ACMxc documentation

E. Fabiano

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1 Theory

Within the Hartree-Fock (HF) adiabatic connection theory [1] the correlation energy (beyond the HF energy) can be obtained as

$$E_c = \int_0^1 W_\lambda d\lambda \ , \tag{1}$$

where λ is a coupling-strength parameter for the electron-electron interaction and

$$W_\lambda = \langle \Psi_\lambda^{HF} | \hat{V}_e e - \hat{J} - \hat{K} | \Psi_\lambda^{HF} \rangle - U[\rho^{HF}] - 2E_x^{HF} \ , \tag{2}$$

with Ψ_λ^{HF} being the HF ground-state wave function at coupling-strength λ, $\hat{V}_e e$ being the bare electron-electron interaction, $\hat{J}$ and $\hat{K}$ being the Coulomb and exchange operators, respectively, ρ^{HF} being the HF electron density, U being the Hartree energy, and E_x^{HF} being the HF exchange energy.

An explicit formula for W_λ is not known, however there are explicit expressions for the asymptotic limits:

$$W_{\lambda\to 0} = E_x^{HF} + \sum_{n=2}^{\infty} n E_c^{MPn} \lambda^{n-1} \ , \tag{3}$$

$$W_{\lambda\to \infty} = W_\infty + \frac{1}{\sqrt{\lambda}} W'_\infty + \cdots \ , \tag{4}$$

where E_c^{MPn} is the Møller-Plesset series and W_∞ and W'_∞ can be approximated as functionals of the HF density [2, 3, 4]. Using these asymptotic limits several interpolation formulas have been proposed for W_λ [5, 6, 7, 8, 9, 10].

2 The acmxclib module

The `acmxclib` module is a library that implements all the tools to perform adiabatic connection models (ACM) calculations.

It is called as

```
acmxclib(program="turbomole", tdir=None, path=".", prog_input="input",
         ncpu=1, formula="isi", wfunc="hpc", metal_mode=False,
         verbose=True)
```

Options are:

- `program`: electronic structure code to use for the calculation of Hartree-Fock, W_∞, and MP2 quantities. Actually the only allowed choices are `program=turbomole` or `program=crystal`.
- `tdir`: full path of the directory where the executalbe code selected by `program` is located. If `tdir=None` global environment variables are used to determine the location of the code.
- `path`: full path of the directory that contains the input files for the electronic structure code (working directory).
- `prog_input`: name of the input file for the electronic structure code. Actually this option is used only when `program=crystal`; in this case the file name does not include the .d12, .d3, and .d4 extensions.
- `ncpu`: number of cpu to use when running the electronic structure code.
- `formula`: ACM formula to use. Actually the allowed options are: `isi, revisi, spl, lb, genisi, dpi, spl2, mpacf1, mp2`.
- `wfunc`: functional to be used for the calculation of W_∞ and W'_∞. Actually allowed options are: `pc, hpc, mpc`.
- `metal_mode`: this flag is used when dealing with systems with zero gap (pure metals). If set to `True` is skips the MP2 calculation and automatically sets $E_{MP2} = -\infty$.
- `verbose`: this flag control whether information and results must be printed to standard output or not.

2.1 acmxclib functions

- `set_tdir(value)`: set up the value of the `self.tdir` variable.
- `set_path(value)`: set up the value of the `self.path` variable.
- `set_prog_input(value)`: set up the value of the `self.baseinput` variable.
- `set_ncpu(value)`: set up the value of the `self.ncpu` variable.
- `set_formula(value)`: set up the value of the `self.acm_formula` variable.

- `set_wfunc(value)`: set up the value of the `self.wfunc` variable.
- `set_metal_mode(value)`: set up the value of the `self.metal_mode` variable.
- `set_program(value)`: set up the value of the `self.program_name` variable and initialize the required program (this includes setting up the `self.tdir` variable).
- `run_program()`: run the electronic structure calculations (HF, W_∞, and MP2) with the selected code.
- `extract_results()`: collect results from the output of the electronic structure calculations.
- `compute_acm_xc_energy()`: compute the correlation energy according to the selected ACM formula.
- `print_results()`: print results to standard output.

3 The acmxc script

`acmxc` is a script which used the `acmxclib` module to perform calculations using adiabatic connection models for the correlation energy. It drives electronic structure calculations from several codes and computes total energies. Actually the following codes are supported: TURBOMOLE, Crystal.

3.1 Prerequisites

To use `acmxc` the following resources are needed:

- python interpreter (version 3 or higher);
- at least one of the following codes:
  - TURBOMOLE (version 7.7 or higher);
  - Crystal (version 3.3 or higher including cryscor);

Note that for calculations with Crystal a development version of the *properties* executable is required. This can be obtained from the developers.

3.2 USAGE

Preparation
To perform calculations with `acmxc` set up a valid input file for the program you are going to use. The input file must define a Hartree-Fock calculation as well a MP2 calculation as usual for the code of choice. In particular:

- for TURBOMOLE the RI approximation must be used (the *ridft* code is employed) and the *control* file must contain the data group `$ricc2 mp2` as well as the proper auxbasis for *ricc2* calculations.

- for Crystal <*file-name*>*.d12*, <*file-name*>*.d3*, and <*file-name*>*.d4* files must be prepared. The ¡*file-name*¿*.d12* must contain the keyword `EXCHGENE`.

Running

To run the script use:

```
acmxc -p <program> [ -i <file_name> ] [ other options ]
```

The `-i` option is required only if `<progam> == crystal`.

If you consider systems with a vanishing gap (e.g. periodic metals) use the `--metal` option (see below).

Options

The following options are available:

- `-p <string>, --prog <string>, --program <string>`: Program to use. Possible options: turbomole, crystal;

- `-f <string>, --formula <string>`: ACM formula to be used. Possible options: isi, revisi, genisi, spl, lb, dpi, spl2, mpacf1, mp2 (default: isi);

- `-w <string>, -wfunc <string>`: W_∞ functional to use. Possible options: pc, hpc, mpc (default: hpc);

- `-n <int>, -nthreads <int>`: Number of threads to use (default: 1);

- `-d <string>, -dir <string>\verb`: Base path of ¡program¿ . (default=set from environment variable);

- `-i <string>, --input <string>`: Specification of <*file-name*> This is required (and mandatory!) only for crystal. <*file-name*> is not including the *.d12*, *.d3* and *.d4* extensions;

- `--metal`: Sets $E_{MP2} = -\infty$. This must be used for calculations of systems with a vanishing gap, e.g. metallic solids (default=False).

References

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