Quantum Monte Carlo tutorial

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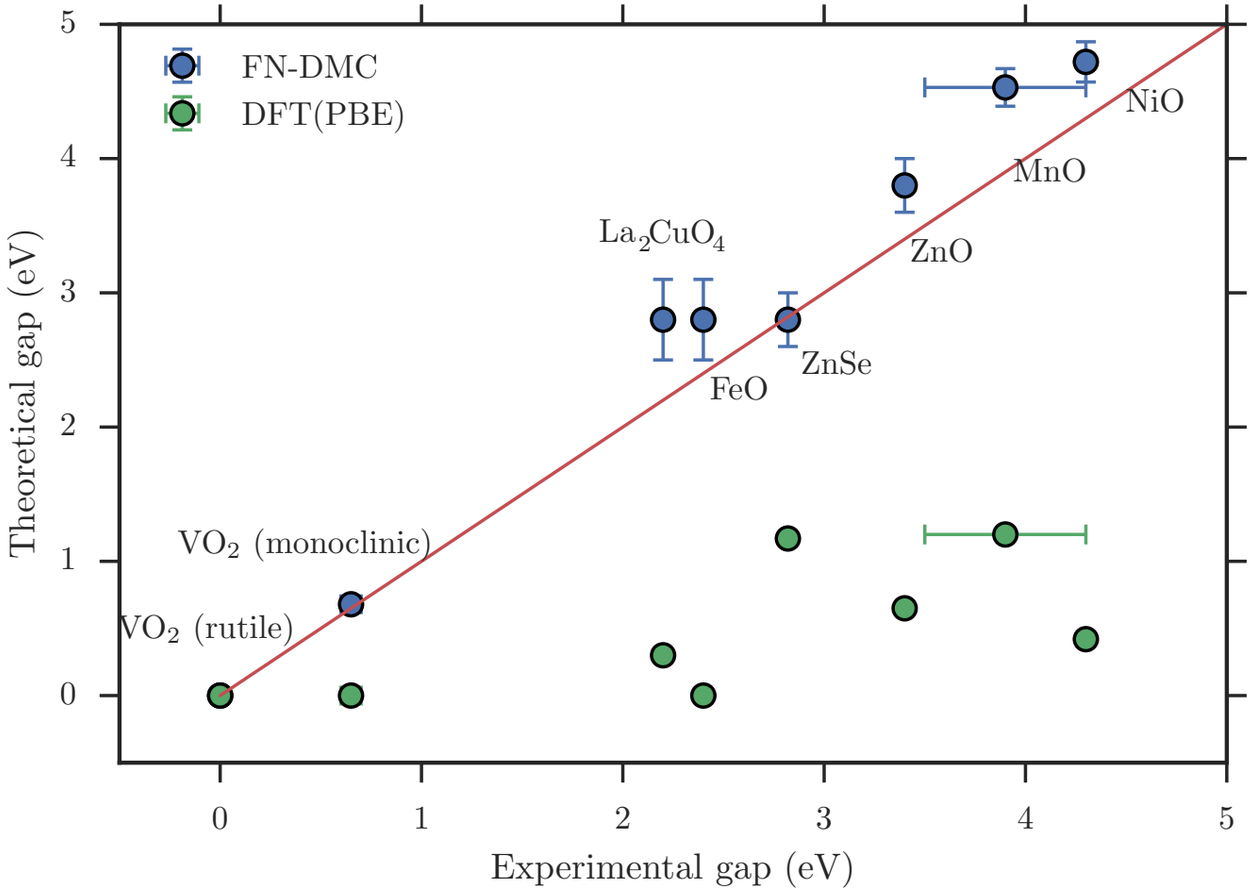
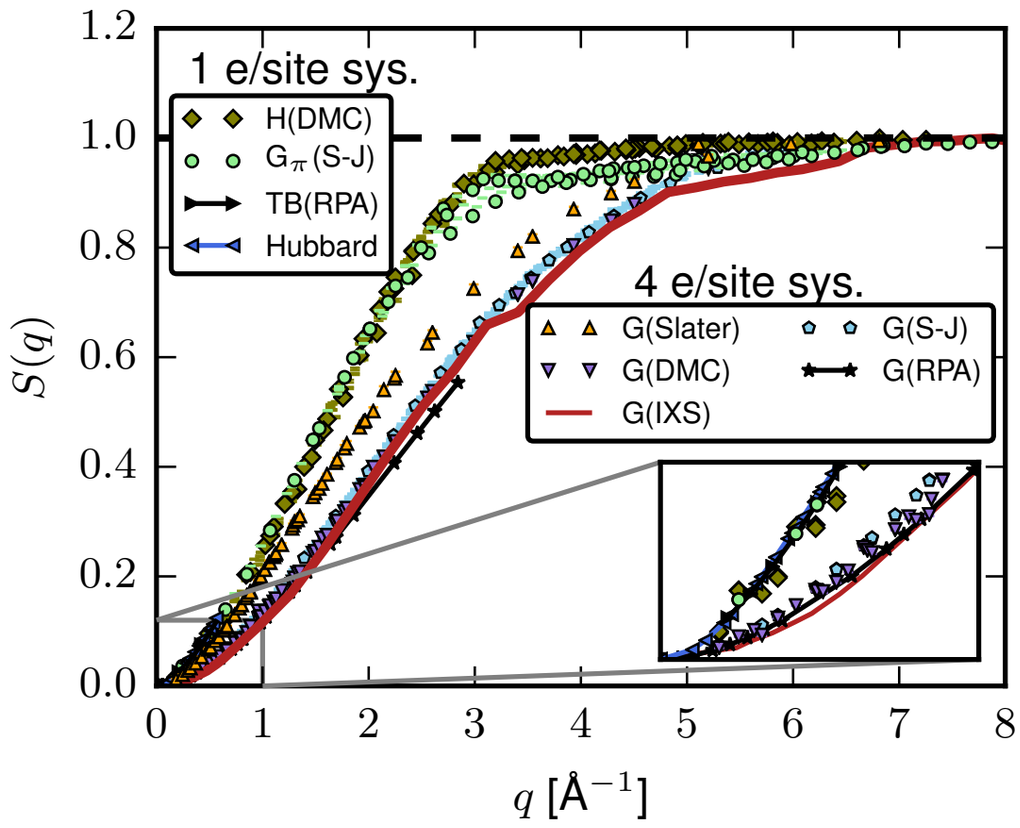
QMC: what is it good for?



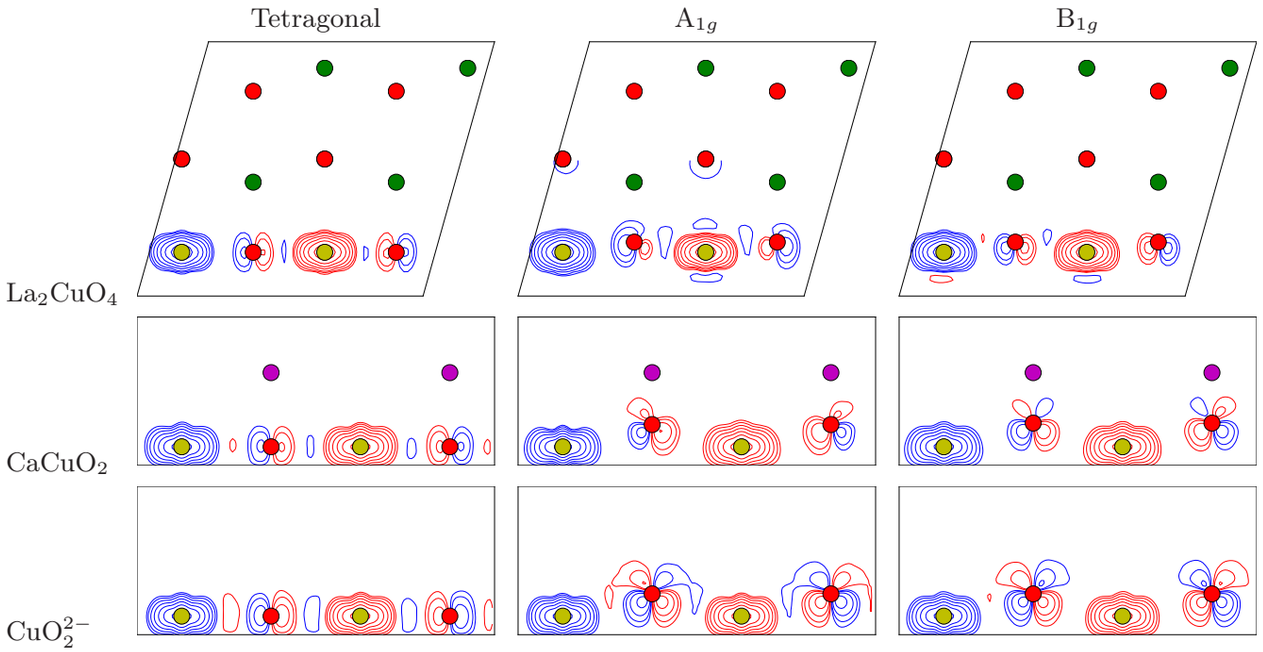
Gaps

Wagner, Ceperley
Rep. Prog. Phys. **79** 094501 (2016)

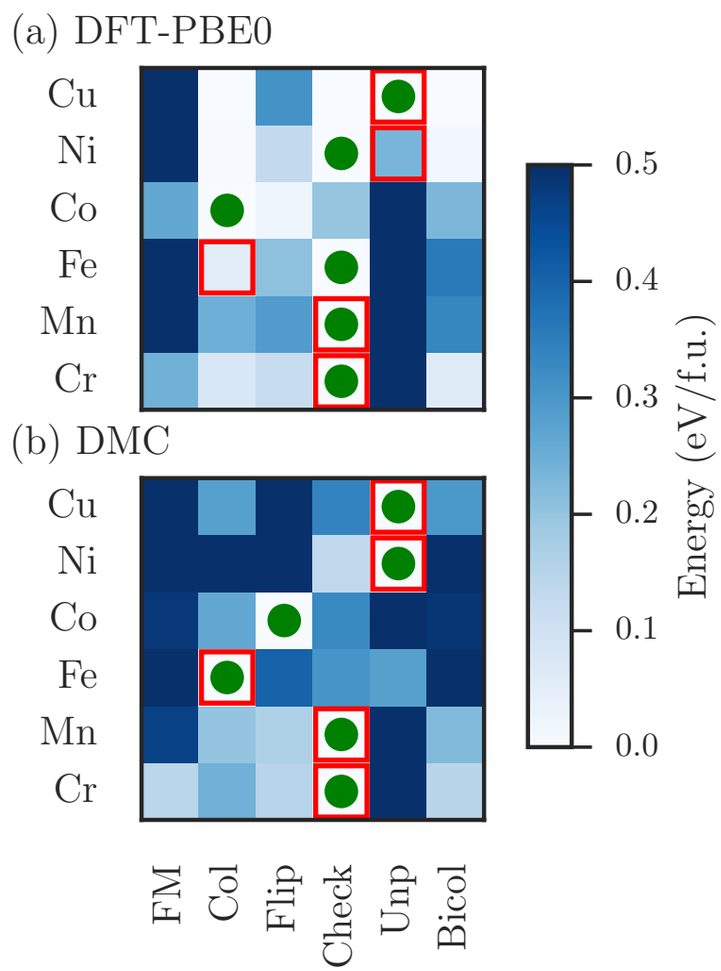


Correlation functions

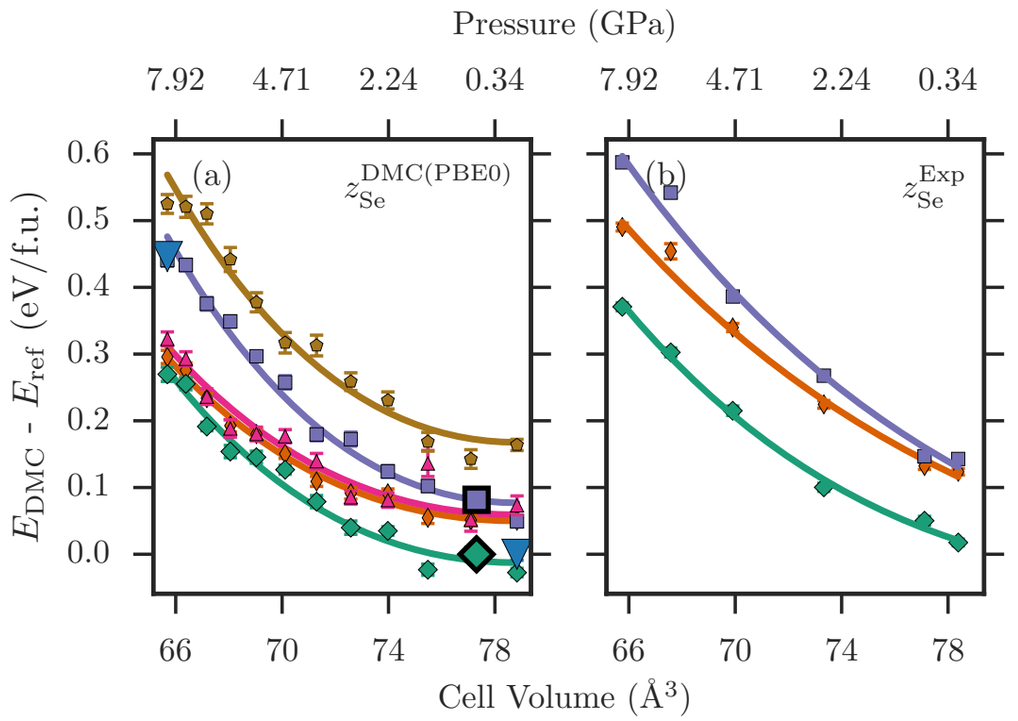
Zheng, Gan,
Abbamonte, Wagner

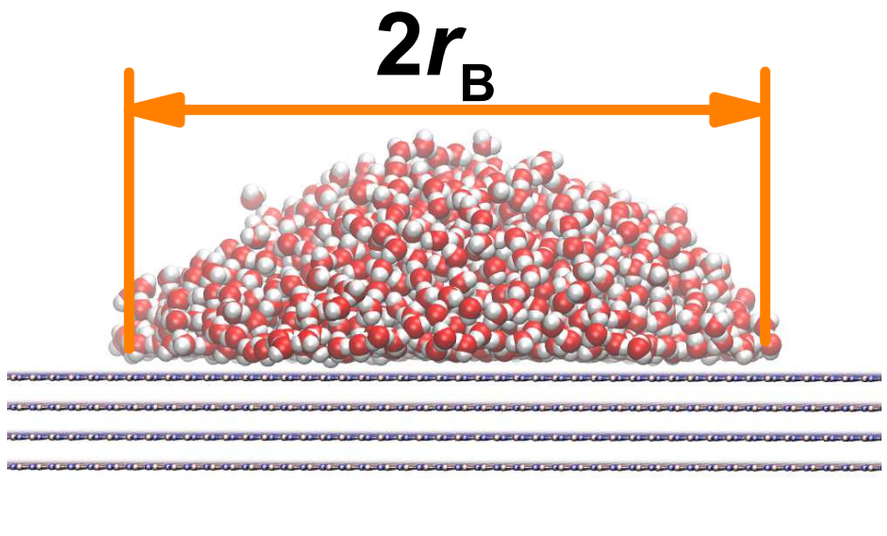


Magneto-phonon coupling
Wagner, Abbamonte
PRB **90** 125129 (2014)



Ground states of magnetic systems
Narayan, Busemeyer, Wagner (in preparation)





Pressure dependence of magnetic energies in FeSe

Busemeyer, Dagrada, Sorella, Casula, Wagner

Phys. Rev. B **94** 035108 (2016)

Water on boron nitride

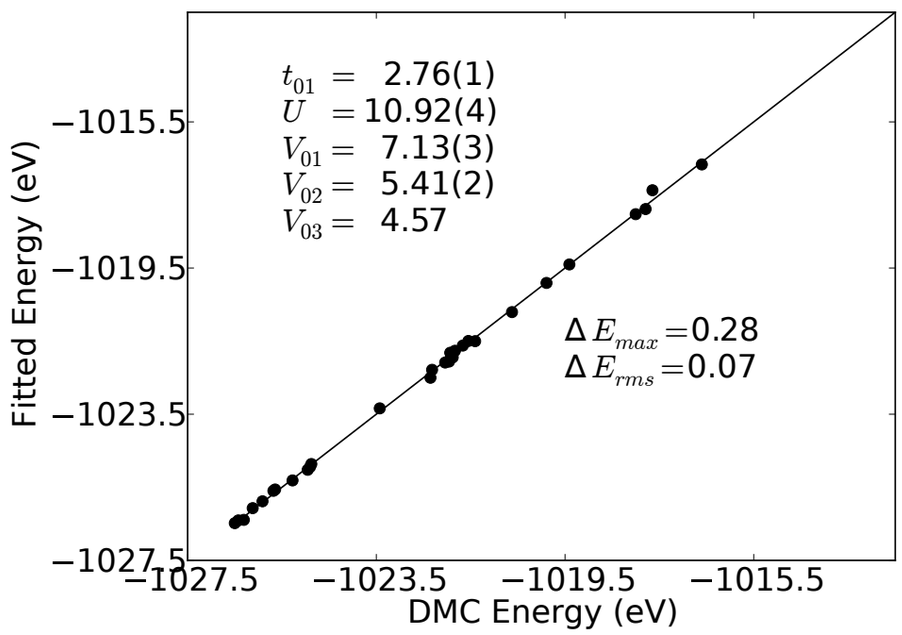
Wu, Aluru, Wagner

J. Chem. Phys. **142**, 234702 (2015), **144** 164118 (2016)

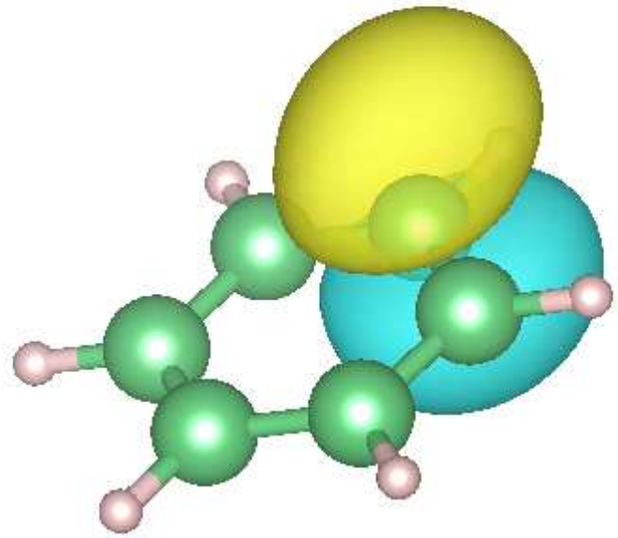
Al-Hamdani, Ma, Alfè, Lilienfeld & Michaelides

J. Chem. Phys. **142**, 181101 (2015).

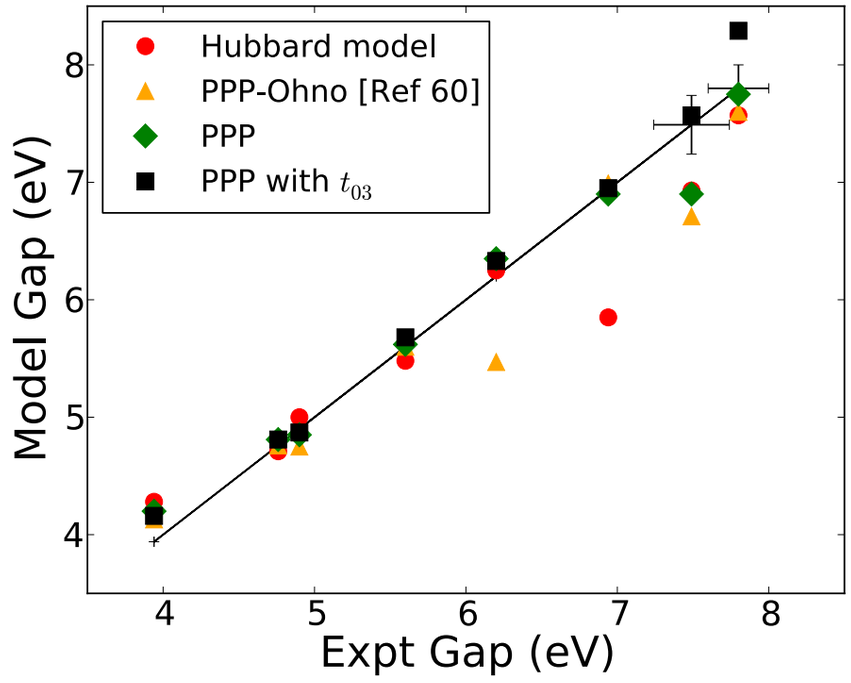
Fitting models



(e)



Excitation spectrum very close to experiment.



Changlani, Zheng, Wagner.
J. Chem. Phys. **143**, 102814 (2015)

Telluride School on Stochastic Approaches to Electronic Structure Calculations

Hands on every day

Time for walks (quantum and classical)

Code QMC algorithms:

Variational
Diffusion
Path integral
Auxiliary field
Full Configuration interaction

telluridescience.org

Starting up

Find 2-3 friends. You are now a group

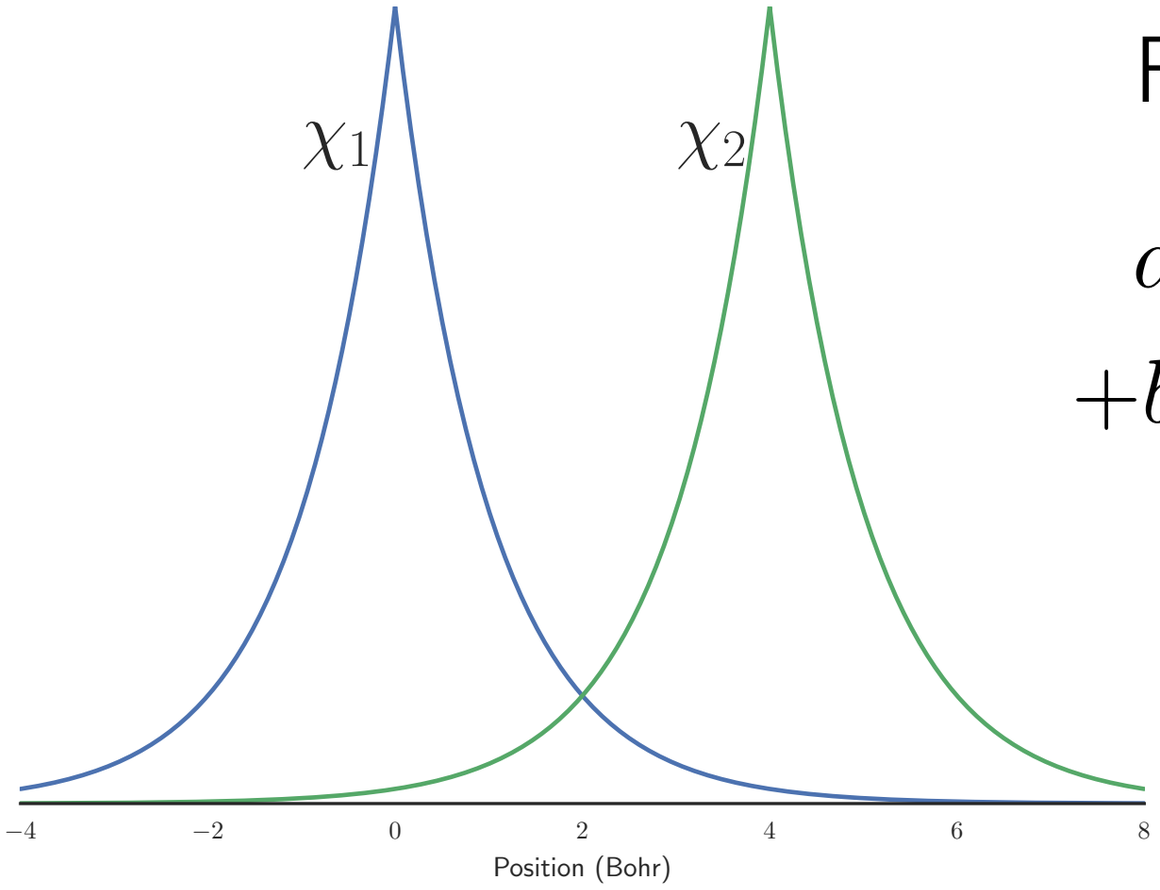
git clone https://github.com/lkwagner/MagLabWinterSchool2017.git qmc_tutorial
modify runqmc.py to point to your QWalk installation.

if you want to run natively on Linux or Mac:

git clone https://github.com/QWalk/mainline qwalk
cd qwalk/src
make install

sudo pip3 install seaborn matplotlib numpy pandas

Approximate wave functions



For an up and down electron:

$$a(\chi_1(r_1)\chi_2(r_2) + \chi_2(r_1)\chi_1(r_2))$$
$$+b(\chi_1(r_1)\chi_1(r_2) + \chi_2(r_1)\chi_2(r_2))$$

Limits:
a=b: non-interacting
b=0: no double occupancy

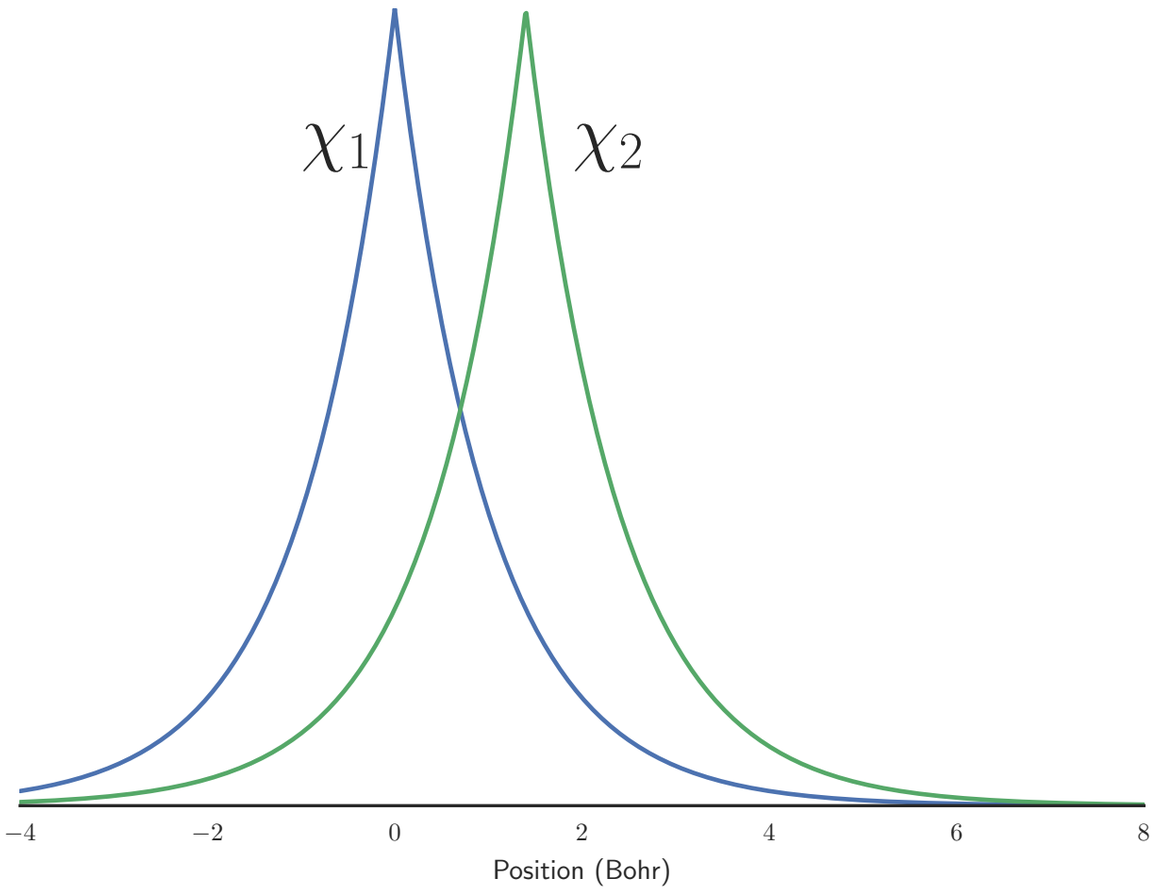
Non-interacting case

$$a(\chi_1(r_1)\chi_2(r_2) + \chi_2(r_1)\chi_1(r_2))$$
$$+b(\chi_1(r_1)\chi_1(r_2) + \chi_2(r_1)\chi_2(r_2))$$

a=b.

This is the Hartree-Fock (RHF) result.
The probability of finding two electrons on a given site is exactly 0.25

Why Jastrow?



When the densities overlap a lot, then the electrons avoid each other on a much smaller scale.

The Jastrow factor includes that kind of correlation.

Measurements

Total energy (Hartrees: ~27 eV)

Double occupancy of atomic orbitals (2-RDM)

Electron-electron radial distribution function

Wave function ansatz	Comment
Restricted Hartree-Fock	No electron correlation at all
Multiple Slater determinants	Reduces double occupancies of orbitals
Multiple Slater-Jastrow	Electrons also avoid one another at small distances
diffusion Monte Carlo	Exact or nearly exact in this situation (everything else!)

File	Purpose
runqmc.py	Interface to QWalk
scan.py	Run an ensemble of jobs -> .pickles
plot.py, plot_gr.py, plot_double.py	Plot scripts
hubbard.py	Find best Hubbard model

Define the Hamiltonian

Define the Hamiltonian (qwsinglet1.0.hf)

```
SYSTEM { MOLECULE
  NSPIN { 1  1 }
  ATOM { H  1  COOR 0   0  0.0 }
  ATOM { H  1  COOR 0   0  1.0 }
}
```

One up, one down

Position in Bohr

Atomic charge

Multiple slater determinant

```
TRIALFUNC {
  SLATER
  ORBITALS {
  CUTOFF_MO
    MAGNIFY 1
    NMO 2
    ORBFILE qwsinglet1.44.orb
    INCLUDE qwsinglet1.44.basis
    CENTERS { USEATOMS }
  }
  STATES { 1 2    2 1    1 1    2 2   }
  CSF { 1.0 1.0 1.0 }
  CSF{ 1.0 1.0 1.0 }
  OPTIMIZE_DET
}
```

χ_1, χ_2

$$a(\chi_1(r_1)\chi_2(r_2) + \chi_2(r_1)\chi_1(r_2))$$
$$+b(\chi_1(r_1)\chi_1(r_2) + \chi_2(r_1)\chi_2(r_2))$$

Procedure: evaluate wave function

```
method { vmc nstep 1000
  average { gr }
  average { tbdm_basis
    npoints 1
    ORBITALS { CUTOFF_MO MAGNIFY 1 NMO 2
               ORBFILE qwsinglet1.44.orb INCLUDE qwsinglet1.44.basis
               CENTERS { USEATOMS }
    }
  }
}
```

Evaluate the wave function and average the radial distribution function and two body density matrix on the atomic basis.

Define Jastrow factor

```
TRIALFUNC { slater-jastrow
wf1 {
  SLATER
  ORBITALS {
  CUTOFF_MO
    MAGNIFY 1
    NMO 2
    ORBFILE qwsinglet1.44.orb
    INCLUDE qwsinglet1.44.basis
    CENTERS { USEATOMS }
  }
  STATES { 1 2    2 1    1 1    2 2   }
  CSF { 1.0 1.0 1.0 }
  CSF{ 1.0 1.0 1.0 }
  OPTIMIZE_DET

}
wf2 {

  JASTROW2
  GROUP {
    TWOBODY_SPIN {
      FREEZE
      LIKE_COEFFICIENTS { 0.25  0   }
      UNLIKE_COEFFICIENTS { 0  0.5   }
    }
    EEBASIS { EE CUTOFF_CUSP GAMMA 24 CUSP 1 CUTOFF 7.5 }
    EEBASIS { EE CUTOFF_CUSP GAMMA 24 CUSP 1 CUTOFF 7.5 }
  }
  GROUP {
    ONEBODY { COEFFICIENTS { H 0. 0. 0. } }
    TWOBODY { COEFFICIENTS { 0. 0. 0. }  }
    EIBASIS { H POLYPADE RCUT 7.5 BETA0 -0.4 NFUNC 3 }
    EEBASIS {  EE POLYPADE RCUT 7.5 BETA0 -0.02 NFUNC 3 }
  }
}
}
```

$$\exp\left[\sum_{i,\alpha}^{(\text{onebody})}\sum_{k} c_k a_k(r_{i\alpha}) + \sum_{i,j}^{(\text{twobody})}\sum_{k} c_k b_k(r_{ij})\right]$$

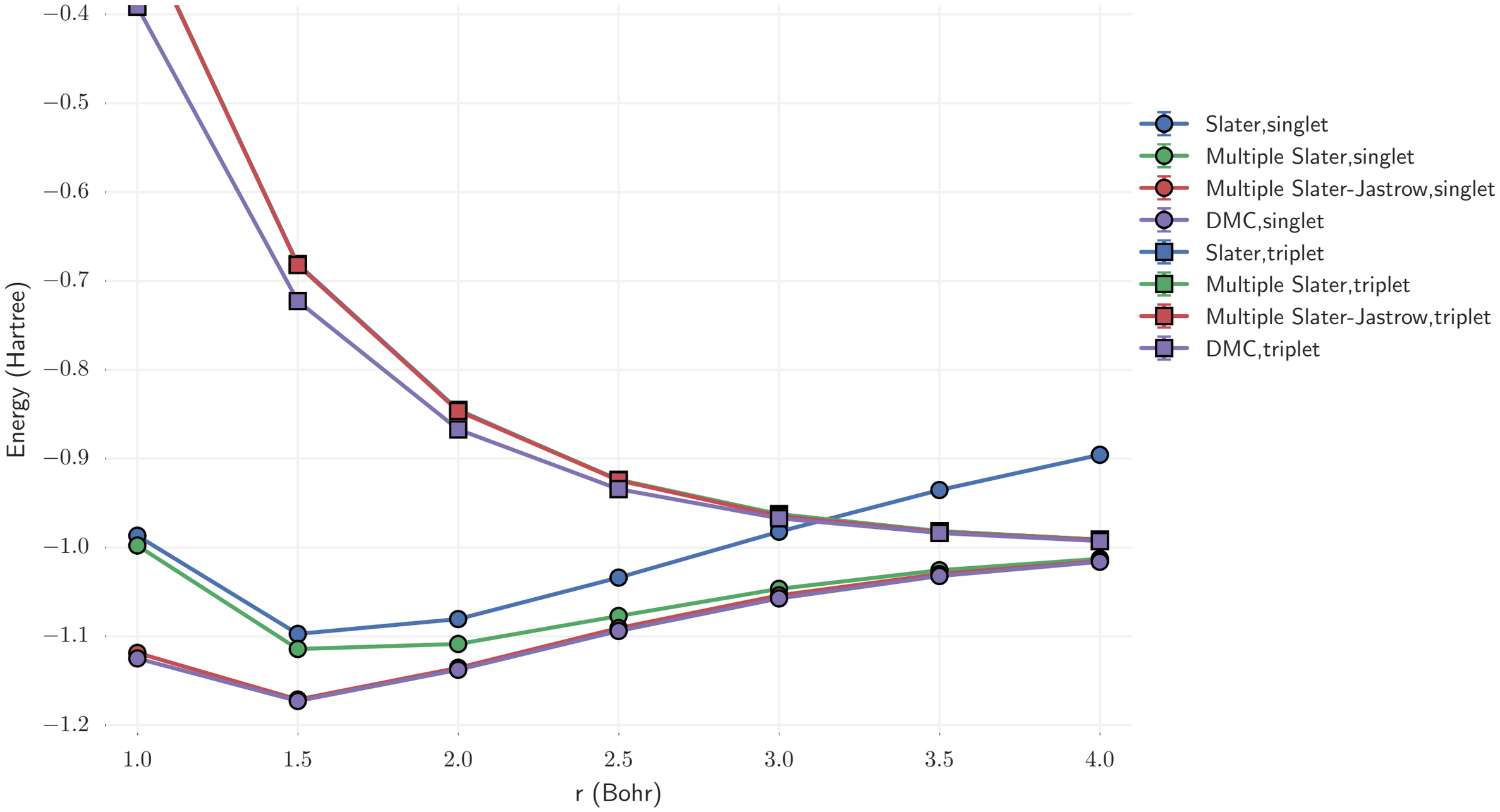
Define a’s and b’s

Optimize:

Optimize and then

```
method { LINEAR total_nstep 250 }
```

```
method { vmc nstep 1000
  average { gr }
  average { tbdm_basis
    npoints 1
    ORBITALS { CUTOFF_MO MAGNIFY 1 NMO 2
               ORBFILE qwsinglet1.44.orb INCLUDE qwsinglet1.44.basis
               CENTERS { USEATOMS }
    }
  }
}
```

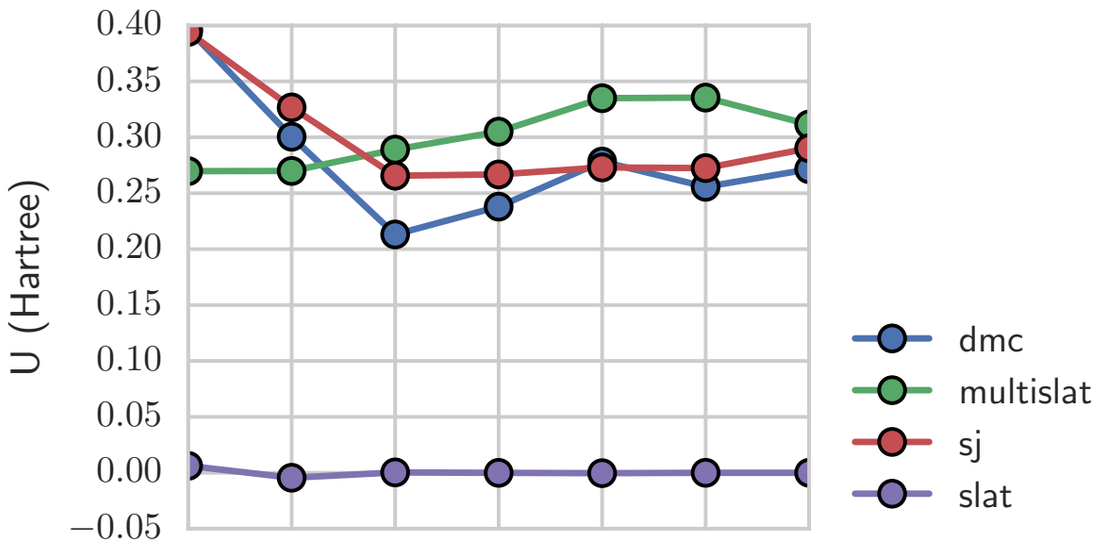

Energy (Hartree)
−0.4
−0.5
−0.6
−0.7
−0.8
−0.9
−1.0
−1.1
−1.2
1.0
1.5
2.0
2.5
3.0
3.5
4.0
r (Bohr)
Slater,singlet
Multiple Slater,singlet
Multiple Slater-Jastrow,singlet
DMC,singlet
Slater,triplet
Multiple Slater,triplet
Multiple Slater-Jastrow,triplet
DMC,triplet

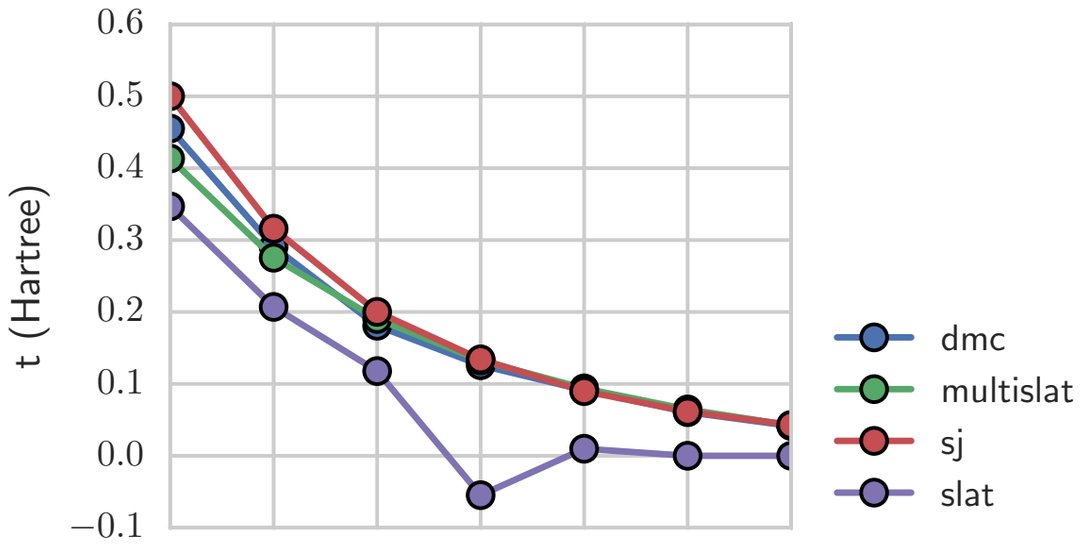
Discussion questions

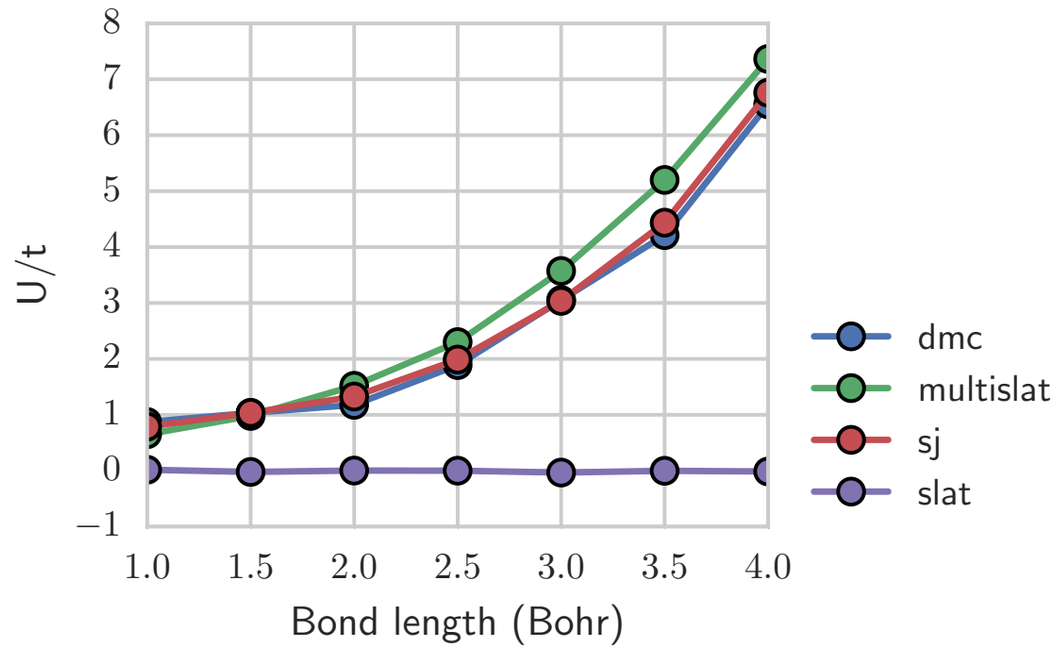
Where do the singlet and triplet state become degenerate for the different wave function ansatz? Why the differences?

Where is the multiple slater without Jastrow good, and where is it poor?

Why does DMC have the highest double occupancy in the singlet state around r=3 Bohr?







Why does RHF always result in zero effective U?

Why does multiple Slater result in larger U values than when short-range correlation is included?