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 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]

$$P_{\sigma\sigma'}(\mathbf{k},\mu) = \left\langle \psi^{(\mathbf{k})}_{\sigma\mu} \middle| \psi^{(\mathbf{k})}_{\sigma'\mu} \right\rangle = \left(c^{(\mathbf{k})\dagger}_{\sigma} S^{(\mathbf{k})} c^{(\mathbf{k})}_{\sigma'} \right)_{\mu\mu}$$

$\mathbf{k}$: a wave vector

μ : states (band indices)

σ : spin indices ($\sigma = \alpha, \beta$)

$\left| \psi^{(\mathbf{k})}_{\sigma\mu} \right\rangle$: Bloch states

c_{σ} : LCPAO expansion coefficients

$S^{(\mathbf{k})}$: The overlap matrix

$$\begin{pmatrix} P_{\alpha\alpha}(\mathbf{k},\mu) & P_{\alpha\beta}(\mathbf{k},\mu) \\ P_{\beta\alpha}(\mathbf{k},\mu) & P_{\beta\beta}(\mathbf{k},\mu) \end{pmatrix}$$

Eigenvalue problems for the Kohn-Sham equation

$H^{(\mathbf{k})}_{\sigma} c^{(\mathbf{k})}_{\sigma} = S^{(\mathbf{k})} c^{(\mathbf{k})}_{\sigma} \varepsilon^{(\mathbf{k})}_{\sigma}$

$H^{(\mathbf{k})}_{\sigma}$: The Hamiltonian

$\varepsilon^{(\mathbf{k})}_{\sigma}$: Energy eigenvalues

[1] H. Kotaka, F. Ishii, and M. Saito, Jpn. J. Appl. Phys. **52**, 035204 (2013).

Decomposition of the k-space spin density matrices

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

where

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

$\mathbf{k}$: a wave vector

μ : states (band indices)

σ : spin indices

i, j : site indices

ia, jb : PAO indices

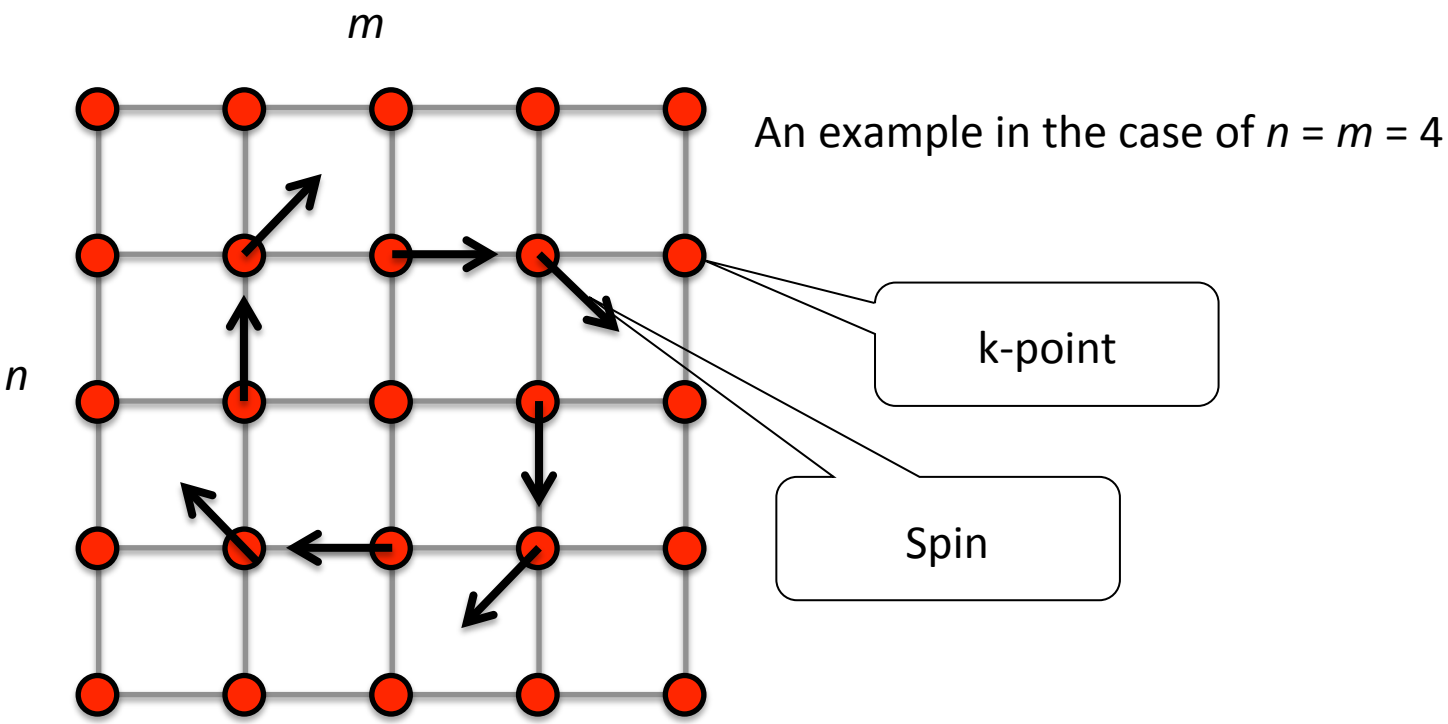
$\left|\psi^{(\mathbf{k})}_{\sigma\mu}\right\rangle$: Bloch states

c_{σ} : LCPAO expansion coefficients

$S^{(\mathbf{k})}$: The overlap matrix

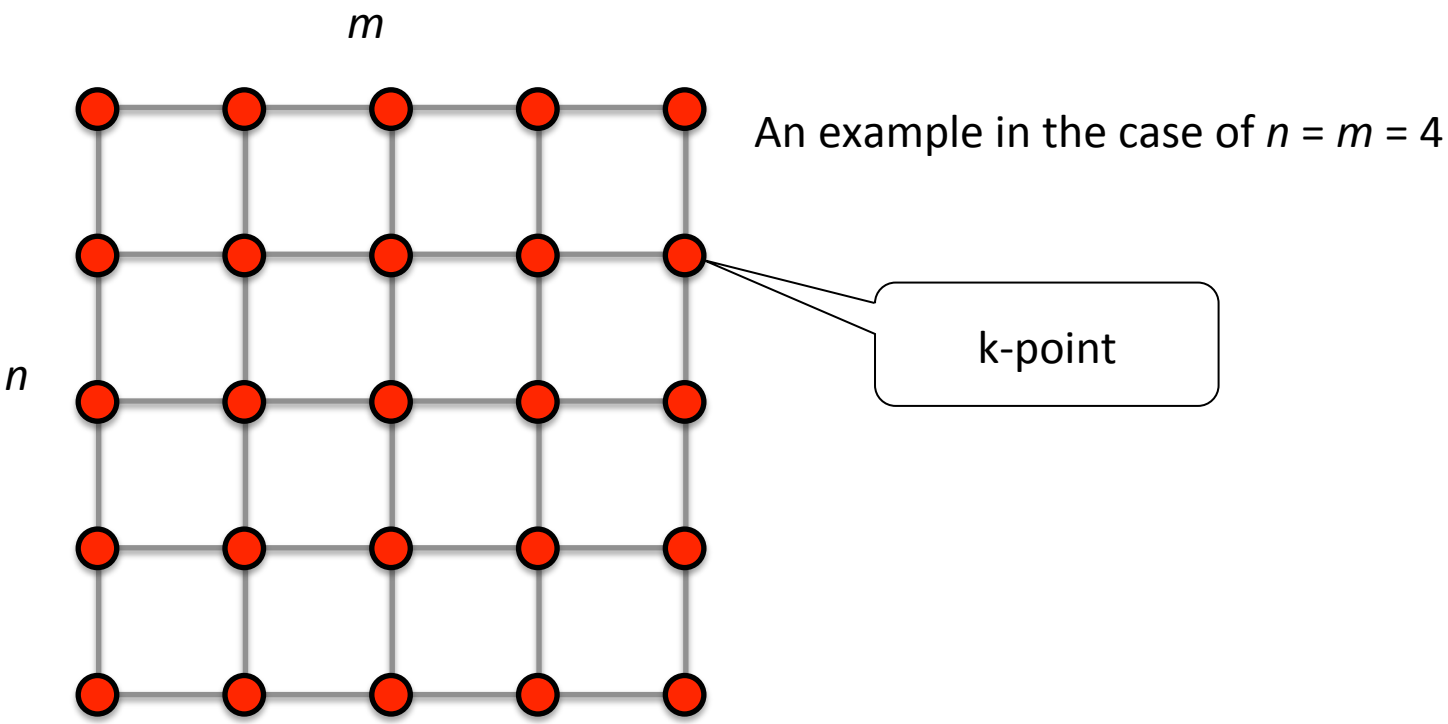
Method 1: GridCalc

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.



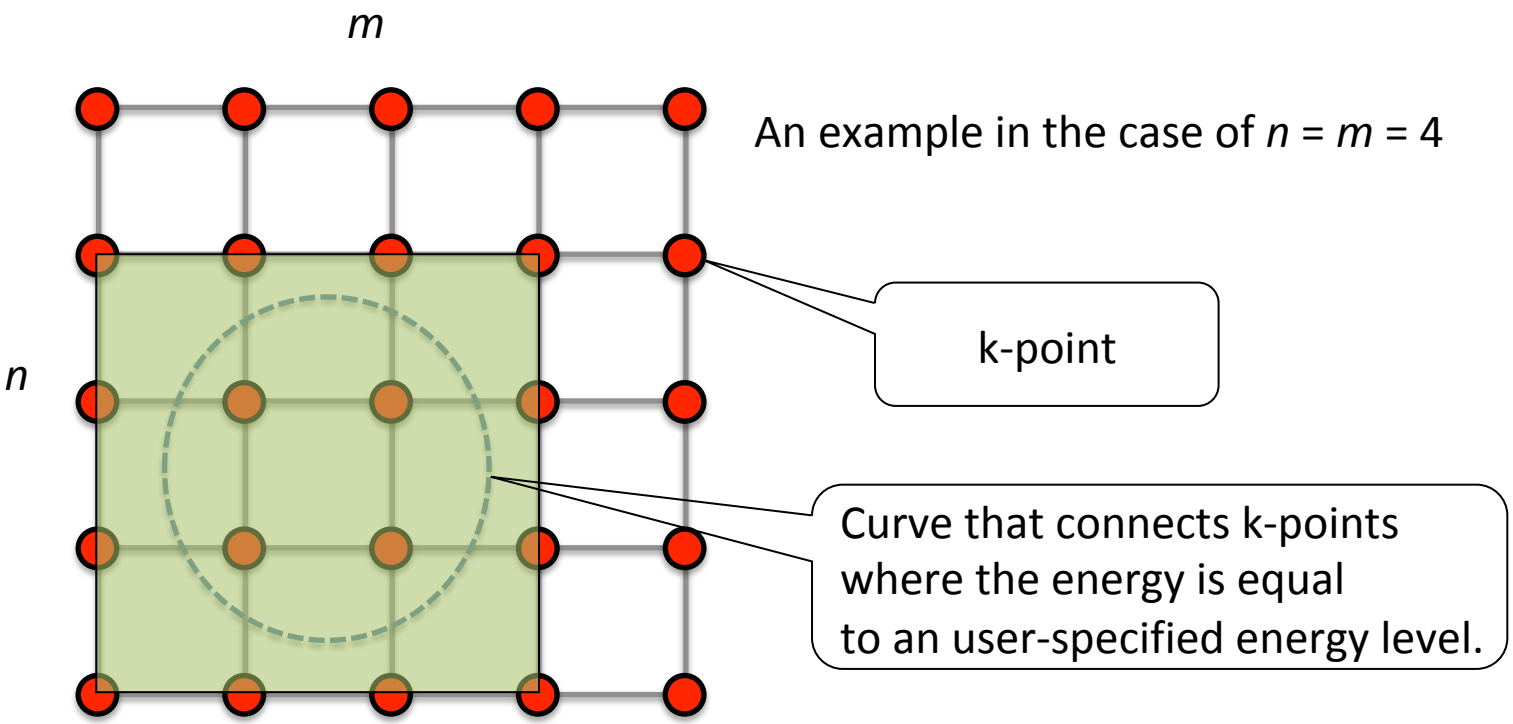
Method 2: FermiLoop – 1st step

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.



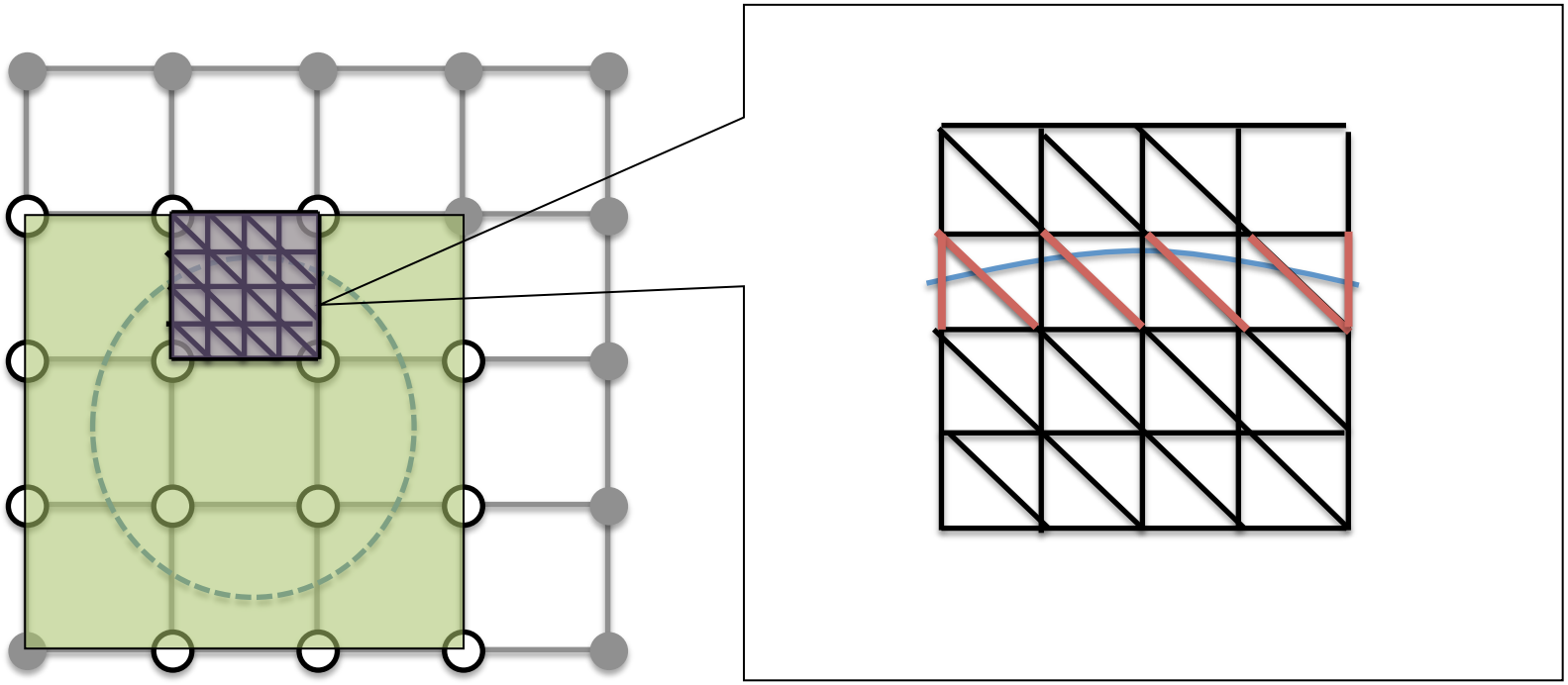
Method 2: FermiLoop – 1st step

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).



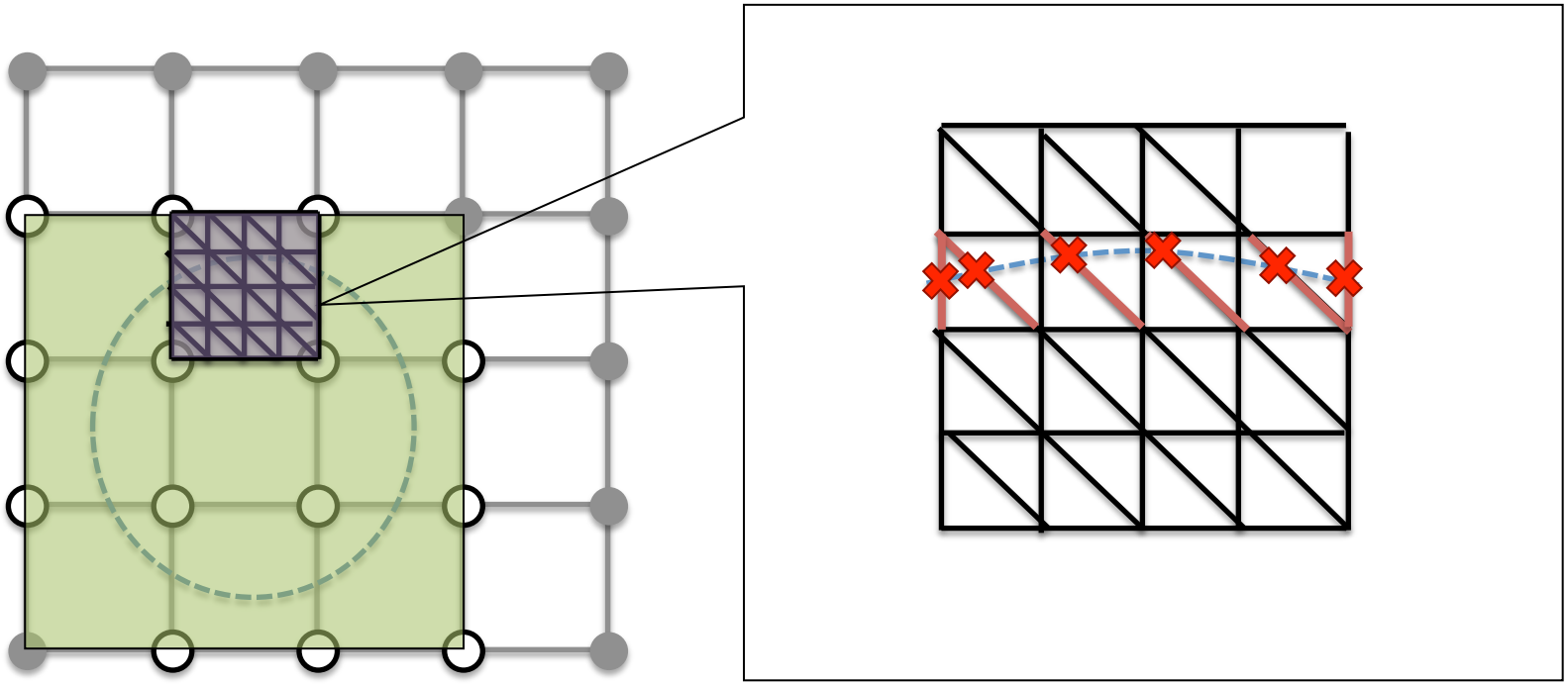
Method 2: FermiLoop – 2nd step

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.



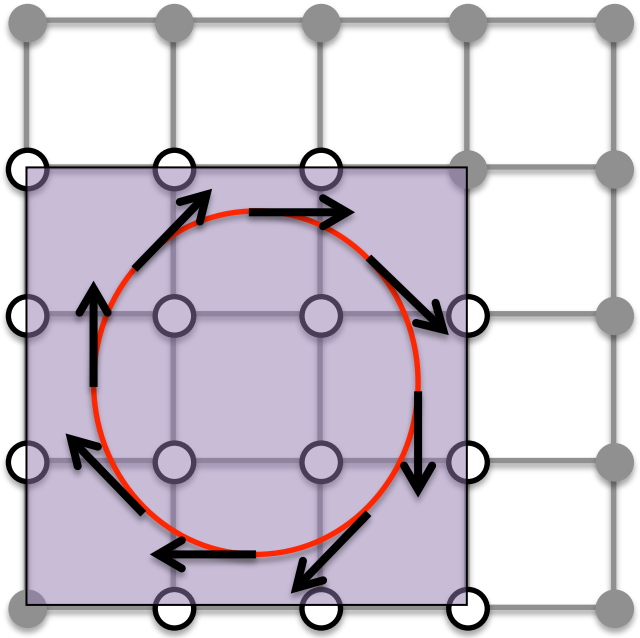
Method 2: FermiLoop – 2nd step

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 – 2nd 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:

k_x	k_y	k_z	μ (State, Band index)
0.00000000000000	0.18000000000000	0.00000000000000	55
0.00000000000000	0.17778390130712	0.02815820370724	55
0.00000000000000	0.17119017293313	0.05562305898749	55
0.00000000000000	0.16038117435391	0.08171828995312	55
0.00000000000000	0.14562305898749	0.10580134541265	55
0.00000000000000	0.12727922061358	0.12727922061358	55
0.00000000000000	0.10580134541265	0.14562305898749	55
0.00000000000000	0.08171828995312	0.16038117435391	55
0.00000000000000	0.05562305898749	0.17119017293313	55