Configuration interactionによるQMC全エネルギーの改善

木野日織（物質・材料研究機構）

共同研究者：Prof. Lubos Mitas (NCSU)

H22.5.7 筑波大学

First-principles study

Difficulty of many body problem <- evaluation of correlation energy

$$\frac{e^2}{|r-r'|}$$

DFT

- Using *model XC potential*, solve as an one-body problem.
- Relatively fast
- Order(N) sometimes

Diffusion Monte Carlo

- Correlation energy, more than 90%
- ~$N^{3.5}$
- Parallel, almost 100%
- time : 1000 folds more than DFT
- Little ambiguity, prediction without exp.

Correlated wavefunciton, Ψ

$$\Psi = e^{J}\Phi$$

- Φ: CISD,MC,CAS,Pfaffian(extention of Slater Determinant),…

  usually carried out mechanically as a study of optimization algorithm.

- J: Jastrow factor (mainly electron electron repulsion)

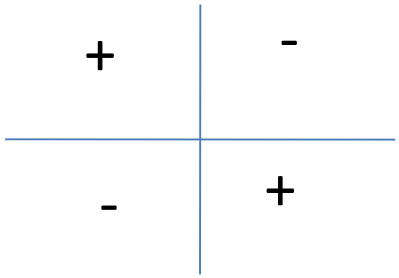
- Few precedent. One must study how good/bad, and its accuracy

Nodes of correlated wavefunctions

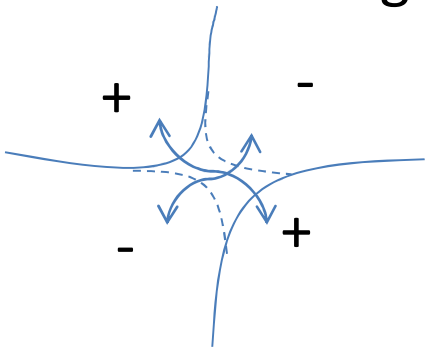
3D harminic well, unpolarized interacting Fermion

fill space with + and -

Non-interacting



interacting



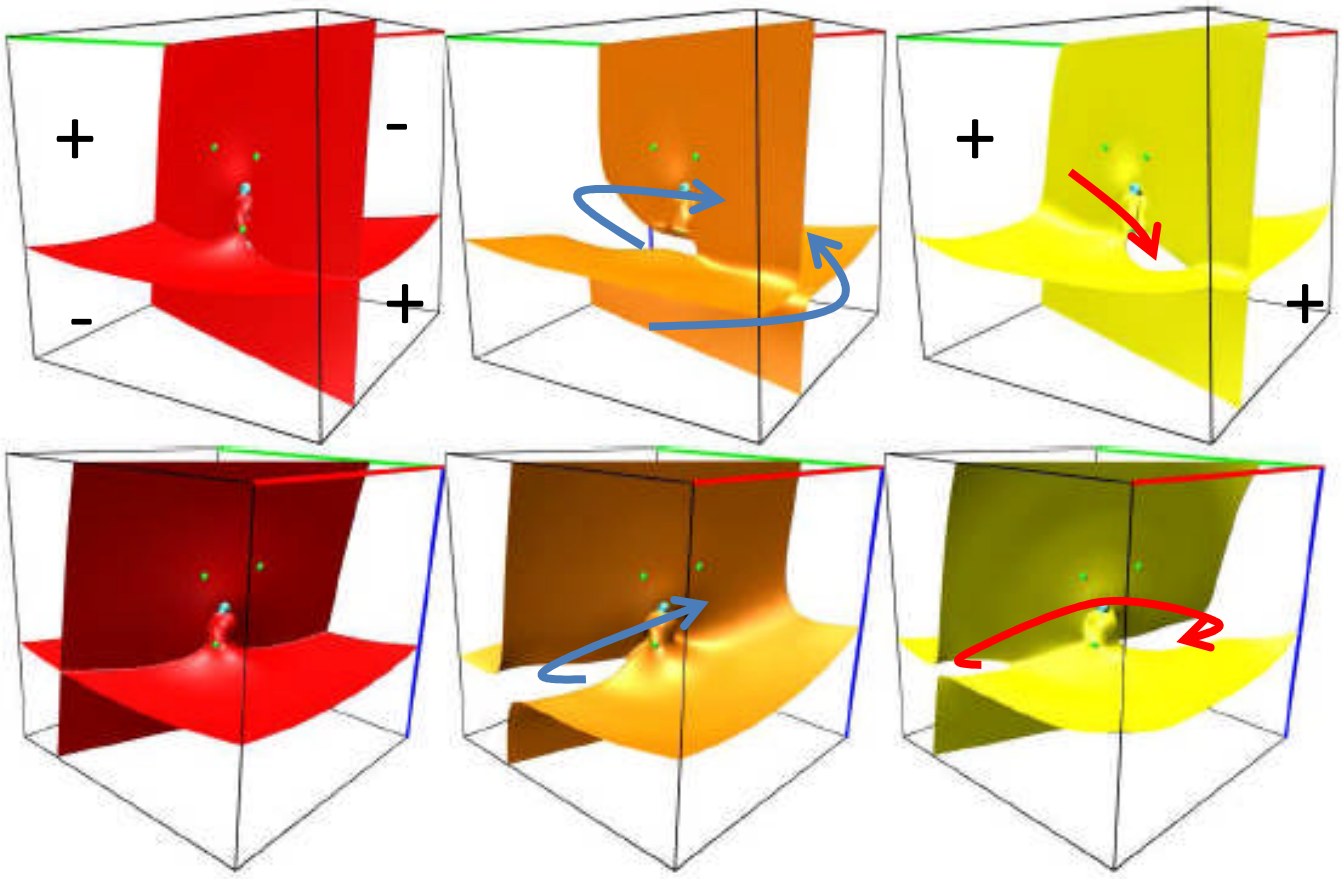
Too symmetric -> higher energy

L. Mitas, PRL 96 240402 (2006).

O atom, nodes

Spin polarized

$$\Psi(r_1, r_2, \ldots, r_N)$$ (fix)



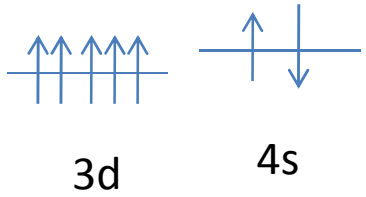
Single Slater Multi Pfaffian CI

(Jastrow factor doesn't change nodal structure.)

M.Bajdich, et al., PRL 96,130201(2006) and his thesis

Mn atom

- Mn: $(3d)^5(4s)^2$, ferromagnetic
- Mn_2: r_e~3.5Å, a van der Waals molecule



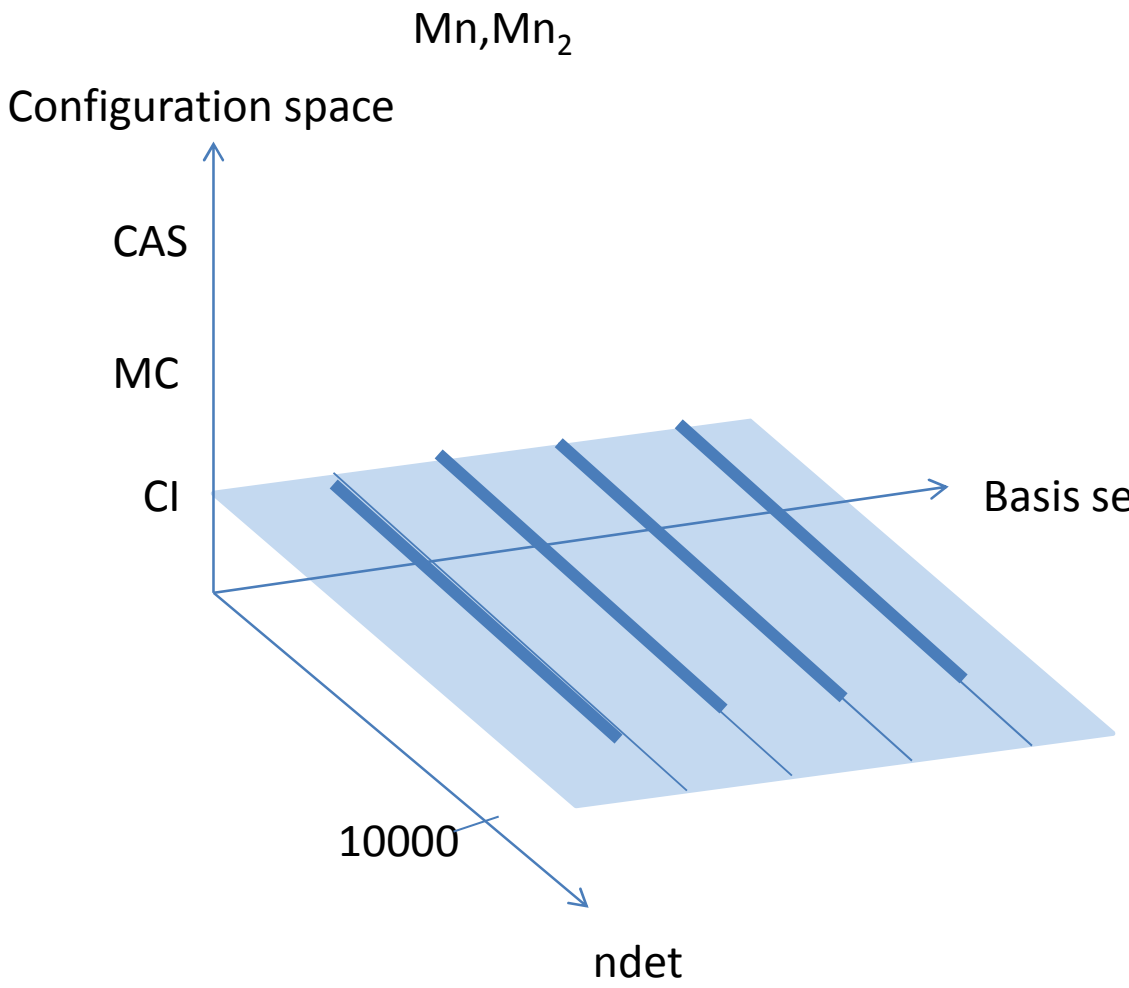
Problems:
any good choice of configuration space?
convergence properties

- Li, Be: near degeneracy problem, E_{2s}~E_{2p}

~97% correlation energy for ~20 configuration

- Mn: E_{4s},E_{4p}?, f?

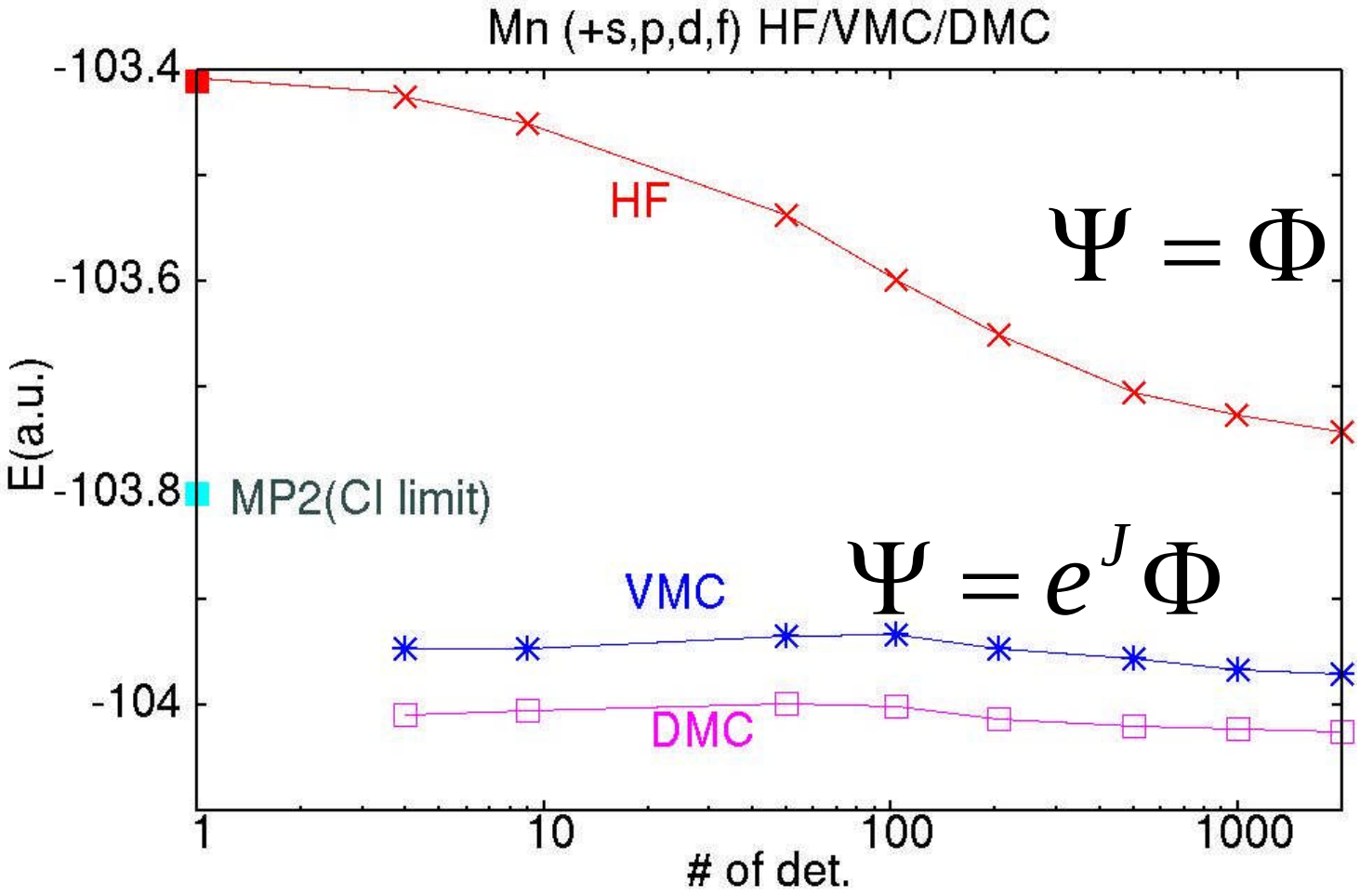
Calculations



$$\Psi = e^{J} \sum^{n\det} c_i \Phi_i$$

$$\Phi_i = | \phi_i(r) |$$

Mn CI/26(+s,p,d,f)



$$\Psi = \Phi$$

$$\Psi = e^{J}\Phi$$

$$\Psi = \sum c_i \Phi_i$$

c_i: CISD