Analysis of spin texture in the k-space: Ver. 1.0

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A postprocessing code “kSpin”

• “kSpin” calculates the k-space spin density matrices from a scfout file for every state at every k-point.
• The k-space spin density matrices are used to analyze spin textures.
• There are four different methods in terms of how to choose k-points.
• From the k-space spin density matrix, the direction and magnitude of the spin for a state at a k-point are calculated to draw spin textures.
• The k-space spin density matrices are decomposed into the contribution to each atom and pseudo atomic orbital (PAO).
**k-space spin density matrix [1]**

\[ P_{\sigma\sigma'}(\mathbf{k}, \mu) = \left\langle \psi_{\sigma\mu}^{(k)} \right| \psi_{\sigma'\mu}^{(k)} \right\rangle = \left( c_{\sigma}^{(k)} \right)^\dagger S^{(k)} c_{\sigma'}^{(k)} \right\rangle_{\mu\mu} \]

**k**: a wave vector  
**\( \mu \)**: states (band indices)  
**\( \sigma \)**: spin indices (\( \sigma = \alpha, \beta \))  
\( \left| \psi_{\sigma\mu}^{(k)} \right\rangle \): Bloch states  
\( c_{\sigma} \): LCPAO expansion coefficients  
\( S^{(k)} \): The overlap matrix


Eigenvalue problems for the Kohn-Sham equation:

\[ H_{\sigma}^{(k)} c_{\sigma}^{(k)} = S^{(k)} c_{\sigma}^{(k)} \varepsilon_{\sigma}^{(k)} \]

\( H_{\sigma}^{(k)} \): The Hamiltonian  
\( \varepsilon_{\sigma}^{(k)} \): Energy eigenvalues
Decomposition of the k-space spin density matrices

\[ M_{\sigma\sigma',ia}(k,\mu) = \sum_{jb} c^{(k)*}_{\sigma\mu,ia} S^{(k)}_{iajb} c^{(k)}_{\sigma',\mu,jb}, \]

where

\[ P_{\sigma\sigma'}(k,\mu) = \sum_{ia} M_{\sigma\sigma',ia}(k,\mu). \]

\( k \): a wave vector
\( \mu \): states (band indices)
\( \sigma \): spin indices
\( i, j \): site indices
\( ia, jb \): PAO indices

\( |\psi^{(k)}_{\sigma\mu}\rangle \): Bloch states
\( c_{\sigma} \): LCPAO expansion coefficients
\( S^{(k)} \): The overlap matrix
Method 1: GridCalc

1. Set an $n$ by $m$ k-point grid in a user-specified two-dimensional reciprocal space.
2. Solve eigenvalue problems at each k-point.
3. Calculate the k-space spin density matrices at each k-point.

An example in the case of $n = m = 4$
Method 2: FermiLoop – 1st step

1. Set an $n$ by $m$ k-point grid in a user-specified two-dimensional reciprocal space.
   (We call it the first k-point grid hereafter.)
2. Solve eigenvalue problems at each k-point.

An example in the case of $n = m = 4$
Method 2: FermiLoop – 1\textsuperscript{st} step

3. Find squares crossing curves that connects k-points where the energy is equal to an user-specified energy level (a green region in the below figure).

An example in the case of $n = m = 4$

Curve that connects k-points where the energy is equal to an user-specified energy level.
Method 2: FermiLoop – 2\textsuperscript{nd} step

4. Set an triangle mesh as the second k-point grid in the squares on the first k-point grid.
5. Solve eigenvalue problems at each k-point on the second k-point grid.
6. Pick up sides of triangles, which compose the k-point grid, that crosses Fermi arcs.
Method 2: FermiLoop – 2\textsuperscript{nd} step

7. Determine k-points on the curves by linear interpolation or Brent’s method for energy eigenvalues. Data of these k-points is stored as it is useful to draw closed curves by connecting them. It is important to constant energy lines for Rashba spin splittings, for example.
Method 2: FermiLoop – 2\textsuperscript{nd} step

8. Calculate the k-space spin density matrices at each k-point on Fermi arcs.
Method 3: BandDispersion

1. Specify k-paths.
2. Solve eigenvalue problems at each of k-points on k-paths.
3. Calculate the k-space spin density matrices at each k-point.

Specification of k-paths:

```
Band.Nkpath 2
<Band.kpath
  135 0.0 0.500000 0.000000 0.0 0.000000 0.000000 M G
  135 0.0 0.000000 0.000000 0.0 -0.500000 0.000000 G -M
Band.kpath>
```
Method 4: MulPOnly

1. Solve eigenvalue problems at each of given sets of a k-point and a state (band index).
2. Calculate the k-space spin density matrices at each k-point.

Specification of sets of a k-point and a state:

<table>
<thead>
<tr>
<th>k_x</th>
<th>k_y</th>
<th>k_z</th>
<th>μ (State, Band index)</th>
</tr>
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<td>0.1800000000000000</td>
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