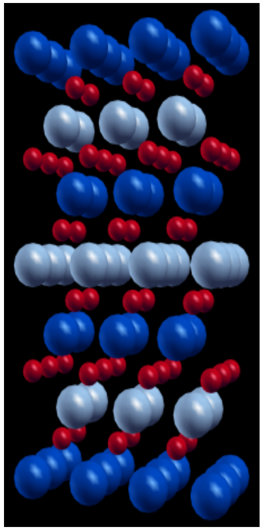
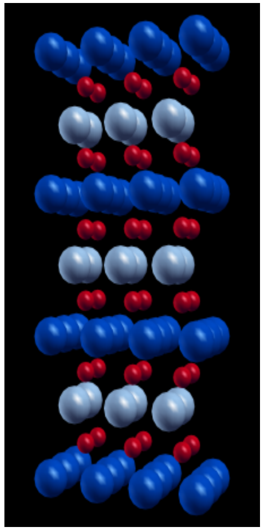
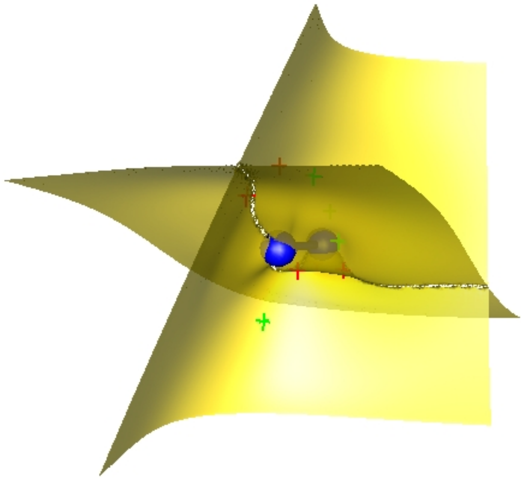
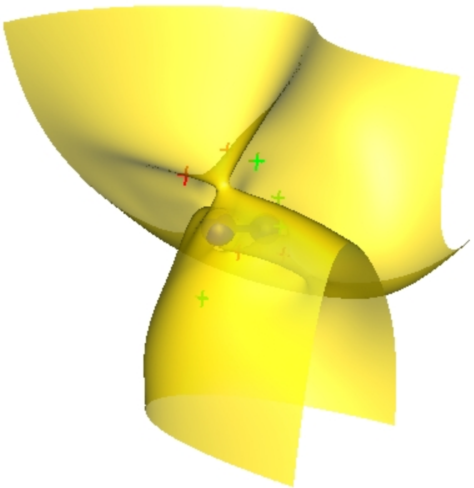
Electronic structure quantum Monte Carlo: pfaffians and many-body nodes of ground and excited states

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KITP, Santa Barbara, January '10

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PetaApps and INCITE
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Project out the ground state → imaginary time Schrodinger eq. (Fermi 1933)

$$\psi(\mathbf{R},t)=\exp(-tH)\psi_T(\mathbf{R}) \quad \rightarrow \quad \psi(\mathbf{R},t\rightarrow\infty) \propto \phi_0(\mathbf{R})$$

projector in parameter *t*

trial wave function

ground state of given symm.

H : electrons + ions and/or other interactions

$\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$: 3N-dim. continuous space

Projection in a differential/integral form (imaginary time Sch. eq.)

$$-\partial_t \psi(\mathbf{R},t)=H\psi(\mathbf{R},t)$$

$$\psi(\mathbf{R},t+\tau)=\int G(\mathbf{R},\mathbf{R}',\tau)\psi(\mathbf{R}',t)\,d\mathbf{R}'$$

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Quantum Monte Carlo (QMC) in a nutshell

Evolution equation $\psi(\boldsymbol{R}, t+\tau) = \int G(\boldsymbol{R}, \boldsymbol{R}', \tau)\psi(\boldsymbol{R}', t)\, d\boldsymbol{R}'$

with transition probability density $G(\boldsymbol{R}, \boldsymbol{R}', \tau) = \langle \boldsymbol{R} | \exp(-\tau H) | \boldsymbol{R}' \rangle$

can be mapped onto an equivalent stochastic process:

Value of the wavefunction ↔ density of sampling points in 3N-space

$$\psi(\boldsymbol{R}, t) = dens[\sum_i^{walkers} \delta(\boldsymbol{R} - \boldsymbol{R}_i(t))] + \epsilon_{statistical}$$

sampling points → "walkers" → eigenstates of position operator

Solution: find $G(\boldsymbol{R}, \boldsymbol{R}', \tau)$ **and iterate**

Exact mapping but fermion sign problem!

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Fix the sign problem by the fixed-node approximation: fixed-node diffusion Monte Carlo (FNDMC)

Consider a product: $f(\boldsymbol{R},t)=\psi_T(\boldsymbol{R})\phi(\boldsymbol{R},t)$

modify Sch. eq. accordingly: $f(\boldsymbol{R},t+\tau)=\int G^*(\boldsymbol{R},\boldsymbol{R}',\tau)f(\boldsymbol{R}',t)d\boldsymbol{R}'$

so that: $f(\boldsymbol{R},t\to\infty)\propto\psi_T(\boldsymbol{R})\phi_{ground}(\boldsymbol{R})$

Fermion node: (3N-1)-dimen. hypersurface defined as $\phi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)=0$

Fixed-node (FN) approximation: $f(\boldsymbol{R},t)>0$

- **antisymmetry (nonlocal) replaced by a boundary (local)**
- **accuracy determined by the nodes of** $\psi_T(\boldsymbol{R})$
- **exact node enables to recover exact energy (in polynomial time)**

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QMC calculations: basic steps

Hamiltonian: - valence e- only, using pseudopots/ECPs
- e-e interactions explicitly
- size: up to a few hundreds valence e-

Explicitly correlated trial wavefunction of Slater-Jastrow type:

$$\psi_{Trial} = det^{\uparrow}[\phi_{\alpha}] det^{\downarrow}[\phi_{\beta}] \exp[\sum_{i,j,I} U_{corr}(r_{ij}, r_{iI}, r_{jI})]$$

(or more sophisticated: BCS, pfaffians, backflow,..., later)

Orbitals: - from HF, DFT, hybrid DFT, possibly CI, etc

Solids: - supercells
- finite size corrections

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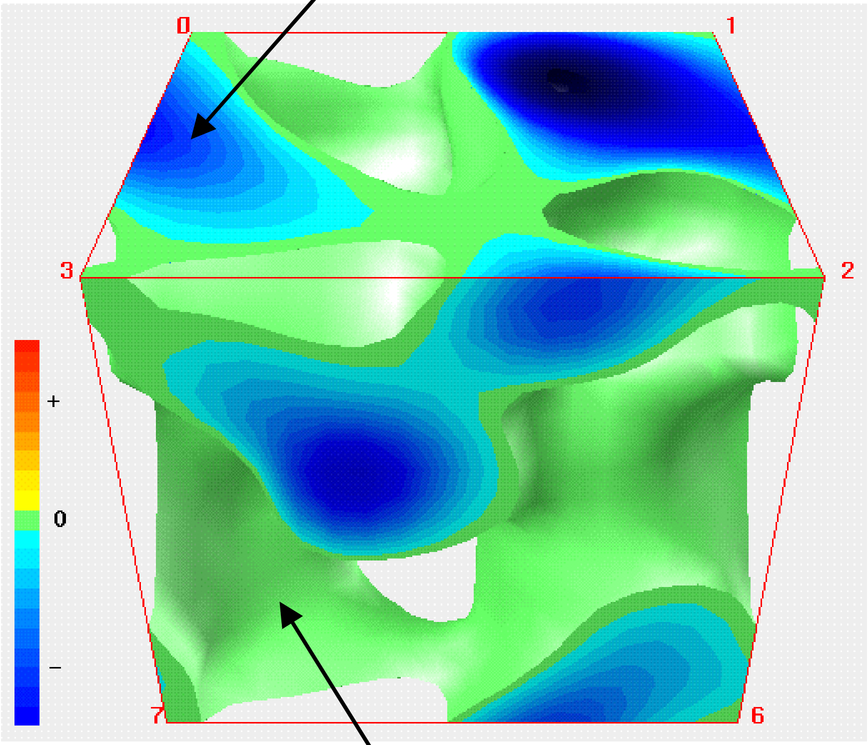
Fixed nodes in reality: complex multi-D hypersurface, impossible to “see”, ...

Wavefunction value



3D subset of 59-dim node

- defined by the antisymmetric part of the trial function → difficult to parametrize efficiently

but

- systematically improvable at least for small systems

- easy to enforce, eg, evaluate the sign of an antisymmetric form, eg, a determinant

Let's see how it works ...

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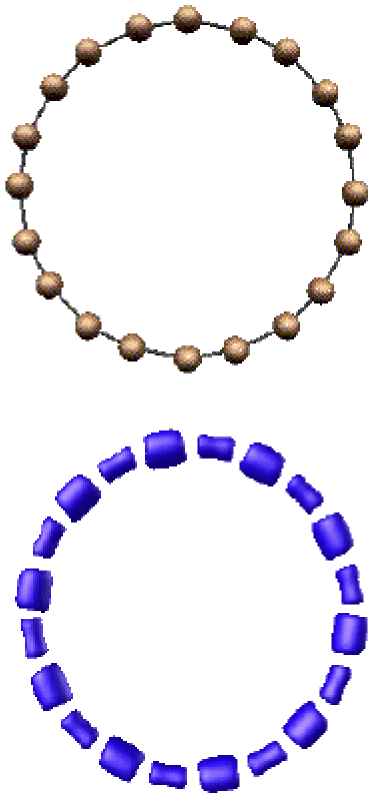
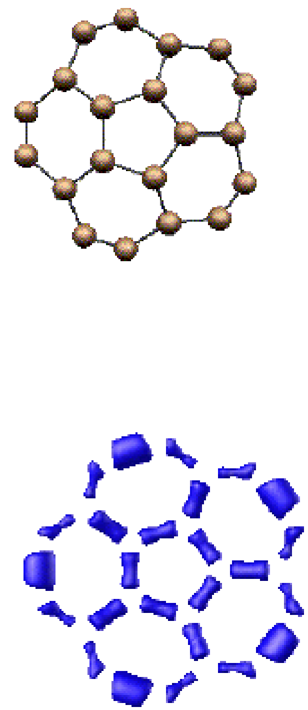
Application example: which is the lowest energy isomer of C_{20} ?

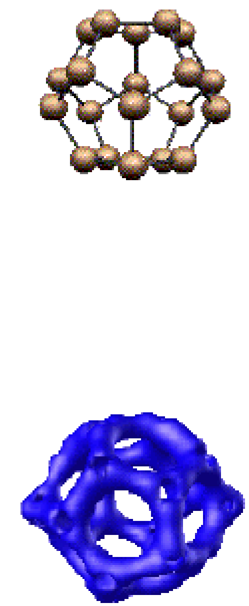
ring



bowl



cage



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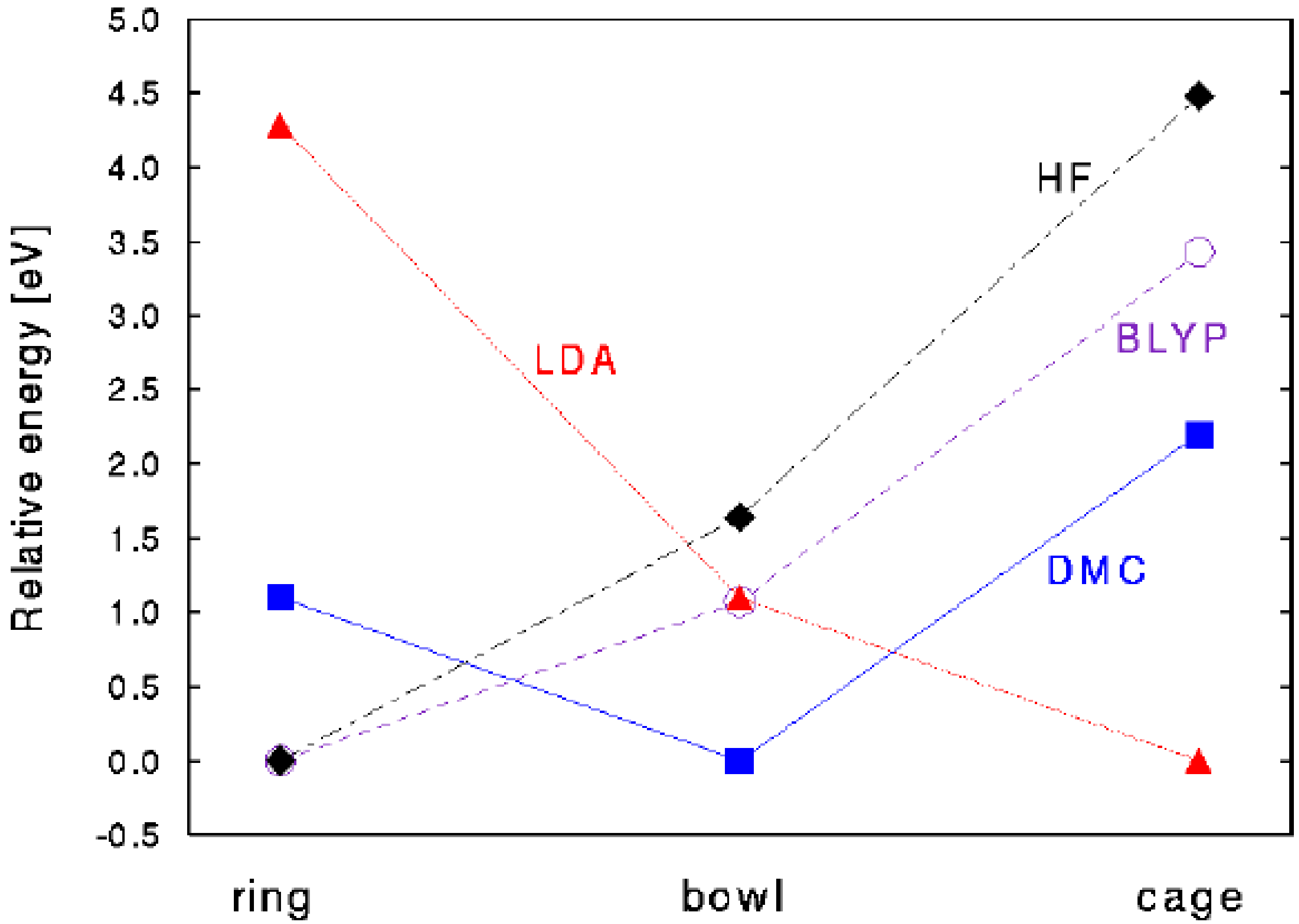
FNDMC/HF nodes: the lowest is the bowl isomer! (later confirmed by independent methods, still used in benchmarking of DFT functionals)



J.C. Grossman, L. M., K. Raghavachari, Phys. Rev. Lett. '95

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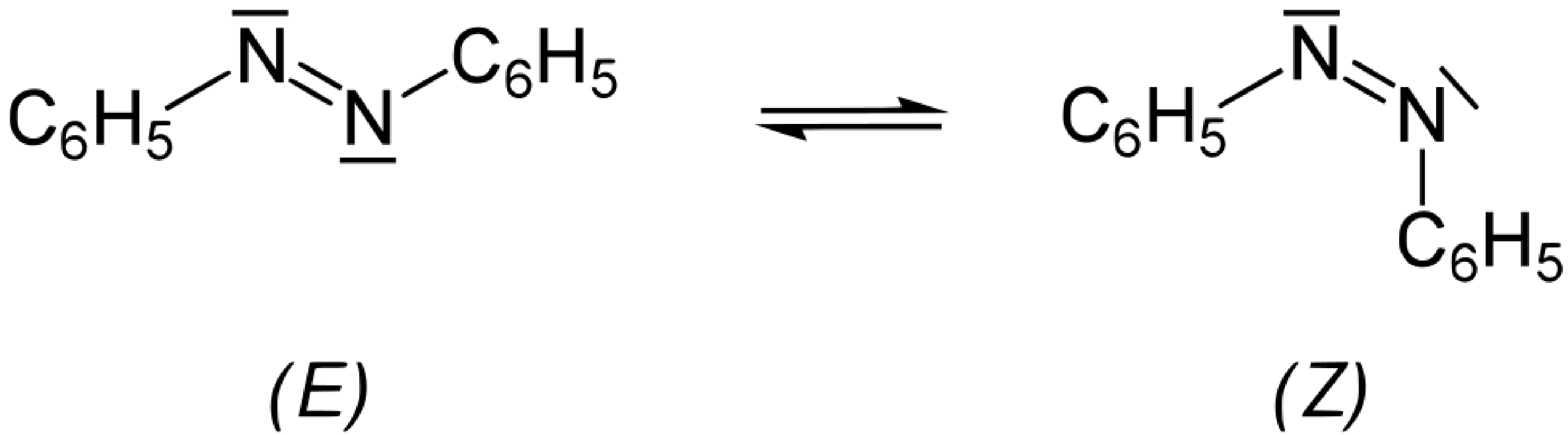
Azobenzene: optically active molecule with photoisomerization



M. Kostolny, R. Derian, I. Stich, L.M. 2010

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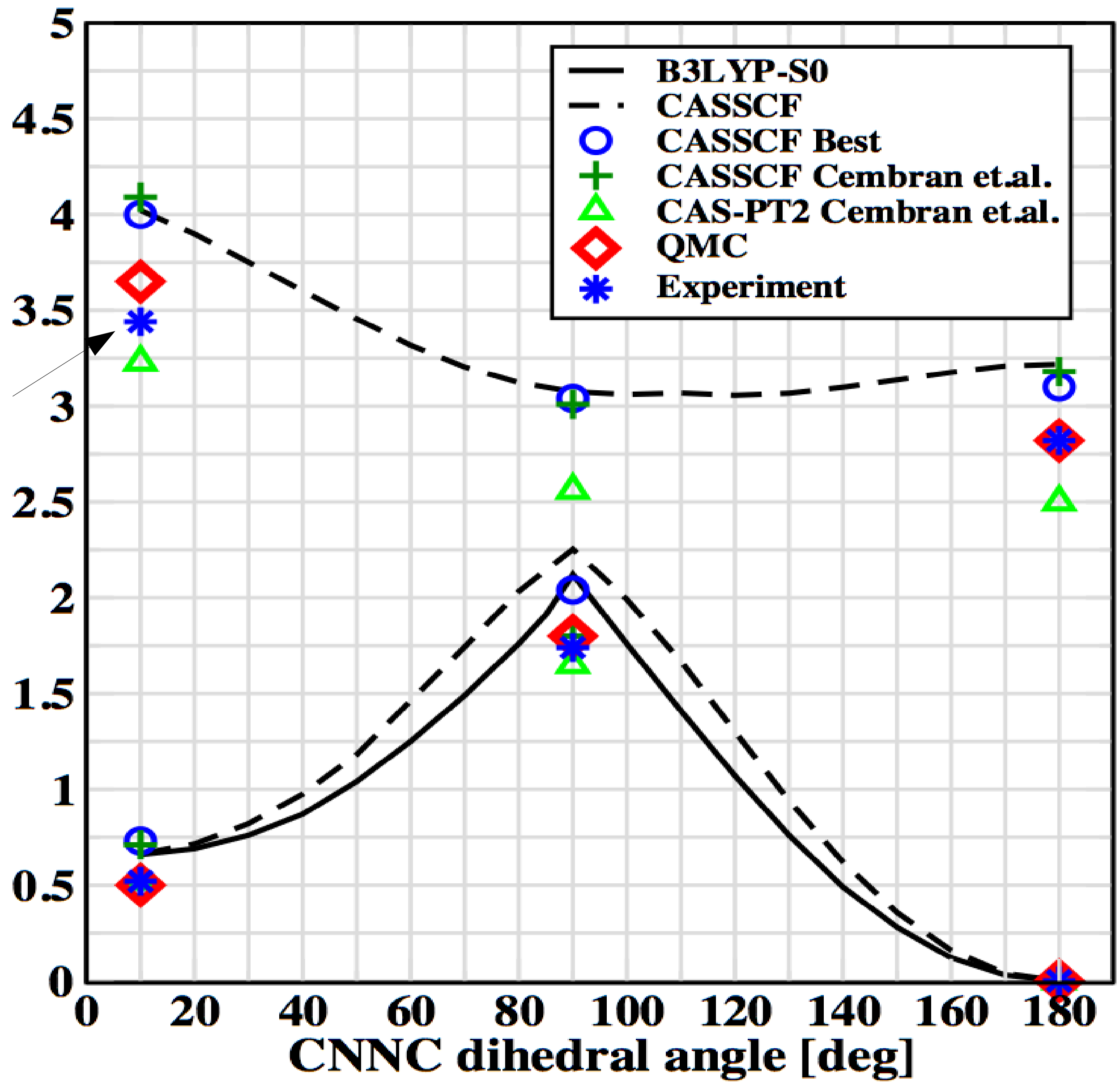
Azobenzene barrier and excitations: better than 0.05 eV accuracy with FNDMC/multi-det.



Experiment not ok (?)

M. Kostolny, R. Derian, I. Stich, L.M. 2010

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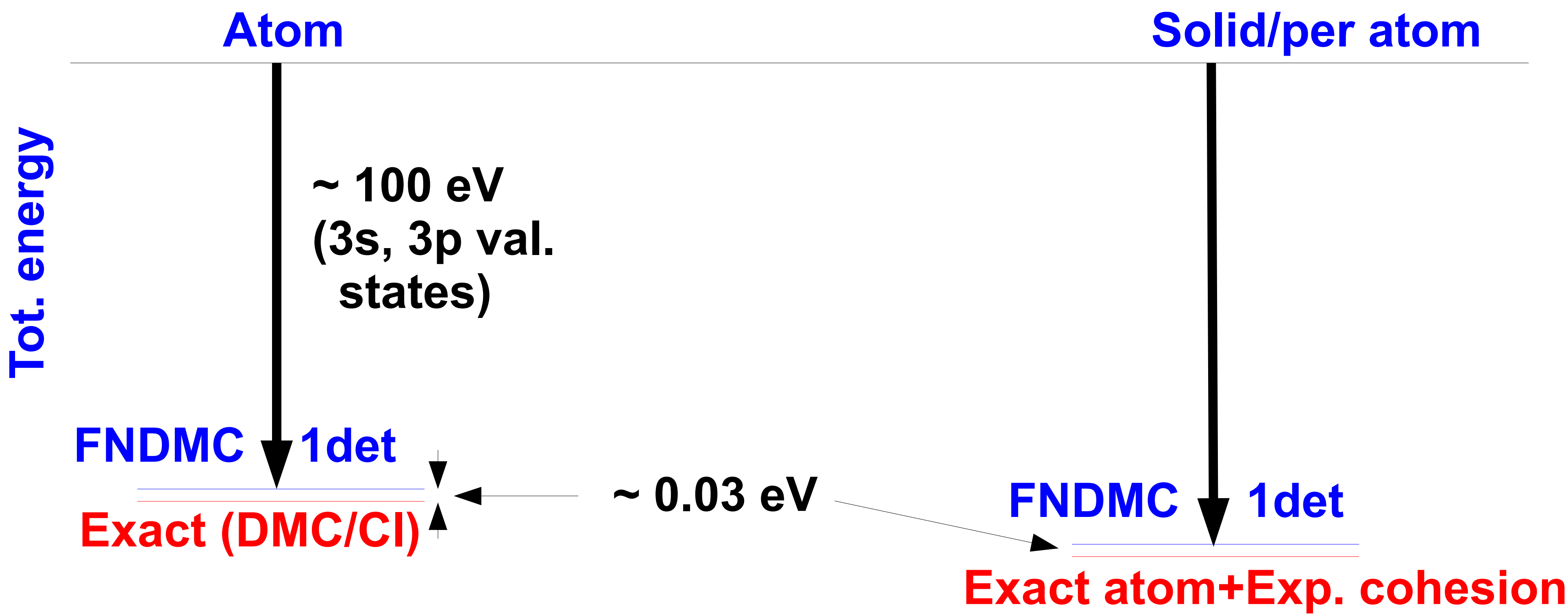
Semiconductor example: solid Si (up to 214 atoms) FNDMC/single-det/PBE nodes: stochastic and systematic errors are small



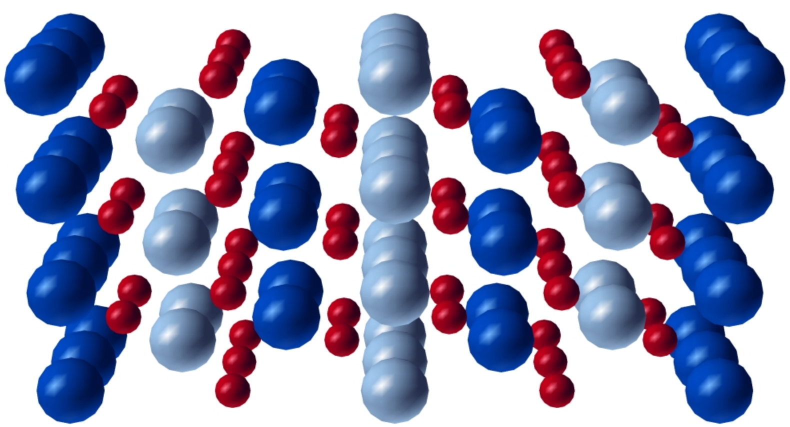
Cohesion:
- rigorous lower bound(!) → 6.58(1) eV
- FNDMC (error canc.) → 4.61(1) eV
- experiment → 4.62(8) eV

FeO solid at high pressures

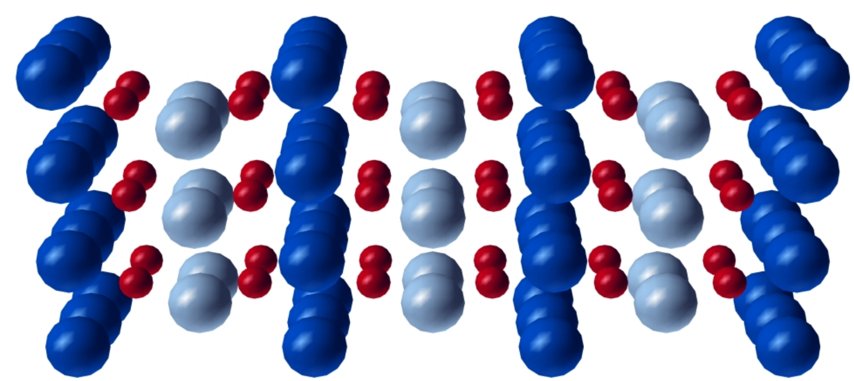
- **large e-e correlations, difficult**: competition of Coulomb, exchange, correlation and crystal-field effects; important **high-pressure physics** (Earth interior, for example)

- mainstream Density Functional Theories (DFT) predict: **wrong** equilibrium structure; and for the correct structure predict a **metal instead of large-gap insulator**

B1/AFII (equil.)



iB8/AFII



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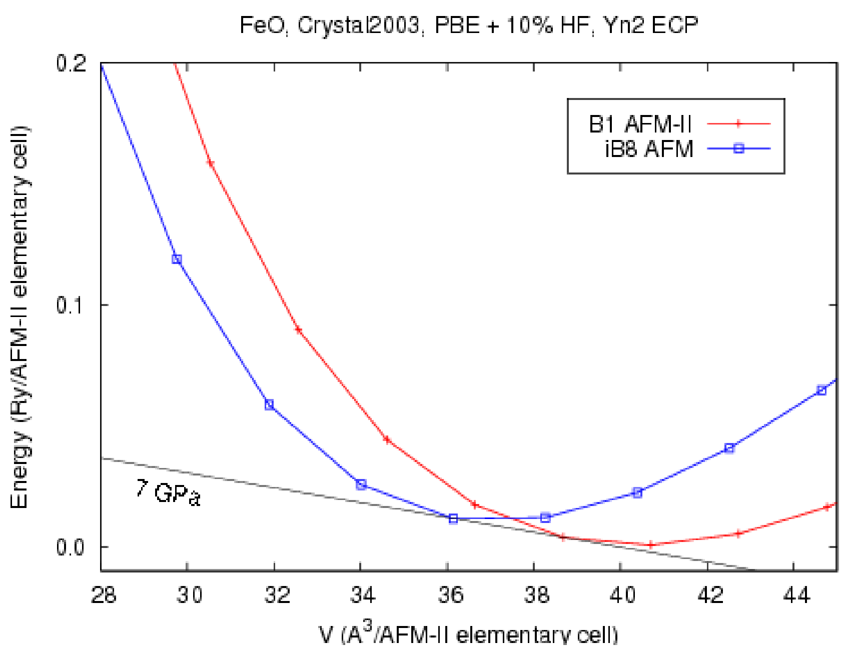
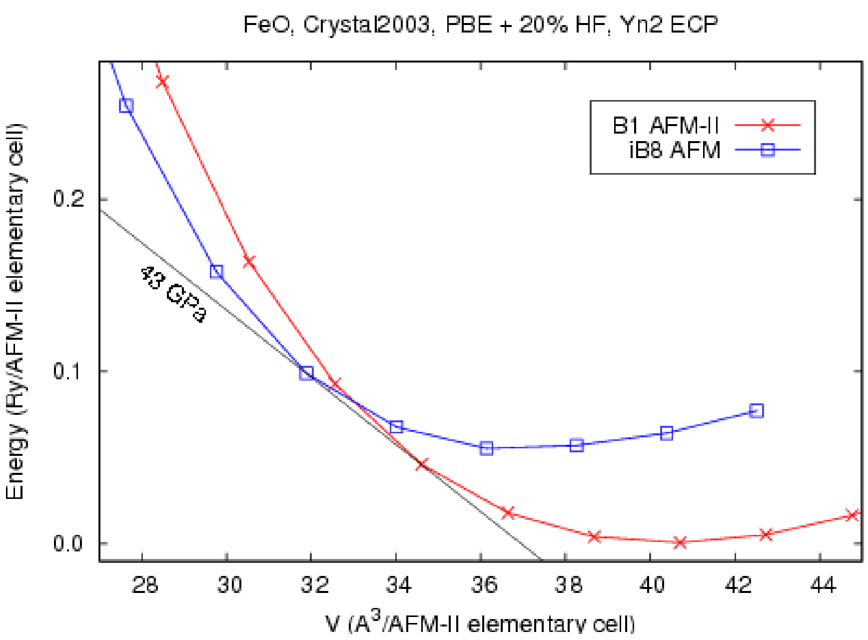
FeO solid at high pressures DFT with HF mixing

In order to reconcile theory with experiment one needs Hubbard U or, alternatively, mixing of an exact exchange into the effective Hamiltonian: non-variational, certain arbitrariness





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Comparisons of the FeO solid equilibrium parameters FNDMC/single det.

	DFT/PBE	FNDMC	Exp.(FeO_{1-x})
iB8-B1/AFMII [eV]	- 0.2	0.5 (1)	>0
Cohesion [eV]	~ 11	9.7 (1)	9.7(2)
a_0 [A]	4.28	4.32	4.33
K_0 [GPa]	180	170(10)	152(10)
Opt. gap [eV]	~ 0 (metal)	2.8(3) eV	~ 2.4 eV

J. Kolorenc & LM, Phys. Rev. Lett. '08

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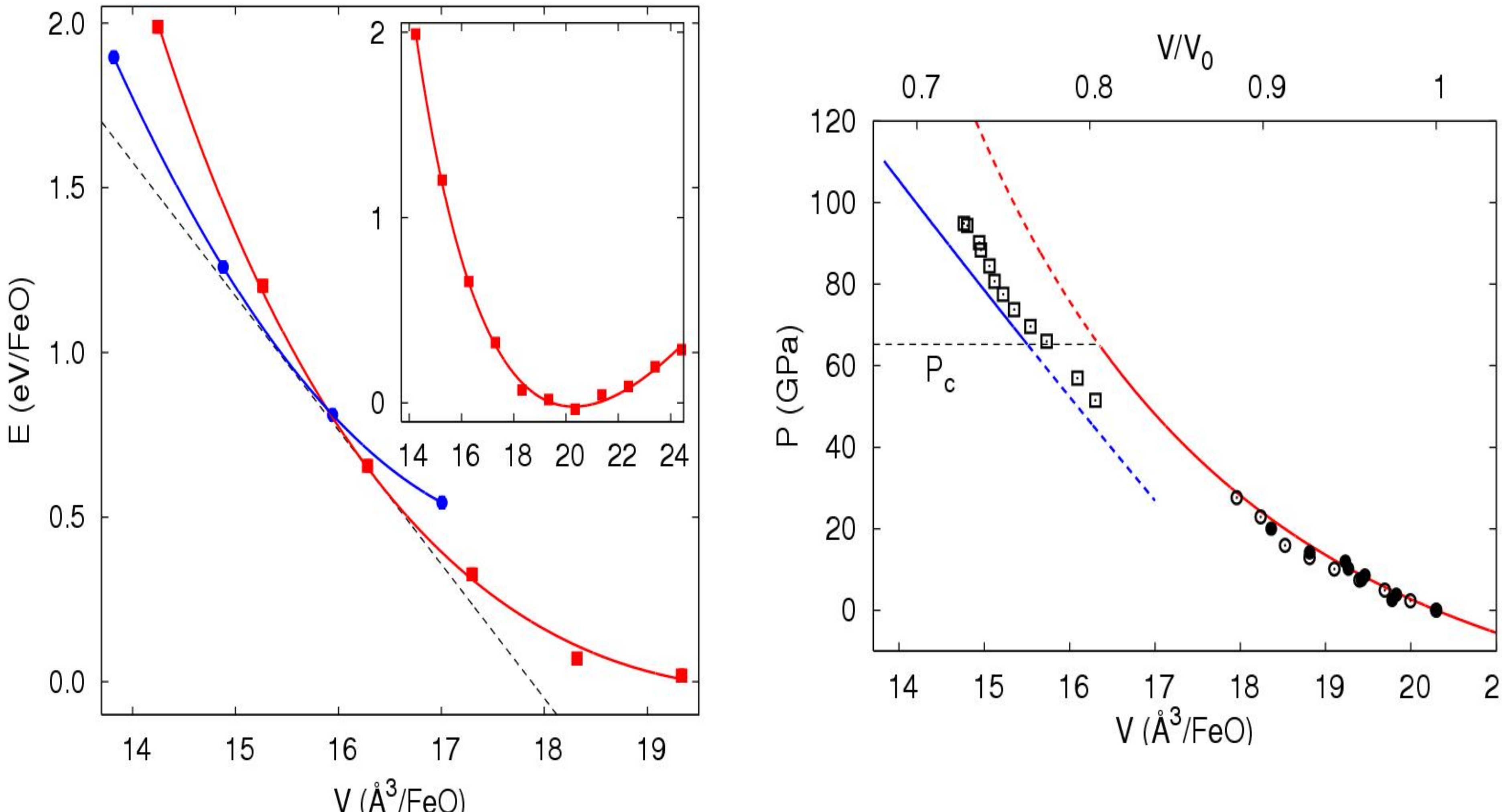
FeO solid at high pressures
QMC shows transition at ~ 65 GPa (Exper. 70-100)



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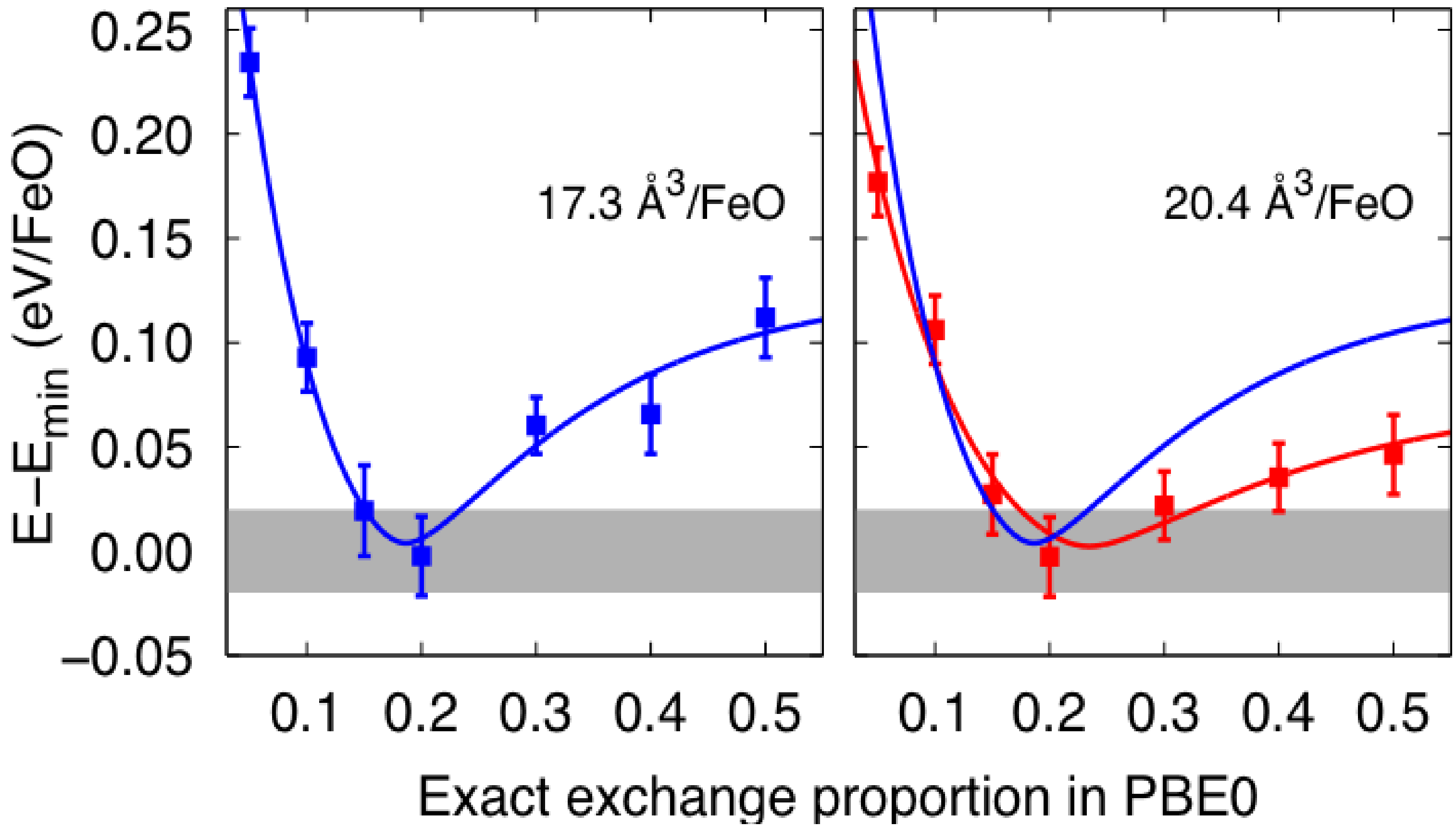
JK & LM, Phys. Rev. Lett. '08

Orbitals from hybrid PBE0 functional
Optimal weight of the Fock exchange found by minimization of the fixed-node DMC energy



HF weight → d-p hybridization: HF "ionic" vs DFT "covalent"

Note: variational FNDMC optimization of the DFT functional!

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QMC byproduct: construction of optimal effective Hamiltonians (one-body or beyond)

The mixing of exact exchange into the effective one-particle (DFT) Hamiltonian is simple, useful and clearly justified:

- variationally optimized fixed-node DMC energy

- orbitals beyond Hartree-Fock → correlated (most of the correlation in QMC is captured: all the bosonic correlations, cusps, etc, captured exactly)

- points out towards a more general idea/tool: variational space includes not only wavefunction but also effective Hamiltonian (more efficient and faster generation of accurate nodes)

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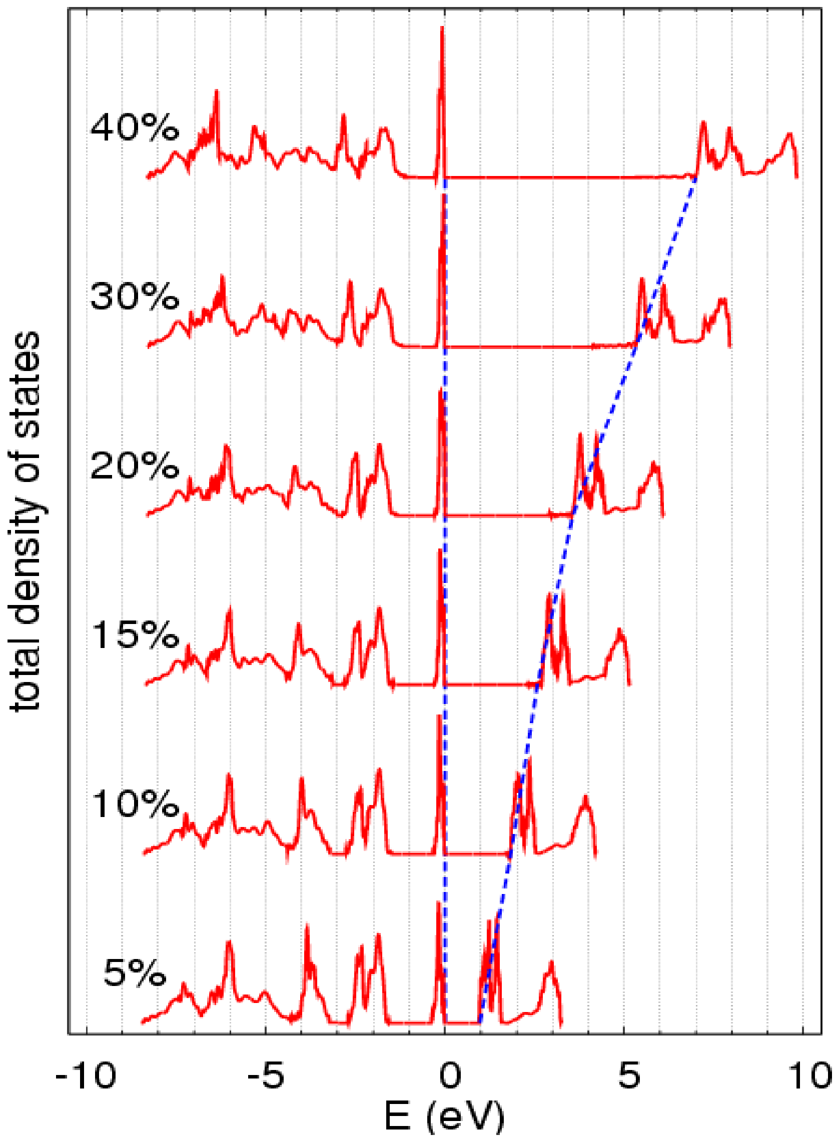
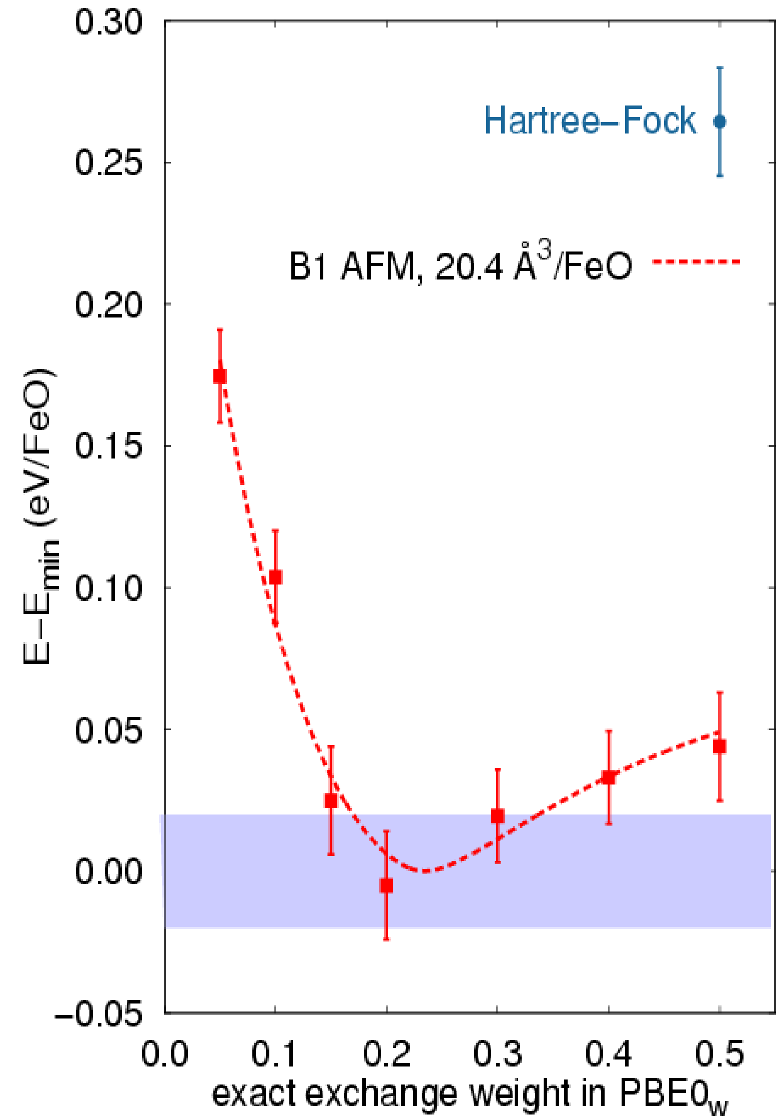
Enables also to look back at the (corrected) one-particle picture, eg, density of states, gap, etc





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Large-scale QMC calculations: performance and cost

FNDMC:
- Ne-core relativistic ECPs for Fe
- orbitals: HF, hybrid DFT
- size: 8 and 16 FeO supercells, up to 352 valence e-
- finite size corrections

Slater-Jastrow wavefunction:

$$\psi_{Trial} = det^{\uparrow}[\phi_{\alpha}]\, det^{\downarrow}[\phi_{\beta}] \exp[\sum_{i,j,I} U_{corr}(r_{ij}, r_{iI}, r_{jI})]$$

Scaling as ~ N^2- N^3, parallel scalability

Computational cost: typical run 30,000 hours (3 orders of magnitude slower than a typical DFT run)

Correlation energy (E_HF – E_exact) recovered: ~ 90 - 95 %

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FeO calculations illustrate a few key points about QMC

Practical:
- systems with hundreds of electrons are feasible
- agreement with experiment within few %
- the simplest, "plain vanilla" FNQMC → single-determinant nodes!

Fundamental:
- note: no ad hoc parameters, no Hubbard U or Stoner J, etc: applicable to solids, nanosystems, BEC-BCS condensates ...

- 90-95 % of correlation is "bosonic"-like (within nodal domains), efficiently captured by algebraically scaling methods

- fixed-node approx. is the only key issue: 5-10% of correlation → enough accuracy for cohesion, gaps, optical excitations, etc

- 5-10% still important: magnetic effects, superconductivity, etc

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Beyond the fixed-node approximation: fermion nodes
What do we need and want to know ?

$\phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_N) = 0$ $\rightarrow$ **(DN-1)-dim. smooth hypersurface**

It divides the space into domains with constant wf. sign ("+" and "- ")

Interest in nodes goes back to D. Hilbert and L. Courant (eg, n-th exc. state has n or less nodal domains). However, ... we need (much) more:

- **nodal topologies, ie, number of nodal cells/domains → important for correct sampling of the configuration space**
- **accurate nodal shapes ? how complicated are they ? → affects the accuracy of the fixed-node energies**
- **nodes ↔ types of wavefunctions ?**
- **nodes ↔ physical effects ?**

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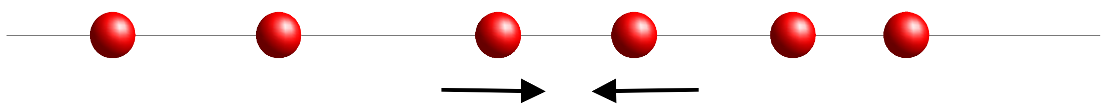
Topology of fermion antisymmetry: what do we know ?

1D: the ground state node of N fermions on a line is known exactly,



since each time two fermions cross each other they hit the node and the system passes from one domain to another $\rightarrow$ N! domains

3D: a few special cases of 2e-, 3e- atoms nodes known exactly:

A) 2e- He atom triplet $^3S[1s2s]$ exact node: $|\mathbf{r}_1|^2 - |\mathbf{r}_2|^2 = 0$

two domains (one +, one -) $\rightarrow$ $r_1 > r_2$ or $r_2 > r_1$

B) 3e- atomic lowest quartet of S symmetry and odd parity

$^4S[2p^3]$: the exact node is $\mathbf{r}_1 \cdot (\mathbf{r}_2 \times \mathbf{r}_3) = 0$

again two domains: $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$ either left-handed or right-handed

Conjecture: for d >1 the ground states have only two nodal cells, one "+" and one "-"

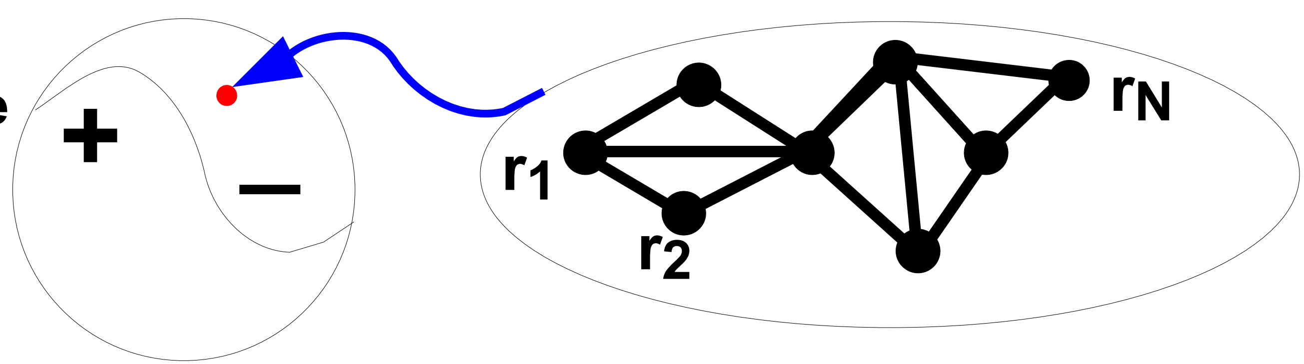
Numerical proof for 200 noninteracting fermions in 2D/3D (Ceperley '92):

Tiling by permutations property for nondegenerate ground states:

$$Let\ Q(R_0)\ be\ the\ nodal\ domain\ around\ R_0 \ \rightarrow$$
$$\sum_P Q(PR_0) \ = \ whole\ configuration\ space$$

Then, for a given $\phi(\boldsymbol{R})$ find a point such that triple exchanges connect all the particles into a single cluster: then there are only two nodal cells

All-particle configuration space



(Why ? Connected cluster of triple exchanges exhausts all even/odd permutations + tiling property $\rightarrow$ no space left)

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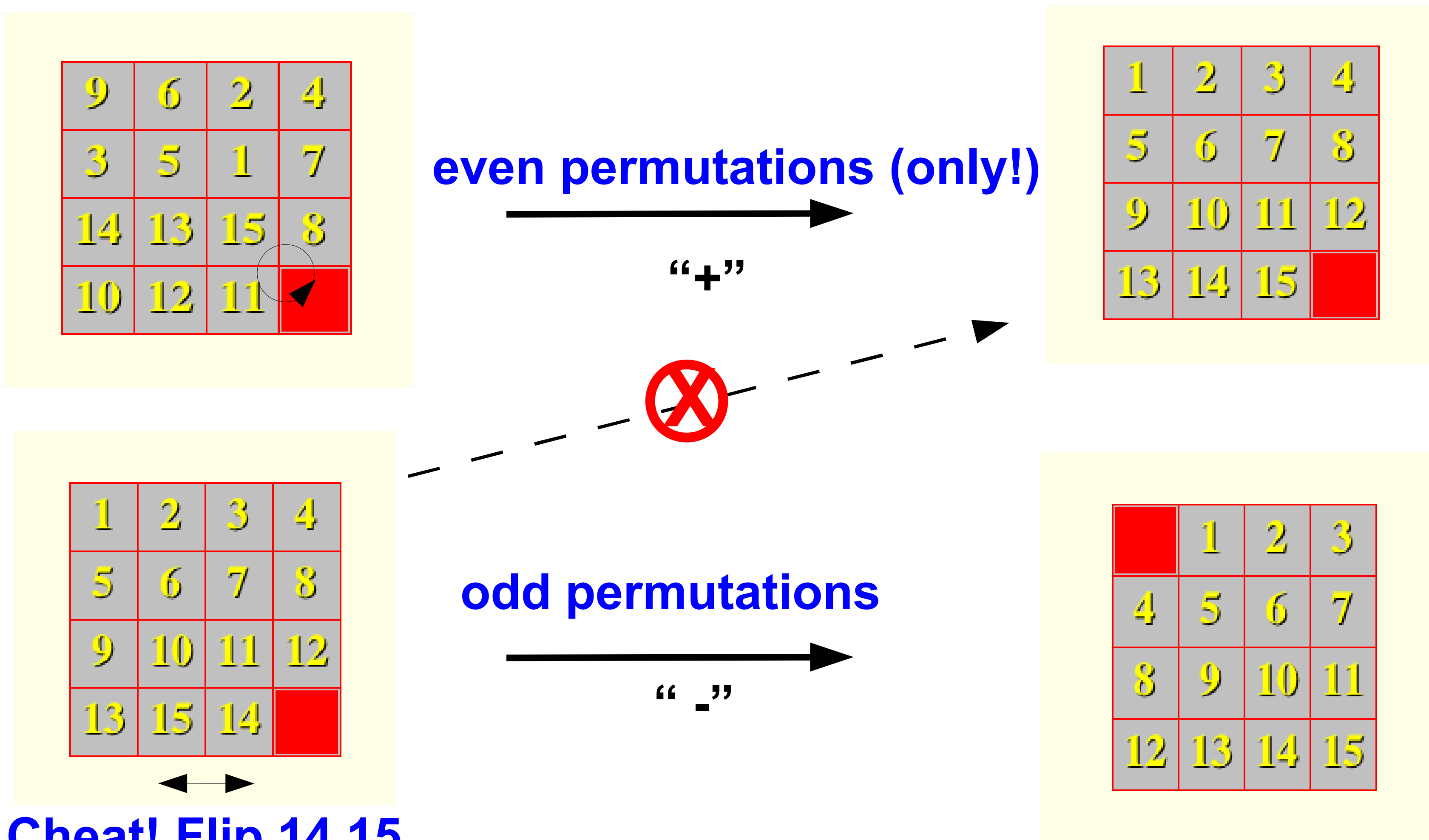
Sliding 15-puzzle: an example of 3-cycle (triple exchange) permutation cluster



Cheat! Flip 14,15

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Is this the case of fermionic ground states for d>1? Yes!

Two nodal cells theorem. **Consider a spin-polarized, closed--shell ground state given by a Slater determinant**

$$\psi_{exact} = C_{symm}(1,\ldots,N)\, det\{\phi_j(i)\}; \quad C_{symm} \geq 0$$

Let the Slater matrix elements be monomials $x_i^n y_i^m z_i^l$ **of positions or their homeomorphic maps in d>1.**

Then the wavefunction has only two nodal cells for any d>1.

(L.M. PRL, 96, 240402; cond-mat/0605550)

Covers many noninteracting models: harmonic fermions, homog. gas (fermions on T^d), fermions on a sphere (S^2), ...

Can be extended also to inhomogeneous polynomials such as atoms, HF atoms, etc

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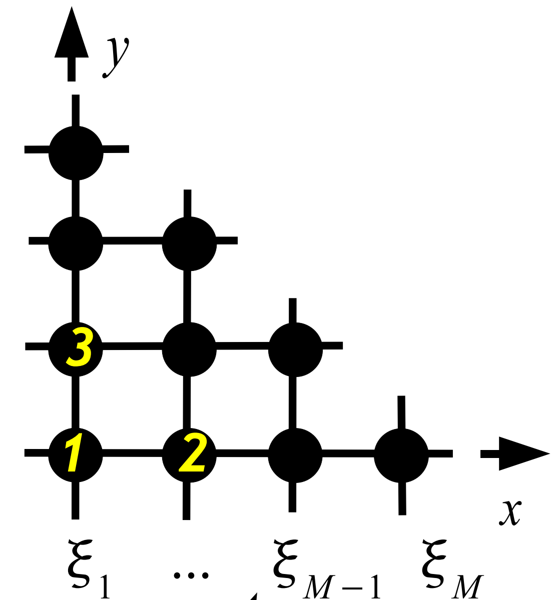
Proof sketch for spin-polarized noninteracting 2D harmonic fermions: Step 1 → Wavefunction factorization

Place fermions on a Pascal-like triangle →

$(M+1)(M+2)/2$ **fermions on** M **lines**



Factorize out the particles on the vertical line:

$$\psi_{\underline{M}}(1,..,N_M)=C_{gauss}\,det\left[1,x,y,x^2,xy,y^2,...,y^M\right]=$$

$$=\psi_{\underline{M-1}}(1,...,N_M/I_{\xi_1})\prod_{i<j}^{i,j\in I_{\xi_1}}(y_j-y_i)\prod_{1<k\le M}(\xi_k-\xi_1)^{n_k}$$

particle coords

lines coords

General: factorizable along *vertical, horizontal* or *diagonal* lines, recursive → "multi-dimensional Vandermonde determinant"

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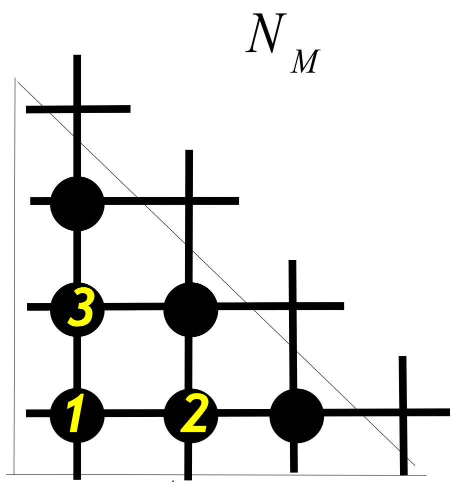
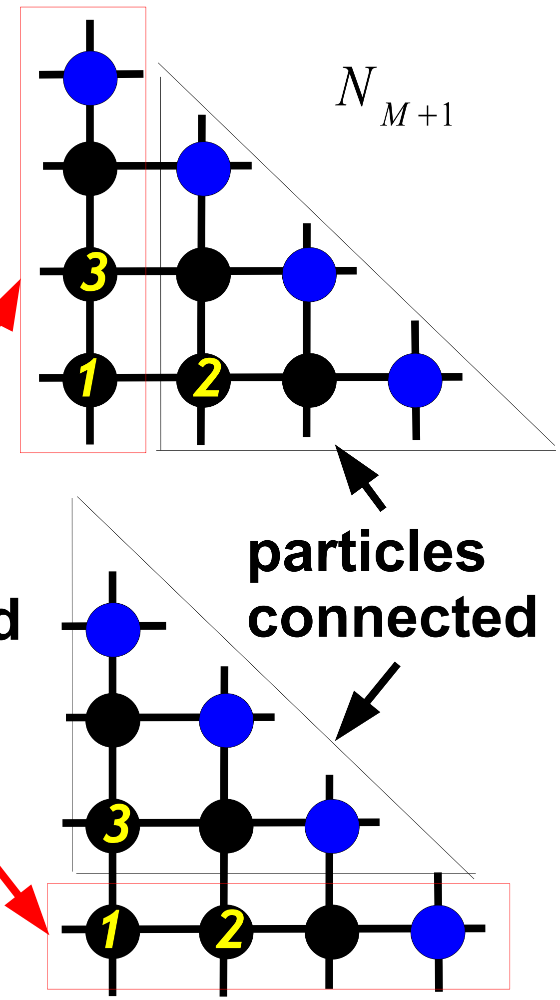
Explicit proof of two nodal cells for spin-polarized harmonic fermions: Step 2 → Induction



assume particles are connected by 3-exchanges

$M \rightarrow M+1$



"lines" factorized out

particles connected

Therefore all particles connected, any size. Q.E.D.

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For noninteracting/HF systems with both spin channel occupied → more nodal cells.
Interactions → minimal number of two cells again!

Unpolarized noninteracting/HF systems: 2*2=4 nodal cells!!!
-> product of two independent Slater determinants

$$\psi_{HF} = det^{\uparrow}\{\phi_\alpha\} det^{\downarrow}\{\phi_\beta\}$$

What happens when interactions are switched on ?

"Nodal domain degeneracy" is lifted → topology change
→ multiple nodal cells fuse into the minimal two again!

Bosonic ground states → global/all-electron S-waves
Fermionic ground states → global/all-electron "P-waves" !

Fundamental and generic property of fermions!

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The same is true for the nodes of temperature/imaginary time density matrix

Analogous argument applies to temperature density matrix

$$\rho(R, R', \beta) = \sum_{\alpha} \exp[-\beta E_{\alpha}] \psi *_{\alpha}(R) \psi_{\alpha}(R')$$

fix R', β $\rightarrow$ nodes/cells in the R subspace

High (classical) temperature: $\rho(R, R', \beta) = C_N det\{\exp[-(r_i - r'_j)^2/2\beta]\}$

enables to prove that R and R' subspaces have only two nodal cells. Stunning: sum over the whole spectrum!!!
L.M. PRL, 96, 240402; cond-mat/0605550

H. Monkhorst: "So what you are saying is that nodes are simple!"
Topology: yes! Shapes: no! $\rightarrow$ better wavefunctions: pfaffians ...

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The simplest case of a nodal topology change from interactions/correlations: three e- in Coulomb pot.

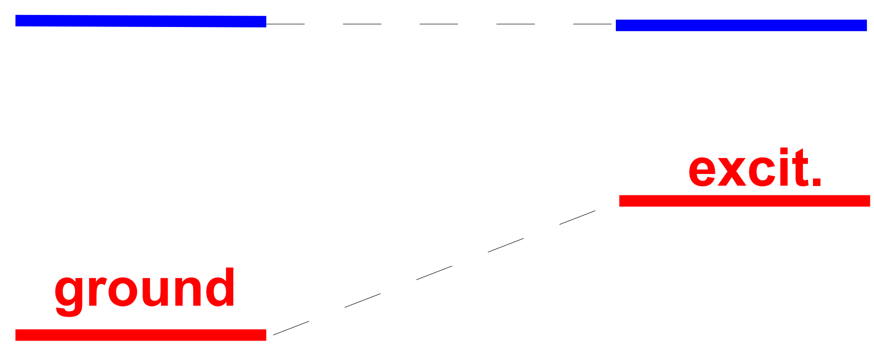
Consider three electrons in Coulomb potential, in the lowest quartet (all spins up) of S symmetry and even parity state

Noninteracting Hamiltonian has two degenerate states:

$$\psi_I = det[1s, 2s, 3s] \qquad \psi_{II} = det[1s, 2p_x, 3p_x] + \; + \; x \rightarrow y \; + \; y \rightarrow z$$

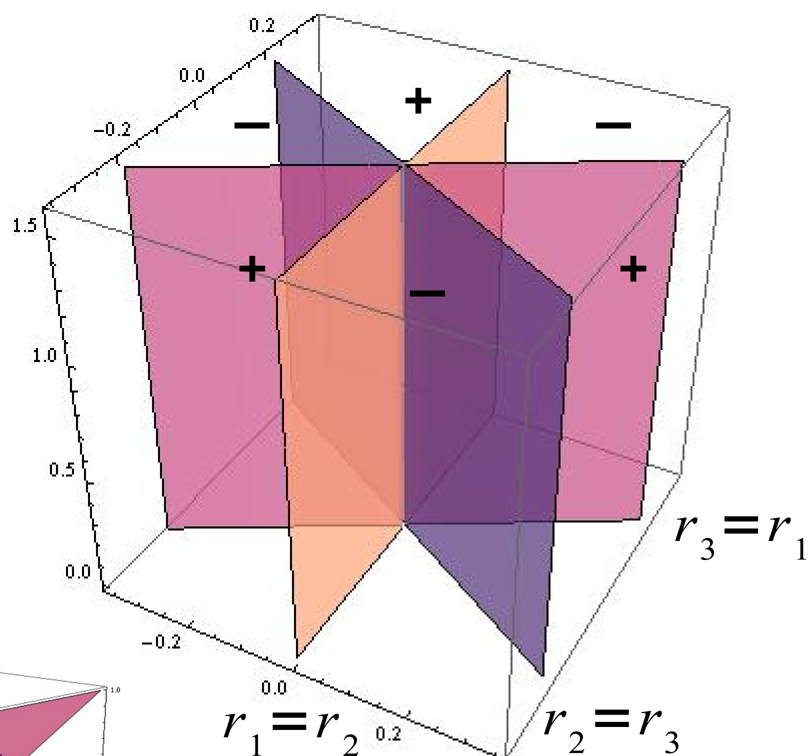
non-interacting

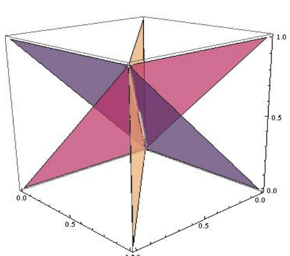
Interaction -> states split
(already in HF)

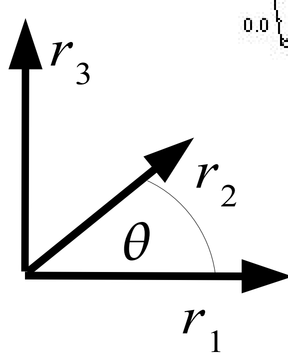


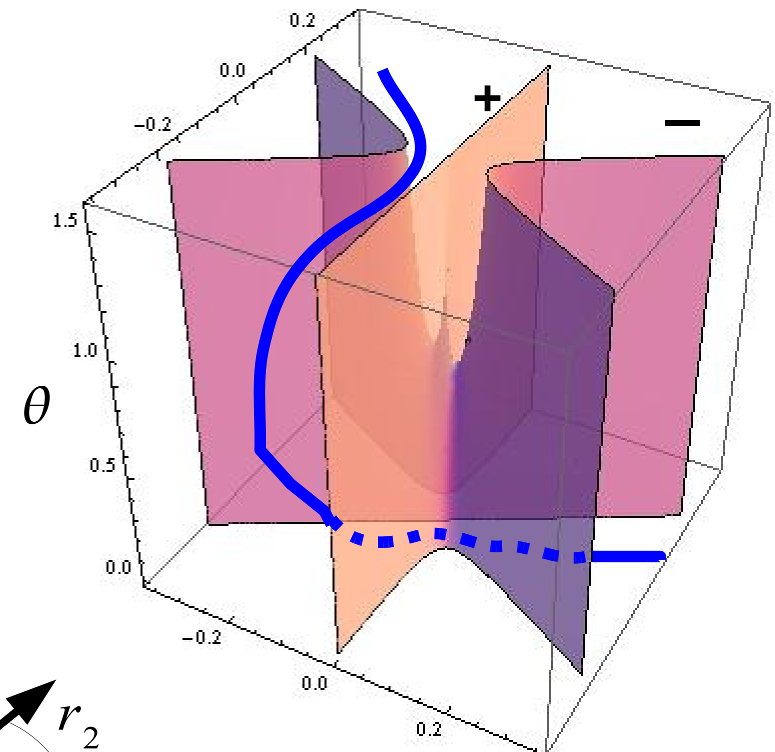
^{4}S(1s2s3s) HF node: $(r_1 - r_2)(r_2 - r_3)(r_3 - r_1) = 0 \;\; \rightarrow$ **6 domains (quasi 1D!)**

Nodal topology change from interactions/correlation (“triplet pairings”: tiny but nonzero effect)









HF node

6 cells

Pfaffian (or expansion in dets) → corr. node

2 cells

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Pfaffian: signed sum of all distinct pair partitions of permutations (Pfaff, Cayley ~ 1850) -> the simplest antisymm. pair spinorbital wavefunction

$$pf[a_{ij}] = \sum_P (-1)^P a_{i_1 j_1} \ldots a_{i_N j_N} \quad , \quad i_k < j_k , \quad k = 1, \ldots, N$$

Pair orbital $\phi(x_1, x_2)$ **+ antisymmetry** $\rightarrow$ **pfaffian***

$$\psi_{PF} = A[\phi(x_1, x_2)\phi(x_3, x_4)\ldots] = pf[\phi(x_i, x_j)] \qquad i, j = 1, \ldots, 2\mathrm{N}$$

- **determinant is a special case of pfaffian (pfaffian is more general)**
- **pfaffian algebra similar to determinants (minors, etc)**
- ψ_{HF} **is a special case of** ψ_{PF}

$$\phi(x_i, x_j) = \phi^{\uparrow\downarrow}(r_i, r_j)(\uparrow\downarrow - \downarrow\uparrow) + \chi^{\uparrow\uparrow}(r_i, r_j)(\uparrow\uparrow) + \chi^{\downarrow\downarrow}(r_i, r_j)(\downarrow\downarrow) + \chi^{\uparrow\downarrow}(r_i, r_j)(\uparrow\downarrow + \downarrow\uparrow)$$

symmetric/singlet **antisymmetric/triplet**

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Pfaffian wavefunctions with both singlet and triplet pairs (beyond BCS!) -> all spin states treated consistently: simple, elegant

$$\psi_{PF} = pf \begin{bmatrix} \chi^{\uparrow\uparrow} & \phi^{\uparrow\downarrow} & \psi^{\uparrow} \\ -\phi^{\uparrow\downarrow T} & \chi^{\downarrow\downarrow} & \psi^{\downarrow} \\ -\psi^{\uparrow T} & -\psi^{\downarrow T} & 0 \end{bmatrix} \times \exp[U_{corr}]$$

- **pairing orbitals (geminals) expanded in one-particle basis**

$$\phi(i,j) = \sum_{\alpha \geq \beta} a_{\alpha\beta} [h_\alpha(i) h_\beta(j) + h_\beta(i) h_\alpha(j)]$$
$$\chi(i,j) = \sum_{\alpha > \beta} b_{\alpha\beta} [h_\alpha(i) h_\beta(j) - h_\beta(i) h_\alpha(j)]$$

- **unpaired** $\psi(i) = \sum_\alpha c_\alpha h_\alpha(i)$

BCS wf. for 2N-particle singlet is a special case: $\psi_{BCS} = det[\phi^{\uparrow\downarrow}]$

Pairing wavefuctions enable to get the correct nodal topologies ...

(M. Bajdich et al PRL '06; PRB '08)

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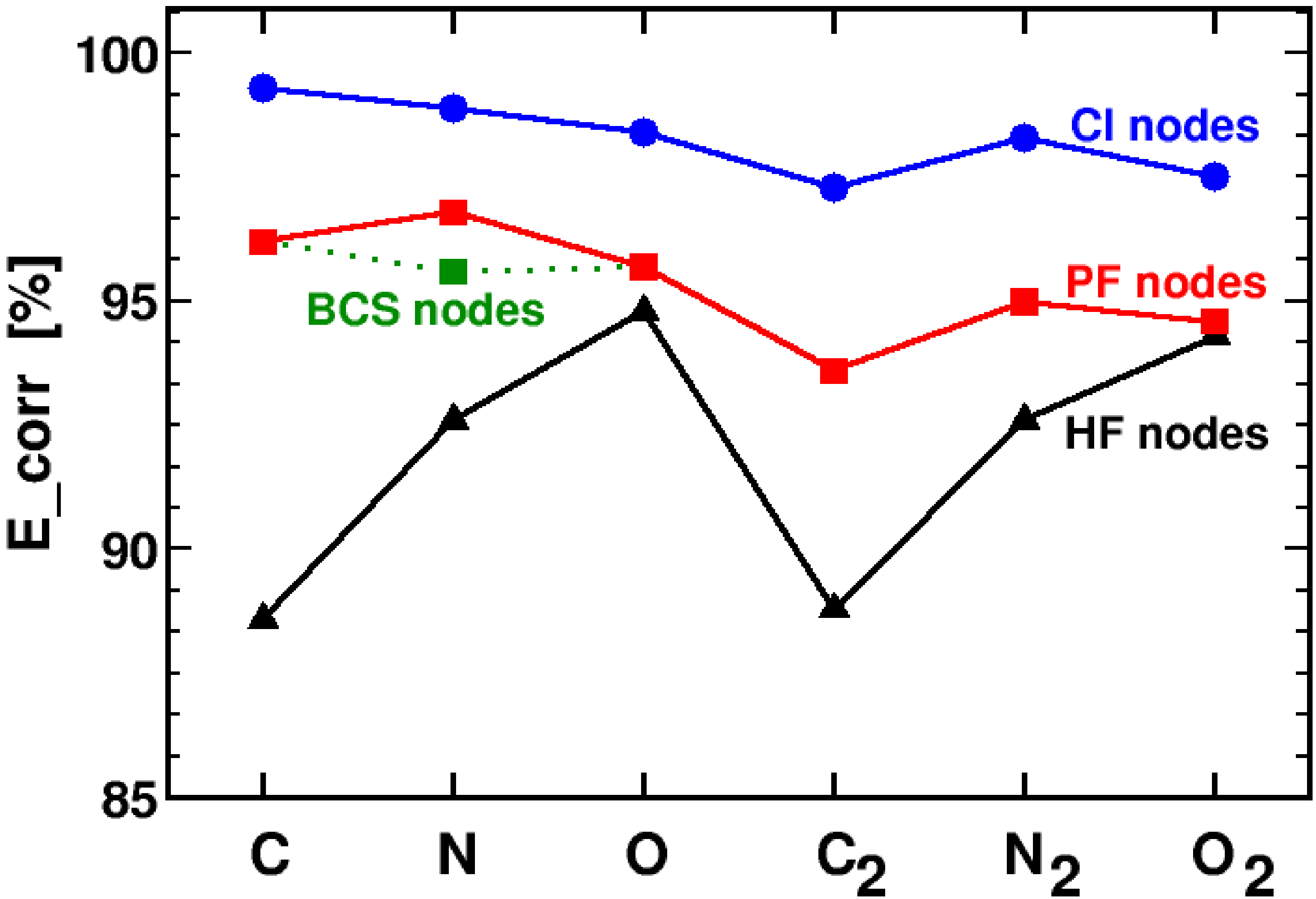
DMC correlation energies of atoms, dimers
Pfaffians: more accurate and systematic than HF while scalable (unlike CI)



Expansions in many pfaffians for first row atoms: FNDMC ~ 98 % of correlation with a few pfaffians

Table of correlation energies [%] recovered: MPF vs CI nodes

n = # of pfs/dets

WF	n	C	n	N	n	O
DMC/MPF	3	98.9	5	98.4	11	97.2
DMC/CI	98	99.3	85	98.9	136	98.4

- further generalizations: pairing with backflow coordinates, independent pairs, etc (M. Bajdich et al, PRL 96, 130201 (2006))

Pfaffians describe nodes more efficiently

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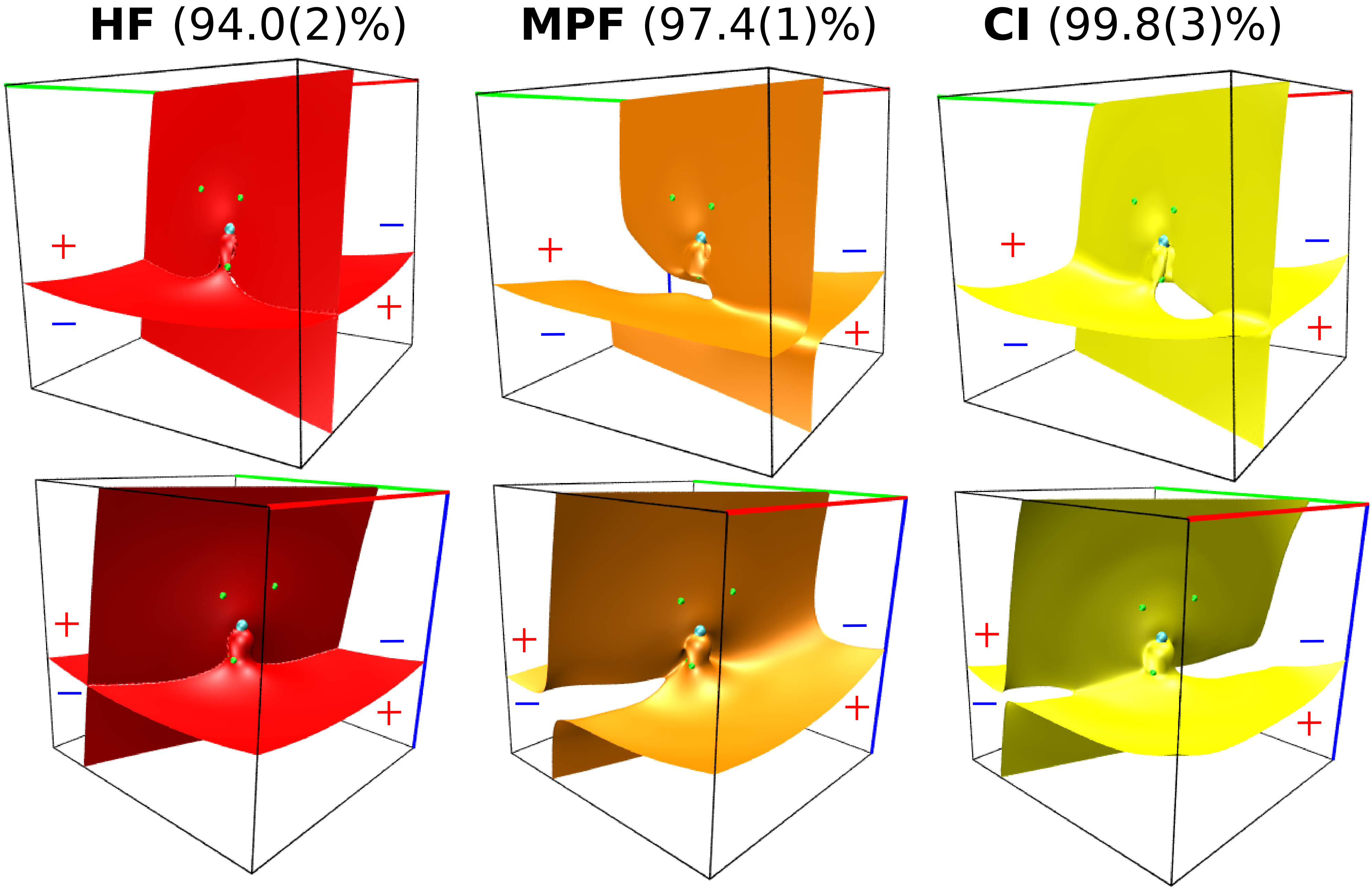
Nodes of different wfs (%E_corr in DMC): oxygen atom wf scanned by 2e- singlet (projection into 3D -> node subset)



Ultracold atoms in a special state: unitary gas
Total energy first calculated by QMC

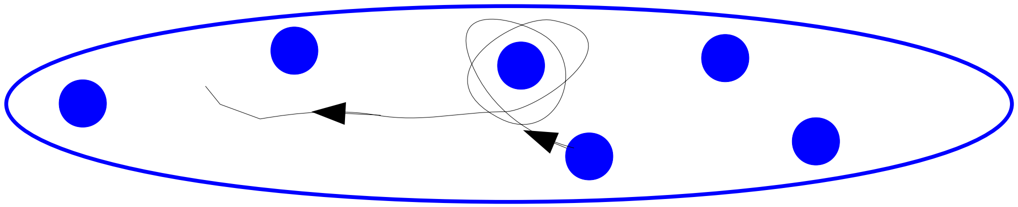
Effective, short-range attractive interaction **Scattering length: a**

1/a > 0 **BCS, weakly paired superconductor**

1/a < 0 **BEC of covalently bonded molecules**

1/a → 0 **unitary limit →** $r_{int} \ll r_s \ll a\,,\qquad E_{tot}^{unitary} = \xi\, E_{tot}^{free}$

Tuned, so that a pair is on the verge of forming a bound state (ie, E=0)



$$\xi_{FNDMC} / HF\ nodes \ = 0.50(1)$$

$$\xi_{FNDMC} / BCS\ nodes = 0.44(1) \qquad J.\ Carlson\ et\ al\ ,\ '03$$

$$\xi_{exact} / release\ nodes \le 0.40(1) \qquad J.\ Carlson\ ,\ unpub.\ ;\ X.\ Li\ ,\ L.M.\ ,\ unpub.$$

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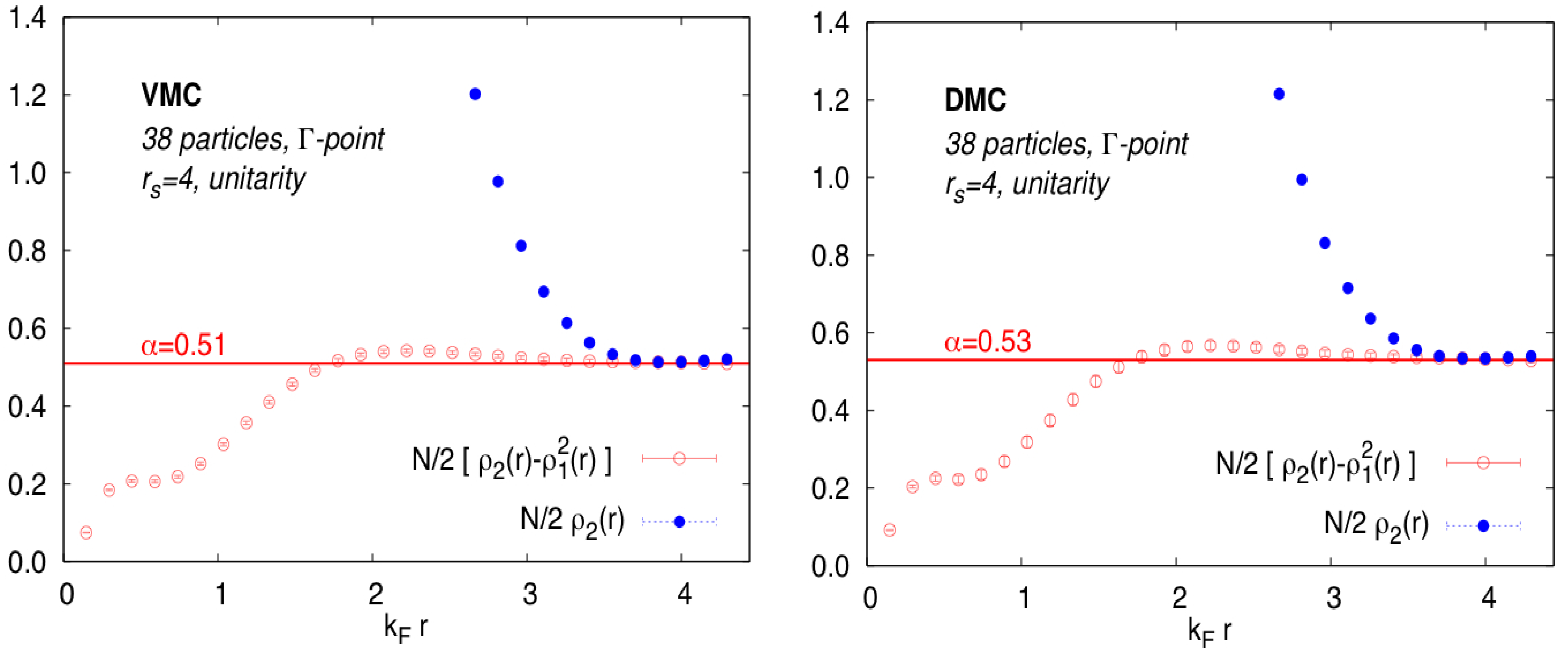
Unitary limit: seemingly a weakly interacting system Opposite is true: strongly interacting regime, large amount of condensate (BEC ↔ unitary ↔ BCS)

Find the amount of the condensate directly: averaged two-body density matrix at long-range (BCS wavefunction)



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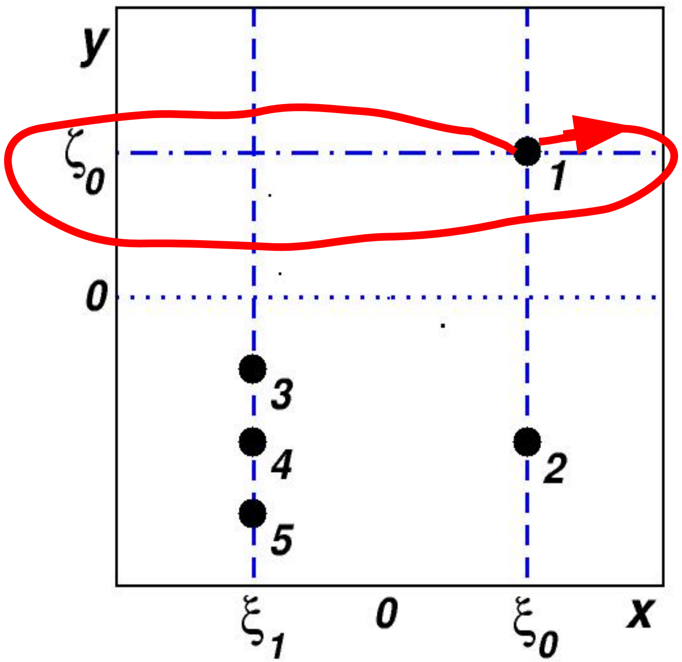
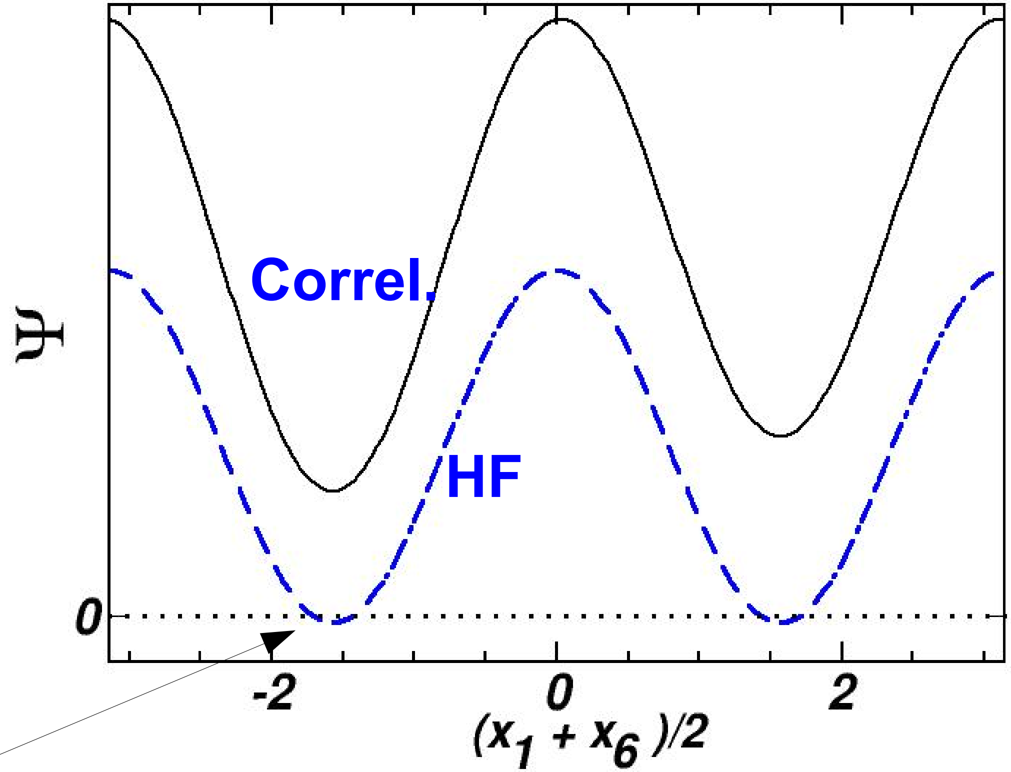
Correlated nodes in a fermion gas: singlet pair of e- winds around the box without crossing the node

$$r_i\uparrow = r_{i+5}\downarrow + offset\,, \quad i=1,\ldots,5$$



Wavefunction along the winding path



HF crosses the node, BCS/pfaffian does not (supercond.)

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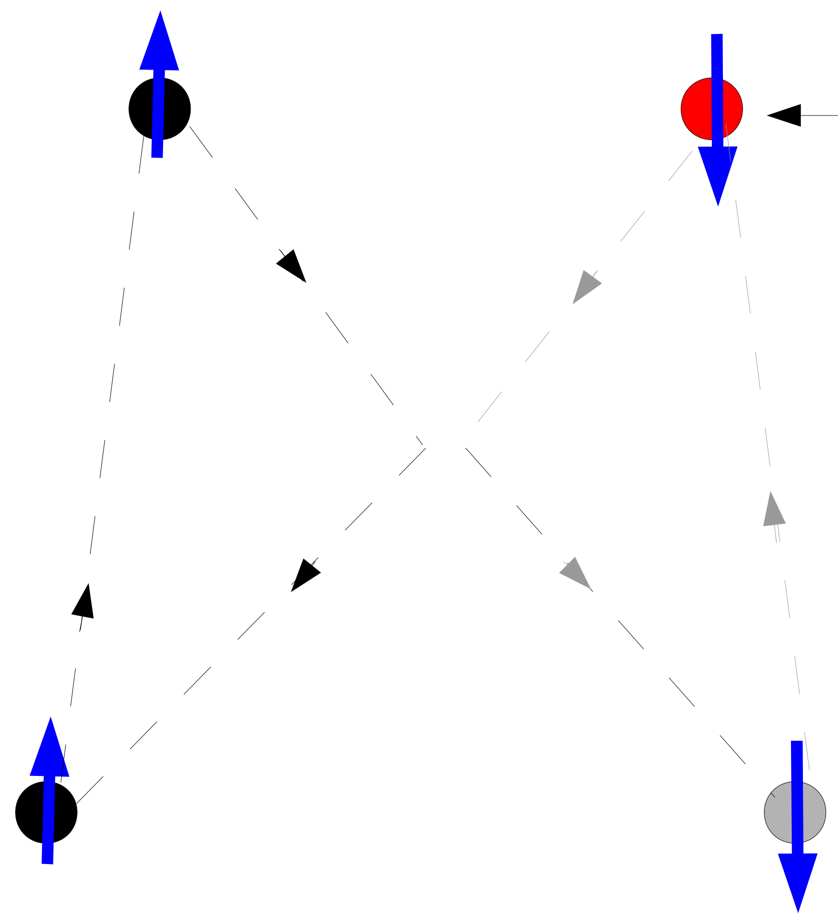
The four particle exchange: illustration of pair exchange without node crossing

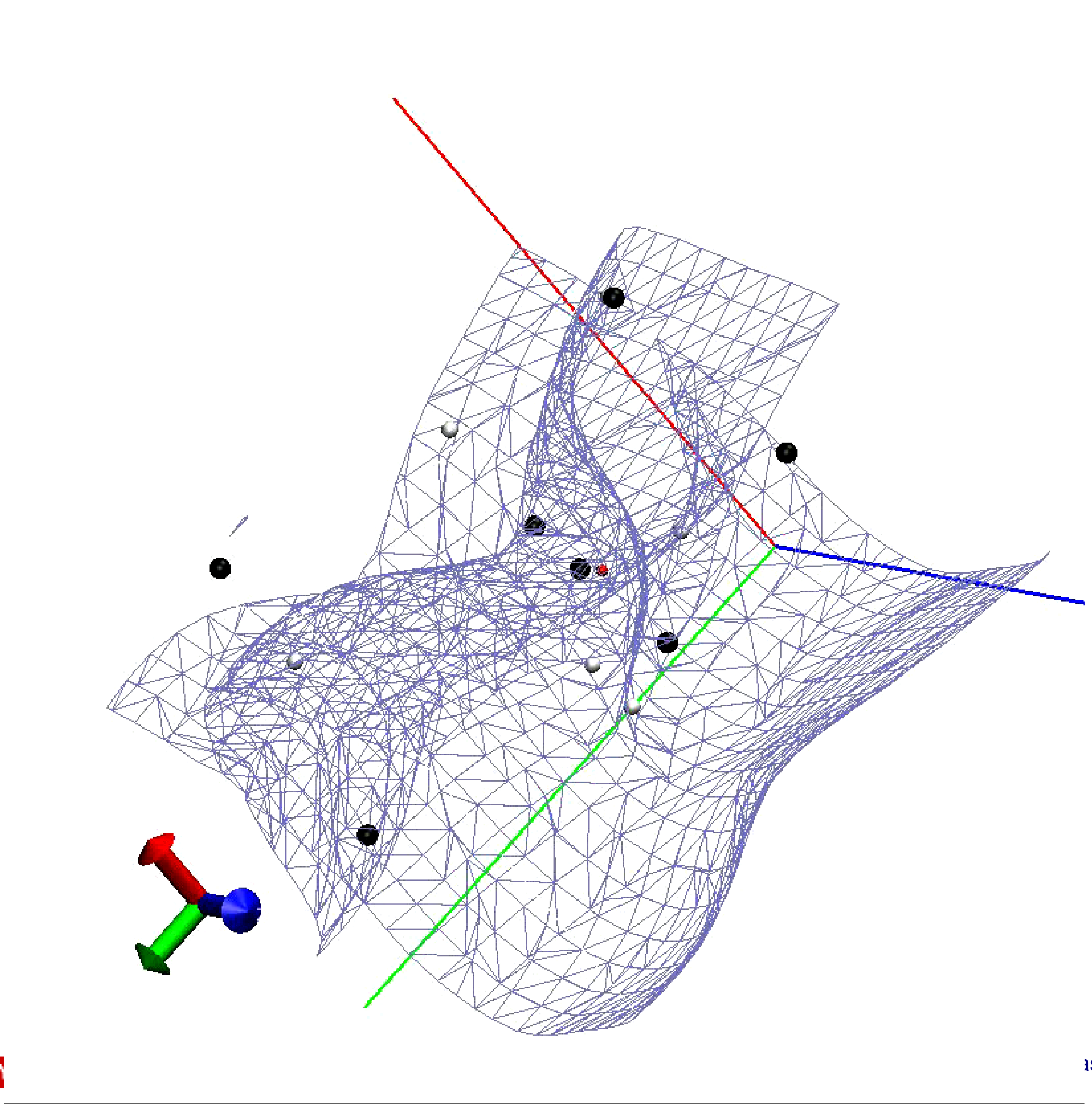
Exchange in each spin channel separately has to cross the node, concerted both spin channels exchange can avoid the node



node scanning particle

(X. Li, LM,'09)

I.



Another type of wavefunction with improved nodes: backflow coordinates

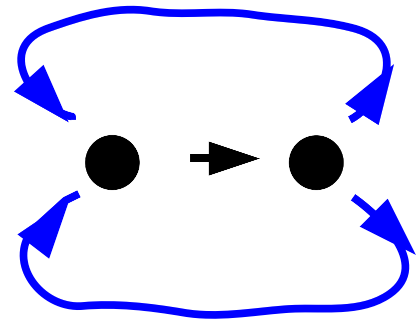
Improve the Slater-Jastrow wf. $\exp(-\tau H)\psi_T \approx \psi_T - \tau H \psi_T$

$$H e^{U_{corr}} det[.] = e^{U_{corr}} (T + V_{eI}) det[.] + det[.] (T + V_{ee}) e^{U_{corr}} - \nabla e^{U_{corr}} \cdot \nabla det[.]$$

"spurious" term

$|\nabla det[.]| \gg |\nabla e^{U_{corr}}|$ $\rightarrow$ **strongly inhomogeneous -> excitations (CI, pfaffians) cancel out the spurious terms**

$|\nabla det[.]| \ll |\nabla e^{U_{corr}}|$ $\rightarrow$ **backflow terms are effective (homogeneous systems)**



$x_i = r_i + \sum_{i<j} \gamma(r_{ij}) r_{ij}$ **backflow described by "dressed" coordinates -> combine with pfaffian wavefunctions**

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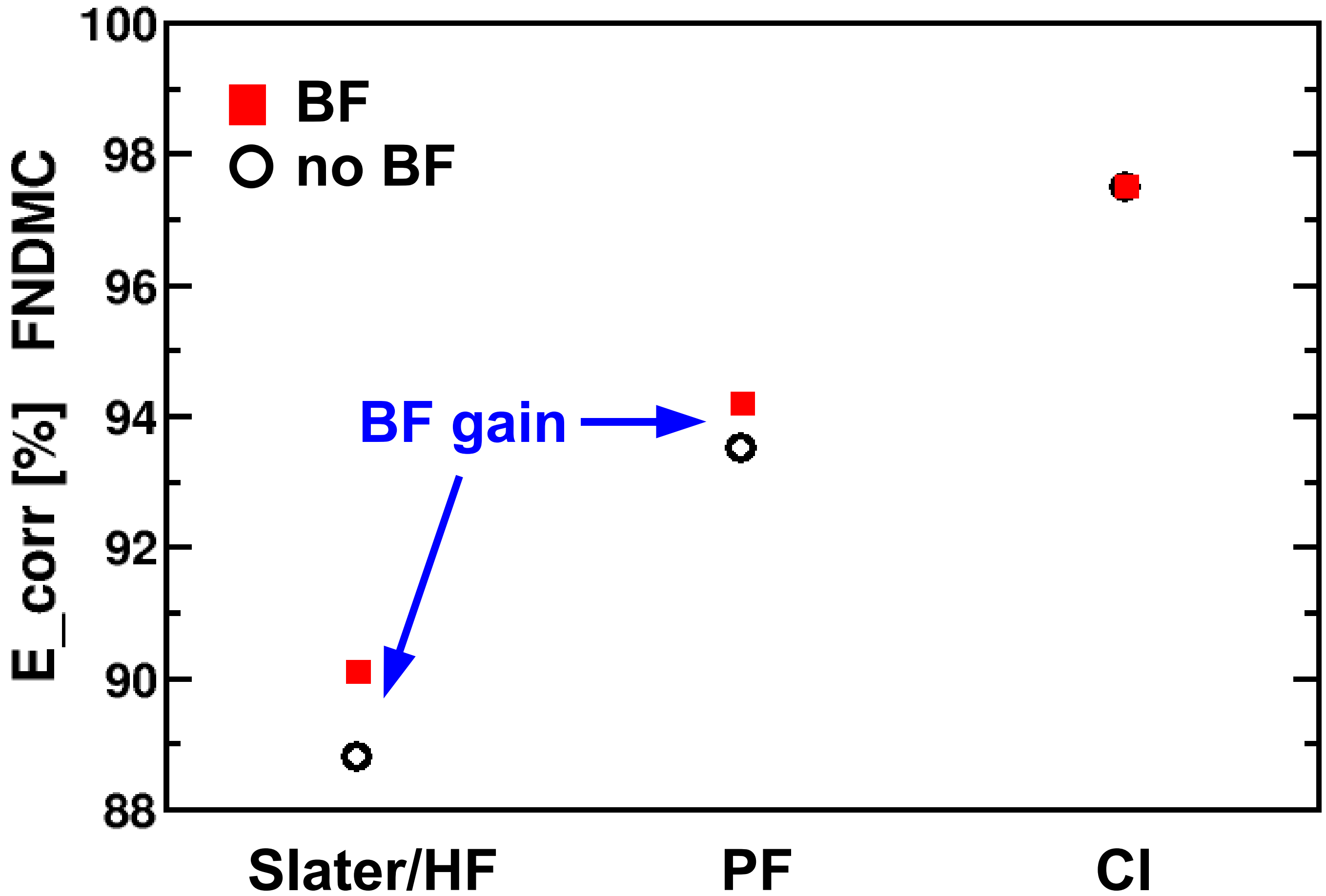
FNDMC correlation energies of C_2 molecule for various wavefunctions with and without the backflow



Gains from backflow are rather small ...

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Backflow for homogeneous periodic electron gas (Coulomb e-e + neutralizing background)

characterized by a single parameter: r_s $\rightarrow$ inverse density

r_s	HF	DMC/HF nodes	DMC/BF nodes
1	0.56925	0.53087(4)	0.52990(4)
5	-0.056297	-0.07862(1)	-0.07886(1)
20	-0.022051	-0.031948(2)	-0.032007(2)

About 1% gain but significant since it cuts the fixed-node error by a factor of 2 or so. Works better for homogeneous systems, as expected. Still, not enough understanding!

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Summary

- QMC: practical for hundreds of interacting quantum particles
  but also
  provides new unique insights into many-body effects

- explicit proof of two nodal cells for d>1 and arbitrary size
  with rather general conditions → fundamental topological
  property of fermionic ground states: global "P-wave" like

- another example of importance of geometry for quantum
  many-body effects

Open source code: QWalk ("Quantum Walk") → www.qwalk.org

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Working hypothesis

Geometry is not the only thing, but it is the most important thing

Connolly

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