Tutorial on using the Semistochastic Heat-bath Configuration Interaction (SHCI) method

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There are presently two SHCI codes available for quantum chemistry (and periodic solids and in fact any system for which an integrals file is available) – one in Fortran developed by the Umrigar group at Cornell (primarily by Adam Holmes, with very efficient parallelisation and other contributions by Matt Otten), and another in C++ developed by the Sharma group at the University of Colorado. There is also an SHCI program for treating the homogeneous electron gas developed in the Umrigar group by Junhao Li. Today, we will install and use the first program, but both the Fortran and C++ chemistry programs are available.

Adam Holmes, showed in his talk the potential energy curves for the 12 lowest energy states of C_2, computed in a cc-pV5Z basis. In this tutorial, we will compute a simplified version of this – we will do the lowest 3 states (you can easily do more if you wish) in a cc-pVDZ basis.

1. Download the code by typing:
   ```
   git clone https://bitbucket.org/sqmc/hci.git --depth=1
   ```

2. Compile the program:
   ```
   cd hci/src
   make
   ```

3. ```
   cd ../C2_v2z_curve
   ```
   There are 2 input files (for $^1\Sigma_g$ and $^3\Pi_u$ symmetries) and integrals files (from PySCF) for 9 different geometries. Take a look at one of these inputs. The one for $^1\Sigma_g$ computes the 2 lowest states of that symmetry and the one for $^3\Pi_u$ computes just the lowest state. Run all these inputs by typing:

   ```
   ./runall
   ./runall_mac (on Macs)
   ```

4. Make tables of all these calculations:
   ```
   ./make_table
   ```

5. Plot the energies in the tables:
   ```
   gnuplot < i.gnu
   evince pes_C2_2z.eps
   ```

Refs:

1) Heat-bath Configuration Interaction: An efficient selected CI algorithm inspired by heat-bath sampling, A. A. Holmes, Norm Tubman and C. J. Umrigar, J. Chem. Theory Comput., **12**, 3674 (2016)

2) Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory, Sandeep Sharma, A. A. Holmes, G. Jeanmairet, A. Alavi and C. J. Umrigar, J. Chem. Theory Comput., **13**, 1595 (2017).
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