Spinwave Calc File

Bill Flynn

May 12, 2010

1

First we generate the spin of each atom in the local coordinate system (using the z-axis as the quantization axis). This yields a list of length = number of atoms with elements of the form:

$$s_i = \begin{pmatrix} \sqrt{\frac{S}{2}}\left(c_i + c_i^\dagger\right) \\ \sqrt{\frac{S}{2}}\left(c_i - c_i^\dagger\right)/i \\ \mathbf{S} - c_i c_i^\dagger \end{pmatrix} \tag{1}$$

where $\mathbf{S}$ is a constant (bolded for emphasis – do not confuse with matrix/vector/etc.). We then transform the local spins into the global coordinate system using a specific rotation matrix determined during the simulated annealing process.

$$S_i = Rot_i s_i \tag{2}$$

Each of the N atoms in the atom array has a vector which describes its anisotropy, or preference to point in a particular direction, and a matrix which describes how that atom interacts with other atoms. We use these to create the hamiltonian:

$$H = -\sum_{i,j=0}^{N} S_i J_{ij} S_j - \sum_{\alpha} D_\alpha S_{i_\alpha}^2 \tag{3}$$

where J_{ij} is the interaction matrix between two interacting atoms and D_α corresponds to preference along the $\{x, y, z\}$ directions. This process yeilds an expression which we then simplify by removing all terms that do not depend on spin, $\mathbf{S}$. For example, the expression

$$A\mathbf{S}^2 + B\mathbf{S} + C + D\mathbf{S}^2 + E + F\mathbf{S} + \ldots \tag{4}$$

is reduced to

$$A\mathbf{S}^2 + B\mathbf{S} + D\mathbf{S}^2 + F\mathbf{S} + \ldots. \tag{5}$$

For the Fourier transform, we make the following substitutions in the Hamiltonian, H:

$$c_i^\dagger c_j^\dagger \rightarrow \frac{1}{2}\left(c_{k,i}^\dagger c_{-k,j}^\dagger e^{-i\vec{k}\cdot\vec{r}} + c_{-k,i}^\dagger c_{k,j}^\dagger e^{i\vec{k}\cdot\vec{r}}\right) \tag{6}$$

$$c_i c_j \rightarrow \frac{1}{2}\left(c_{k,i} c_{-k,j} e^{i\vec{k}\cdot\vec{r}} + c_{-k,i} c_{k,j} e^{-i\vec{k}\cdot\vec{r}}\right) \tag{7}$$

$$c_i^\dagger c_j \rightarrow \frac{1}{2}\left(c_{k,i}^\dagger c_{k,j} e^{-i\vec{k}\cdot\vec{r}} + c_{-k,i}^\dagger c_{-kj} e^{i\vec{k}\cdot\vec{r}}\right) \tag{8}$$

$$c_i c_j^\dagger \rightarrow \frac{1}{2}\left(c_{k,i} c_{k,j}^\dagger e^{i\vec{k}\cdot\vec{r}} + c_{-k,i} c_{-k,j}^\dagger e^{-i\vec{k}\cdot\vec{r}}\right) \tag{9}$$

$$c_j^\dagger c_j \rightarrow \frac{1}{2}\left(c_{k,j}^\dagger c_{k,j} + c_{-k,j}^\dagger c_{-k,j}\right) \tag{10}$$

Additionally, we substitute in the following commutation relations:

$$c_{k,i} c_{k,j}^\dagger \rightarrow c_{k,j}^\dagger c_{k,i} + \delta_{ij} \tag{11}$$

$$c_{-k,i}^\dagger c_{-k,j} \rightarrow c_{-k,j}^\dagger c_{-k,i} + \delta_{ij} \tag{12}$$

$$c_{k,i} c_{-k,j} \rightarrow c_{-k,j} c_{k,i} \tag{13}$$

$$c_{-k,j}^\dagger c_{k,i}^\dagger \rightarrow c_{k,i}^\dagger c_{-k,j}^\dagger \tag{14}$$

We then create the two arrays

$$O = \left[c_{k,1}, c_{k,2}, \ldots, c_{k,N}, c_{-k,1}^\dagger, c_{-k,2}^\dagger, \ldots, c_{-k,N}^\dagger\right] \tag{15}$$

and

$$O^\dagger = \left[c_{k,1}^\dagger, c_{k,2}^\dagger, \ldots, c_{k,N}^\dagger, c_{-k,1}, c_{-k,2}, \ldots, c_{-k,N}\right] \tag{16}$$

which we use to rewrite the Hamiltonian:

$$H = X_{ij} O_i O_j^\dagger \tag{17}$$

We take these coefficients, the X_{ij}, and construct the matrix X from them. We also construct a matrix G that is the same size as X which has a diagonal that looks like $\{1, 1, \ldots, 1, -1, -1, \ldots, -1\}$. The product GX is our diagonalized Hamiltonian.