Backflow transformations in QMC: extension to inhomogeneous systems

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Backflow transformations in QMC

The backflow transformation

Motivation:

- **Backflow can change nodal surface; may overcome the fixed-node approximation**
- **Application of backflow to homogeneous systems successful**

Backflow transformations in QMC

The backflow transformation

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

$$\Psi_{SJ} = e^{J(\boldsymbol{R})} \Psi_S(\boldsymbol{R})$$

with Ψ_S = Slater (multi-) determinant part, and J = Jastrow factor

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

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

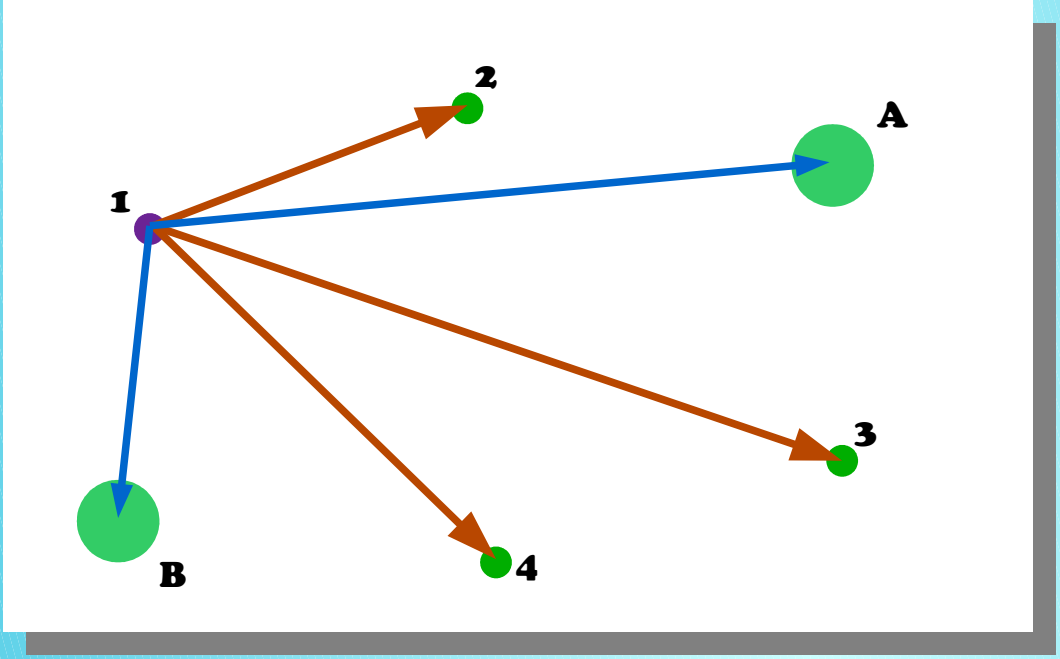
ξ_i = backflow displacement of i-th electron

Backflow transformations in QMC

The backflow transformation

Generalized 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

Backflow transformations in QMC

The backflow transformation

Generalized backflow transformation:

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

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

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

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

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

Backflow transformations in QMC

The backflow transformation

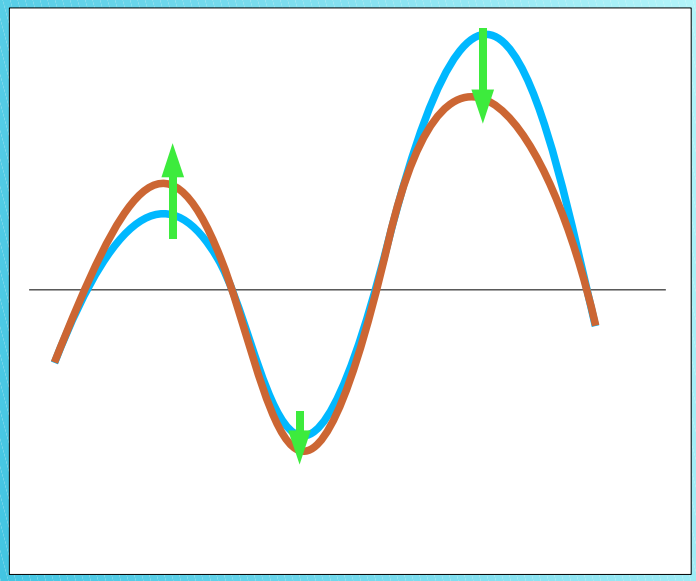
Generalized backflow transformation:

- **Use power expansions to parametrize the backflow functions**
- **Smoothly cut off the backflow functions at optimizable 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**

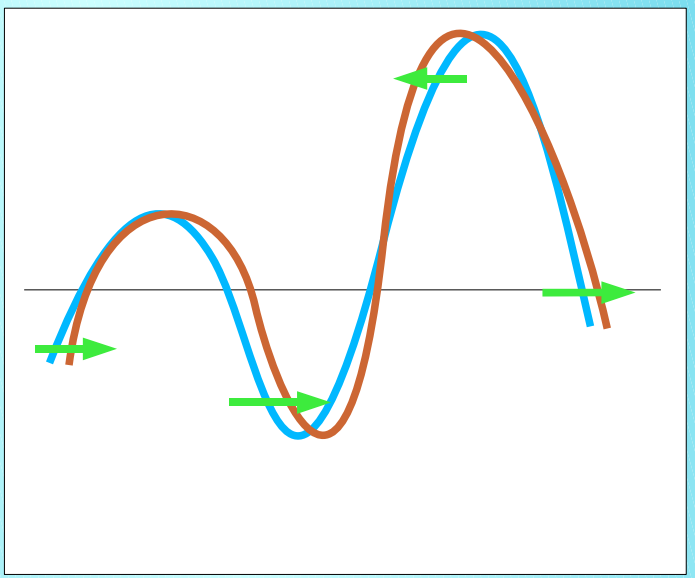
Backflow transformations in QMC

The backflow transformation

Backflow complementary to Jastrow:



Effect of a Jastrow factor

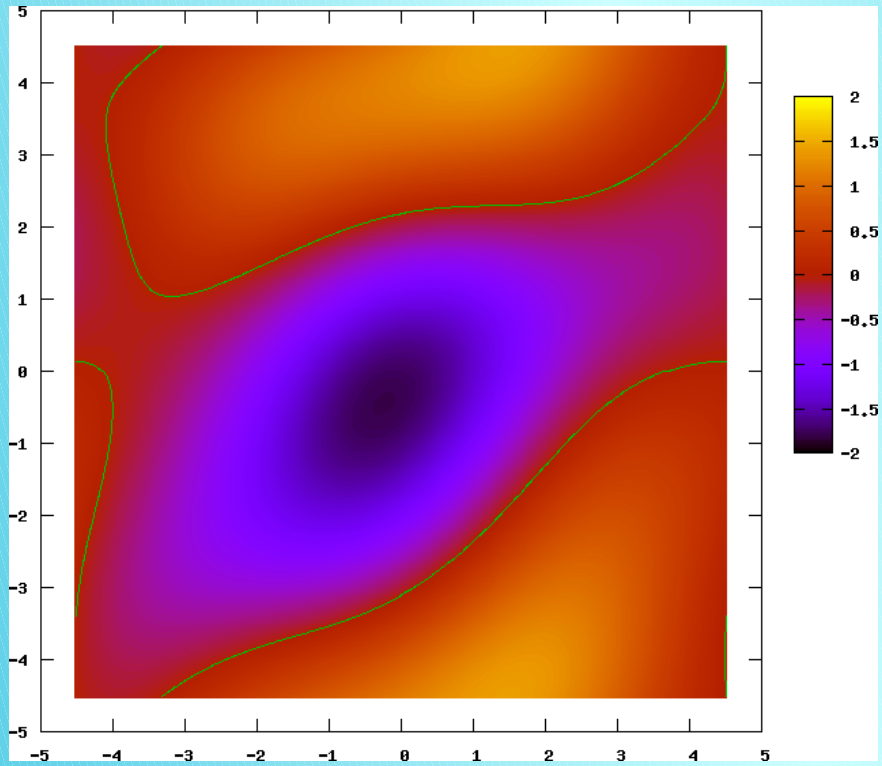


Complementary effect

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:



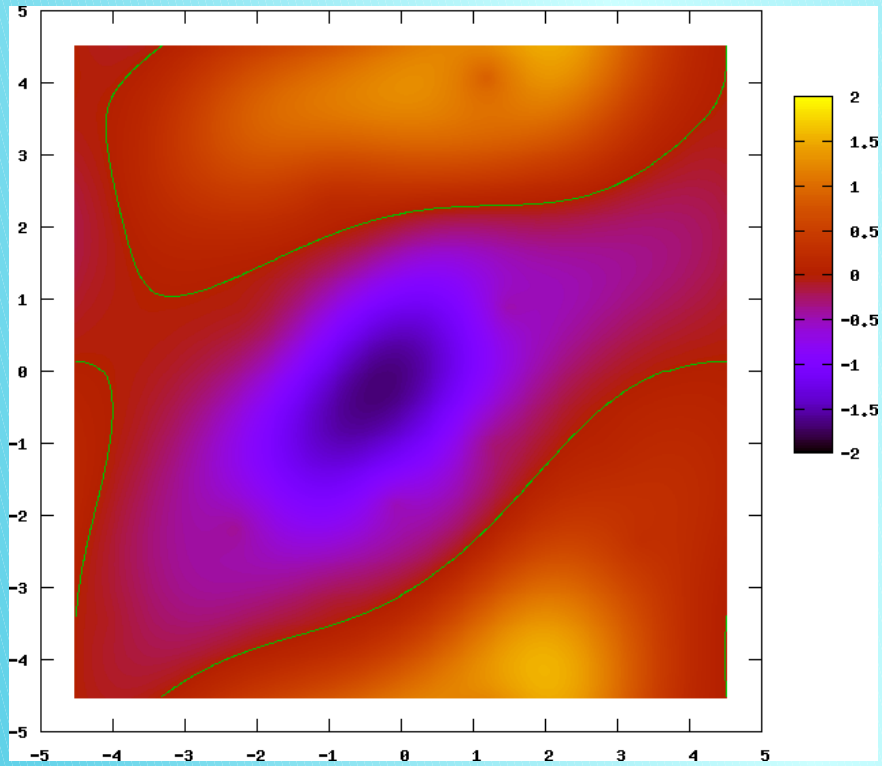
HF wave-function

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

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:



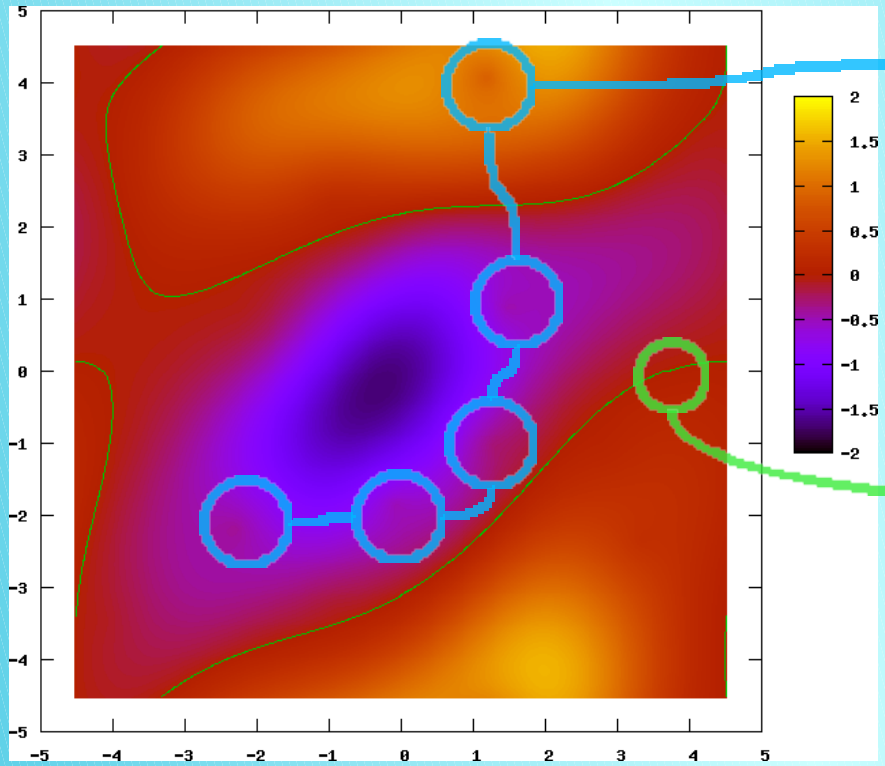
SJ wave-function

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

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:

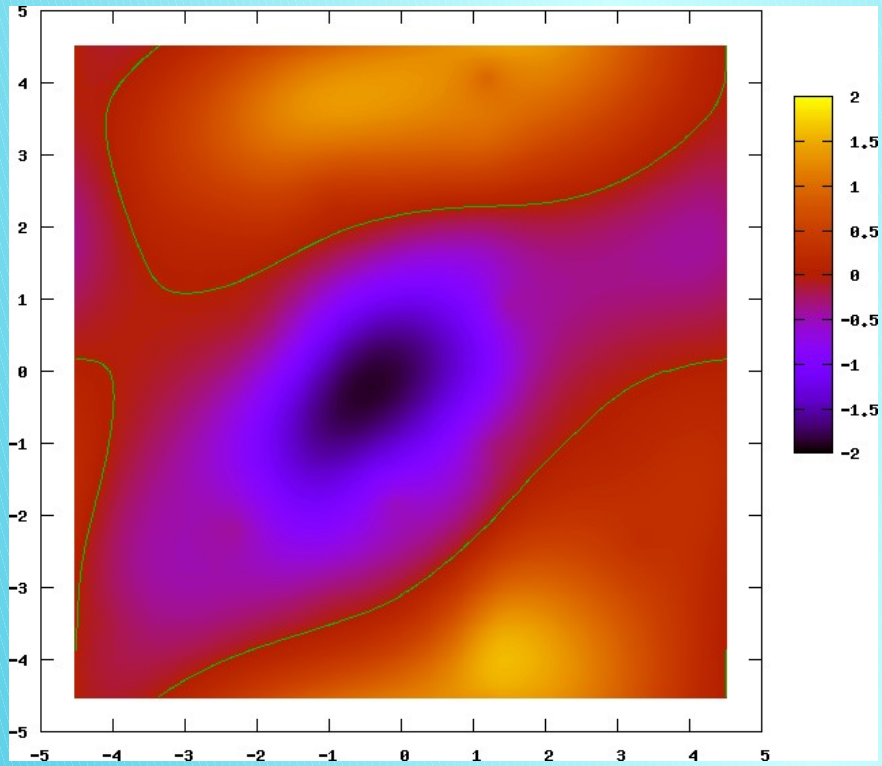


26-electron 2D HEG at rs= 1.0
Moving one electron with the rest fixed.

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:



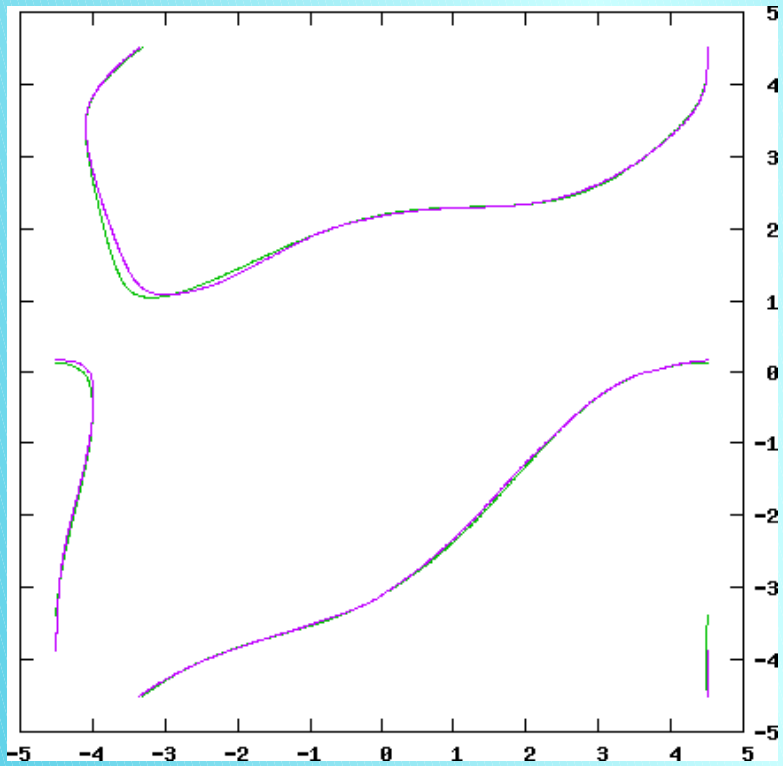
BF wave-function

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

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:



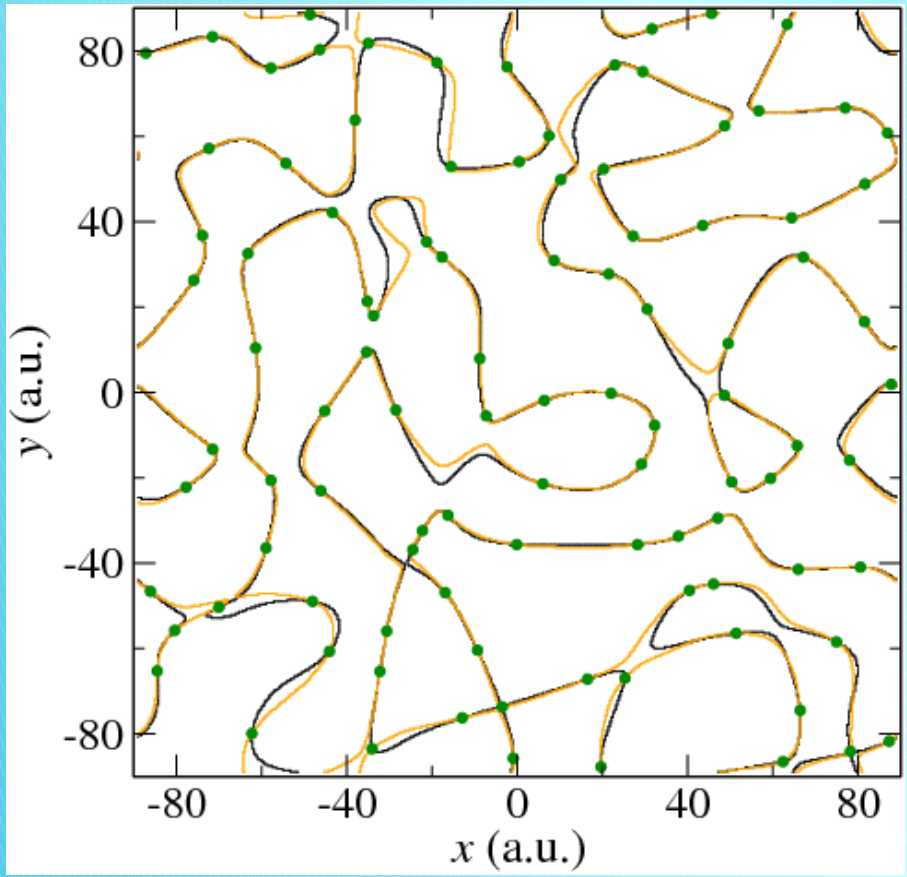
26-electron 2D HEG at rs=1.0
projected HF (green) and BF (purple) nodal surfaces

HF and BF nodes

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:



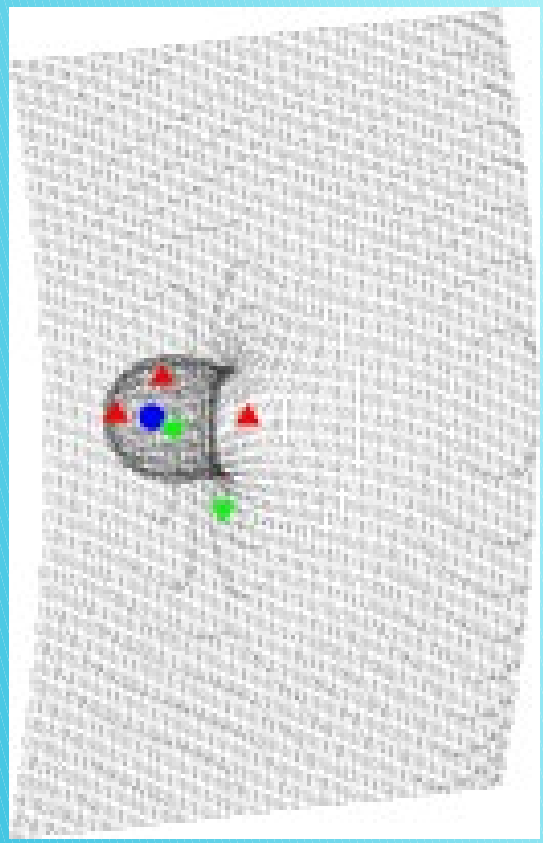
101-electron 2D HEG at rs=10.0
projected HF (black) and BF (orange) nodal surfaces

HF and BF nodes

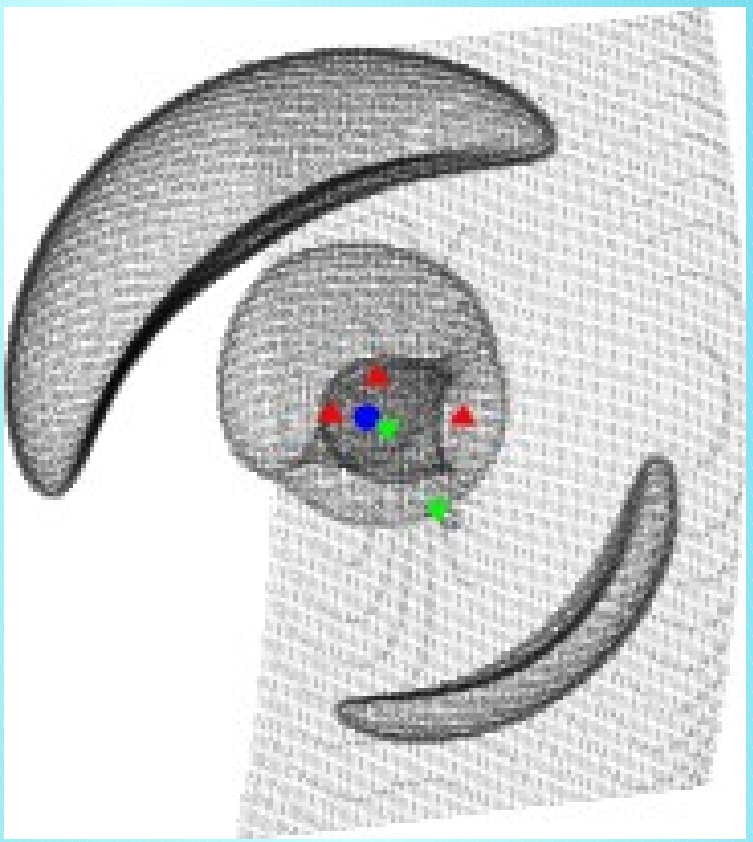
Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:



Carbon atom, projected
HF nodal surface

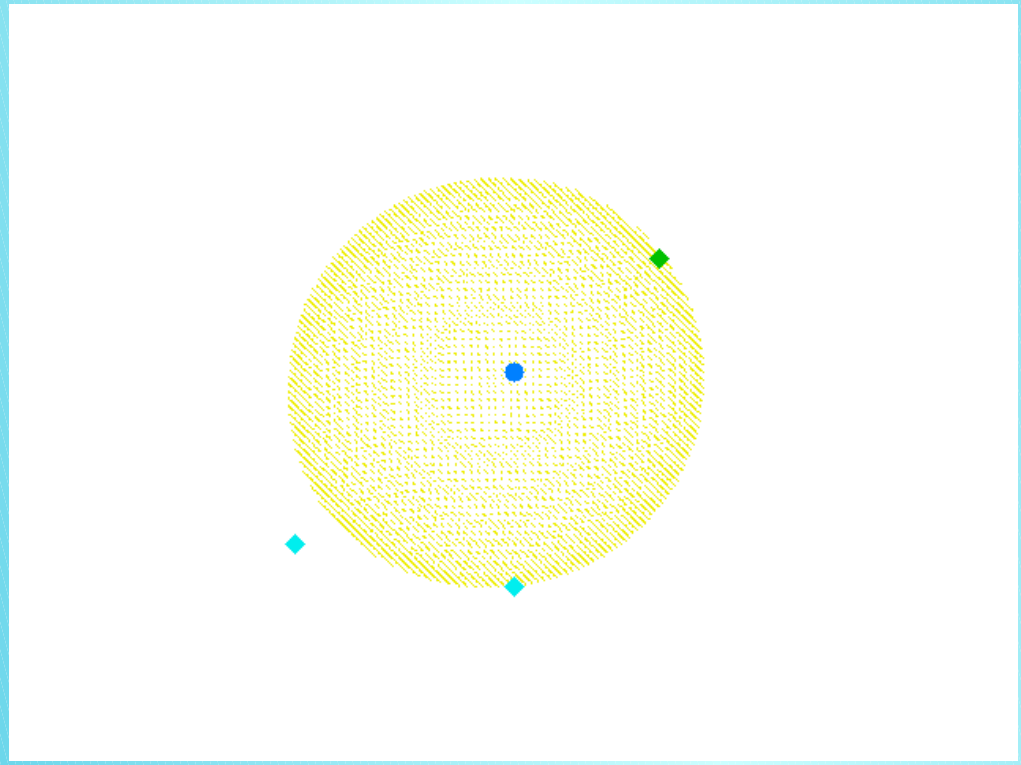


Carbon atom, projected
BF nodal surface

Backflow transformations in QMC

The backflow transformation

Changing the nodal surface:

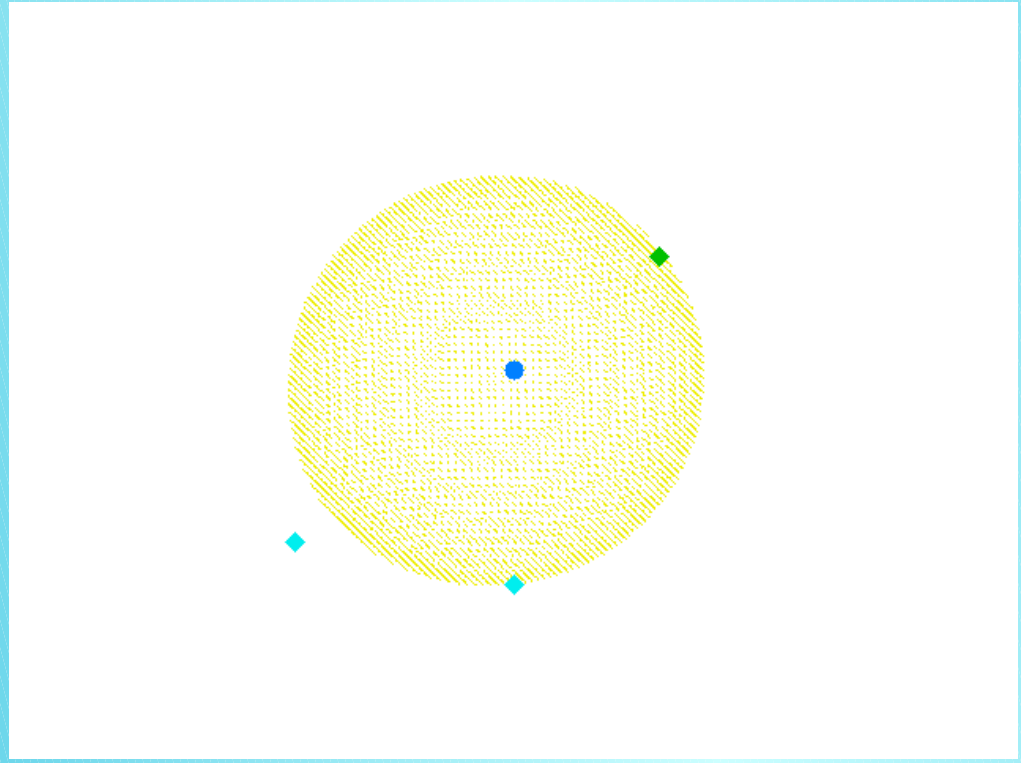


Beryllium atom, projected MD-BF nodal surface

Backflow transformations in QMC

The backflow transformation

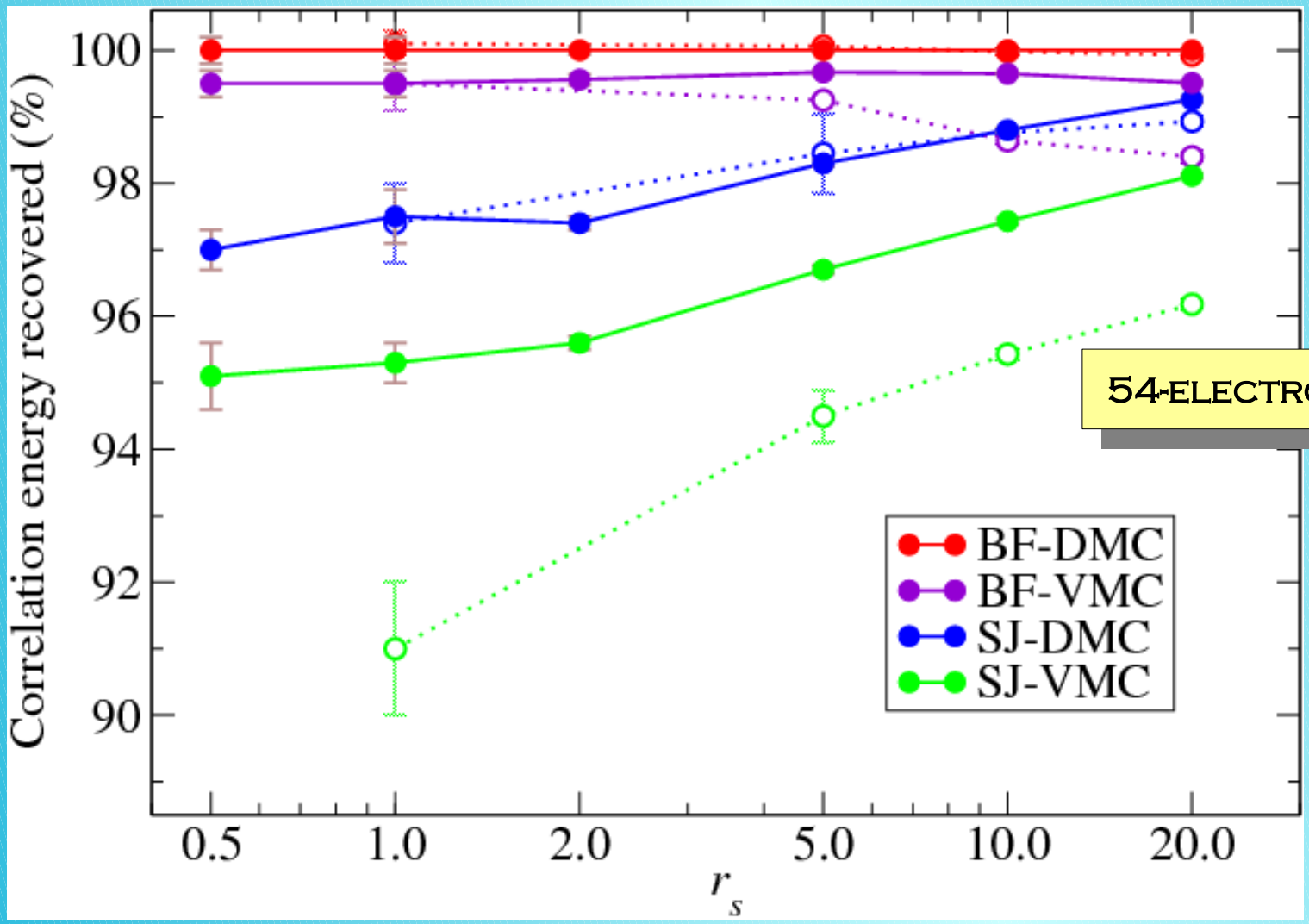
Changing the nodal surface:



Beryllium atom, projected MD-BF nodal surface

Backflow transformations in QMC

Application and results

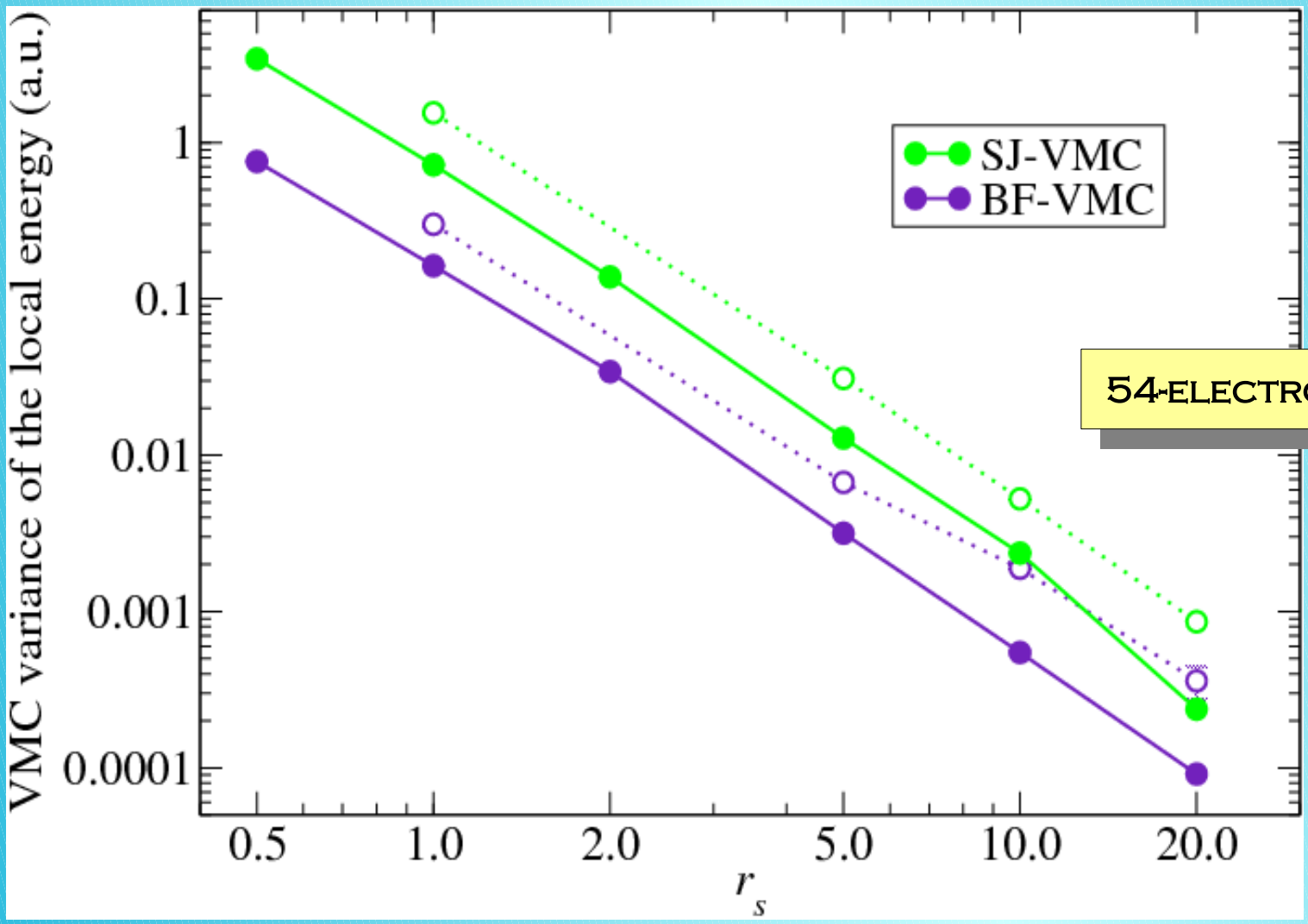


54-electron 3D HEG

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

Backflow transformations in QMC

Application and results



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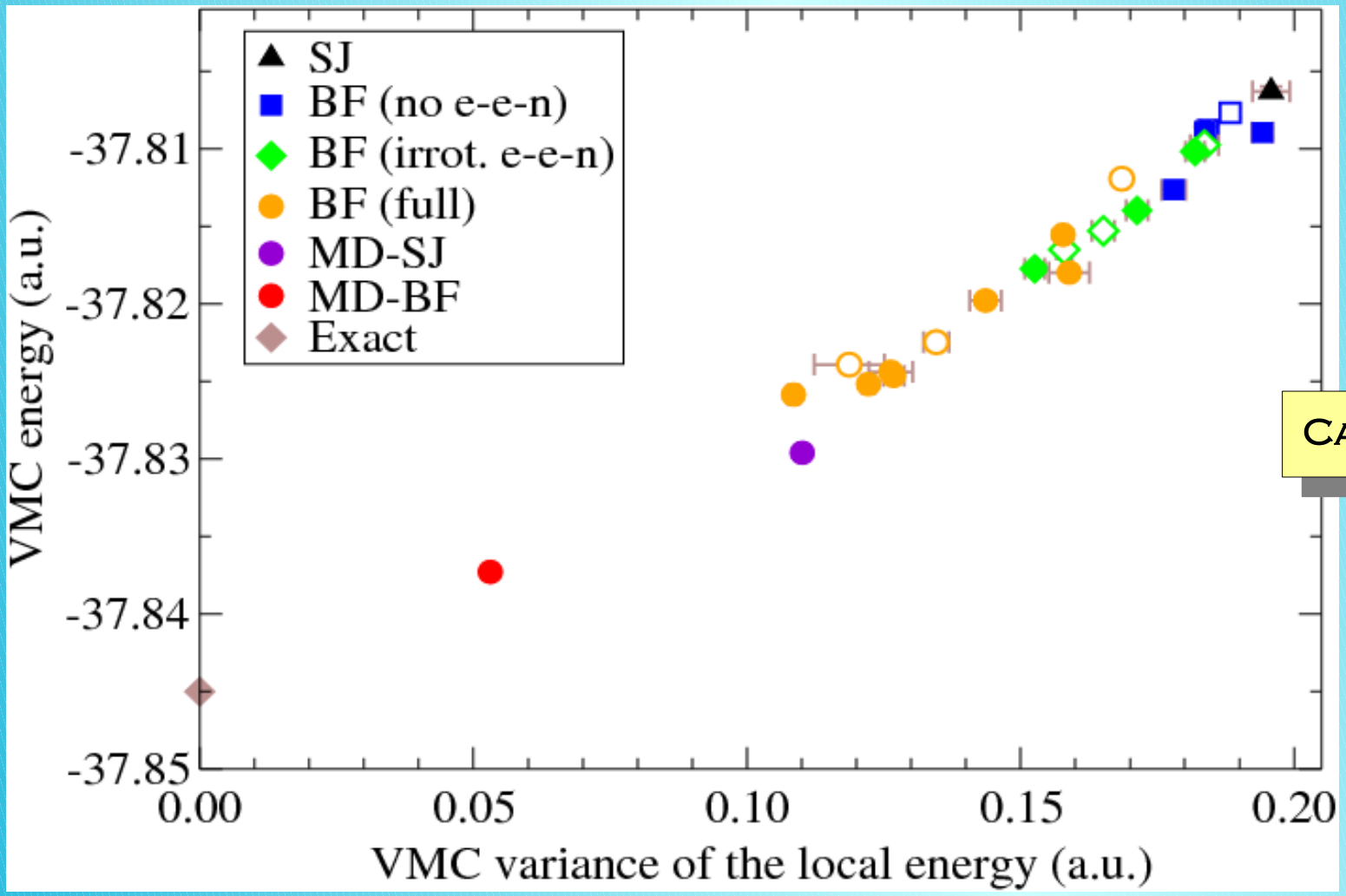
Backflow transformations in QMC

Application and results

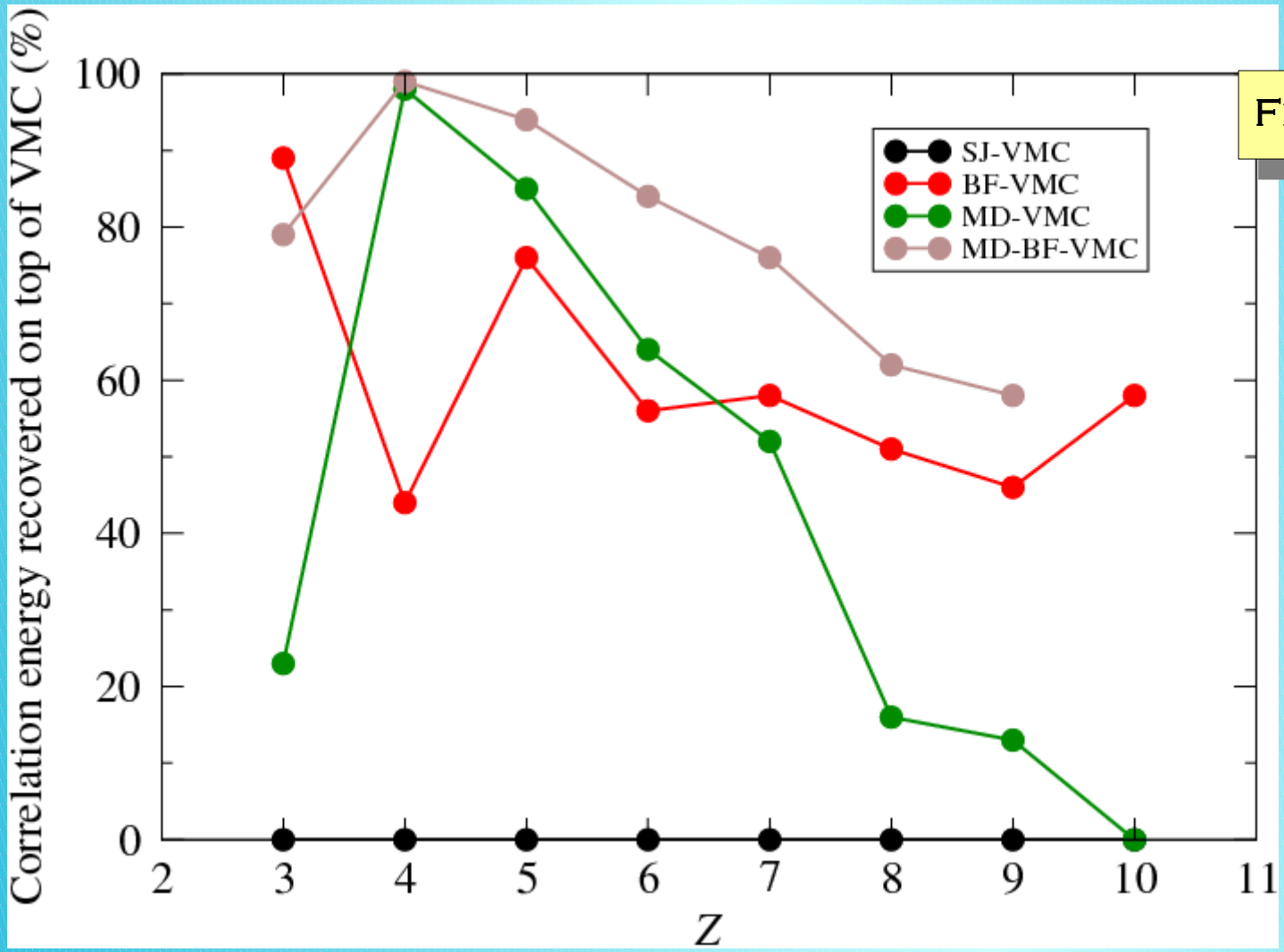


Carbon atom (AE)

*MD (18 CSFs) performed by John Trail.

Backflow transformations in QMC

Application and results

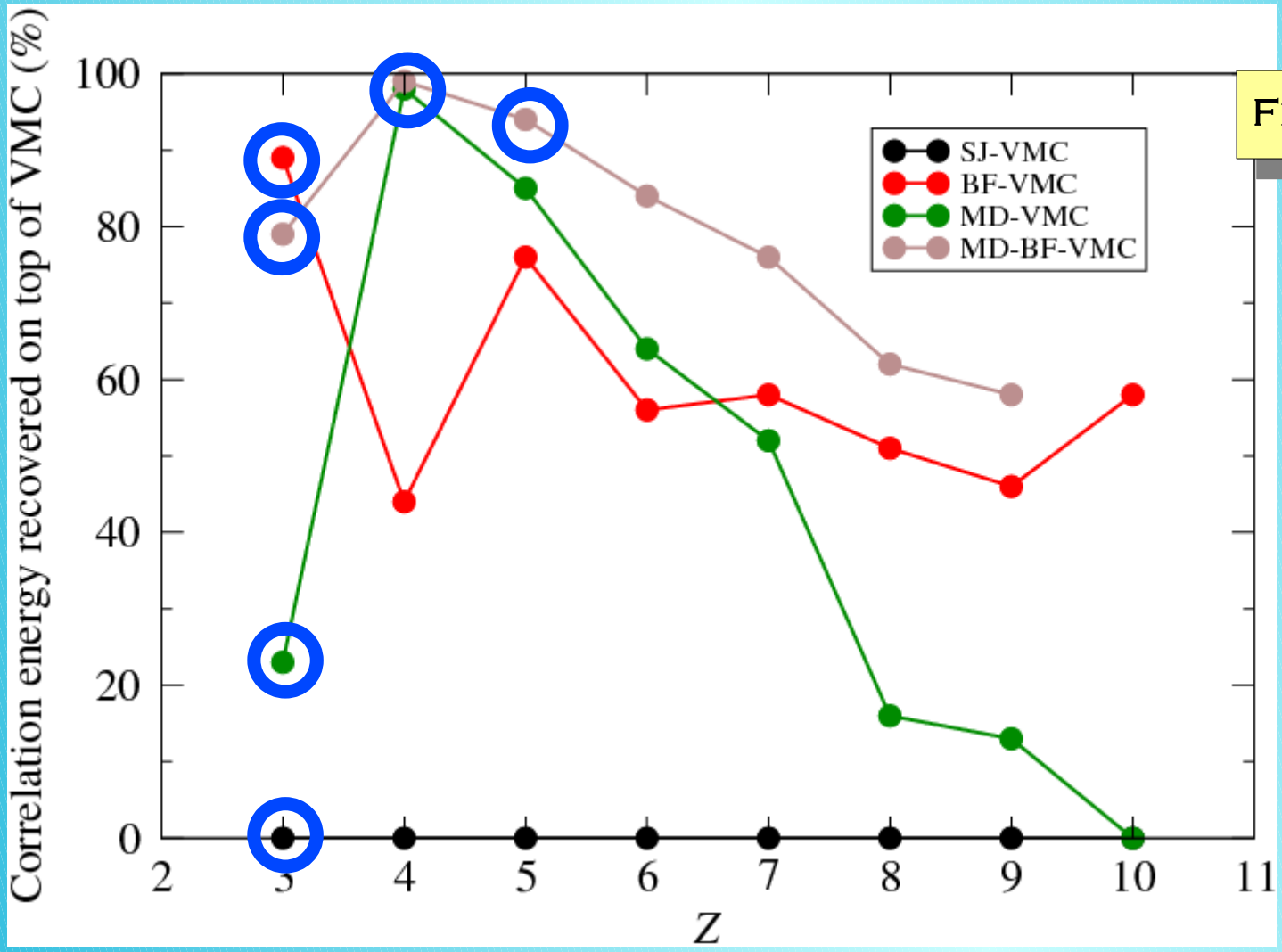


First-row AE atoms

*Calculations performed by John Trail.

Backflow transformations in QMC

Application and results



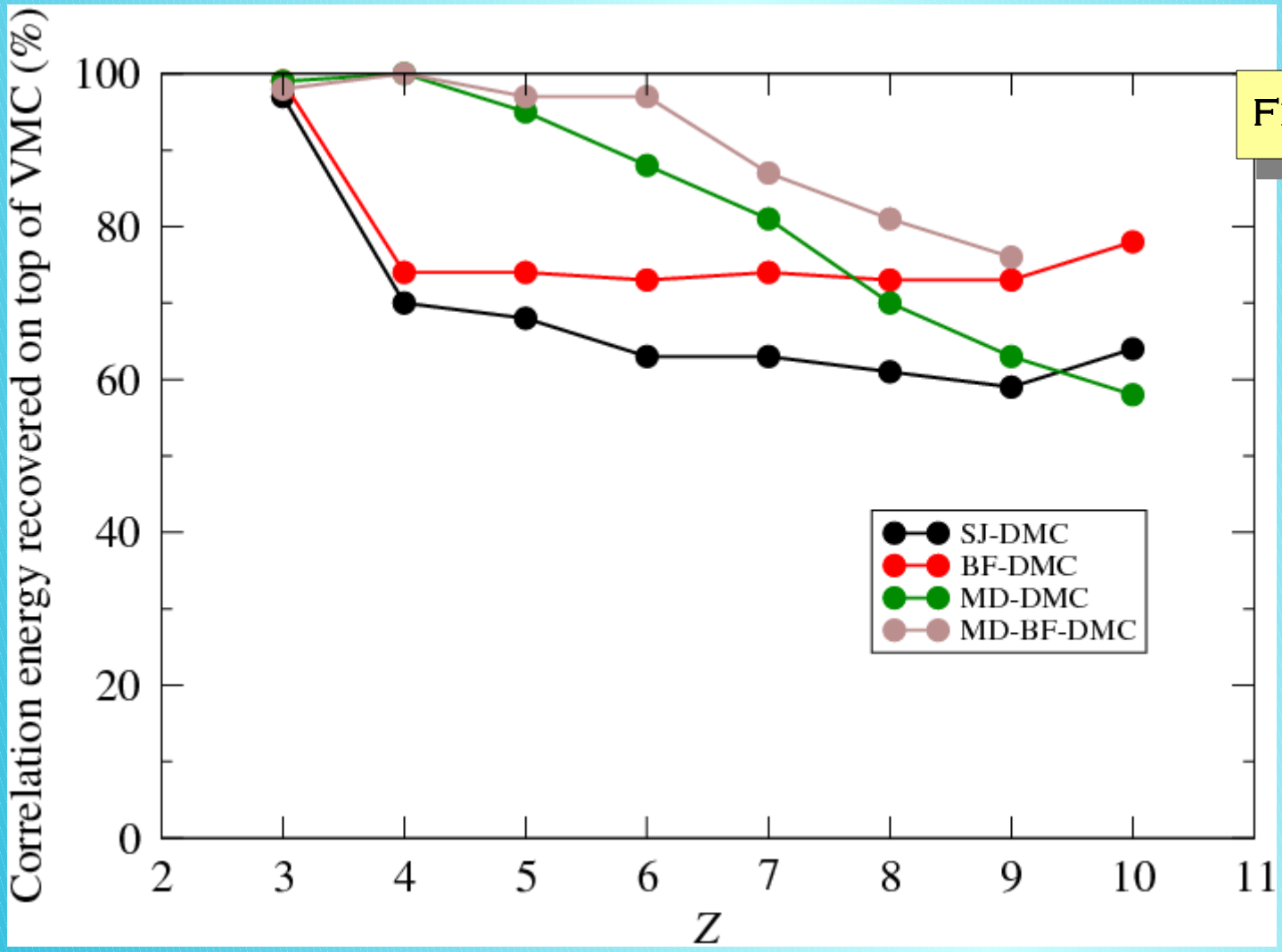
First-row AE atoms

: chem. acc.

*Calculations performed by John Trail.

Backflow transformations in QMC

Application and results



First-row AE atoms

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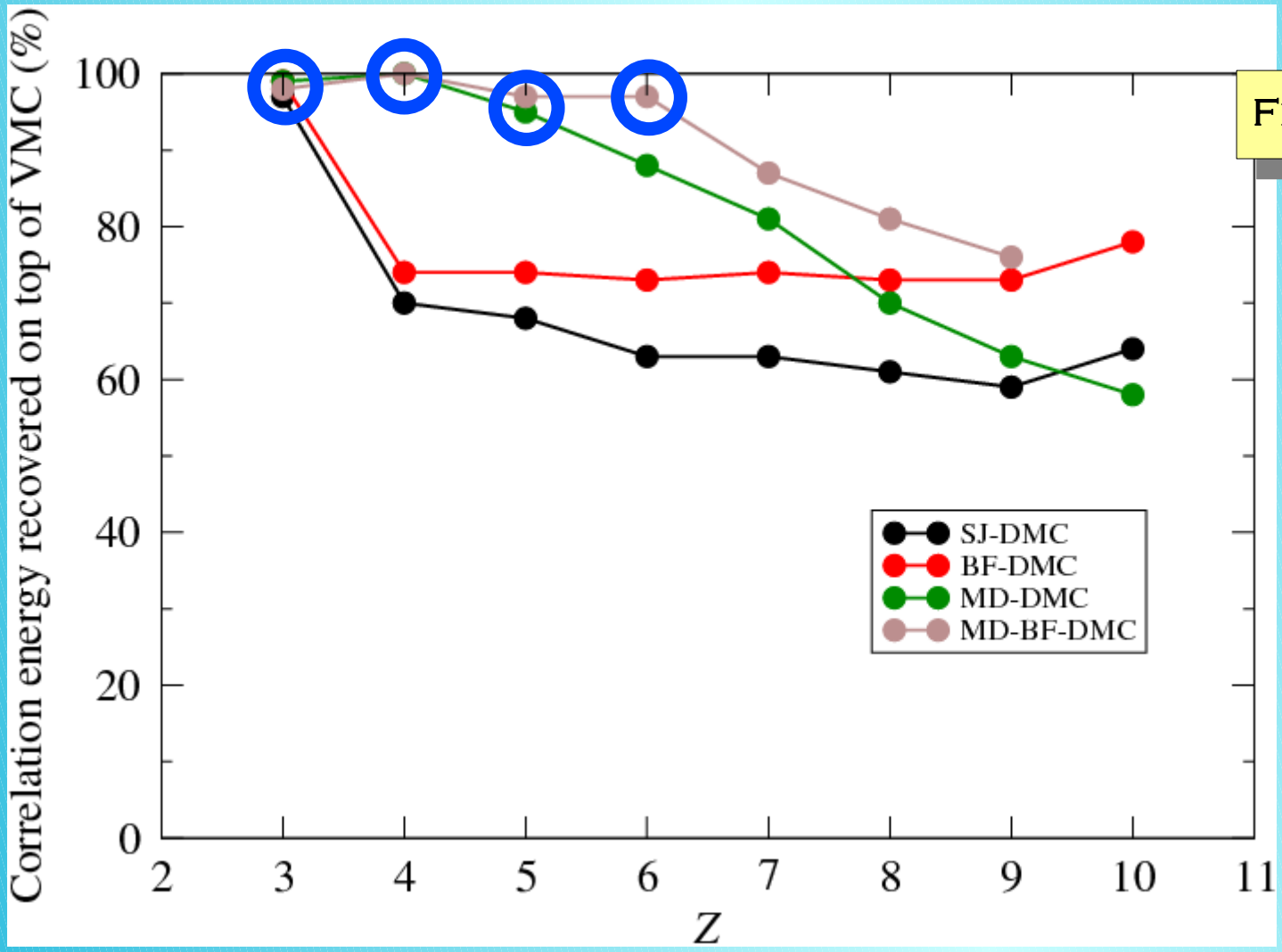
Backflow transformations in QMC

Application and results



First-row AE atoms

: chem. acc.

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Backflow transformations in QMC

Application and results

		Si diamond 2x2x2	
Method	Wfn	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)	-
	BF	(running)	-

		Si betatin 2x2x2	
Method	Wfn	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)	-
	BF	(running)	-

		C diamond 2x2x2	
Method	Wfn	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)	-
	BF	-11.4141(3)	-

Crystalline systems (Pseudopotentials)

Backflow transformations in QMC

Application and results

- **Implementation detail: electron-by-electron sampling is <u>much cheaper</u> than configuration-by-configuration sampling.**
- **Timing for fixed number of configs is increased.**
- **Lower errorbars provide large compensation.**
- **It is actually cheaper to get to a fixed errorbar with BF than SJ in the HEG and lithium atom!**

  Other systems: 2 to 8 times more expensive

Backflow transformations in QMC

Application and results

- **The closer VMC and DMC are for a given Ψ, the lower the DMC variance is, as:**

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

- **Backflow generally lowers VMC more than DMC**

- **Hence DMC statistics are better: good for DMC even if the energy is unchanged**

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 in full** (G. Spink et al, unpublished)

Backflow transformations in QMC

Conclusions

- Excellent results, good scaling properties, wide applicability
- Successfully combined with MD (not a substitute in all cases)
- Gets on well with orbital optimization too
- Combine with Pfaffians?
- BF-VMC is a powerful level of theory in many cases. BF-DMC statistics are hugely improved as a result
- Optimization method focused on nodes would help a lot [1]

[1] Work in Progress by J. R. Trail

Backflow transformations in QMC

Acknowledgements

- All calculations performed using CASINO v2.0 [1]
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  Jesus College, Cambridge (NDD)

  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)