Spinwave Calculations

Michael Yang[1,2], William Ratcliff II[2]
[1]Thomas Jefferson High School for Science and Technology
[2]National Institute of Standards and Technology Center for Neutron Research

Significance

- Underlying assumptions
- Colossal magneto-resistant materials
- Multiferroics

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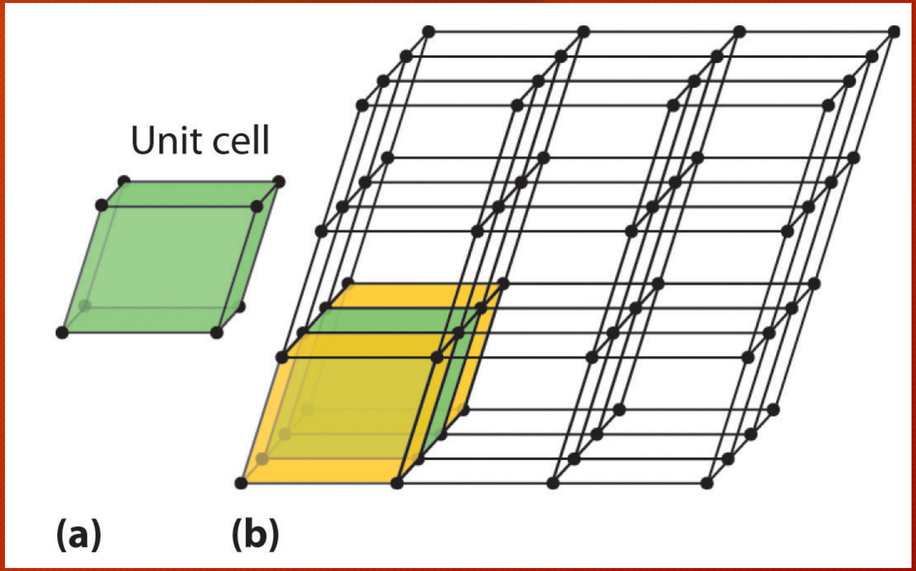
Crystal Lattice

- Lattice structure
  - Repeated unit cell
- Space groups
  - Symmetry



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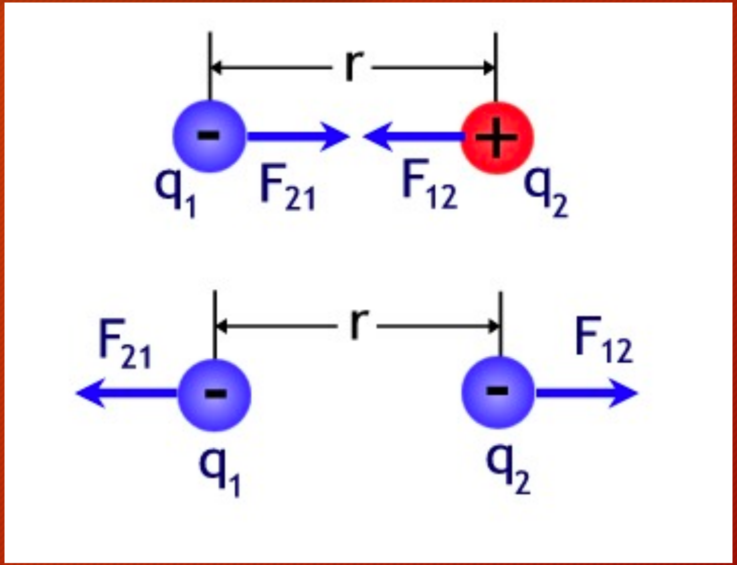
Electron Spin

- Pauli exclusion principle
- Coulomb repulsion
- Magnetic order
- Spin angular momentum
  - Operators: $\{S_x, S_y, S_z\}$



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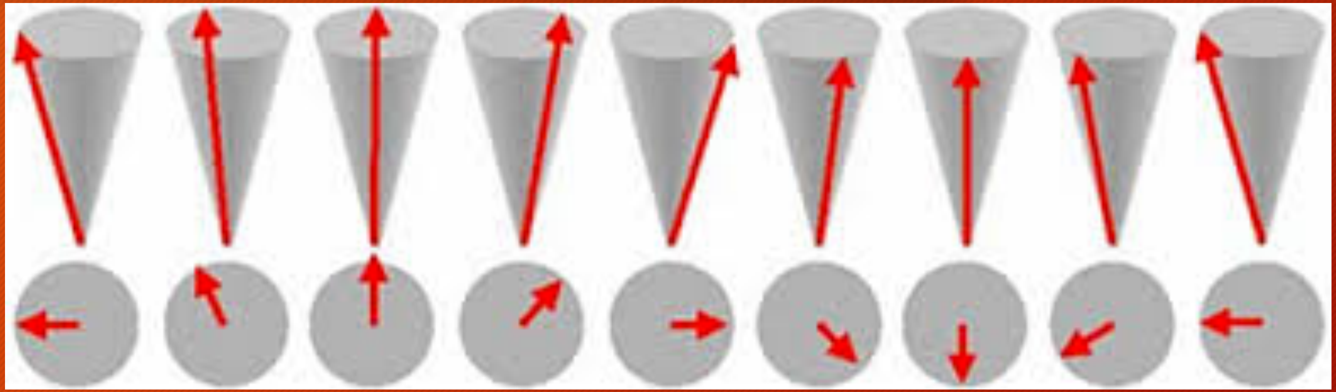
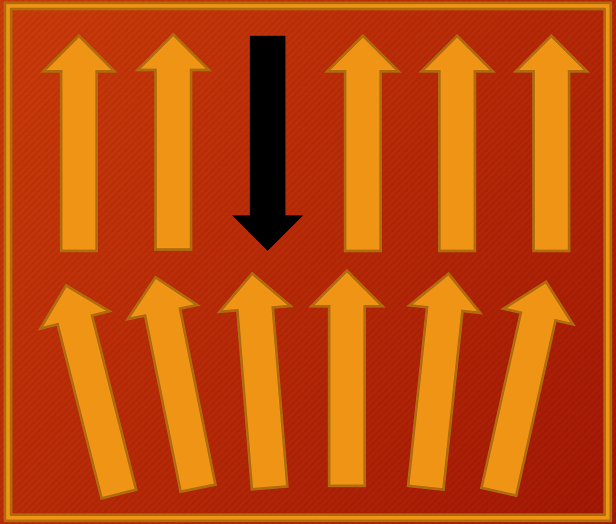
Spinwaves

- Magnetic moments
  - Ferromagnet
  - Paramagnet
- Small deviation along moments
- Causes





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Spinwave Energy Hamiltonian

$$H = \sum_{i,j} S_i J_{i,j} S_{nj} + \sum_i S_i A_i S_i + B \sum_i g_i S_i$$

- 1st Term:
  - Exchange spin interactions
- 2nd Term:
  - Anisotropic interactions
- 3rd Term:
  - Applied magnetic field

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SpinW (Paul Scherrer Institute)

- Crystal lattice
- Space groups
- Symmetry

- Invariance under rotations
- Common coordinate system
- **Linear spin wave theory**
- Holstein-Primakoff
- Fourier transform

- New spin operators
- Substitutions
- New Hamiltonian expression

- More substitutions
- Diagonalization
- Eigenvalues = spin wave energies

$$\mathsf{H} = \sum_{\substack{mi\\nj}} \left\{ \sqrt{\frac{S_i}{2}} (\overline{\mathbf{u}}_i^{\mathsf{T}} b_{mi} + \mathbf{u}_i^{\mathsf{T}} b_{mi}^{\dagger}) + \mathbf{v}_i^{\mathsf{T}} (S_i - b_{mi}^{\dagger} b_{mi}) \right\} \mathsf{R}_m^{\mathsf{T}} \mathsf{J}_{mi,nj} \mathsf{R}_n \left\{ \sqrt{\frac{S_j}{2}} (\overline{\mathbf{u}}_j b_{nj} + \mathbf{u}_j b_{nj}^{\dagger}) + \mathbf{v}_j (S_j - b_{nj}^{\dagger} b_{nj}) \right\}$$

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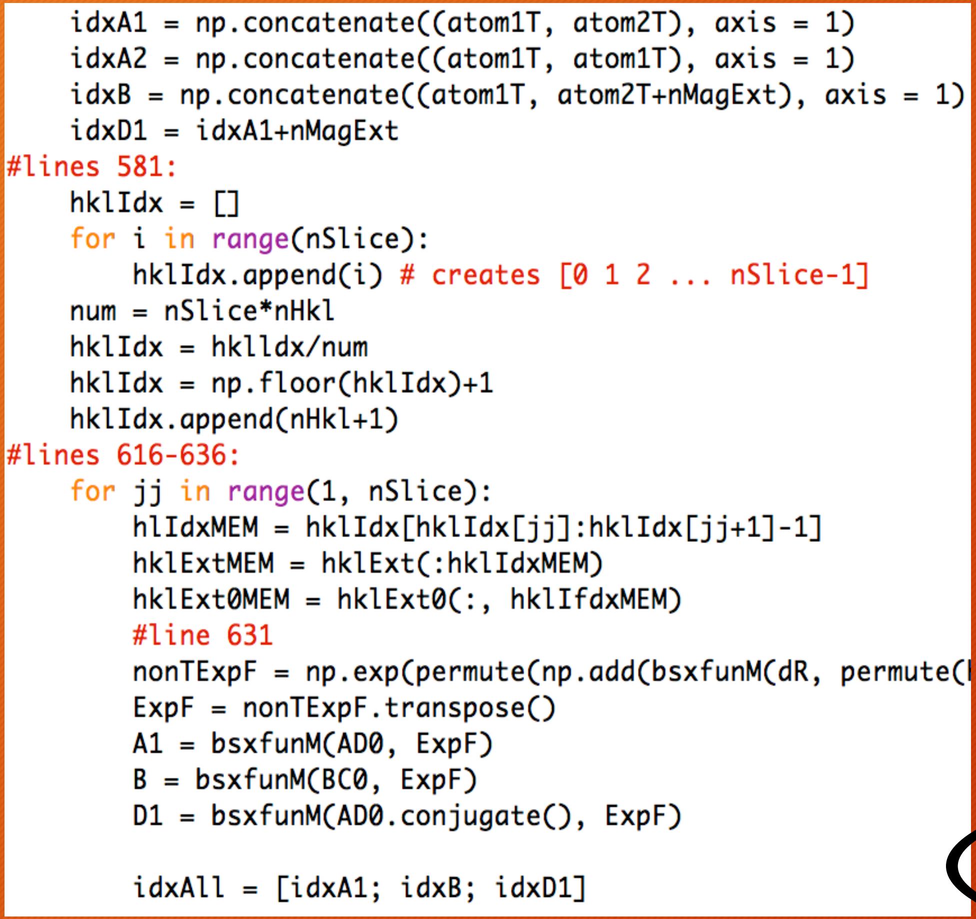
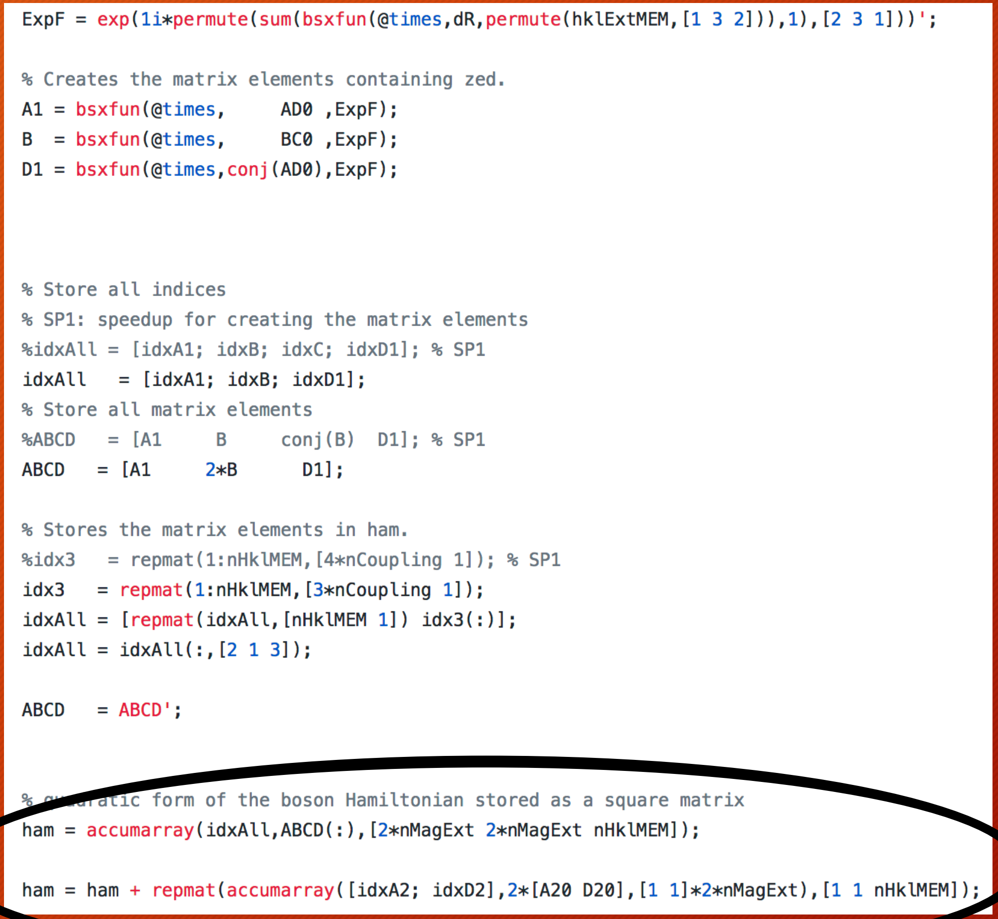
Progress



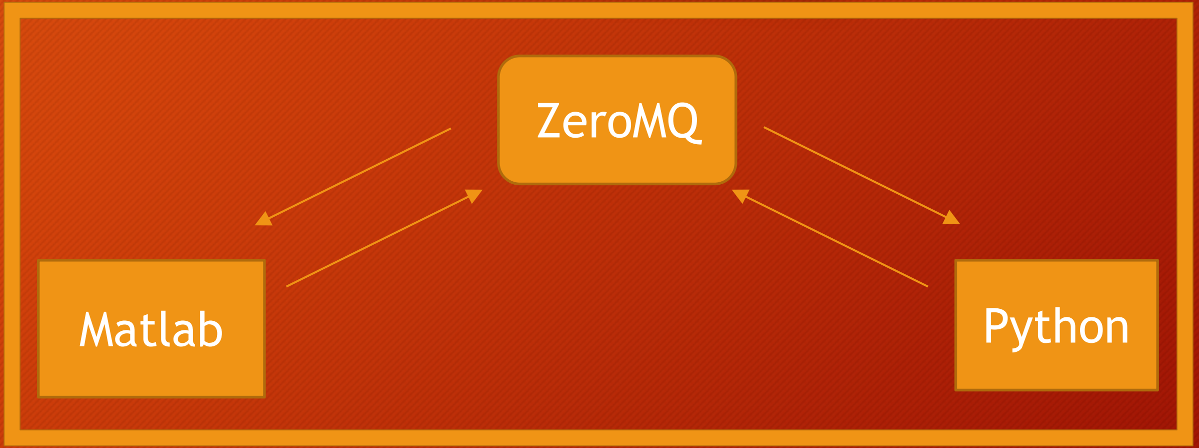
```
    idxA1 = np.concatenate((atom1T, atom2T), axis = 1)
    idxA2 = np.concatenate((atom1T, atom1T), axis = 1)
    idxB = np.concatenate((atom1T, atom2T+nMagExt), axis = 1)
    idxD1 = idxA1+nMagExt
#lines 581:
    hklIdx = []
    for i in range(nSlice):
        hklIdx.append(i) # creates [0 1 2 ... nSlice-1]
    num = nSlice*nHkl
    hklIdx = hklldx/num
    hklIdx = np.floor(hklIdx)+1
    hklIdx.append(nHkl+1)
#lines 616-636:
    for jj in range(1, nSlice):
        hlIdxMEM = hklIdx[hklIdx[jj]:hklIdx[jj+1]-1]
        hklExtMEM = hklExt(:hklIdxMEM)
        hklExt0MEM = hklExt0(:, hklIfdxMEM)
        #line 631
        nonTExpF = np.exp(permute(np.add(bsxfunM(dR, permute(
        ExpF = nonTExpF.transpose()
        A1 = bsxfunM(AD0, ExpF)
        B = bsxfunM(BC0, ExpF)
        D1 = bsxfunM(AD0.conjugate(), ExpF)

        idxAll = [idxA1; idxB; idxD1]
```

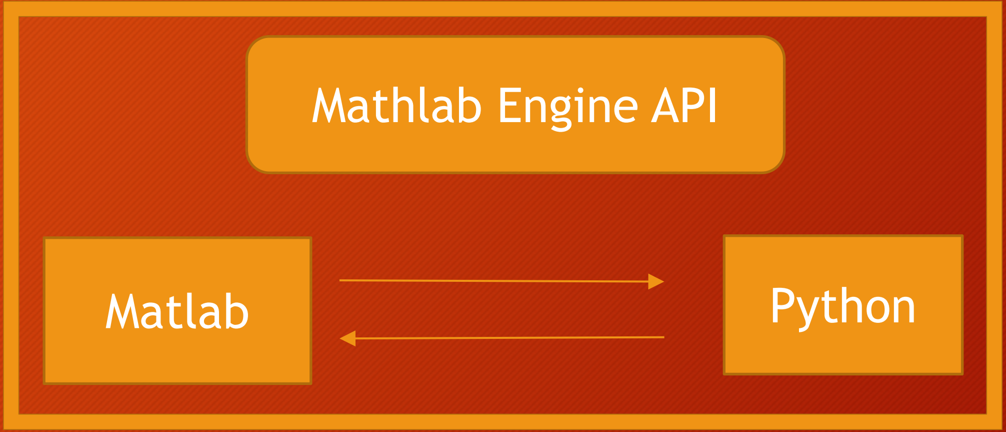


```
ExpF = exp(1i*permute(sum(bsxfun(@times,dR,permute(hklExtMEM,[1 3 2])),1),[2 3 1]))';

% Creates the matrix elements containing zed.
A1 = bsxfun(@times,     AD0 ,ExpF);
B  = bsxfun(@times,     BC0 ,ExpF);
D1 = bsxfun(@times,conj(AD0),ExpF);



% Store all indices
% SP1: speedup for creating the matrix elements
%idxAll = [idxA1; idxB; idxC; idxD1]; % SP1
idxAll   = [idxA1; idxB; idxD1];
% Store all matrix elements
%ABCD   = [A1     B     conj(B)  D1]; % SP1
ABCD   = [A1     2*B      D1];

% Stores the matrix elements in ham.
%idx3   = repmat(1:nHklMEM,[4*nCoupling 1]); % SP1
idx3   = repmat(1:nHklMEM,[3*nCoupling 1]);
idxAll = [repmat(idxAll,[nHklMEM 1]) idx3(:)];
idxAll = idxAll(:,[2 1 3]);

ABCD   = ABCD';


% quadratic form of the boson Hamiltonian stored as a square matrix
ham = accumarray(idxAll,ABCD(:),[2*nMagExt 2*nMagExt nHklMEM]);

ham = ham + repmat(accumarray([idxA2; idxD2],2*[A20 D20],[1 1]*2*nMagExt),[1 1 nHklMEM]);
```

Future Actions

- ZeroMQ and Mathlab Engine API
- Future goals





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