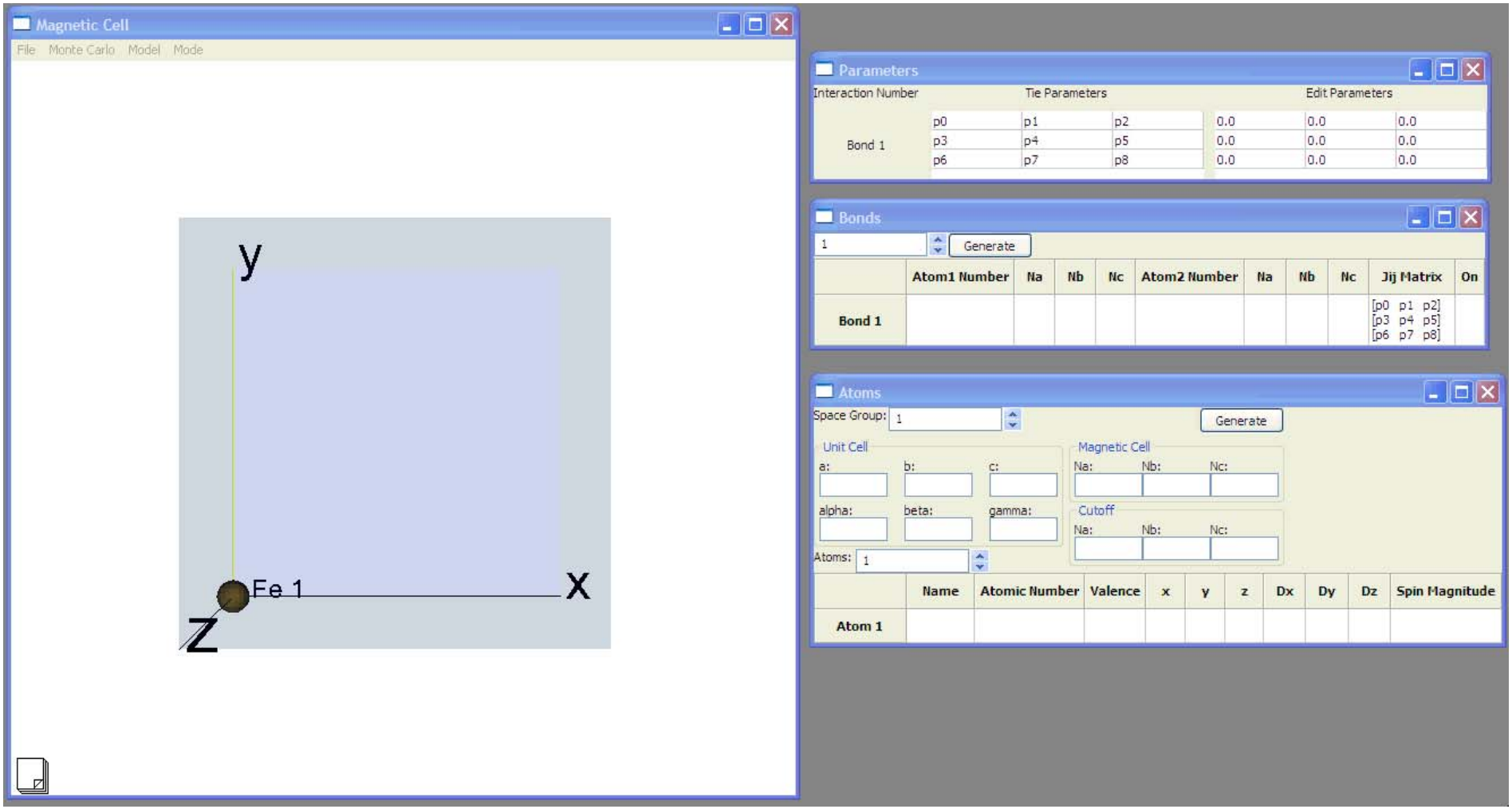


Note:
Not actual data

Starting Point

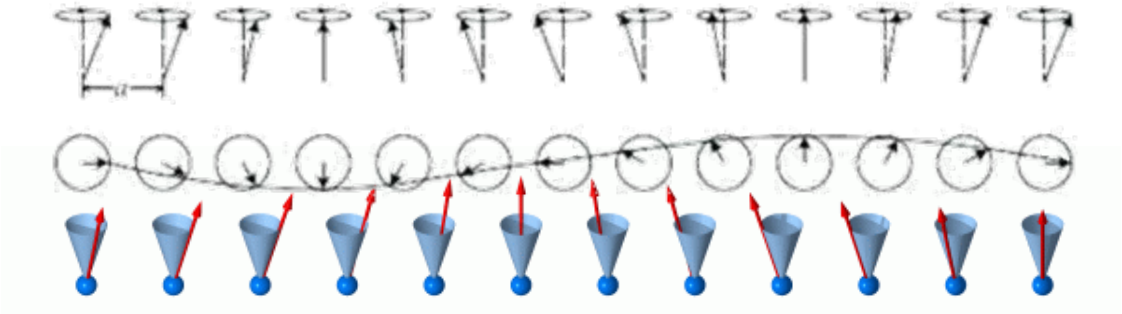
- Tom Sarvey
  - 1,000s of lines of code!
  - Open source; python & C
  - Graphical interface
- Needs:
  - Expansion – capability to calculate spin wave dispersion, cross-section, fits, optimization, etc.
  - Testing – fixing bugs, establishing testing suite
  - Maintenance – updating code

Program Demo: Lattice Creation, Bond Forming, Spin Ground State Simulation

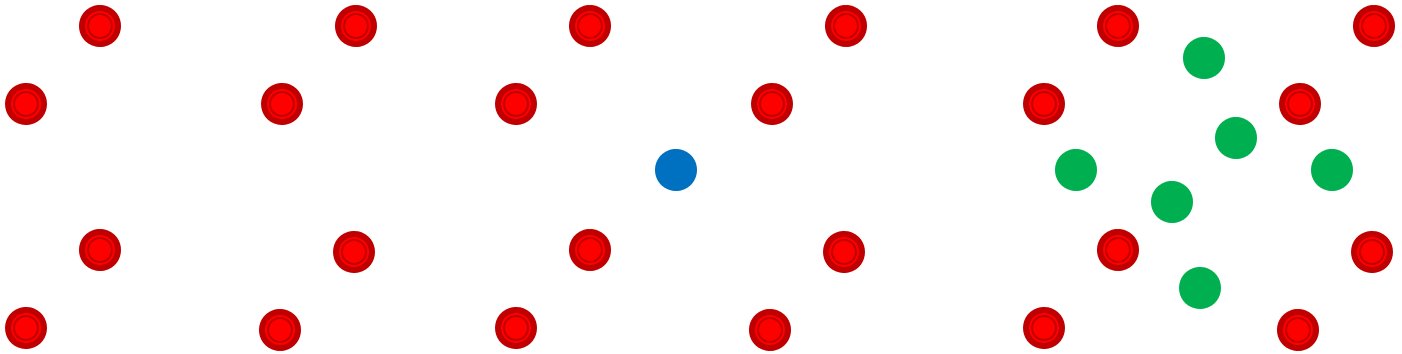


Excited states

- *Naïve excitation:* Flip direction of one spin
  - **High energy cost**
- *Reality:* Spread spin reversal over many spins
  - **Much lower energy cost**
  - Superposition of states with one reduced spin
- Spin waves are the propagation of this misalignment of near-neighbors' spins



Dispersion Calculation



Simple Body Centered Face Centered

```
\section{eigs}

$- 5.78889782593128e-5 S
\mbox{sin}\left(kz\right) + \frac{1}{2}
\sqrt{- 127.999997575541 S^{2}
\mbox{cos}\left(kz\right) -
-63.9999986229848 S^{2} -
-63.9999989525566 S^{2}
\mbox{cos}^{2}\left(kz\right)}$

$- 5.78889782593128e-5 S
\mbox{sin}\left(kz\right) - \frac{1}{2}
\sqrt{- 127.999997575541 S^{2}
\mbox{cos}\left(kz\right) -
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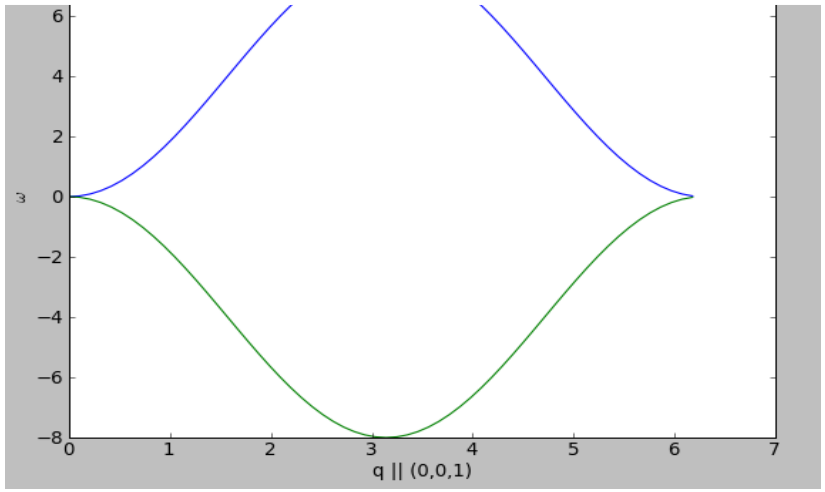
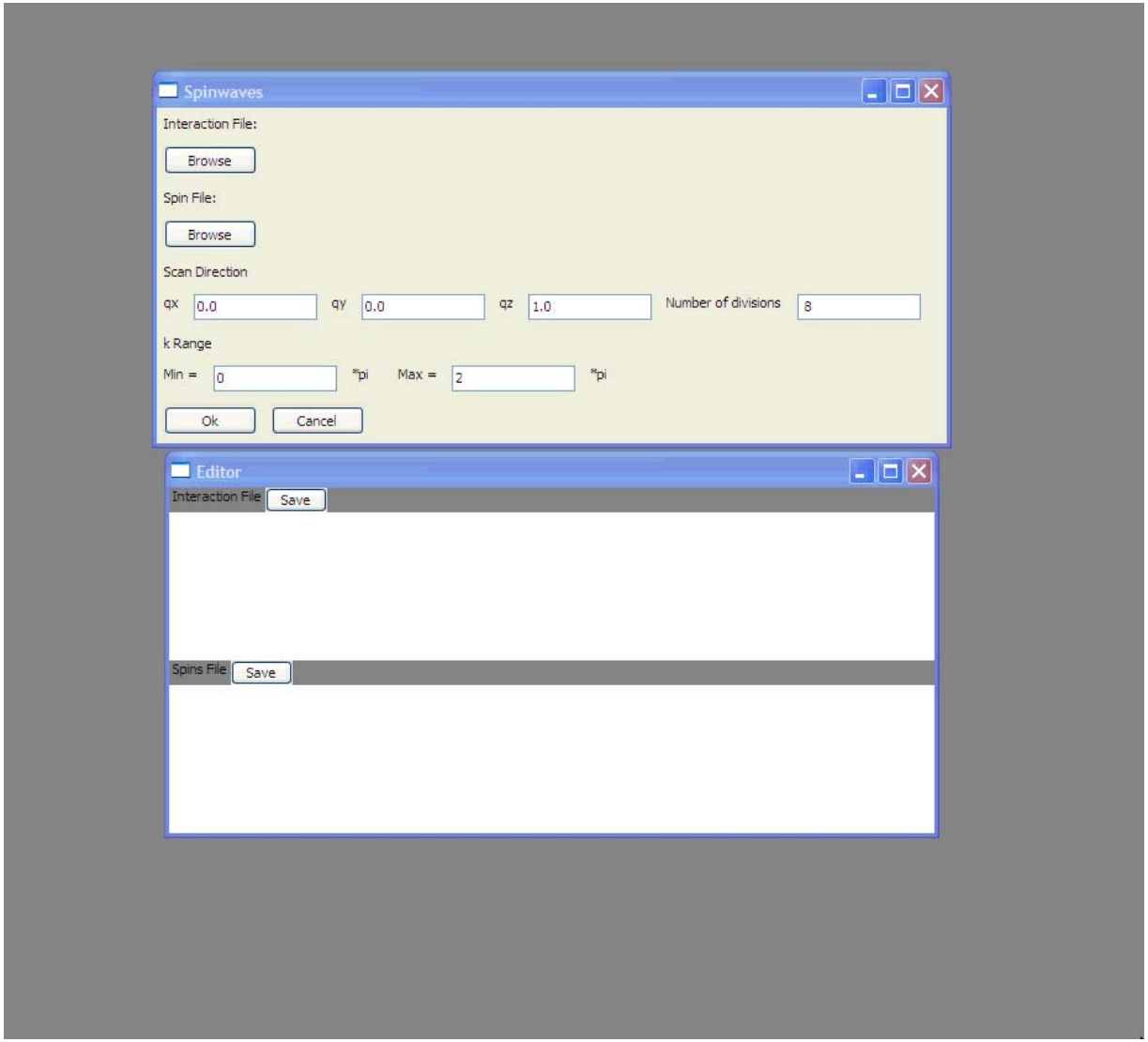


Program Demo: Dispersion Calculation



The Cross Section

- Number of neutrons scattered per second into an angle Ω with energy in [E,E+dE']
- Measurable in scattering experiment
- One magnon cross section
- One Magnon – quantized spin wave with energy of ±ħω
- We take Linear Approximation

Example: Simple ferromagnet quantized along z – axis

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{(\gamma r_0)^2}{2\pi\hbar}\frac{k'}{k}\frac{(2\pi)^3}{v_0}\frac{1}{2}\left|\langle\kappa_1|\hat{\kappa}\cdot\mathbf{M}_\perp(\mathbf{Q})|\kappa_2\rangle\right|^2 \exp\left(-2W(\mathbf{Q})\right)\sum_{\alpha\beta}\left(\delta_{\alpha\beta}-\hat{\kappa}_\alpha\hat{\kappa}_\beta\right)\sum_{\tau,\mathbf{q}}\delta(\mathbf{Q}-\boldsymbol{\tau}-\mathbf{q})\int_{-\infty}^{\infty}\langle S^\alpha_{-\mathbf{q}}(0)S^\beta_{\mathbf{q}}(t)\rangle\exp(-i\omega t)\,dt$$

What did I actually do?

TASKS

- Cross-section Calculation
- Optimization
- Fitting – Mpfit
- Testing Suite
- General code updates
- Pretty printing

COMPLICATIONS

- SymPy has little support for non-commutative algebra
  - Rewrote substitution evaluation methods in core multiplication file
  - Sent in patch for review
    - Not accepted
      - Complications with newest version of SymPy
    - Currently rewriting

Pretty printing

LATEX GUI OUTPUT

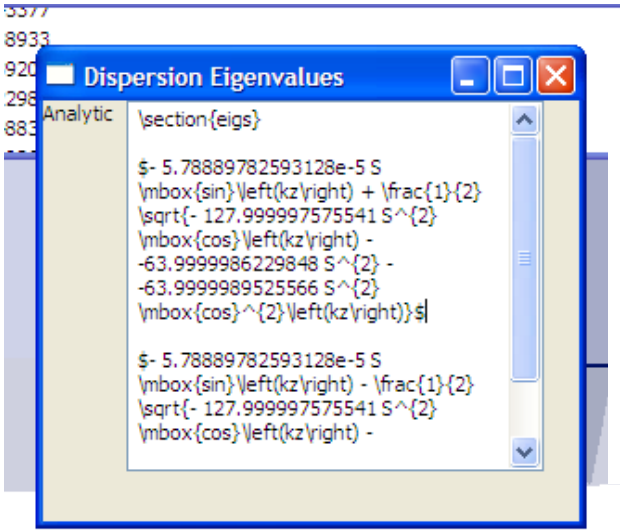
- Generates GUI text field containing LaTeX-ified output
- Uses Python Multiprocessing Module
- Complications
  - MainLoop() control
  - Processes Not Completely Independent

LATEX COMPILER

- Generates .tex, .pdf, .dvi file containing expression
- Uses Python Subprocessing Module
- Complications
  - Equation Breaking
  - Overfull Boxes
  - Requires LaTeX on machine
  - Package use
    - amsmath vs. revtex4

Pretty Printing Example

GUI POP-UP



COMPILED LATEX DOCUMENT

1 Dispersion Eigenvalues

$$-5.78889782593128e{-}5S\sin\left(kz\right)+\tfrac{1}{2}\sqrt{-127.999997575541S^{2}\cos\left(kz\right)+63.9999986229848S^{2}+63.9999895255566S^{2}\cos^{2}\left(kz\right)}$$
$$-5.78889782593128e{-}5S\sin\left(kz\right)-\tfrac{1}{2}\sqrt{-127.999997575541S^{2}\cos\left(kz\right)+63.9999986229848S^{2}+63.9999895255566S^{2}\cos^{2}\left(kz\right)}$$

Future

- Fitting data
- Resolution convolution
- Powder average
- Domain average
- Better non-commutative algebra system
- Comprehensive testing
- Widespread distribution

Acknowledgements

- William Ratcliff
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