

README for constrmag.F

Pui-Wai Ma
Culham Centre for Fusion Energy, Abingdon, Oxfordshire, OX14 3DB
United Kingdom

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1 Introduction

We added a new constrained non-collinear magnetism method to VASP. It can be implemented easily by recompiling VASP with our modified constrmag.F. Please cite the following if you are using this method.

Pui-Wai Ma and S. L. Dudarev, *Constrained density functional for noncollinear magnetism*, Physical Review B 91, 054420 (2015)

2 Theory

We define the magnetic moment of an atom as

$$\mathbf{M}_I = \int_{\Omega_I} \mathbf{m}(\mathbf{r}) d^3r, \quad (1)$$

where $\mathbf{m}(\mathbf{r})$ is a spatially varying magnetization density, and Ω_I is a sphere centred at atom I .

Instead of using \mathbf{M}_I directly, we use an alternative definition of the local magnetic moment, namely

$$\mathbf{M}_I^F = \int_{\Omega_I} \mathbf{m}(\mathbf{r}) F_I(|\mathbf{r} - \mathbf{r}_I|) d^3r \quad (2)$$

where $F_I(|\mathbf{r} - \mathbf{r}_I|)$ is a scalar function decreasing monotonically to zero towards the boundary of the atomic sphere. Such definition of \mathbf{M}_I^F was adopted in VASP for other constrained method.

The constrained total energy functional has the form:

$$E = E_0 + E_p \quad (3)$$

$$= E_0 + \sum_I \lambda_I (|\mathbf{M}_I^F| - \mathbf{e}_I \cdot \mathbf{M}_I^F) \quad (4)$$

where E_0 is the DFT energy of the material, E_p is the penalty energy term, \mathbf{e}_I is a unit vector in the desired direction of the local magnetic moment, and λ_I is a Lagrange multiplier associated with site I . The dimensionality of λ_I is the same as of external magnetic field.

The penalty energy term in (4) introduces an effective extra potential inside each sphere Ω_I centred at atom I , given by

$$V_I(\mathbf{r}) = -\mathbf{b}_p(\mathbf{r}) \cdot \sigma \quad (5)$$

where σ is the vector of Pauli matrices, and

$$\mathbf{b}_p(\mathbf{r}) = -\frac{\delta E_p}{\delta \mathbf{m}(\mathbf{r})} \quad (6)$$

$$= -\lambda_I \left(\frac{\mathbf{M}_I^F}{|\mathbf{M}_I^F|} - \mathbf{e}_I \right) F_I(|\mathbf{r} - \mathbf{r}_I|) \quad (7)$$

is an additional penalty “field” in the Kohn-Sham equations. Equations 4 and 7 show that both E_p and $V_I(\mathbf{r})$ terms vanish only if vector \mathbf{M}_I^F points in the same direction as \mathbf{e}_I .

From equation (6) we see that functions $F_I(|\mathbf{r} - \mathbf{r}_I|)$ eliminate discontinuities of the effective potential at the boundaries of atomic spheres Ω_I . We do not need to separate the core and interstitial regions. The part played by the penalty term in this respect is similar to the action of local spatially-varying external magnetic field.

For more details, please refer to our Phys. Rev. B paper.

3 Controls

Our constrained method can be activated by using:

`I_CONSTRAINED_M=4`

Other details of setup are the same as using `I_CONSTRAINED_M=1`.

Additionally, if VASP is compiled with “-Dconstrmagtanh”, it replaces the function

$$F_I(|\mathbf{r} - \mathbf{r}_I|) = \sin(x)/x, \quad (8)$$

where $x = \pi(|\mathbf{r} - \mathbf{r}_I|)/R_I$ by

$$F_I(|\mathbf{r} - \mathbf{r}_I|) = -\tanh((x/\pi - 1)/c) \quad (9)$$

where we set $c = 0.01$. It is useful for `I_CONSTRAINED_M=2`.