Backflow transformations in QMC

Pablo López Ríos
Theory of Condensed Matter group
Cavendish Laboratory. University of Cambridge

Wave functions in QMC

- The quality of the VMC energy depends on the quality of the trial wave function
- The quality of the DMC energy depends on the quality of the nodes of the trial wave function
- Expectation values other than the energy depend more strongly on the trial wave function, even in DMC
- It is very important to have flexible wave-function forms

Backflow transformations in QMC

Wave functions in QMC

- **The Slater determinant:**

$$\Psi_S = D_\uparrow(\boldsymbol{R}_\uparrow)\, D_\downarrow(\boldsymbol{R}_\downarrow) \quad ; \quad D_\sigma(\boldsymbol{r}_1^\sigma, \ldots, \boldsymbol{r}_{N_\sigma}^\sigma) = \begin{vmatrix} \phi_1^\sigma(\boldsymbol{r}_1^\sigma) & \phi_2^\sigma(\boldsymbol{r}_1^\sigma) & \vdots & \phi_{N_\sigma}^\sigma(\boldsymbol{r}_1^\sigma) \\ \phi_1^\sigma(\boldsymbol{r}_2^\sigma) & \phi_2^\sigma(\boldsymbol{r}_2^\sigma) & \vdots & \phi_{N_\sigma}^\sigma(\boldsymbol{r}_2^\sigma) \\ \ldots & \ldots & \ddots & \ldots \\ \phi_1^\sigma(\boldsymbol{r}_{N_\sigma}^\sigma) & \phi_2^\sigma(\boldsymbol{r}_{N_\sigma}^\sigma) & \vdots & \phi_{N_\sigma}^\sigma(\boldsymbol{r}_{N_\sigma}^\sigma) \end{vmatrix}$$

*** Correct anti-symmetry (exchange)**
*** Constructed from one-particle orbitals**

*** No correlations taken into account (except multi-determinants)**
*** Local energy diverges when two particles coincide**

Wave functions in QMC

- **The Slater-Jastrow wave function:**

$$\Psi_{SJ} = e^{J(\boldsymbol{R})} \Psi_S(\boldsymbol{R}) \quad ; \quad J(\boldsymbol{R}) = J_{e-e}(\boldsymbol{R}) + J_{e-N}(\boldsymbol{R}) + J_{e-e-N}(\boldsymbol{R}) + \ldots$$

*** Ability to introduce arbitrary correlations (2-body, 3-body, ...)**
*** Ability to remove divergencies, giving stable calculations**
*** Simple, well-tested functional forms**

*** Inability to modify the nodal surface**

Wave functions in QMC

- **The Slater-Jastrow-backflow wave function is:**

$$\Psi_{BF} = e^{J(\boldsymbol{R})} \Psi_S(X) \quad , \quad \boldsymbol{x}_i = \boldsymbol{r}_i + \boldsymbol{\xi}_i$$

ξ_i **= backflow displacement of** i**-th electron**

*** Ability to move the nodes**

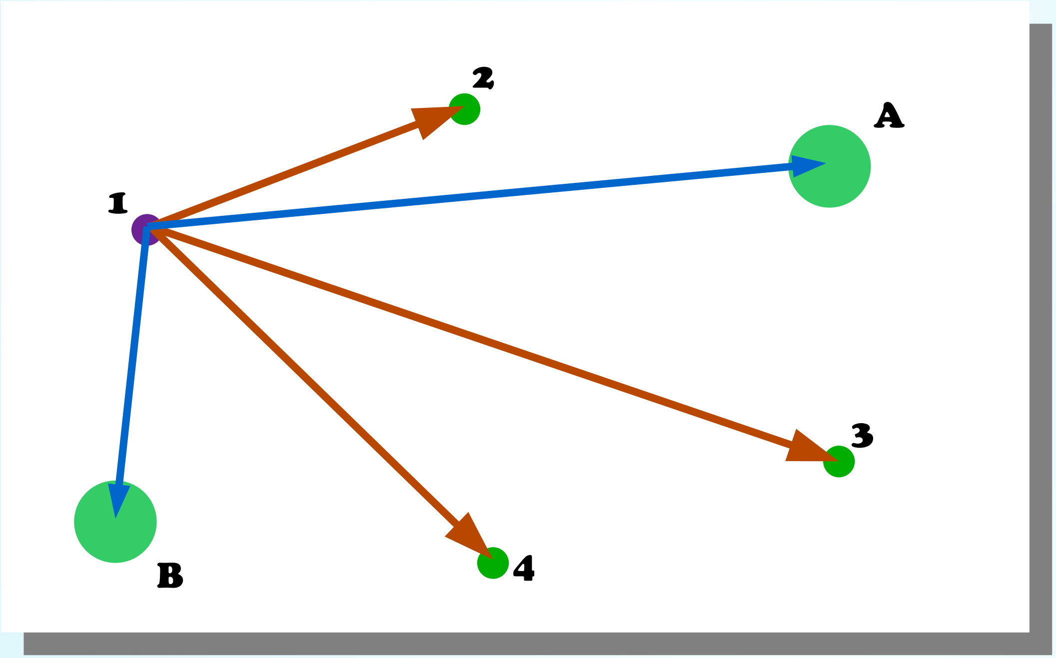
*** Makes all orbitals despend on the coordinates of all the electrons.**

Backflow transformations in QMC

The backflow transformation

Inhomogenous backflow transformation:

- Consider set of "preferred directions" seen by each electron



Set of directions seen by particle 1 in the presence of particles 2, 3 and 4, and nuclei A and B

The backflow transformation

Generalized backflow transformation:

- **Write most general (isotropic) vector field in terms of such vectors**

$$\boldsymbol{\xi}_i = \boldsymbol{\xi}_i^{e-e} + \boldsymbol{\xi}_i^{e-N} + \boldsymbol{\xi}_i^{e-e-N}$$

$$\boldsymbol{\xi}_i^{e-e} = \sum_{j \neq i}^{N} \eta(r_{ij}) \boldsymbol{r}_{ij}$$

$$\boldsymbol{\xi}_i^{e-N} = \sum_{I}^{N_{ion}} \mu(r_{iI}) \boldsymbol{r}_{iI}$$

$$\boldsymbol{\xi}_i^{e-e-N} = \sum_{j \neq i}^{N} \sum_{I}^{N_{ion}} \left[\Phi(r_{ij}, r_{iI}, r_{jI}) \boldsymbol{r}_{ij} + \Theta(r_{ij}, r_{iI}, r_{jI}) \boldsymbol{r}_{iI} \right]$$

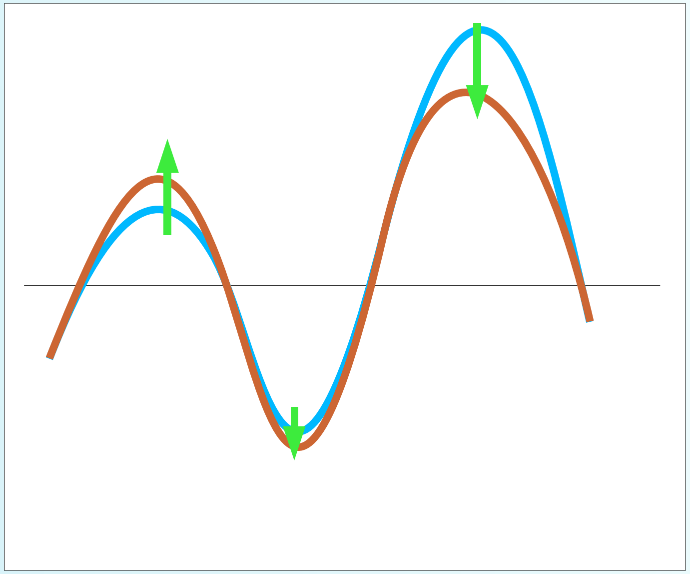
The backflow transformation

Generalized backflow transformation:

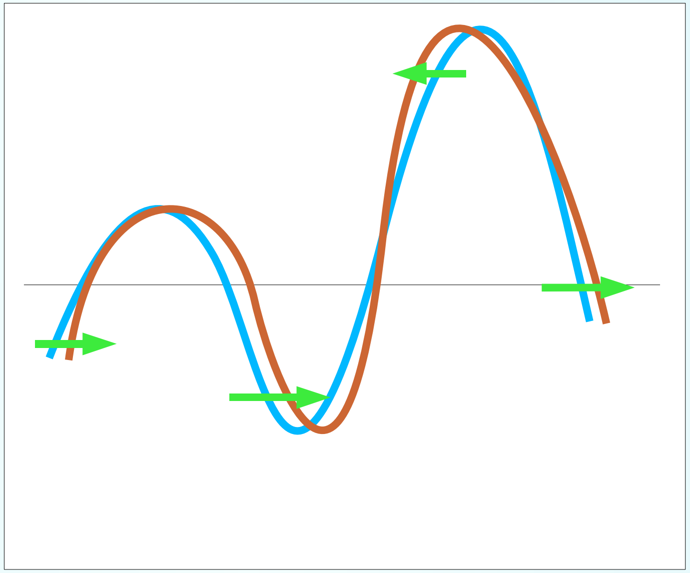
- Use power expansions to parametrize the backflow functions
- Smoothly cut off the backflow functions at variable distances
- Apply cusp conditions (choice: backflow not to alter conditions applied by Jastrow and orbitals)
- All-electron atoms delicate as orbitals are to cancel divergencies of potential; this must not be modified

The backflow transformation

Backflow complementary to Jastrow:



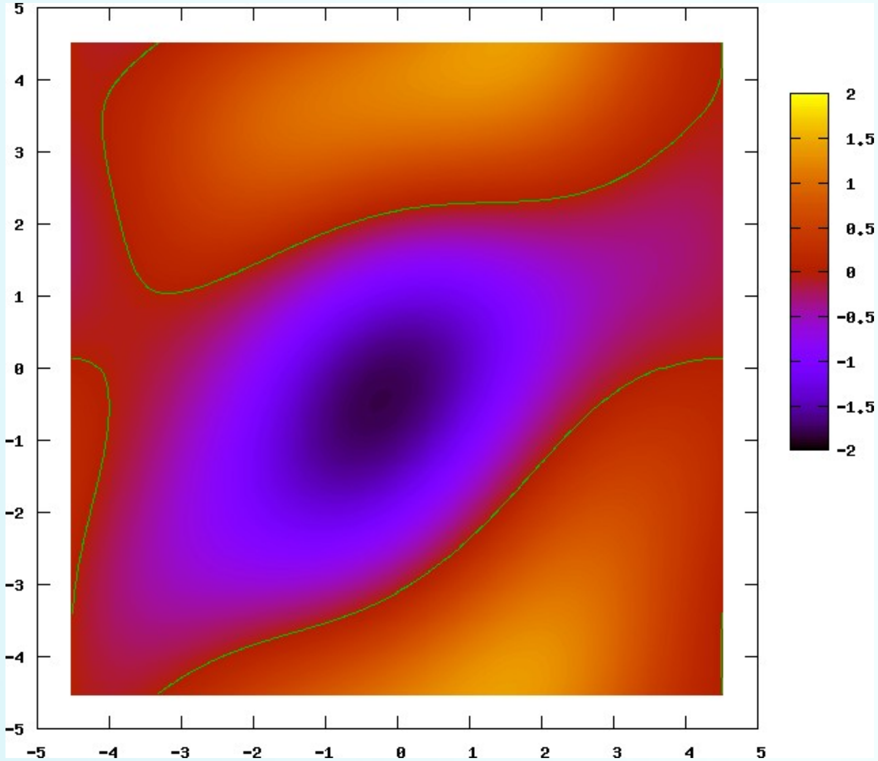
Effect of a Jastrow factor



Complementary effect

The backflow transformation

Changing the nodal surface:

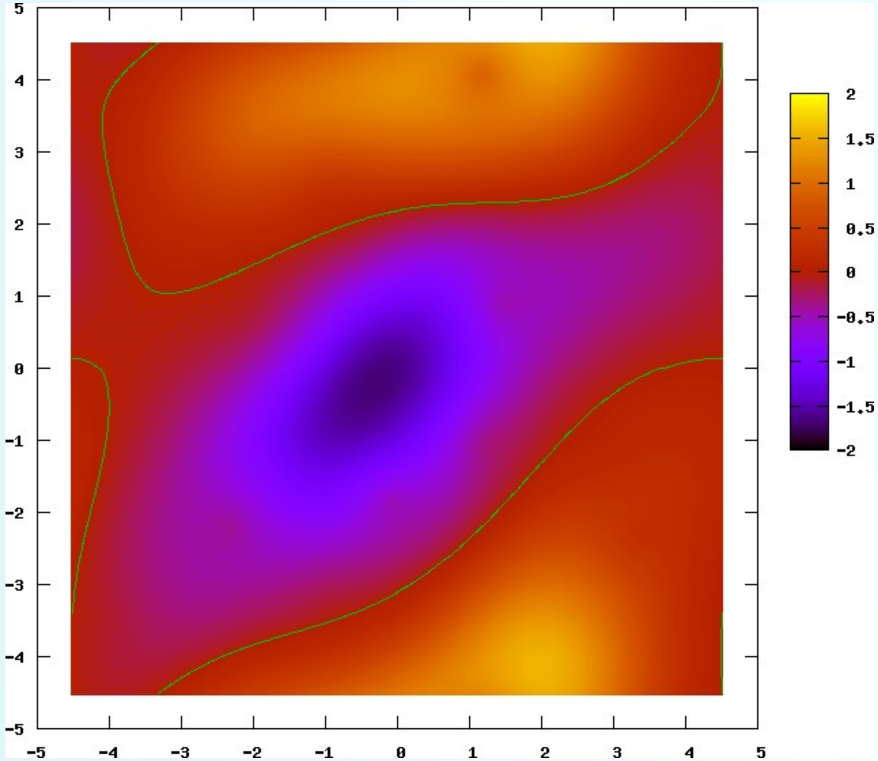


26-electron 2D HEG at rs=1.0
Moving one electron with the rest fixed.

HF wave-function

The backflow transformation

Changing the nodal surface:



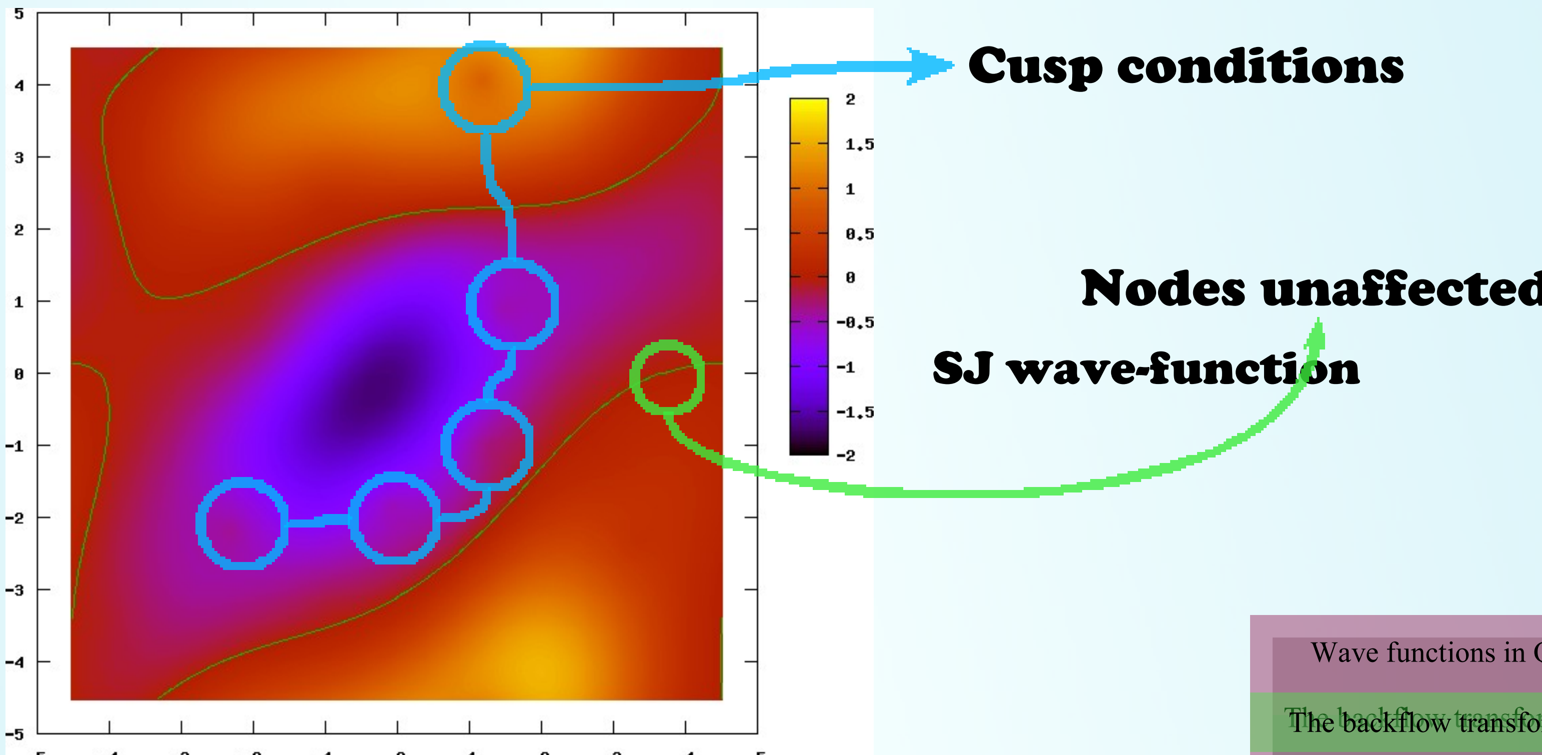
26-electron 2D HEG at rs=1.0
Moving one electron with the rest fixed.

SJ wave-function

Backflow transformations in QMC

The backflow transformation

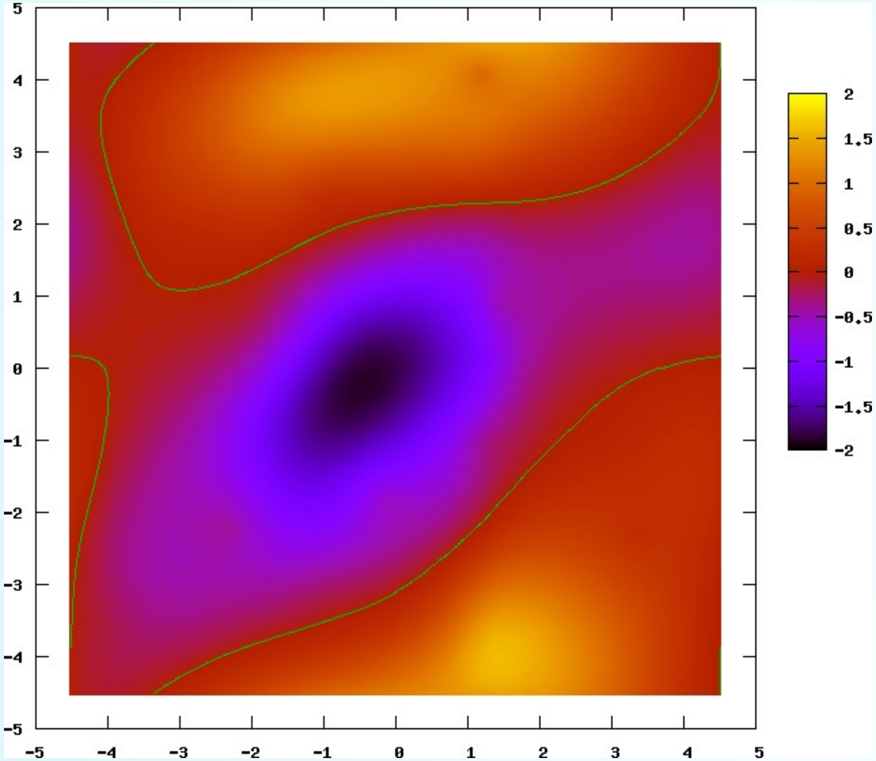
Changing the nodal surface:



26-electron 2D HEG at rs=1.0
Moving one electron with the rest fixed.

The backflow transformation

Changing the nodal surface:

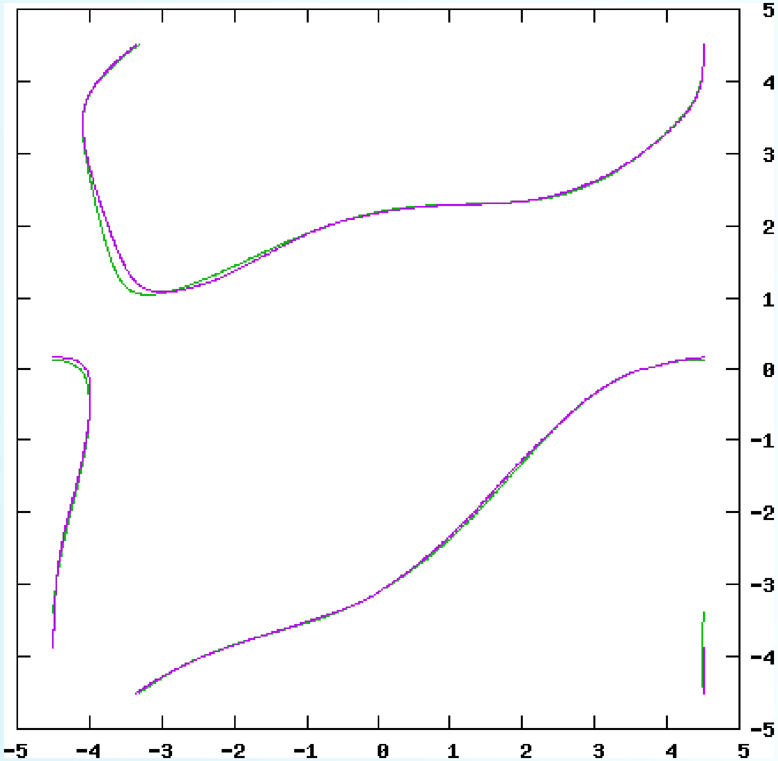


26-ELECTRON 2D HEG AT RS=1.0
MOVING ONE ELECTRON WITH THE REST FIXED.

BF wave-function

The backflow transformation

Changing the nodal surface:



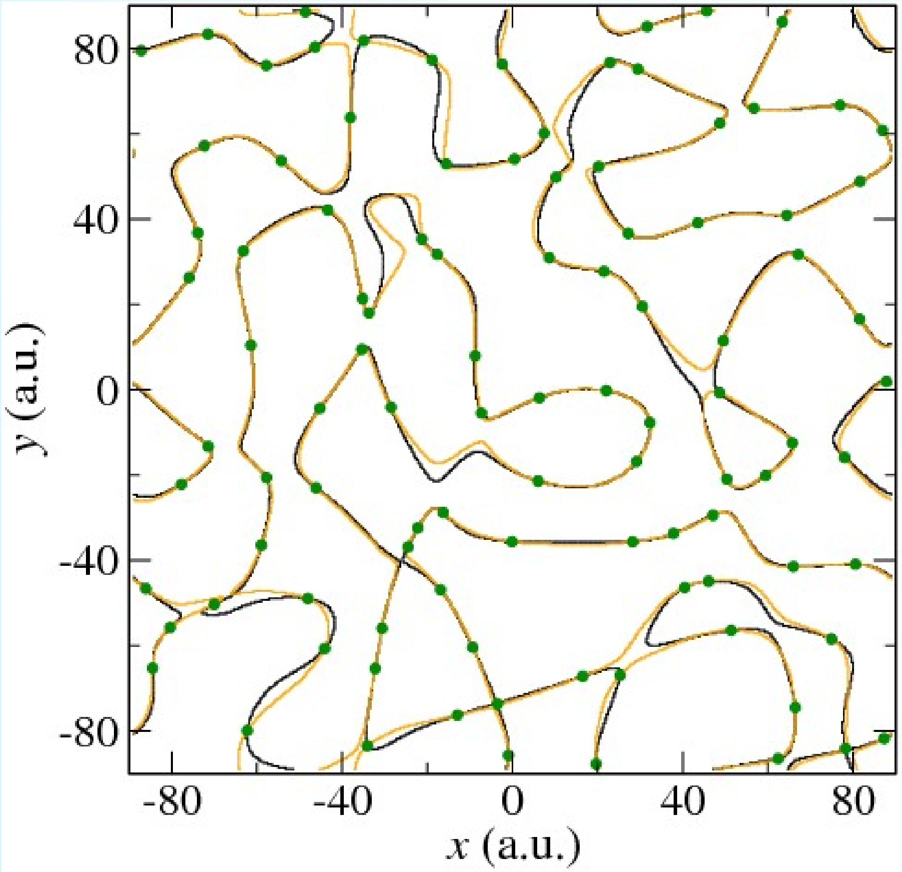
26-electron 2D HEG at rs=1.0
projected HF (green) and BF (purple) nodal surfaces

HF and BF nodes

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:

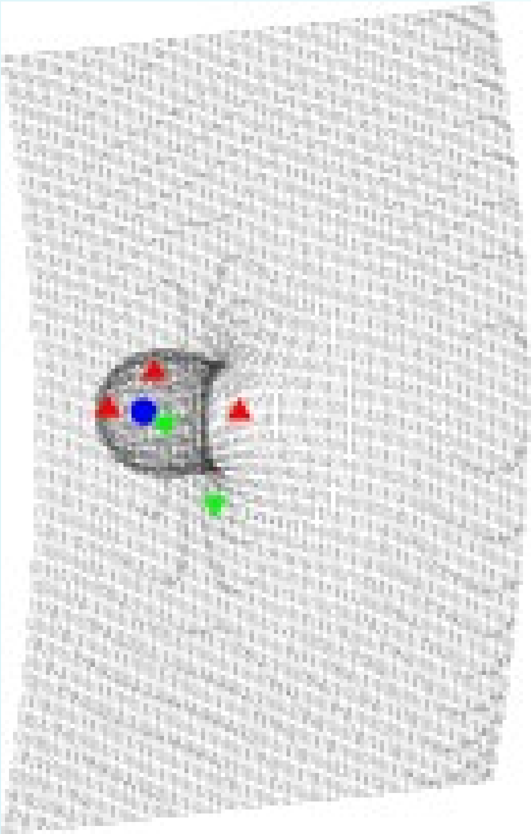


101-electron 2D HEG at rs=10.0
projected HF (black) and BF (orange) nodal surfaces

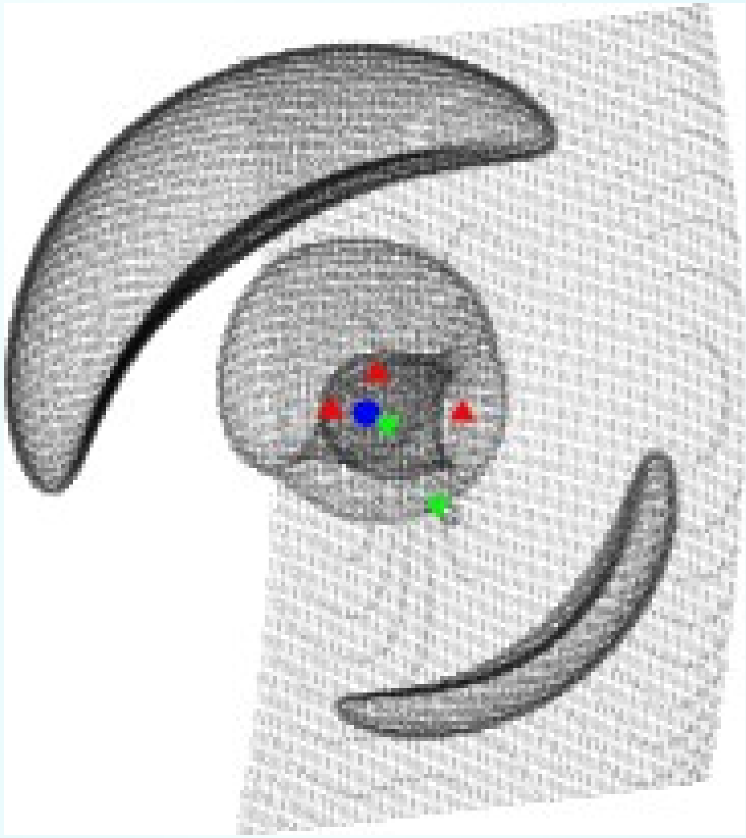
HF and BF nodes

The backflow transformation

Changing the nodal surface:



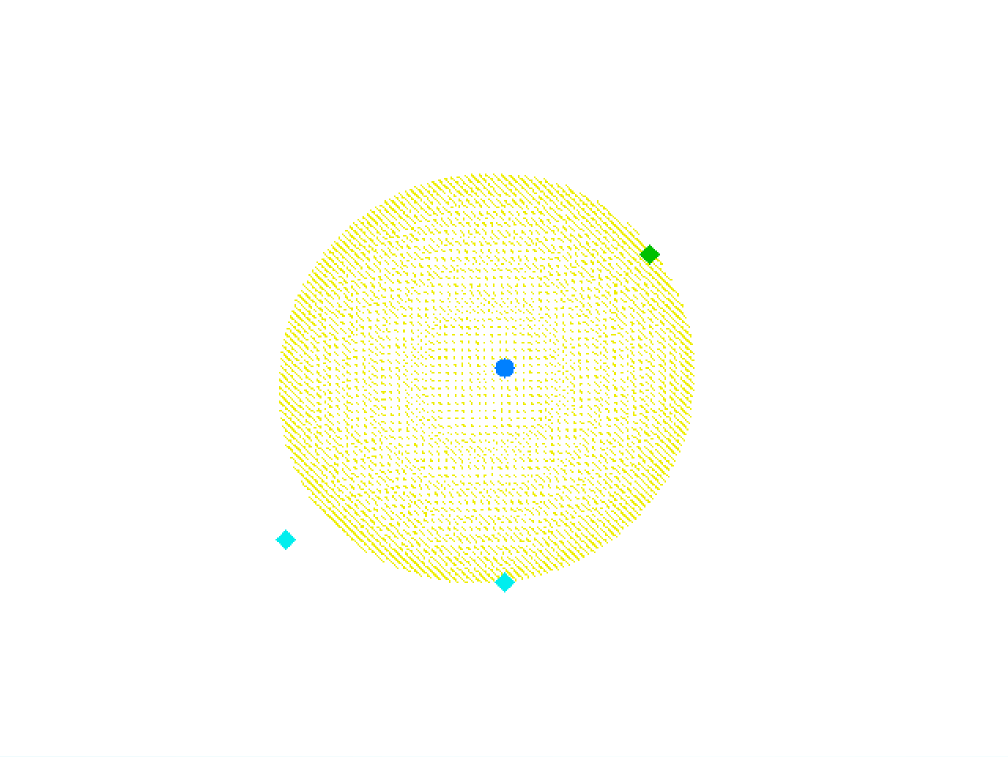
Carbon atom, projected
HF nodal surface



Carbon atom, projected
BF nodal surface

The backflow transformation

Changing the nodal surface:

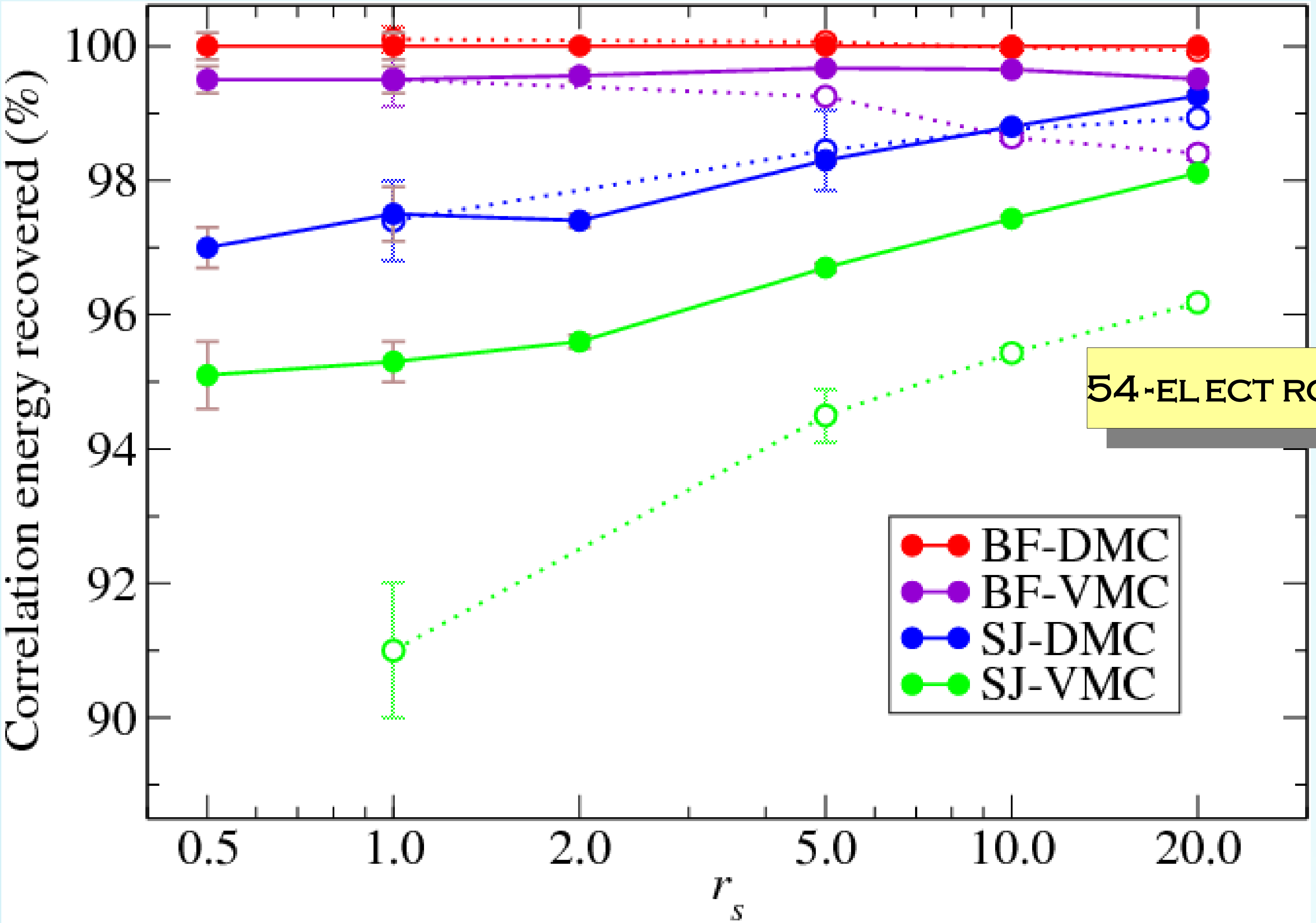


Berillium atom, projected
MD-BF nodal surface

Animation at www.tcm.phy.cam.ac.uk/~pl275/nodes.gif

Backflow transformations in QMC

Application and results

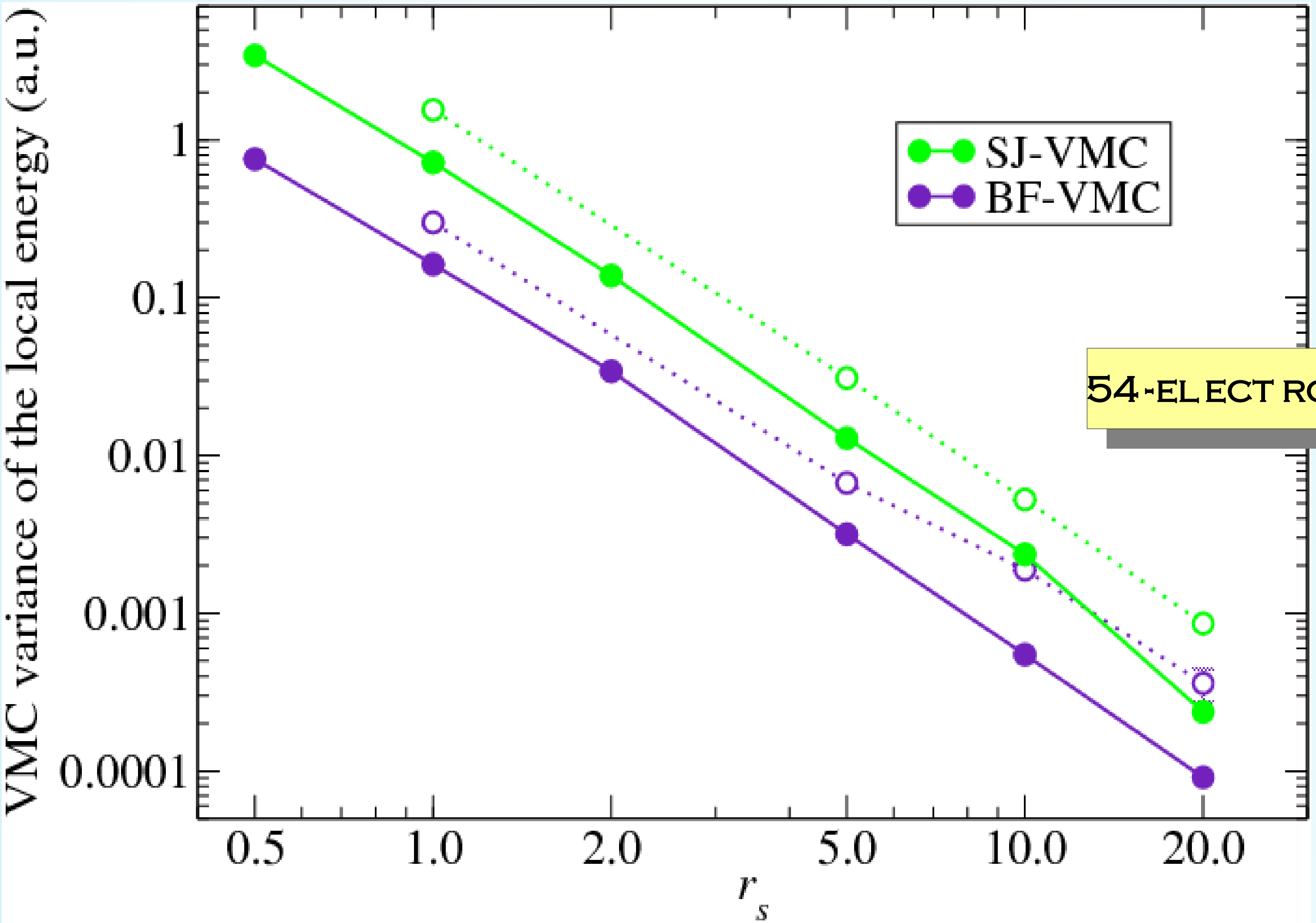


54-electron 3D HEG

Dotted lines: Holzmann, Ceperley, Pierleoni, Esler; Phys Rev E **68**, 046707 (2003)

Backflow transformations in QMC

Application and results

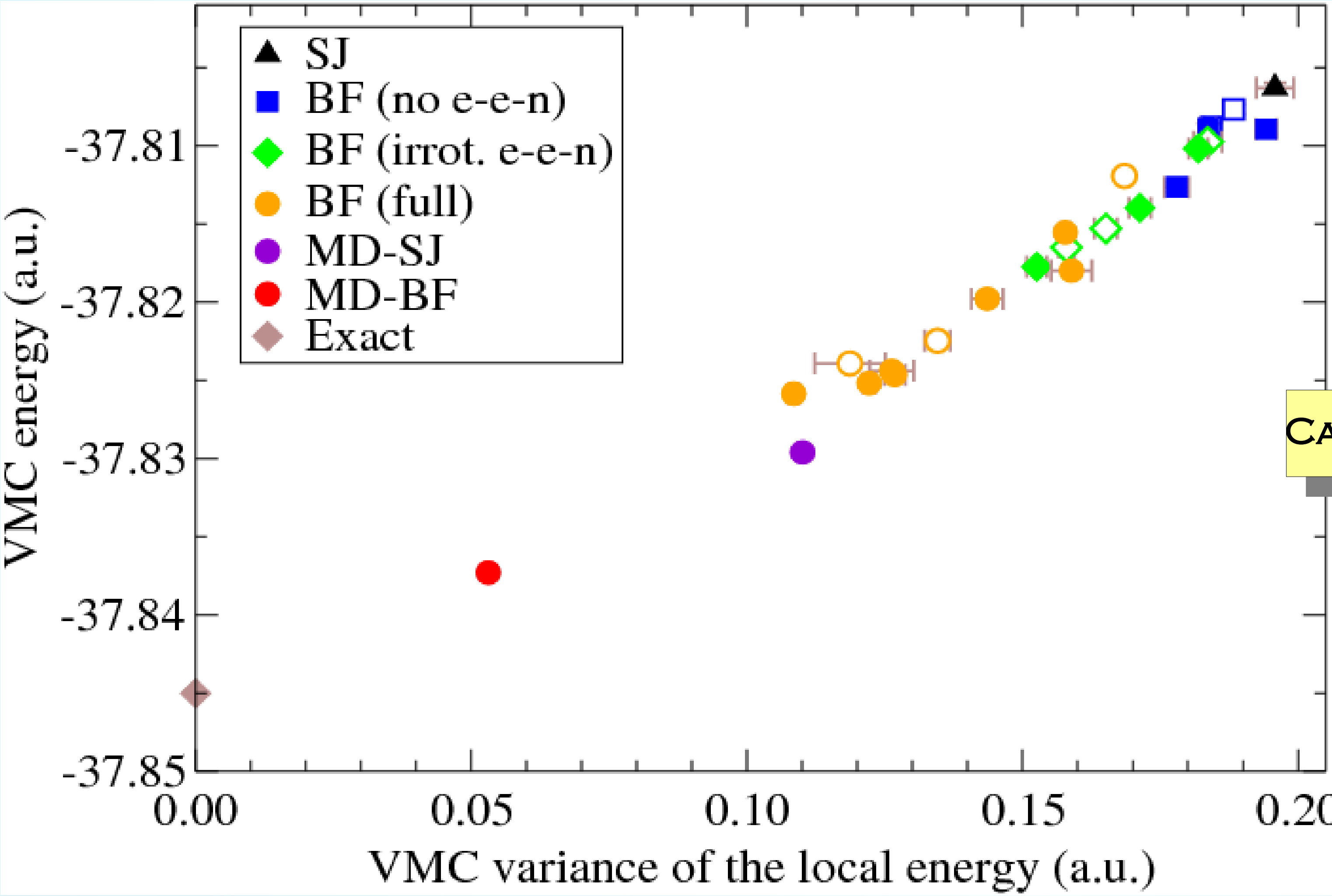


54-electron 3D HEG

Dotted lines: Holzmann, Ceperley, Pierleoni, Esler; Phys Rev E **68**, 046707 (2003)

Backflow transformations in QMC

Application and results

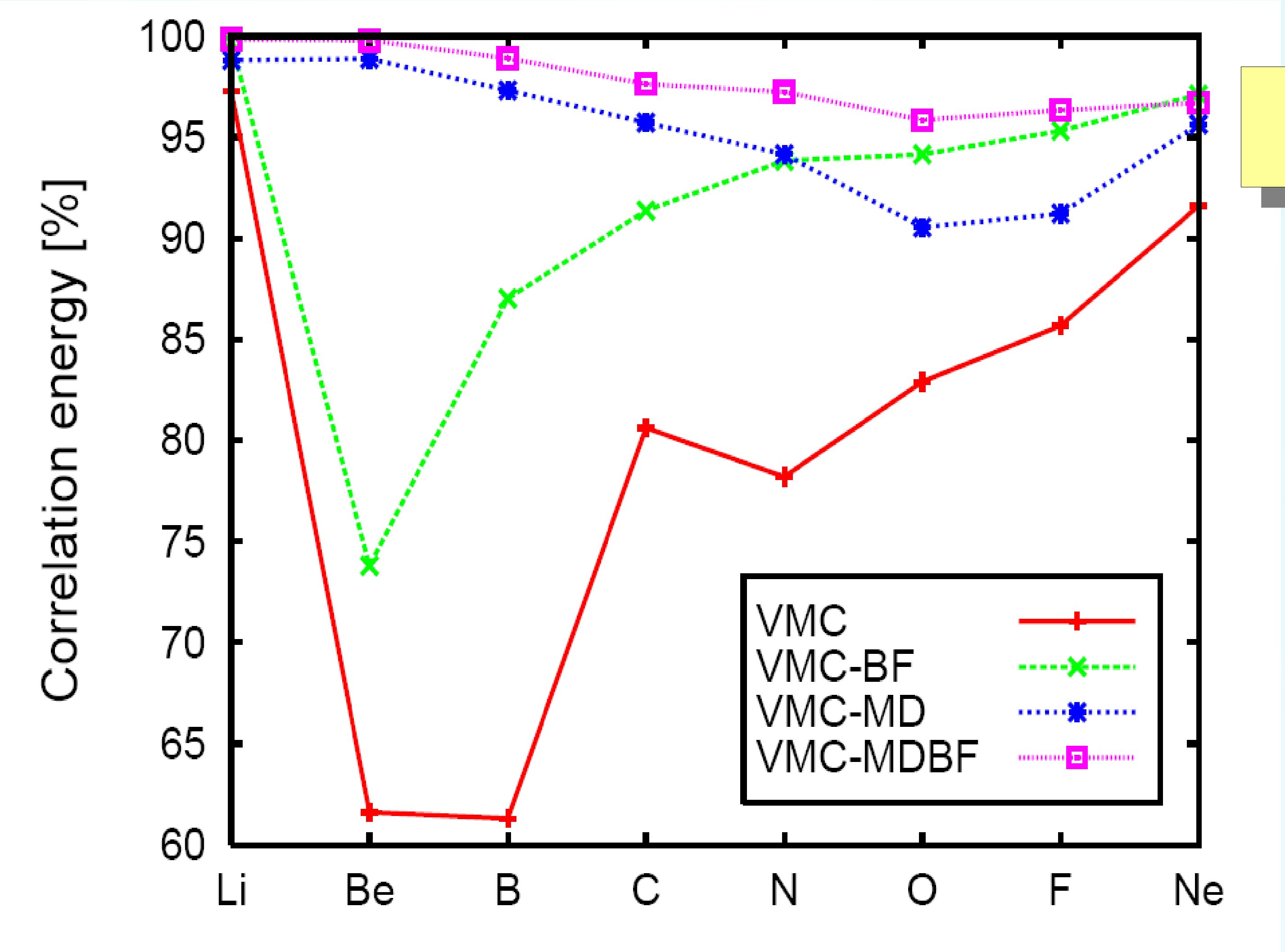


Carbon atom (AE)

*MD (18 CSFs) performed by John Trail.

Backflow transformations in QMC

Application and results

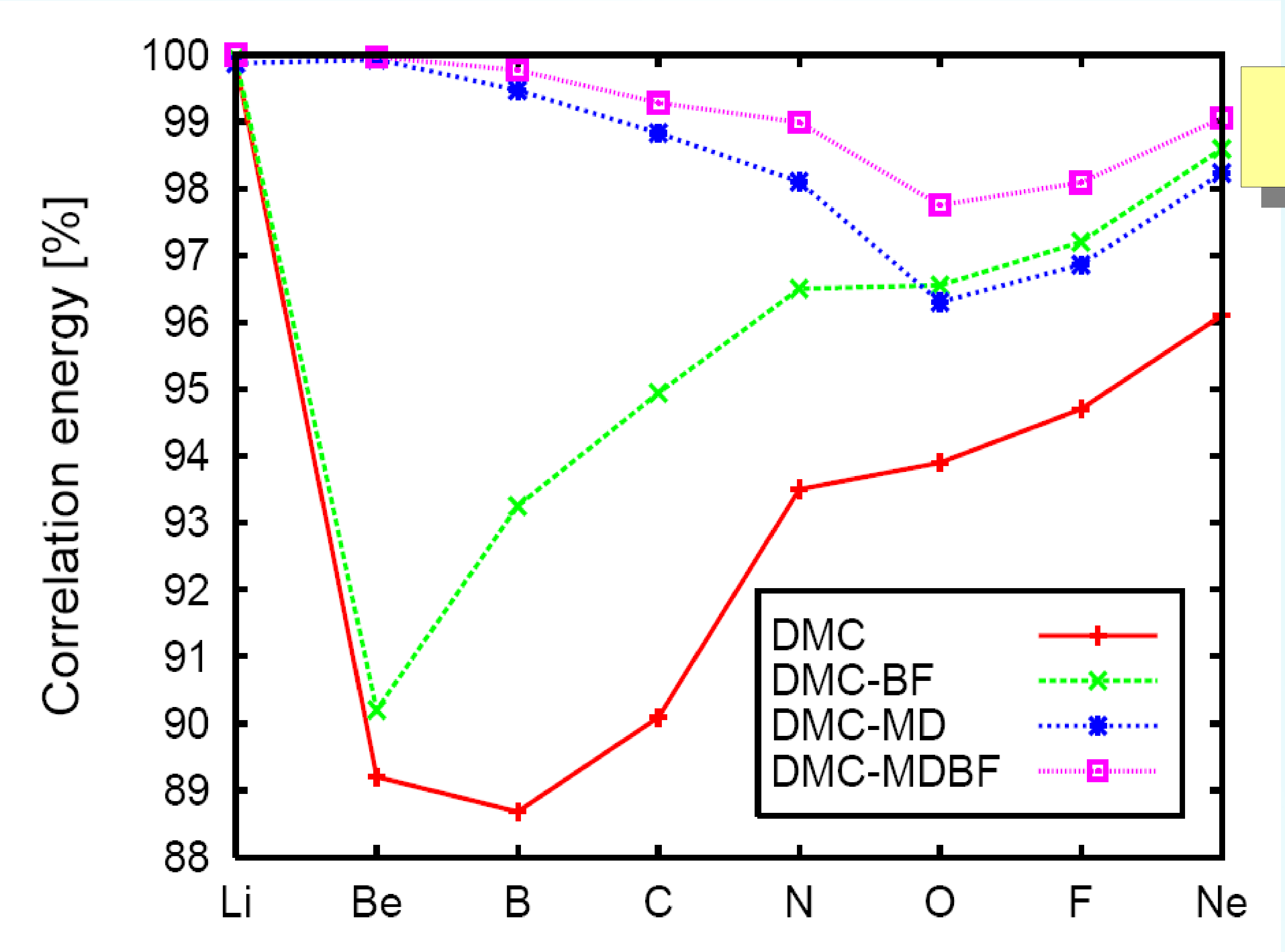


First-row AE atoms

Pablo López Ríos

Backflow transformations in QMC

Application and results



First-row AE atoms

*Calculations performed by John Trail.

Backflow transformations in QMC

Application and results

Method	Wfn	Si diamond 2x2x2 Energy (au)	σ^2 (au)
VMC	SJ	-7.87026(9)	0.591(2)
	BF	-7.8875(3)	0.237(3)
DMC	SJ	-7.8878(1)	-

Method	Wfn	Si betatin 2x2x2 Energy (au)	σ^2 (au)
VMC	SJ	-62.0063(3)	0.74(2)
	BF	-62.180(5)	0.346(6)
DMC	SJ	-62.175(1)	-

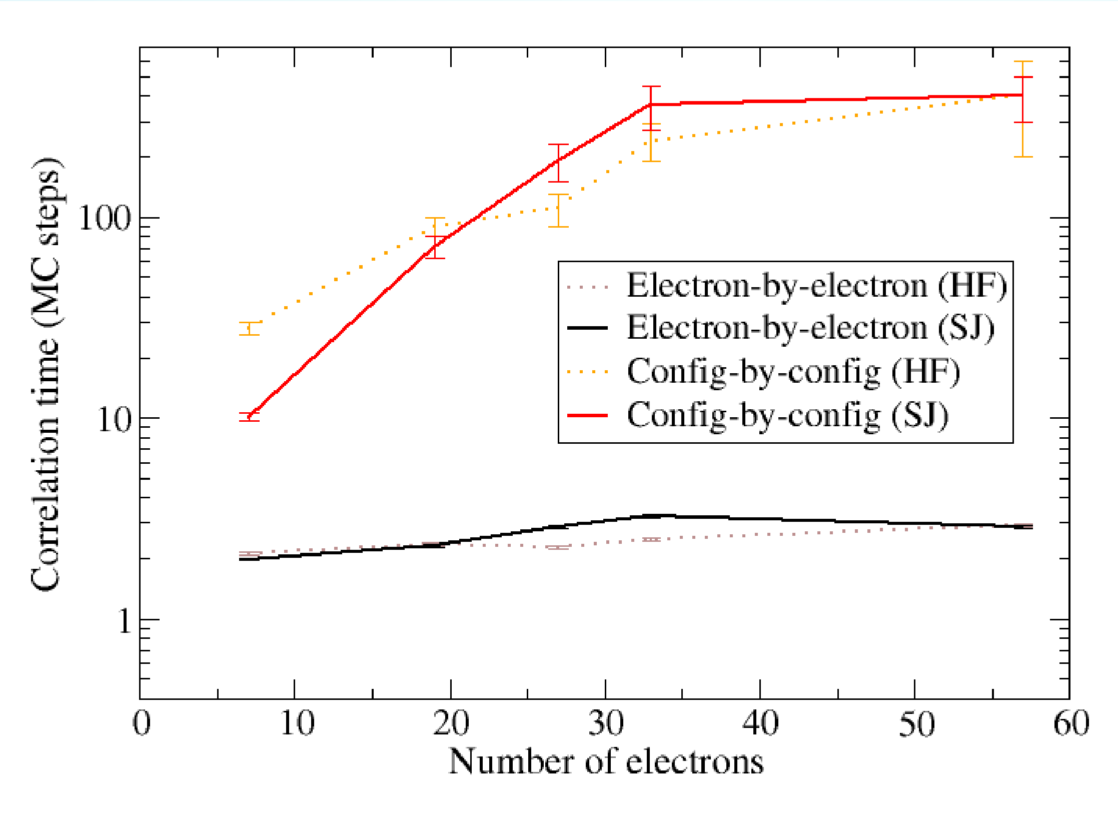
Method	Wfn	C diamond 2x2x2 Energy (au)	σ^2 (au)
VMC	SJ	-11.3708(2)	1.51(8)
	BF	-11.3970(3)	0.897(8)
DMC	SJ	-11.40717(8)	-

CRYSTALLINE SYSTEMS (PSEUDOPOTENTIALS)

Backflow transformations in QMC

Application and results

- **Side issue: electron-by-electron sampling is <u>much cheaper</u> than configuration-by-configuration sampling.**



Backflow transformations in QMC

Application and results

- Scaling goes from N^3 (SJ) to N^4 (BF).
- Timing for fixed number of configs increases.
- Lower errorbars largely compensate higher cost per config.
- E.g., cheaper to achieve fixed errorbars with BF than with SJ in the HEG and lithium atom.

  For other systems this varies...

Backflow transformations in QMC

Application and results

- The closer VMC and DMC energies are for a given Ψ, the lower the variance of the energies encountered during DMC is, as:

$$\sigma^2_{DMC} \sim |E_{VMC} - E_{DMC}|$$

- Backflow generally lowers VMC energy more than DMC energy
- DMC statistics improved: DMC efficiency may be enhanced even if DMC energy is unchanged
- “Sparse” backflow: for large systems with size-independent backflow cutoffs, scaling can be lowered from N^4 back to N^3 by using fast update formulas.

Backflow transformations in QMC

Application and results

Other systems successfully treated so far include:

- **Water molecule and water clusters** (I. García de Gurtubay, unpublished)
- **Electron-hole systems** (P. López Ríos, unpublished)
- **Neon and Neon+** (N. D. Drummond et al, J. Chem. Phys. 124, 224104 (2006).)
- **HEG, full study** (G. Spink et al, unpublished)

Backflow transformations in QMC

Conclusions

- Excellent results, good scaling properties, wide applicability
- Successfully combined with other wave-function parameters
- BF-VMC is a powerful level of theory.
- In DMC, at the very least, statistics are greatly improved.

Acknowledgements

- All calculations performed using CASINO v2.0 [1] or later

- Computing resources provided by the Cambridge HPC service

Funding from the Engineering and Physical Sciences Research Council of the United Kingdom

[1] R. J. Needs, M. D. Towler, N. D. Drummond, P. López Ríos, Casino v2.0 User Manual, University of Cambridge (2006)