MagInt

Manual

version 1.0

Contents

1 Introduction

1.1 GitHub

The latest release of `MagInt` , the developer version and the documentation can be downloaded from the GitHub repository:

  `https://github.com/orgs/MagInteract/repositories/MagInt.git`

1.2 Citations

We ask you to cite the following paper when using `MagInt` :

L.V. Pourovskii *Two-site fluctuations and multipolar intersite exchange interactions in strongly correlated systems*, Phys. Rev. B **94**, 115117 (2016).

If `MagInt` is used in combination with VASP spinor projectors, the following paper should be also cited:

D. Fiore Mosca *et al. The Mott transition in the $5d^1$ compound Ba_2NaOsO_6: A DFT+DMFT study with PAW spinor projectors*, Computational Materials Science, **233**, 112764 (2024).

1.3 Credits

The `MagInt` Developer Group includes Leonid V. Pourovskii (CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, France and Collège de France, Université PSL, Paris, France) and Dario Fiore Mosca (University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria).

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2 `MagInt` formalism

`MagInt` implements the Force-Theorem in Hubbard-I (FT-HI) method that has been introduced in Ref. [1]. In the following, we briefly outline the theory implemented in by the present code; a more complete description is to be found in Ref. [1].

2.1 Intersite exchange by Force Theorem in Hubbard-I (FT-HI)

Force-theorem methods have been extensively used for calculations of intersite exchange interactions in magnetically ordered systems from first principles, see, e.g., Ref. [2] for review. That framework, usually implemented in conjunction with DFT(+U/DMFT) spin-polarized calculations, consists in evaluating the response of the system's free energy to simultaneous small tilting of two ordered moments. The magnetic degrees of freedom in the system are assumed to be describable by an effective classical Heisenberg-like Hamiltonian, thus allowing one to extract effective intersite exchange coupling between classical spins from the DFT free energy response. One may show that only the one-electron DFT band energy contributes to that response (the so-called "force theorem").

The FT-HI method implemented by `MagInt` is similar in spirit, but considers perturbations around the symmetry-unbroken (paramagnetic) state. Evaluating the intersite exchange from the paramagnetic state is preferable for strongly correlated systems, where the paramagnetic high-temperature state is typically much more accessible computationally than low-temperature ordered phases. This is obviously advantageous when dealing with a rich space of possible competing order parameters, like high-rank charge and magnetic multipoles in systems with strong spin-orbit, since, instead of running self-consistent calculations for multiple ordered phases, one needs to carry out only a single paramagnetic calculation.

The FT-HI method considers fluctuations on two neighboring correlated sites in otherwise paramagnetic state. Their correlated atomic shells are assumed to be strongly localized and described within the quasi-atomic Hubbard-I (HI) approximation. Relevant fluctuations are then those within the ground state multiplet of a given correlated shell labeled by an (effective) angular momentum J. In the most general form, such fluctuations are trace-conserving infinitesimal changes $\delta\rho$ of the J-multiplet density matrix ρ. Ref. [1] derived a force-theorem expression for the response of DFT+DMFT grand potential to such two-site fluctuations in ρ; the corresponding intersite coupling between density matrix fluctuations reads

$$\langle M_1 M_3 | V(ij) | M_2 M_4 \rangle = \mathrm{Tr}\left[G(\Delta\mathbf{R}_{ij}) \frac{\delta\Sigma_i^{at}}{\delta\rho_i^{M_3 M_4}} G(\Delta\mathbf{R}_{ji}) \frac{\delta\Sigma_j^{at}}{\delta\rho_j^{M_1 M_2}} \right], \tag{2.1}$$

where $\Delta\mathbf{R_{ij}}$ is the lattice vector connecting the sites i and j, $M = -J...J$ is the projection quantum number, $\rho_{\mathbf{R}}^{MM'}$ is the MM' element of the J-multiplet density matrix on the site i, $\frac{\delta\Sigma_i^{at}}{\delta\rho_i^{MM'}}$ is the derivative of atomic (Hubbard-I) self-energy Σ_i^{at} over a fluctuation of the $\rho_i^{MM'}$ element, $G_{\Delta\mathbf{R}_{ij}}$ is the inter-site Green's function. The self-energy derivatives are calculated with analytical formulas from atomic Green's functions [1]; the inter-site Green's function is calculated by a Fourier transform of the lattice DFT+HI Green's function.

The FT-HI method implemented by `MagInt` is applied as a post-processing on top of DFT+HI calculations. All quantities in the right hand side of eq. 2.1 are evaluated from the fully converged DFT+HI electronic structure of a given system.

2.2 Multipolar Formalism

Rather than focusing on effective inter-site couplings between density matrices ρ given by (2.1), it is preferable to represent local degrees of freedom as moments (spin, orbital or total dipole moments as well as quadrupoles, octupoles etc.). The inter-site interactions can then be naturally described as couplings between the corresponding operators associated with these moments The general form of such quantum inter-site effective Hamiltonian

is:

$$H = \sum_{\langle ij \rangle} V_{KK'}^{QQ'}(ij) O_K^Q(i) O_{K'}^{Q'}(j), \tag{2.2}$$

where $O_K^Q(i)$ is the multipolar operator acting on the J-multiplet on site i of the rank $K = 0...2J$ and projection $Q = -K...K$. The moment expansion and usual matrix representations of ρ are directly related [3, 4]; any density matrix can be exactly represented by its moment expansion.

`MagInt` implements the transformation between the inter-site interactions (2.1) and (2.2) as follows:

$$V_{KK'}^{QQ'}(ij) = \sum_{\substack{M_1 M_2 \\ M_3 M_4}} \langle M_1 M_3 | V(ij) | M_2 M_4 \rangle \left[O_Q^K \right]_{M_2 M_1} \left[O_{Q'}^{K'} \right]_{M_4 M_3}, \tag{2.3}$$

where $\left[O_Q^K(J) \right]_{M_1 M_2}$ is the $M_1 M_2$ matrix element of the corresponding multipolar operator.

The multipolar operators utilized in `MagInt` are the real-valued tensor operators $O_Q^K(J)$ constructed from the multipole tensors defined as [4]:

$$T_{KQ}(J) = \sum_{MM'} (-1)^{J-M} (2K+1)^{\frac{1}{2}} \times \begin{pmatrix} J & J & K \\ M' & -M' & Q \end{pmatrix} |JM\rangle\langle JM'| \tag{2.4}$$

via linear combinations (for $Q > 0$) as:

$$O_Q^K(J) = \frac{1}{\sqrt{2}} \left[(-1)^Q T_{KQ}(J) + T_{K-Q}(J) \right] \tag{2.5}$$

$$O_{-Q}^K(J) = \frac{i}{\sqrt{2}} \left[T_{KQ}(J) - (-1)^Q T_{K-Q}(J) \right] \tag{2.6}$$

The operators O are in fact proportional to the usual definition of multipole operators as (non-normalized) polynomials of the angular momenta, also called Stevens operators[1]. `MagInt` generally uses the normalized form, $\mathrm{Tr} \left[O_K^Q \cdot O_{K'}^{Q'} \right] = \delta_{KK'} \delta_{QQ'}$, as specified in Refs. [4, 1], but the usual angular momentum operators $\hat{S}_Q \propto \hat{O}_1^Q$ can be also employed for dipoles.

The final result of `MagInt` calculation is a set of inter-site couplings $V_{KK'}^{QQ'}(ij)$ for a given J-multiplet and a desired set of lattice vectors $\{\mathbf{R}_{ij}\}$. We stress that the resulting effective Hamiltonian is quantum, in contrast to the standard "magnetic force theorem" methods [2] mapping to a classical Hamiltonian.

2.3 Pseudo-Spin basis

The result of the mapping (2.3) into intersite coupling between multipoles depends on the choice for phases of $|JM\rangle$ eigenstates that form the basis in the space of the J multiplet. Different choices for the phases will lead to different forms of the effective Hamiltonian (2.2). Though all such choices are formally equivalent and will lead to the same values of observables, it is usually preferable to work with operators O_K^Q having well defined symmetry properties (e. g., under time reversal and transforming as well defined representations of the relevant rotation or point group). To achieve this, the J-multiplet basis needs be chosen in an optimal way.

In the case when the J-multiplet coincides with the true atomic ground state (when one evaluates the couplings for the full ground state multiplet, e. g., in an f-electron system), the choice for the phases is trivial. The phases are defined by the requirement for the matrix elements of the ladder operator $\langle JM+1|\hat{J}_+|JM\rangle$ to be real positives.

In the case when the J-multiplet is really "pseudo-spin", i.e. its basis functions are not true eigenstates of any angular momentum, choosing an optimal basis is more complex. The phases need be chosen to have proper symmetry in the pseudo-spin space, as discussed in the literature (see, e. g., Supplementary of Ref. [5] for the phase choice in context of a `MagInt` application, or Ref. [6] for a more general discussion).

`MagInt` does not provide a dedicated module to generate pseudo-spin bases, since the choice for the pseudo-spin basis depends on the problem at hand and no general scheme exists, to our awareness. Instead we provide some script examples to demonstrate the pseudo-spin construction for several typical cases.

2.4 Scope and limitations of `MagInt`

The principal application of `MagInt` is to inter-site exchange interactions (IEI) in correlated (Mott) insulators. All IEI between the ground state multiplets of correlated shells in a compound can be simultaneously evaluated,

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[1]Explicit expressions for Stevens operators can be found in many references and on-line resources, see, e. g. McPhase manual

including IEI between high-rank multipoles. The coupling mechanism can be any type of kinetic exchange between correlated shells (e. g., direct exchange or superexchange).

The method permits various choices for the ground-state J-multiplet adapted to the problem at hand. For example, one may calculate IEI only for the lowest crystal-field level (forming the corresponding pseudo-spin). Alternatively, the IEI can be calculated for the full atomic multiplet with the crystal field subsequently included into the effective Hamiltonian as a one-site term (see examples of `MagInt` applications to multipolar orders using full atomic multiplets in Refs. [7, 8] and using a pseudo-spin in Ref. [5]).

The FT-HI has certain limitations and will not be suitable to all magnetic correlated systems. `MagInt` needs to be applied with care. These limitations are detailed below:
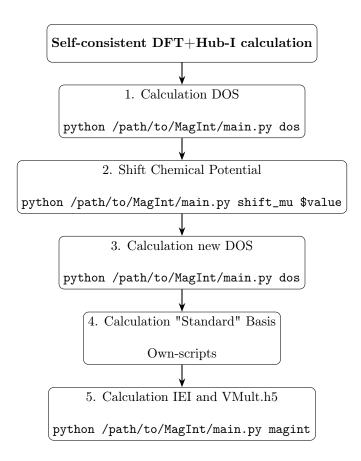
- The target correlated shells should be localized, i. e., in the Mott insulating regime with their spectral function gaped. Metallic systems can be treated, as far as the partial spectral function of the target correlated shell is gaped (see, for example, Ref. [9] for `MagInt` application to a metal).

  The method will break down if the target shell is metallic. `MagInt` will not crash, but the calculated IEI will diverge assuming nonphysical values.

- Due to drawbacks of the HI approximation, even in correlated insulators the converged DFT+HI chemical potential may happen to be pinned right at the lower or upper edges of a well-developed insulating gap. Even a small non-zero spectral weight of the target shell at the Fermi level will cause `MagInt` to break down producing nonphysical IEI. Hence, the DFT+HI spectral function should be always inspected before running `MagInt` calculations. If necessary, the chemical potential should be shifted into the gap by hand, as detailed in this manual later on.

- In some systems (e. g. rare-earth intermetallics), IEI between correlated shells are mainly due to on-site exchange coupling between the localized shell and itinerant ones (e.g., $4f$-$5d$ Hund's rule coupling in rare-earth ions). The kinetic exchange between correlated shells (which is due to $4f$-itinerant shells hopping in the example above) may then play a minor role. In those cases it is important to remember that only this kinetic exchange contribution will be taken into account by `MagInt`.

3 `MagInt` usage

The `MagInt` is a Fortran90 and python based program based on classes. In the following plot the workflow of a `MagInt` calculation is schematized, with the corresponding command lines.

Important For the convention used for the Green's functions, file names and more, please check the Conventions section.

Workflow

```
┌─────────────────────────────────────────────┐
│   Self-consistent DFT+Hub-I calculation       │
└─────────────────────────────────────────────┘
                      │
                      ▼
┌─────────────────────────────────────────────┐
│            1. Calculation DOS                 │
│                                               │
│   python /path/to/MagInt/main.py dos          │
└─────────────────────────────────────────────┘
                      │
                      ▼
┌─────────────────────────────────────────────┐
│         2. Shift Chemical Potential           │
│                                               │
│  python /path/to/MagInt/main.py shift_mu $value│
└─────────────────────────────────────────────┘
                      │
                      ▼
┌─────────────────────────────────────────────┐
│          3. Calculation new DOS               │
│                                               │
│   python /path/to/MagInt/main.py dos          │
└─────────────────────────────────────────────┘
                      │
                      ▼
┌─────────────────────────────────────────────┐
│       4. Calculation "Standard" Basis         │
│                                               │
│               Own-scripts                     │
└─────────────────────────────────────────────┘
                      │
                      ▼
┌─────────────────────────────────────────────┐
│        5. Calculation IEI and VMult.h5        │
│                                               │
│   python /path/to/MagInt/main.py magint       │
└─────────────────────────────────────────────┘
```

Workflow Explained

1. Calculation DOS:

   After completing a fully converged DFT+HI calculation, it is recommended to compute the Density of States (DOS) to ensure that the chemical potential lies within the gap.

2. Shift Chemical Potential:

   If the chemical potential is not within the gap, apply a shift to adjust it accordingly.

3. Calculation new DOS:

   Repeat the DOS calculation as described in step 1.

4. At this stage, the pseudo-spin basis (Standard_Basis.h5) must be calculated. Refer to Section 2.3 for theoretical details. Note that this is a problem-specific step, requiring a custom script tailored to the specific problem.

5. Calculation IEI and VMult.h5

   Finally, calculate the IEI and convert them to the Multipolar formalism. The result is stored in the VMult.h5 file.

3.1   Parameters

For implementing the workflow outlined in the previous section `MagInt` makes use of an input file called `maginteract.ini`.
An example of complete `maginteract.ini` file is given, followed by the explanation of all the parameters implemented. (Note that many values have defaults and do not need to be specified, if not necessary.)

```
[GENERAL]

dft_filename = 'Ba2MgReO6'
dft_exec = 'Wien2k'
folder = './'
verbosity = 2
use_symmetries = True
tol_shells = 0.001

[SOLVER]

U_int = [3.2, 3.2]
J_hund = [0.5, 0.5]
beta = 40
Kanamori = False
n_moments = 4
n_iomega = 1025
use_spin_orbit = True
DC_type = 0
chemical_potential_init = 0.0
LS = [2, 2]
n_el = [1, 1]
n_omega = 1025
ommin = -10
ommax = 10
broadening = 0.05
tol_eal = 0.0005

[BASIS]

ps_j = [1.5, 1.5]
split = 1e-6
action = 'merge'

[MAGINT]

correlated_atoms = ['Re0', 'Re1']
atom1 = 'Re0'
atom2 = 'Re1'
n_shells = 3
calc_all_sites = False
mult_conv = 'sph_tensor'
```

Parameter	Type	Description
GENERAL		
DFT_EXEC	string	DFT executable. Options are 'VASP', 'Wien2k'. `Default : 'VASP'`
NAME	string	Name of the folder.
VERBOSITY	string	Verbosity of the output. Options are 0, 1, 2 `Default : 1`
FOLDER	string	Folder where the files are located.
DFT_FILENAME	string	Filename of the DFT hdf5 output (without '.h5').
USE_SYMMETRIES	bool	Whether symmetries are switched on or not in Wien2k. They must be switched off in case of more than one correlated site or when MULT > 1.
TOL_SHELLS	float	Tolerance on the shells boundary.
SOLVER		
U_INT	list of float	Coulomb U parameter in eV. `Default : [0.0]`
J_HUND	list of float	Hund's J parameter in eV. `Default: [0.0]`
BETA	float	Inverse of temperature `Default : 40.0`
KANAMORI	bool	Whether the Kanamori-reduced Coulomb matrix is calculated or not. `Default: True`
N_MOMENTS	int	Number of moments. `Default: 4`
N_IOMEGA	int	Number of Matsubara frequencies. `Default : 1025`
USE_SPIN_ORBIT	bool	Whether SOC is used or not. `Default: True`
DC_TYPE	int	Which type of double counting is considered. `Default: 0`
CHEMICAL_POTENTIAL_INIT	list of floats	Initial chemical potential. `Default: [0.0]`
LS	list of int	Orbital number L = 0 (s), 1 (p), 2 (d) and 3 (f). If Kanamori is used for a d orbital LS = 1. `Default: [2]`
N_EL	list of int	Number of correlated electrons. `Default : [1]`
N_OMEGA	int	Number of real frequencies. `Default: 2050`
OMMIN	float	Minimum value of frequency with respect to $\omega = 0$ eV.
OMMAX	float	Maximum value of frequency with respect to $\omega = 0$ eV.

Parameter	Type	Description
SOLVER		
BROADENING	float	Broadening of the DOS.
EAL_READ	bool	Whether the Effective Atomic Levels (EALs) are read from file called "eal_last_site_$i.dat" or not. `Default : False`
N_LEV	list of int	Number of levels to be included in the GSM calculation. `Default: True`
TOL_EAL	float	Tolerance on the EAL. Values lower than this parameter are automatically set to zero. `Default: 1e-5`
BASIS		
SPLIT	float	Splitting of the GSM with applied magnetic field. `Default: 1e-6`
PS_J	list	List of effective total angular momenta J for each correlated shell. The list can be also nested, $[[\#.\#, \#.\#], [\#.\#, \#.\#],$ etc.], in that case each entity is a list of two effective J to be combined. `Default: [0]`
ACTION	string	Defines the way of combining two Js in the case of combined pseudospins, see above. Two options are possible: `dirprod`: the combined operators are direct products of the operators for each J, $O = O(J_1) \times O(J_2)$; `merge`: $O(J_1, J_2)$ are two-J multipolar operators [3]. `Default: 'merge'`
MAGINT		
ATOM1	string	Name of the first correlated atom.
ATOM2	string	Name of the second correlated atom.
		See Section 3.2 for the convention used.
N_SHELLS	int	Maximum number of shells (n-nearest-neighbors) to be included in the `MagInt` calculation. `Default: 3`
CALC_ALL_SITES	bool	Whether not only *atom1-atom2* interactions need to be calculated, but also *atom1-atom1*, *atom2-atom2* and *atom2-atom1*. `Default: False`

Parameter	Type	Description
MULT_CONV	string	Convention used for the Multipolar operators. See Section 2.2 for the formalism. Options are : `sph_tensor` : orthonormal spherical tensors O^Q_K for all K; `operator` : non-normalized angular momenta J are used for the dipole operators, $K{=}1$. `Default:  sph_tensor`
INCLUDED_ATOMS	list	Whether one wants to restrict the `MagInt` calculation to a specific subset of correlated sites. In that case a list of correlated atoms from SK.correl_to_inequiv should be initialized. `Default:  None`

3.2 Conventions

HDF5 input

`MagInt` reads the atomic Green's function, Self-Energy, EALs, and other inputs from the HDF5 file case.h5. Many of these inputs follow the DFTTools structure of the TRIQS package.

However, `MagInt` can automatically read the Self-Energy from the case.h5 file only if a specific group is present.

```
"['dmft_output']['Sigma_iw_$i']".
```

with $i being the number of the correlated shell. The atomic Green's function is saved in

```
"['dmft_output']['G_iw_$i']".
```

Correlated atoms labels

The `atom1`, `atom2` parameters in `[MAGINT]` have specific labels, in order to allow for precise calculation of magnetic interactions with respect to an atom considered as origin (`atom1`). The convention is 'ATOM'+position in the structure file.

When unsure of the actual names it is sufficient to call

```
python /path/to/magint/main.py shell
```

This will output the

```
Ion names for [MAGINT] :

['Ir0', 'Ir1', 'K2', 'K3', 'K4', 'K5', 'Br6', 'Br7', 'Br8', 'Br9', 'Br10',
    'Br11', 'Br12', 'Br13', 'Br14', 'Br15', 'Br16', 'Br17']
```

Therefore the `[MAGINT]` parameters for calculating interactions of ion `Ir1` with respect to `Ir0` can be set as

```
correlated_atoms = ['Ir0', 'Ir1']
```
```
atom1 = 'Ir0'
```
```
atom2 = 'Ir1' .
```

Additional Key Information

`MagInt` has been generalised to different cases and possible scenarios, however, some things need to be kept in mind when calculating the IEI, especially when it comes to sites with different symmetry or different ground state multiplet (GSM) multiplicity.

1. The interactions between `Ir0` and its equivalent sites will not be calculated, unless explicitly stated with the `calc_all_sites` parameter.

2. When calculating interactions between atoms of different symmetry and/or GSM, one should treat the atoms as non-equivalent.

3.3 Reading the `MagInt` output

`MagInt` generates two output files after calculating the interactions: *V_Mult_Ion0_Ion1.dat* and *Vmult.h5*. The details of these files and their content are explained below.

The *V_Mult_Ion0_Ion1.dat* File

Below is an illustrative excerpt from a real *V_Mult_Ion0_Ion1.dat* file, showcasing interactions between two Cr atoms designated as Ion0 and Ion1. The line labeled `--INTERACTION:` identifies the ions participating in the interaction. The subsequent line, `Ion0_mult0 - Ion1_mult1`, specifies the multiplicity of each ion, accounting for multiple equivalent sites.

Following this, the entry `Shell =` identifies the neighbor shell (e.g., nearest neighbor, next-nearest neighbor, etc.), while `Coor_num =` indicates the number of interacting ions within each shell.

The interaction data is presented using multipolar operator nomenclature, with values expressed in meV. Interaction matrices with elements below 10^{-5} meV are excluded for clarity. Before each interaction matrix, two vectors, `R` and `T`, are provided:

- `R`: The vector connecting the interacting ions.

- `T`: The translation vector linking the unit cells containing the respective ions.

```
 -----INTERACTION: Ion0_0 - Ion0_0

Shell=0

Coor_num = 6

Monopole-Monopole interactions

Monopole-Dipole interactions

Monopole-Quadrupole interactions

Monopole-Octupole interactions

Dipole-Monopole interactions

Dipole-Dipole interactions
 R = [-10.76323 -4.36668 5.78615]
 T = [-10.76345 -4.36700 5.78550]


             y           z           x
     y        0.835      -0.101      -0.178
     z        0.077       0.884      -0.045
     x        0.162      -0.001       0.854

 R = [-10.76323 7.24901 0.00064]
 T = [-10.76345 7.24869 -0.00000]


             y           z           x
     y        0.851       0.095       0.172
     z       -0.091       0.880      -0.030
     x       -0.166      -0.032       0.842
```

The *Vmult.h5* file

Together with the *V_Mult_Ion0_Ion1.dat* file, another file is produced, called *Vmult.h5*, which can be accessed via hdf5. The file has the following tree structure

Subgroup	Description
Multipol_Int	
GSM	Ground state multiplet multiplicity.
Kmax	Maximum value of K in the multipolar expansion.
R_vecs_Ion0-Ion1	Vectors connecting each couple of interacting ions.
TKQ	Multipolar tensor operators for a given J.
T_vecs_Ion0-Ion1	Translational vectors connecting unit cells for each couple of interacting ions considered.
<u>Vmult</u>	Matrices of intersite exchange interactions.
coor_nums_Ion0-Ion1	Coordination numbers for each couple of interacting ions and shell.
ifproduct	Whether the direct product of multipolar operators is considered.
interactions	List of interacting ions.
multipole_names	The list of multipolar operators names divided by rank K.
prn_bas	Corresponding names of multipolar operators by projection Q.
shells_Ion0-Ion1	The number of shells considered in the calculation.

In the following an example of a tree structure for a material whose interactions are up to dipole-dipole interactions. The name of the actual ion has been replaced by Ion0/Ion1 for sake of generality.

The `Vmult` convention follows this structure: Name first interacting ion, corresponding multiplicity, name of the second interacting ion, its corresponsing multiplicity, index of the connecting vector, index of first multipole and index of the second multipole operators.

So for example `Ion0_0_Ion0_0_0_1_1_1` represents the matrix of interactions between ion `Ion0` with multiplicity index `0` and the ion `Ion0` with multiplicity index `0` whose connecting vector index is `0_1` and the interaction is of dipole-dipole `1_1` type. (The corresponding actual vectors `R, T` with index `0_1` can be found at `R_vecs_Ion0-Ion1`, `T_vecs_Ion0-Ion1`)

```
|-- Multipol_Int/
    |-- GSM/
      |-- Ion0
      |-- Ion1
    |-- Kmax
    |-- R_vecs_Ion0-Ion1/
      |-- (('Ion0', 0), ('Ion0', 0))/
      |-- (('Ion0', 0), ('Ion1', 0))/
    |-- TKQ/
      |-- 0_0
      |-- 1_-1
      |-- 1_0
      |-- 1_1
    |-- T_vecs_Ion0-Ion1/
      |-- (('Ion0', 0), ('Ion0', 0))/
      |-- (('Ion0', 0), ('Ion1', 0))/
    |-- Vmult/
      |-- Ion0_0_Ion0_0_0_0_0_0
      |-- Ion0_0_Ion0_0_0_0_0_1
      |-- Ion0_0_Ion0_0_0_0_1_0
      |-- Ion0_0_Ion0_0_0_0_1_1
      |-- Ion0_0_Ion0_0_0_1_0_0
      |-- Ion0_0_Ion0_0_0_1_0_1
      |-- Ion0_0_Ion0_0_0_1_1_0
      |-- Ion0_0_Ion0_0_0_1_1_1
    |-- coor_nums_Ion0-Ion1/
      |-- (('Ion0', 0), ('Ion0', 0))/
      |-- (('Ion0', 0), ('Ion1', 0))/
    |-- ifproduct
    |-- interactions/
      |-- 0/
    |-- multipole_names/
    |-- prn_bas/
      |-- 0_0
      |-- 1_-1
      |-- 1_0
      |-- 1_1
    |-- shells_Ion0-Ion1
```

4 Appendix

4.1 Wien2k Interface

Important Files

The `MagInt` - Wien2k interface relies on reading the following files:

- `case.outputnn`

- `case.dmftsym`

- `case.outputkgen`

- `case.h5`

It employs the Wannier basis construction provided using `dmftproj` program of `dft_tools` package of `TRIQS`. For the standard DFT+DMFT/DFT+HI calculations with this interface see `dft_tools` documentation and Ref. [10].

Important Steps in running `MagInt`-Wien2k

- Newer versions of Wien2k contain a bug rendering DFT+HI calculations with spin-orbit using the `dmftproj` interface impossible. For running `MagInt` with spin-orbit we recommend using Wien2k v. ≤ 14.

- The `nn` program of Wien2k package needs to be recompiled with `nn.f` provided, since additional information for `MagInt` needs to be included into `case.outputnn`. This modification of `nn` will not affect the use of Wien2k for other types of calculations.

  Moreover, since the nearest-neighbors vectors are read by `MagInt` from the `case.outputnn` file, it is recommended to re-run the `nn` program of Wien2k via `x nn` with a high number of nearest neighbors (10 or more depending on the system, please inspect `case.outputnn` after running `nn`). This can be also done after initial DFT+HI self-consistent calculations are completed.

- The calculation of intersite exchange interactions requires the computation of the intersite Green's function via a Fourier transform. The implementation of the k-symmetries in case of multi-correlated sites is not yet implemented; therefore, in order to achieve a correct calculation of the intersite exchange interactions, we recommend to re-calculate the full Brillouin zone (FBZ) k-mesh.

  To generate this mesh, copy `case.struct` file into `case.ksym`, reduce the number of symmetry operations in `case.ksym` to 1 and delete all symmetry operations apart from the identity. Then generate the FBZ mesh via `x kgen -so`. You may first converge DFT+HI with the standard mesh, and then rerun one final DFT+HI interation starting from the FBZ k-mesh (and having deleted or renamed the previous `h5` file).

4.2 VASP Interface

Important Files

The `MagInt` - VASP interface relies on reading the following files:

- `POSCAR`

- `IBZKPT`

- `vasp.h5`

Important Steps

The calculation of intersite exchange interactions is performed in the DFT+DMFT paramagnetic phase. To achieve a correct non-magnetic solution is VASP with SOC a four-step procedure is recommended:

1. High convergence of collinar non-magnetic (`ISPIN=1`) DFT calculation.

2. Collinear magnetic DFT calculation starting from point 1. with magnetic moments set to zero and high convergence criteria.

3. Non-collinear DFT+SOC calculation starting from point 2. with non-collinear magnetic moments set to zero and high convergence.

   Attention! At this step the number of bands `NBANDS` has to be set to the double of the number of bands of the previous calcualtions.

4. Final non-collinear DFT+SOC+PLO calculation `LORBIT = 14` where the window of projection is set according to `EMIN, EMAX`.

For more information please refer to the VASP - TRIQS interface.

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