Self consistency in TD-DMET

0.1 Self consistency in DMFT

There are certainly differences between the self-consistency in DMET and DMFT, but it will be worth recaping the DMFT formulation in the(my?!) adopted DMET language so that analogies can be drawn. In DMFT, I *believe* the flow is as follows:

1. Calculate 'non-interacting' greens-functions $g = [(\omega + i\delta)I - h - \Sigma]^{-1}$ projected over the impurity sites. The quotes are included since it is not really non-interacting, and potentially exact since the self-energy is included (in the atomic limit), but the nomenclature will remain. The sigma is repeated in each unit cell.

2. Construct a hybridization function, which will define the bath states, as $\Delta = (\omega + i\delta)I - h_{imp} - \Sigma - g^{-1}$, where h_{imp} is the bare one-electron hamiltonian over the impurity space.

3. Fit the hybridization over ω to a set of one-electron bath states to define both the coupling to these states from the impurity, and the diagonal hamiltonian block of these states.

4. Solve impurity + bath system to obtain G_{imp} (no explicit self-energy contribution).

5. From G_{imp}, form the local self-energy function, Σ, from $\Sigma = (\omega + i\delta)I - h_{imp} - \Delta - G_{imp}^{-1}$.

0.2 Self consistency in DMET

I will try to maintain the same structure of DMET self-consistency, although there are obviously key differences. Firstly, the 'bath' in DMET will refer to the part of the many-body basis constructed from the non-interacting part of the perturbation acting in the environment space. It will not refer to the one-electron bath orbitals formed in the ground-state DMET, which will remain unchanged. Obviously, since this bath is now a many-electron space, it is fundamentally different to the bath in DMFT. In addition, it is to be updated at each frequency point and on the real-axis, rather than fitted across frequency on the imaginary axis. Despite these differences, a reasonably similar algorithm might proceed as follows:

1. Calculate 'non-interacting' greens-functions as $g = [(\omega + i\delta)I - h - \Sigma]^{-1}$. We assume everywhere that the one-electron hamiltonian also includes the correlation potential from the ground state optimization. As in DMFT, the Σ is copied through the space, and the resultant function projected over the impurity sites.

2. Construct the bath, parameterized by the function $[(\omega+i\delta)I-h-\Sigma-\Delta]^{-1}$ and projecting this into the core and virtual space of the Schmidt basis of the ground state DMET. Unlike previously, the bath orbitals are also parametrized by the action of the hybridization potential, to be defined later (though we could just use the non-interacting greens-function as before).

3. Solve the embedded + bath system to obtain G_{imp}. Unlike DMFT, there are some choices to be made here about the hamiltonian. The hamiltonian should include the hybridization function in the one-electron space that couples the embedded space to the bath functions, and in the diagonal bath blocks of the hamiltonian. The self-energy should not be included. Note that this will change the core energy of the bath states relative to the embedded space, which was previously overlooked - this should be key in coupling the states more effectively.

4. Calculate a new self-energy as $\Sigma = (\omega + i\delta)I - h_{imp} - \Delta - G_{imp}^{-1}$.

5. Calculate a hybridization function as $\Delta = (\omega + i\delta)I - h_{imp} - \Sigma - g^{-1}$

6. Repeat. Self-consistency achieved when G_{imp} is no longer changing?

There are some choices here, such as whether the hybridization is used in the construction of the bath states, rather than just defining the coupling, but these small points should be able to be worked out. Nicely, this also only requires one lattice diagonalization per iteration. Does this sound at all reasonable?