DIPAN
Classical Dipolar Field and Anisotropy in Magnetic Systems

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1 Dipolar field

Magnetic moment $\vec{\mu}_i$ at the point $\vec{r_i}$ gives rise to magnetic field at $\vec{r}\,'$=0, where the nucleus in question is located

$$\vec{b}^i_{dip} = \frac{3(\vec{\mu}_i\,\vec{r}_i)\vec{r}_i - r_i^2\vec{\mu}_i}{r_i^5}. \tag{1}$$

Assume that system is magnetic with $\vec{\mu}_i \parallel \vec{M}$ and we calculate projection of $\vec{b}^i_{dip}$ on the direction of $\vec{M}$. It follows

$$b^i_{dip} = c_{dip}\frac{\mu_i\,[3\,\cos^2\theta_i - 1]}{r_i^3} \tag{2}$$

where θ_i is the angle which magnetization $\vec{M}$ makes with $\vec{r}_i$. If μ_i is in Bohr magnetons, r_i in a.u. and b^i_{dip} in T then
$c_{dip} = -0.53963\ \mathrm{T}\,(\mathrm{a.u.})^3\,\mu_B^{-1}$
Total B_{dip} is the sum over all moments in the system except the moment of atom with nucleus in question.

$$B_{dip} = \sum_{r_i \neq 0} b^i_{dip} \tag{3}$$

In systems with cubic or spherical symmetry B_{dip} is zero. If the sample has nonspherical shape there is a contribution from the surface connected to the demagnetization field and that is not treated here and must be calculated separately.

Program DIPAN calculates B_{dip} by 'brute force' - summing contributions from all magnetic moments in a sphere with radius R_{max}. The calculation is performed for all atoms in the unit cell.

2 Classical dipolar anisotropy energy

In calculation of dipolar anisotropy energy the sum over all atoms in the unit cell is made:

$$E_{an} = -(c_{an}/2V) \sum_j B^j_{dip}\, \mu_j \tag{4}$$

factor 1/2 because of the double summation. V is the volume of the unit cell. with μ_j in Bohr magnetons, B^j_{dip} in T, V in (a.u.)$^{-3}$ the coefficient is
c_{an}= 62584.2.10^5 J/m^3 (μ_B= 9.2740154.10^{-24} J/T, a.u.=5.291772.10^{-11} m).

3 Main limitations

- Spins are collinear and hyperfine field is collinear with the spin.
- Spin density is approximated by point magnetic dipoles located at lattice sites. This implies that any contribution from the interstitial is neglected.

4 Implementation

Program DIPAN is based on the NN program of WIEN2k package. To check the convergency of results with increasing radius R_{max} of the sphere, the contributions of spherical slabs S_n are calculated. S_n are defined as

$$S_n : \quad R^{(n)}_{min} \le r_j < R^{(n)}_{max}$$
$$R^{(n)}_{min} = R^{(n-1)}_{max};\ R^{(n)}_{max} = 2 * R^{(n-1)}_{max}$$

$R^{(0)}_{min}$, R^0_{max} are given in input together with the number N_r that determines maximum number of slabs. Denoting ΔE^n_{an} the contribution of the last slab to E_{an}, the convergency is reached when

$$|\Delta E^n_{an}/E_{an}| < \varepsilon \tag{5}$$

ε being another input parameter.

Calculation is performed for number N_{dir} of directions of magnetization. Note that if the symmetry is axial, single direction is sufficient, for orthorhombic symmetry two directions must be considered.

5 Input data

Similarly as in NN program the information about crystal structure are read from the file case.struct linked to fort.20.

Input is read from case.indip:
1st line $R^{(0)}_{min}$, $R^{(0)}_{max}$, N_r, ε, ipr
2nd line μ_i

3rd line V
4th line N_{dir}
5th line n_x, n_y, n_z

1st line: $R_{min}^{(0)}$, R_{max}^0, N_r, ε are explained above, ipr is the printing option ($ipr = 1$ normal choice, higher values produce longer output).
2nd line: μ_i magnetic moment in μ_B of i-th type of atom (repeated N_{at} times).
3rd line: Volume of unit cell in (a.u.)^3.
4th line: Number N_{dir} of magnetization directions.
5th line: Direction of $\vec{M}$ expressed in lattice vectors as in LAPWSO (repeated N_{dir} times).

All data are in free format, μ_i and V may be taken from case.scf file.
Example of the input data for hcp Co.

```
0.001 5. 7 0.01  1        Rmin0 Rmax0 (a.u.) Nr eps ipr
1.701                     Magnetic moment of Co atom in mu_B
167.48971                 Volume in a.u.**(-3)
2                         Number of magnetization directions
0. 0. 1.                  first direction for the magnetization
1. 0. 0.                  second direction (for testing only -
                                  because of axial symmetry not needed)
```

6 Output

Minimal output ($ipr \leq 0$):
Input data with explanation
Information whether required precision was achieved
Dipolar energy repeated Ndir times
Dipolar field for all atoms in unit cell (repeated Ndir times).
Example of output with the above data for Co:

```
   Dipolar field and magnetic anisotropy - lattice contribution
Co
 Initial Rmin and Rmax of spherical slab =  0.00010  5.00000 a.u.
 Number NR of steps in which Rmax is doubled=   7
 Required precision |(sum_NR - sum_NR-1)|/sum_NR=     0.10000
 atom type   1 has mag. moment   1.7010 Bohr magneton
 volume of unit cell in a.u**(-3)     167.48971
 Required precision achieved, difmax=  0.099065<eps=  0.100000
 M||  0.0  0.0  1.0 Dipolar energy     0.22988 .10**5 J/m**3
 M||  1.0  0.0  0.0 Dipolar energy    -0.11494 .10**5 J/m**3
 Atom   1 Equiv.   1 M||  0.0  0.0  1.0 Bdip    -0.00036 T
 Atom   1 Equiv.   1 M||  1.0  0.0  0.0 Bdip     0.00018 T
 Atom   1 Equiv.   2 M||  0.0  0.0  1.0 Bdip    -0.00036 T
```

```
 Atom   1 Equiv.   2 M||  1.0  0.0  0.0 Bdip     0.00018 T
```

Recommended output $ipr = 1$:
To the above output the contributions from individual slabs are added with number of atoms in the slab that contribute to B_{dip}.
Output for hcp Co is:

```
    Dipolar field and magnetic anisotropy - lattice contribution
Co
 Initial Rmin and Rmax of spherical slab =  0.00010  5.00000 a.u.
 Number NR of steps in which Rmax is doubled=   7
 Required precision |(sum_NR - sum_NR-1)|/sum_NR=     0.10000
 atom type   1 has mag. moment   1.7010 Bohr magneton
 volume of unit cell in a.u**(-3)     167.48971
 Required precision achieved, difmax=  0.099065<eps=  0.100000
  Dipolar energy convergency
  slab  Rmin    Rmax  Edip(.10**5 J/m**3) Natom       M along
   1   0.000   5.000     0.10661             12  0.0  0.0  1.0
   2   5.000  10.000     1.27660             44  0.0  0.0  1.0
   3  10.000  20.000    -2.02787            344  0.0  0.0  1.0
   4  20.000  40.000     0.66540           2802  0.0  0.0  1.0
   5  40.000  80.000     0.21835          22420  0.0  0.0  1.0
   6  80.000 160.000    -0.03197         179210  0.0  0.0  1.0
   7 160.000 320.000     0.02277        1433842  0.0  0.0  1.0
  slab  Rmin    Rmax  Edip(.10**5 J/m**3) Natom       M along
   1   0.000   5.000    -0.05330             12  1.0  0.0  0.0
   2   5.000  10.000    -0.63830             44  1.0  0.0  0.0
   3  10.000  20.000     1.01394            344  1.0  0.0  0.0
   4  20.000  40.000    -0.33270           2802  1.0  0.0  0.0
   5  40.000  80.000    -0.10918          22420  1.0  0.0  0.0
   6  80.000 160.000     0.01599         179210  1.0  0.0  0.0
   7 160.000 320.000    -0.01139        1433842  1.0  0.0  0.0
  Dipolar field convergency
 Atom   1 Equiv.   1
  slab  Rmin    Rmax    Bdip(Tesla)      Natom       M along
   1   0.000   5.000    -0.00017             12  0.0  0.0  1.0
   2   5.000  10.000    -0.00201             44  0.0  0.0  1.0
   3  10.000  20.000     0.00319            344  0.0  0.0  1.0
   4  20.000  40.000    -0.00105           2802  0.0  0.0  1.0
   5  40.000  80.000    -0.00034          22420  0.0  0.0  1.0
   6  80.000 160.000     0.00005         179210  0.0  0.0  1.0
   7 160.000 320.000    -0.00004        1433842  0.0  0.0  1.0
  slab  Rmin    Rmax    Bdip(Tesla)      Natom       M along
   1   0.000   5.000     0.00008             12  1.0  0.0  0.0
   2   5.000  10.000     0.00100             44  1.0  0.0  0.0
   3  10.000  20.000    -0.00160            344  1.0  0.0  0.0
```

```
   4  20.000  40.000     0.00052           2802  1.0  0.0  0.0
   5  40.000  80.000     0.00017          22420  1.0  0.0  0.0
   6  80.000 160.000    -0.00003         179210  1.0  0.0  0.0
   7 160.000 320.000     0.00002        1433842  1.0  0.0  0.0
 Atom    1 Equiv.   2
  slab  Rmin    Rmax    Bdip(Tesla)      Natom       M along
   1   0.000   5.000    -0.00017             12  0.0  0.0  1.0
   2   5.000  10.000    -0.00201             44  0.0  0.0  1.0
   3  10.000  20.000     0.00319            344  0.0  0.0  1.0
   4  20.000  40.000    -0.00105           2802  0.0  0.0  1.0
   5  40.000  80.000    -0.00034          22420  0.0  0.0  1.0
   6  80.000 160.000     0.00005         179210  0.0  0.0  1.0
   7 160.000 320.000    -0.00004        1433842  0.0  0.0  1.0
  slab  Rmin    Rmax    Bdip(Tesla)      Natom       M along
   1   0.000   5.000     0.00008             12  1.0  0.0  0.0
   2   5.000  10.000     0.00100             44  1.0  0.0  0.0
   3  10.000  20.000    -0.00160            344  1.0  0.0  0.0
   4  20.000  40.000     0.00052           2802  1.0  0.0  0.0
   5  40.000  80.000     0.00017          22420  1.0  0.0  0.0
   6  80.000 160.000    -0.00003         179210  1.0  0.0  0.0
   7 160.000 320.000     0.00002        1433842  1.0  0.0  0.0

 M||  0.0  0.0  1.0 Dipolar energy     0.22988 .10**5 J/m**3
 M||  1.0  0.0  0.0 Dipolar energy    -0.11494 .10**5 J/m**3
 Atom    1 Equiv.   1 M||  0.0  0.0  1.0 Bdip    -0.00036 T
 Atom    1 Equiv.   1 M||  1.0  0.0  0.0 Bdip     0.00018 T
 Atom    1 Equiv.   2 M||  0.0  0.0  1.0 Bdip    -0.00036 T
 Atom    1 Equiv.   2 M||  1.0  0.0  0.0 Bdip     0.00018 T
```

7 Tests

Symmetry tests
For system with axial symmetry both the dipolar field and dipolar anisotropy must follow the dependence:

$$B_{dip} \sim 3\cos^2\Theta - 1; \;\; E_{dip} \sim 3\cos^2\Theta - 1 \tag{6}$$

where Θ is the angle that $\vec{M}$ makes with the symmetry axis. We checked that in all cases the above dependence is indeed obtained.
Check of correct sphere size When performing the lattice sum, the summation begins with the unit cell centered at $-n_a\vec{a}, -n_b\vec{b}, -n_c\vec{c}$ and it finishes with cell at $n_a\vec{a}, n_b\vec{b}, n_c\vec{c}$. Problem how to choose minimal set of n_a, n_b, n_c such that sphere with radius R_{max} is fully contained in corresponding parallelipoid is discussed in the Appendix. For general case we still do not have an analytic

solution, but a test may be performed by putting $ntest = 1$ at line 83 of program DIPAN. As a consequence n_a, n_b, n_c is changed to n_a+1, n_b+1, n_c+1, the results must remain the same.

8 Could we do better?

Consider the two limitations listed in section **??**. First limitation - assumption that spins are collinear would be easy to remove. The second limitation - approximation of spin density by point dipoles is more tricky. For calculation of the dipolar field this would still be possible to generalize to a continuously changing density, including the interstitial (note that 'on site' dipolar field is calculated by LAPWDM). To this end approach analogous to the calculation EFG will be needed The real problem arises with the dipolar energy. First, note that this energy is not contained in any of presently used DFT functionals. The reason is that it is the spin density - spin density (or equivalently current-current) interaction that could only be correctly treated in a fully relativistic DFT scheme and no such scheme is available.

9 Appendix A: Nonorthogonal co-ordinate systems

Problem not contained in NN program is how to choose in a nonorthogonal co-ordinate systems parallelipoid in which a sphere with given radius may be inserted. Solution of this geometrical problem is given below.

In a nonorthogonal co-ordinate system with the basis vectors $\vec{a}, \vec{b}, \vec{c}$ and angles α, β, γ

$$\cos\alpha = \frac{\vec{b}\,\vec{c}}{|\vec{b}\,\vec{c}|} \ldots \tag{7}$$

any vector $\vec{r}$ is expressed as

$$\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}. \tag{8}$$

Problem to be solved
Given a sphere with radius R centered at the origin. Find planes parallel to $(\vec{a}\vec{b})$, $(\vec{a}\vec{c})$, $(\vec{b}\vec{c})$ planes that touch the sphere.

Equation of the sphere is:

$$R^2 = r^2 = x^2a^2 + y^2b^2 + z^2c^2 + 2xyab\cos\gamma + 2xzac\cos\beta + 2yzbc\cos\gamma. \tag{9}$$

Plane parallel to $(\vec{a}\vec{b})$ plane is:

$$z = c\,\zeta \tag{10}$$

with ζ fixed.

In (9) we put

$$ax = r\cos\varphi;\ by = r\sin\varphi. \tag{11}$$

To get intersection of the sphere (9) and the plane (10) an equation is to be solved:

$$r^2[1+\sin(2\varphi)\cos\gamma] + 2\zeta r(\cos\varphi\cos\beta + \sin\varphi\cos\alpha) + \zeta^2 - R^2 = 0. \tag{12}$$

This may be regarded as a quadratic equation for r - whenever it has solution, the intersection exists. The discriminant of the equation is

$$D = 4\zeta^2(\cos\varphi\cos\beta + \sin\varphi\cos\alpha)^2 - 4[1+\sin(2\varphi)\cos\gamma](\zeta^2 - R^2). \tag{13}$$

Touching will occur when $D = 0$ that leads to

$$(\cos\varphi\cos\beta + \sin\varphi\cos\alpha)^2 - [1+\sin(2\varphi)\cos\gamma](1 - R^2/\zeta^2) = 0. \tag{14}$$

Analogous equations may be constructed for planes $\parallel (\vec{a}\vec{c})$, $(\vec{b}\vec{c})$. Denoting

$$\kappa_c = R/\zeta,\ \kappa_b = R/\eta,\ \kappa_a = R/\xi \tag{15}$$

and denoting the solutions as φ_c, φ_b, φ_a the three equation to be solved are:

$$\begin{aligned}
(\cos\varphi_c\cos\beta + \sin\varphi_c\cos\alpha)^2 - [1+\sin(2\varphi_c)\cos\gamma](1-\kappa_c^2) &= 0\\
(\cos\varphi_b\cos\alpha + \sin\varphi_b\cos\gamma)^2 - [1+\sin(2\varphi_b)\cos\beta](1-\kappa_b^2) &= 0\\
(\cos\varphi_a\cos\gamma + \sin\varphi_a\cos\beta)^2 - [1+\sin(2\varphi_a)\cos\alpha](1-\kappa_a^2) &= 0.
\end{aligned} \tag{16}$$

These are implicit equations for $\varphi_a, \varphi_b, \varphi_c$ and we seek the situation where the solution ceases to exist. In a general case, with given α, β, γ and R each equation may be considered separately and the critical values of κ's may be found. In a special cases the solution may be found analytically.

Special cases

- $\alpha = \beta = \gamma = \pi/2$: orthogonal system
  All three equations have the same structure and they reduce to

  $$\kappa^2 = 1;\ \text{i.}e.\ \zeta = \pm R;\ \eta = \pm R;\ \xi = \pm R \tag{17}$$

  and that is of course correct.

- $\alpha = \beta = \pi/2;\ \ \gamma \neq \pi/2$ (e.g. hcp lattice). First equation in (16) then gives again

  $$\zeta = \pm R. \tag{18}$$

  Third equation is

  $$\cos^2\varphi_a = \frac{1-\kappa_a^2}{\cos^2\gamma}. \tag{19}$$

Its solution is lost, if the absolute value of the right side is larger than 1. Touching situation is thus obtained for

$$1 = \frac{1-\kappa_a^2}{\cos^2\gamma} \ \ thus \ \ \xi = \pm\frac{R}{\gamma}. \tag{20}$$

Touching for the third case leads to the same equation. Summarizing we have:

$$\xi = \eta = \pm\frac{R}{\gamma}; \ \ \zeta = \pm R. \tag{21}$$

10 Appendix B

Connection of vectors in orthogonal and nonorthogonal systems.
Let $\vec{a}, \vec{b}, \vec{c}, \ \vec{i}, \vec{j}, \vec{k}$ are unit vectors in nonorthogonal and orthogonal systems, respectively. Any vector $\vec{r}$ may be expressed as

$$\vec{(r)} = r_a\vec{a} + r_b\vec{b} + r_c\vec{c} \equiv x\vec{i} + y\vec{j} + z\vec{k} \tag{22}$$

Both systems are connected by the Bravais matrix $\hat{B}$:

$$(r_a, r_b, r_c) = \hat{B}\begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{23}$$

In WIEN (subroutine DIRLAT) $\hat{B}$ is determined for all lattices and called BR2. In the output of DIRLAT $\hat{B}$ is printed as:

$$\begin{pmatrix} B_{11} & B_{21} & B_{31} \\ B_{12} & B_{22} & B_{32} \\ B_{13} & B_{23} & B_{33} \end{pmatrix} \tag{24}$$