Modelmb implementation in Octopus

22.10.2012 | N. Helbig, M.J. Verstraete

The idea

N electrons in one dimension

$$H = \sum_{j=1}^{N} -\frac{d^2}{dx_j^2} + v_{\mathrm{ext}}(x_j) + \sum_{\substack{j,k=1 \\ j \neq k}}^{N} v_{\mathrm{int}}(|x_j - x_k|)$$

is identical to the hamiltonian for one electron in N dimensions

$$v_{\mathrm{ext}}^{Nd}(x_1 \ldots x_N) = \sum_{j=1}^{N} v_{\mathrm{ext}}(x_j) + \sum_{\substack{j,k=1 \\ j \neq k}}^{N} v_{\mathrm{int}}(|x_j - x_k|)$$

Solve $H\Psi(x_1 \ldots x_N) = E\Psi(x_1 \ldots x_N)$ for the one electron

The problem

- Single electron in *N* dimensions doesn't know about antisymmetry of Ψ
- Some of our solutions will not be possible for fermions
- Octopus generally calculates only spatial part of the wave function

For more than 2 electrons

$$\Psi(x_1\sigma_1, \ldots x_N\sigma_N) = \sum_j \Phi_j(x_1 \ldots x_N)\chi_j(\sigma_1 \ldots \sigma_N)$$

only for fully polarized states can the sum have only one entry

Separation in space and spin

- We are only dealing with $\Phi(x_1 \ldots x_N)$
- Ensure that we only keep those Φ that can appear in a sum for a fermionic wave function

Not possible:

$$\Phi(x_1, x_2, x_3) = \varphi(x_1)\varphi(x_2)\varphi(x_3)$$

Solution

Project Φ on fermionic Young diagrams to exclude those wave functions that cannot be fermionic

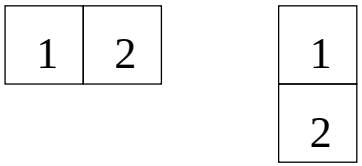
Young diagrams

Goal: find all allowed fermionic configurations

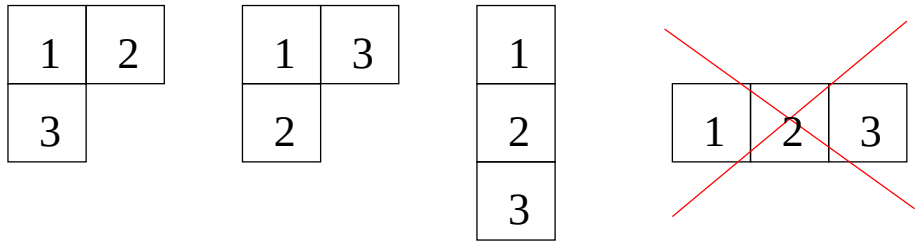
Arrange particles such that

- Number of columns corresponds to number of possible spin directions (electrons: 2)
- Numbers increase from left to right and top to bottom

Two particles

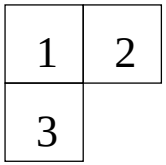


Three particles



Project $\Phi(x_1 \ldots x_N)$ onto Young diagram and $\chi(\sigma_1 \ldots \sigma_N)$ onto corresponding diagram (rows and columns interchanged)

Young diagrams



Explicit symmetrization

1. symmetrize pairs of up-down particles (same row)

$$\tilde{\Phi}(x_1, x_2, x_3) = \frac{1}{2}\left[\Phi(x_1, x_2, x_3) + \Phi(x_2, x_1, x_3)\right]$$

2. antisymmetrize up particles (first column)

$$\Phi_{\text{final}}(x_1, x_2, x_3) = \frac{1}{2}\left[\tilde{\Phi}(x_1, x_2, x_3) - \tilde{\Phi}(x_3, x_2, x_1)\right]$$

3. antisymmetrize down particles (second column)
4. Normalize Φ_{final} unless its norm is smaller than a threshold

Removes all wave functions that cannot be used by fermions

Note of caution

$\Phi_{\mathrm{final}}(x_1..x_N)$ has a specific symmetry under interchange of some variables but not all

- needs always to be multiplied with corresponding χ
- appears in a summation, terms with interchanged variables can appear in a different term in that sum
- the Young diagrams do not correspond to S^2 eigenstates

This is the best we can do

Modelmb calculations in Octopus

For 3 electrons in 1 dimension

```
TheoryLevel = independent_particles
CalculationMode = gs
Dimensions = 3
NDimModelmb = 1
NParticleModelmb = 3
NTypeParticleModelmb = 1
%DescribeParticlesModelmb
'electron' | 1 | 1.0 | 1.0 | 'fermion'
'electron' | 1 | 1.0 | 1.0 | 'fermion'
'electron' | 1 | 1.0 | 1.0 | 'fermion'
%
Output = modelmb + wfs
OutputHow = axis_x
```

Modelmb calculations in Octopus

```
%DescribeParticlesModelmb
'electron' | 1 | 1.0 | 1.0 | 'fermion'
'electron' | 1 | 1.0 | 1.0 | 'fermion'
'electron' | 1 | 1.0 | 1.0 | 'fermion'
%
```

name | # type of particle | mass | charge | fermion/boson/anyon

- Octopus gives variables according to order in the list (x,y,z,w)
- only particles of the same type are interchanged in Young diagrams
- bosons are not implemented yet, anyons can have any symmetry
- output into /static/modelmb folder

Problem

With increasing N the number of non-fermionic states increases dramatically

- for $N = 3$ the second state is the first fermionic one
- for $N = 4$ the first fermionic state is somewhere around the 20th state
- we are calculating a lot of states just to throw them away afterwards

It would make more sense to solve the SE in the subspace of wave functions with the correct symmetry