An overview of the HANDE QMC project

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http://www.hande.org.uk

Highly Accurate N-DEterminant QMC

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Stochastic diagonalisation

Stochastic coupled cluster

Software development

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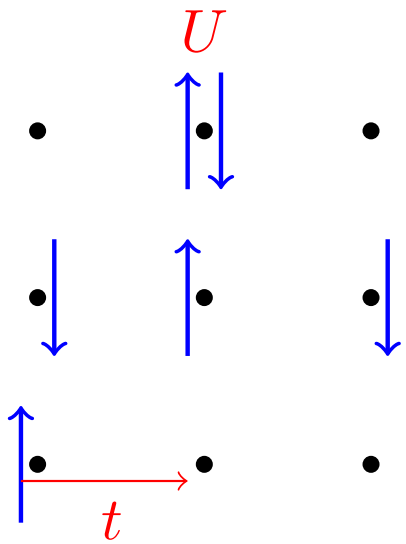
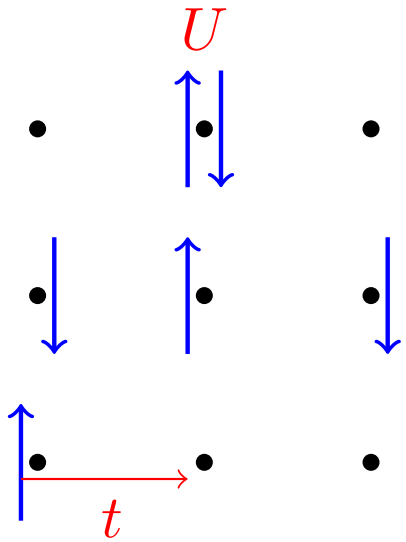
Systems



Hubbard model

Systems



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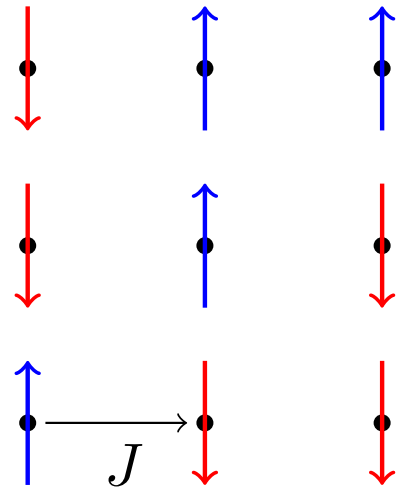

Heisenberg model

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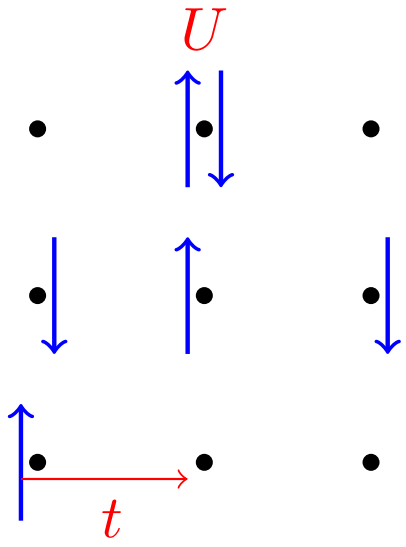

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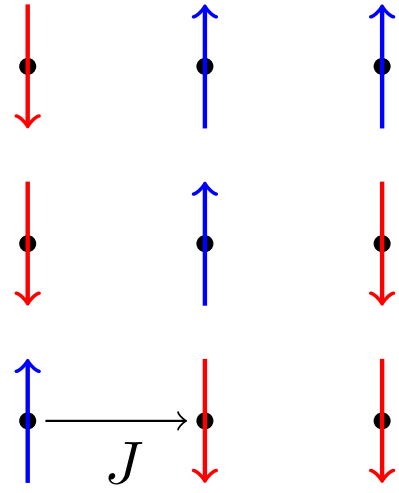
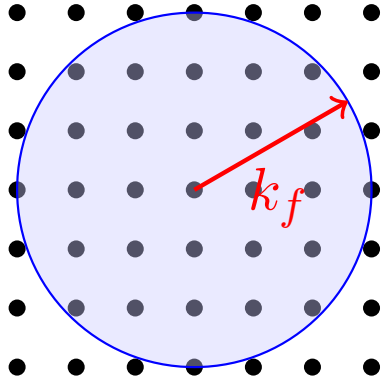
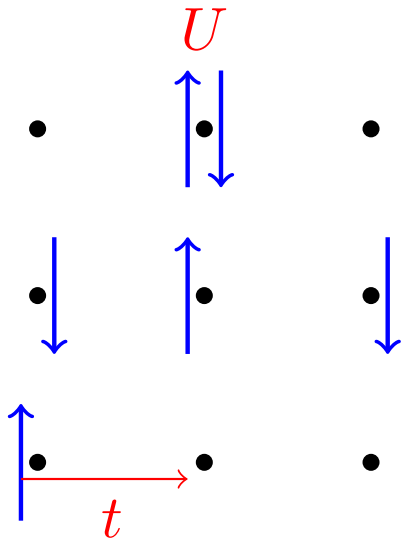


Heisenberg model



uniform electron gas

Systems



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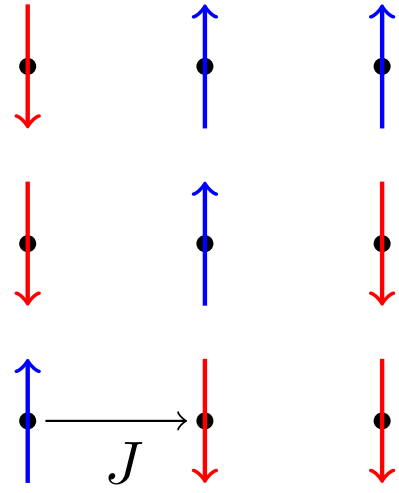

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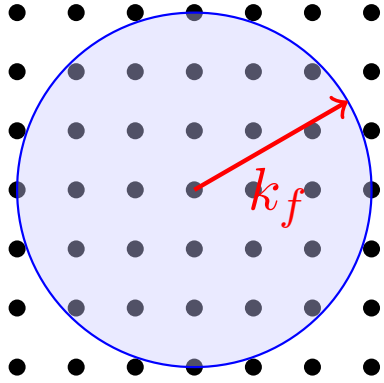

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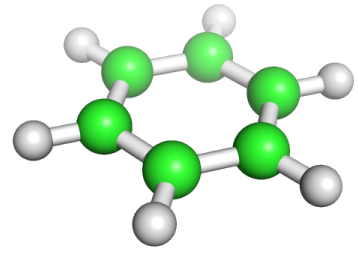
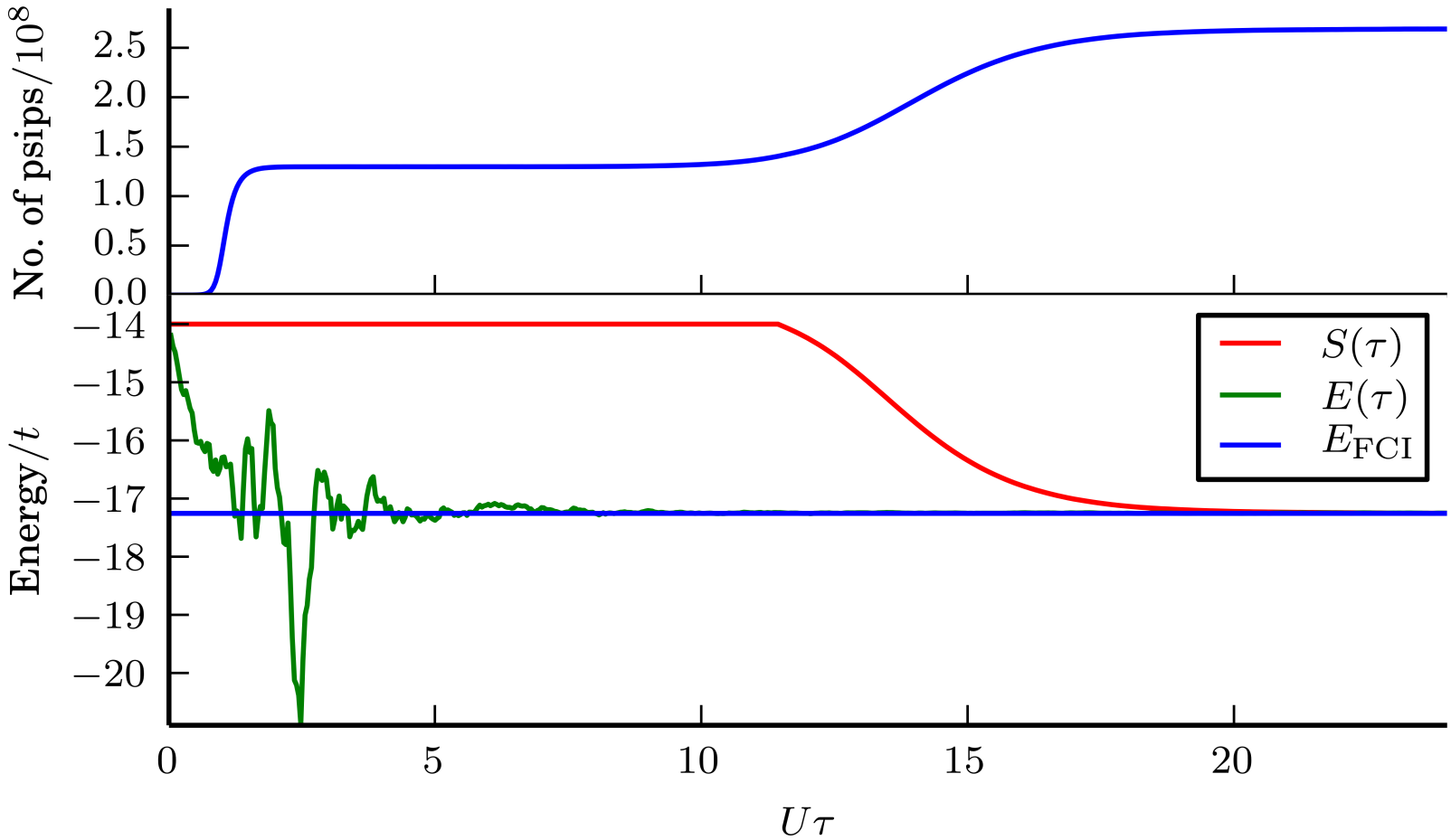


benzene…

Outline

FCIQMC[1]

Stochastically evolve $\frac{\partial \Psi}{\partial \tau} = -\hat{H}\Psi$.

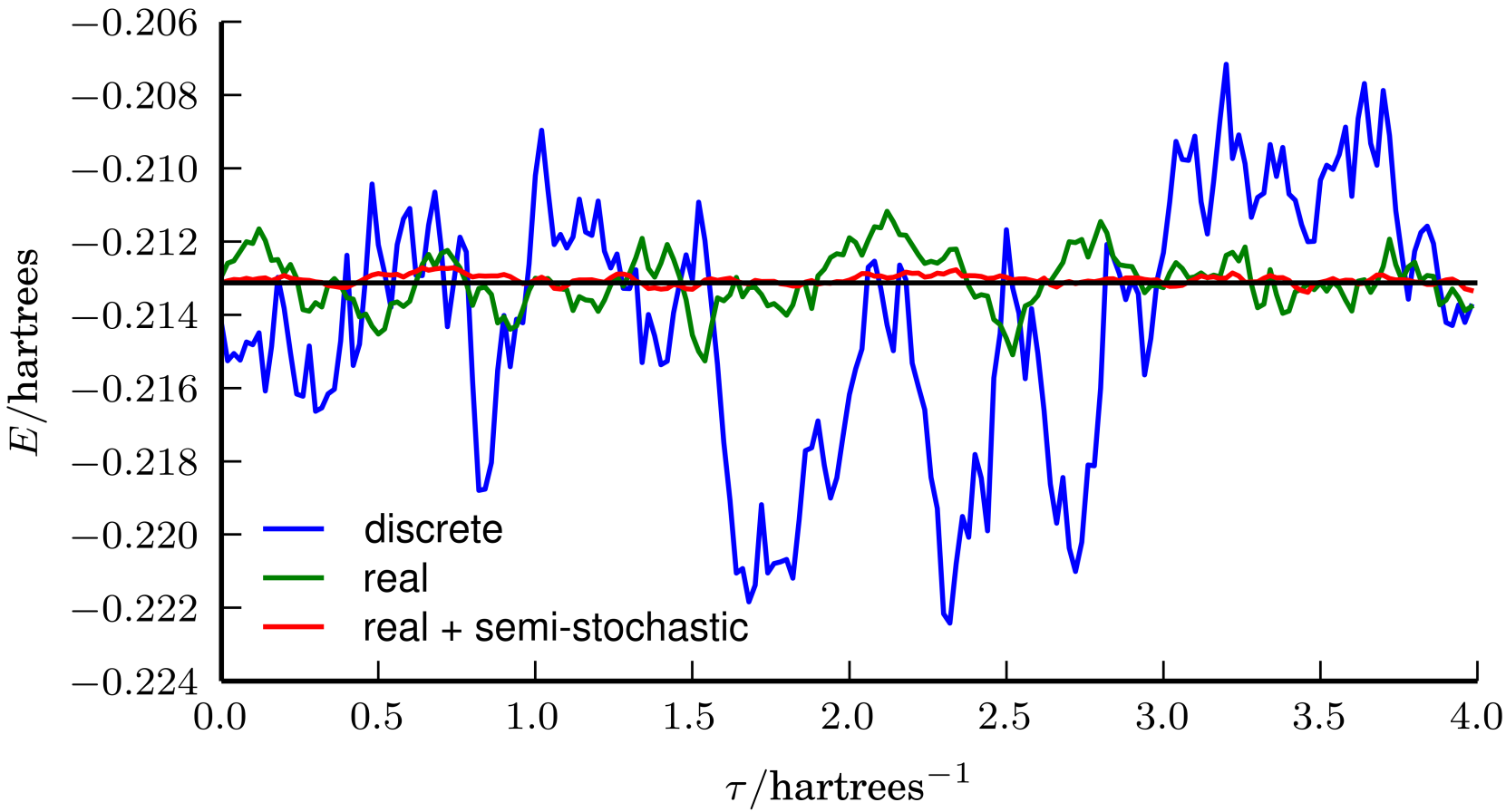


[1] Booth, Thom, Alavi, JCP 131 054106 (2010); JSS, Blunt, Foulkes, JCP 136 054110 (2012)

Semi-stochastic Projection[3]

Deterministically evolve core subspace.

Stochastically evolve remainder of Hilbert space[2].

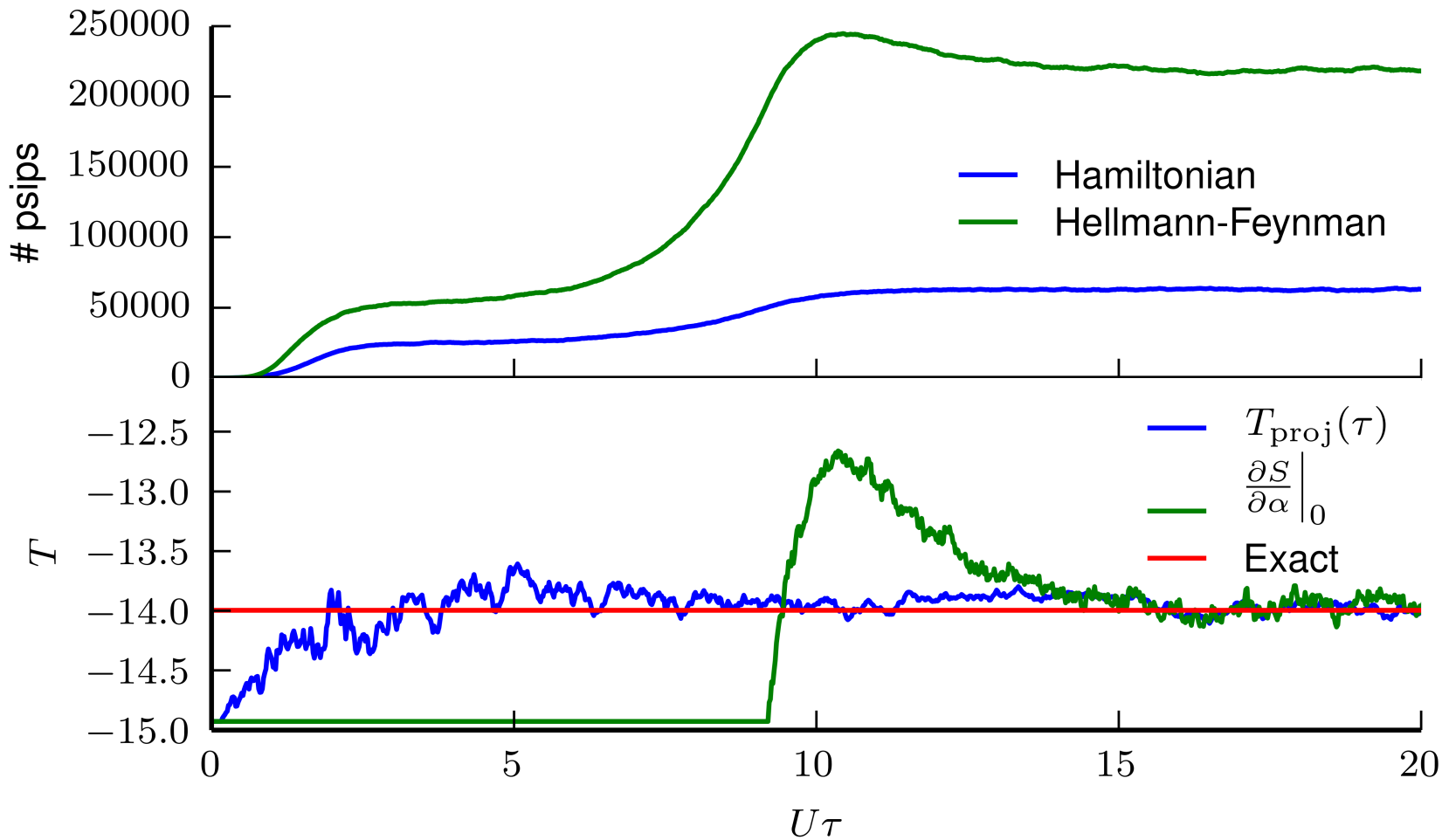


[2]F.R. Petruzielo, A.A. Holmes, H.J. Changlani, M.P. Nightingale, C.J. Umrigar, PRL, 109 230201 (2012)

Hellmann–Feynman sampling

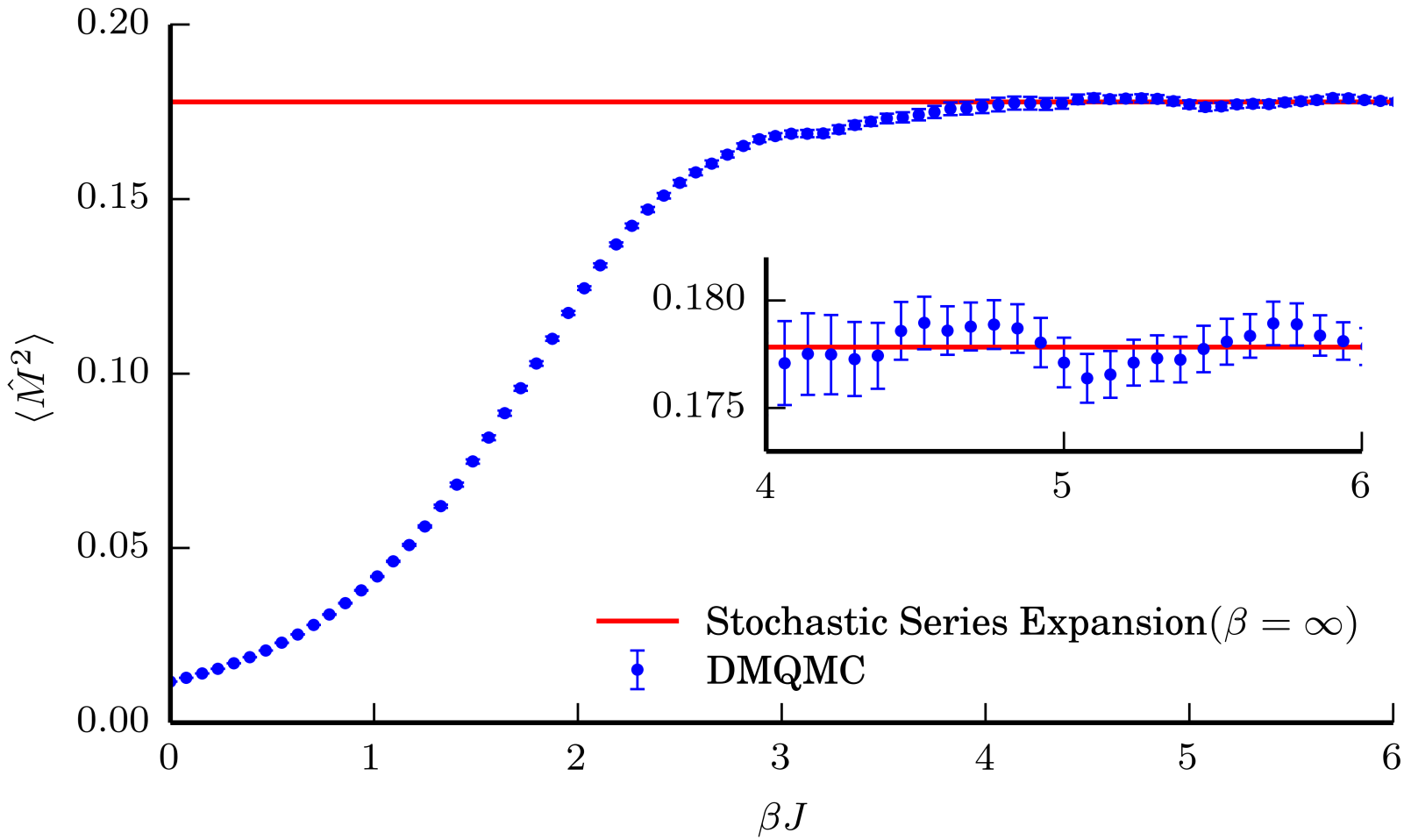
$$\hat{H}(\lambda) = \hat{H} + \lambda\hat{O} \quad \Rightarrow \quad \langle \hat{O} \rangle = \left. \frac{\partial E(\lambda)}{\partial \lambda} \right|_{\lambda=0}.$$

$\rightarrow$ Sample $\left. \frac{\partial \Psi}{\partial \tau \partial \lambda} \right|_{\lambda=0}$.



Density Matrix Quantum Monte Carlo[4]

Stochastically evolve $\frac{\partial \rho}{\partial \beta} = -\hat{H}\rho = -\frac{1}{2}\{\hat{H}, \rho\}$.



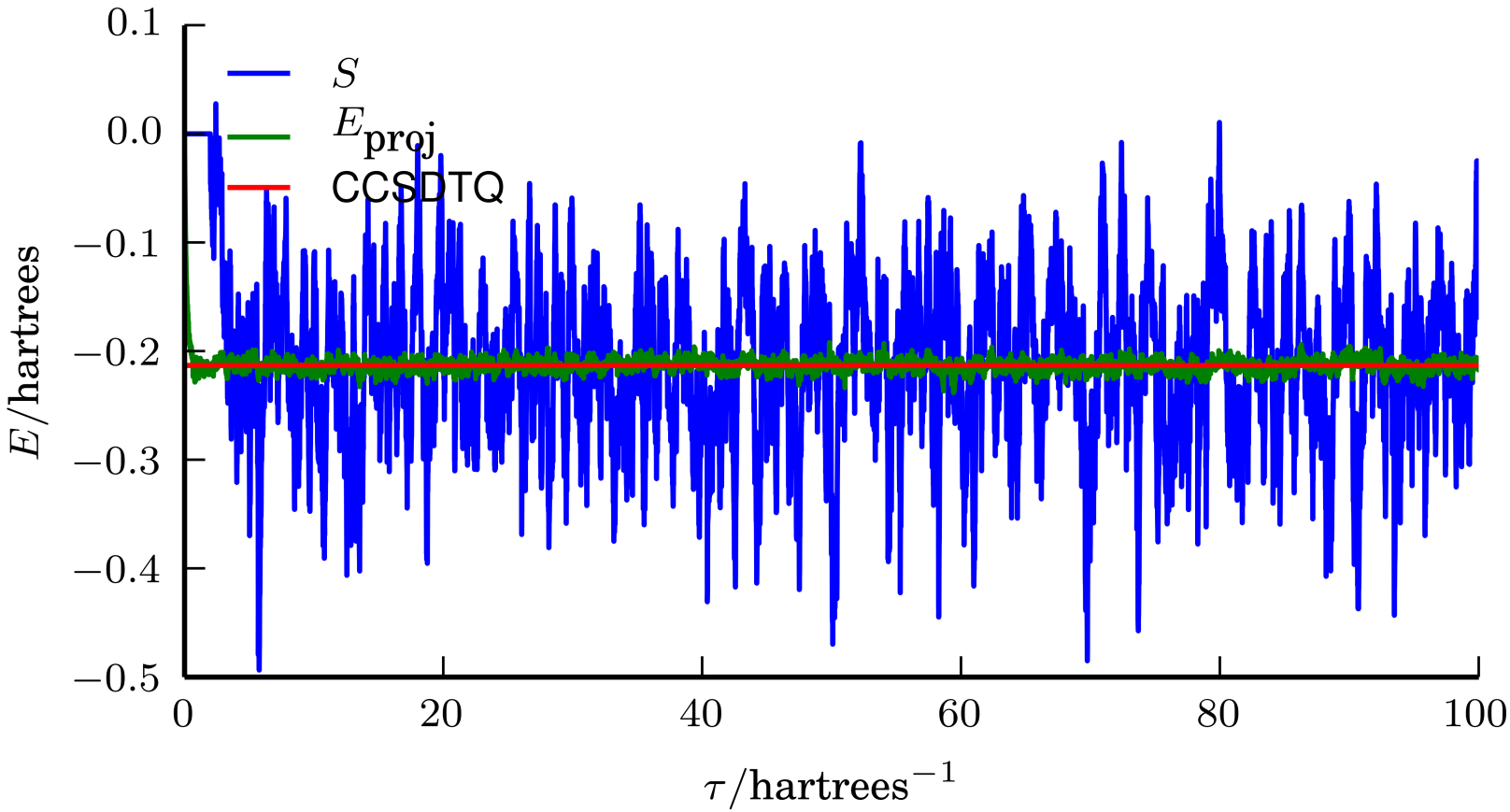
[4] N.S. Blunt, T.W. Rogers, W.M.C. Foulkes

Outline

Coupled Cluster Monte Carlo[5]

Stochastically evolve $\frac{\partial \Psi}{\partial \tau} = -\hat{H}\Psi$.

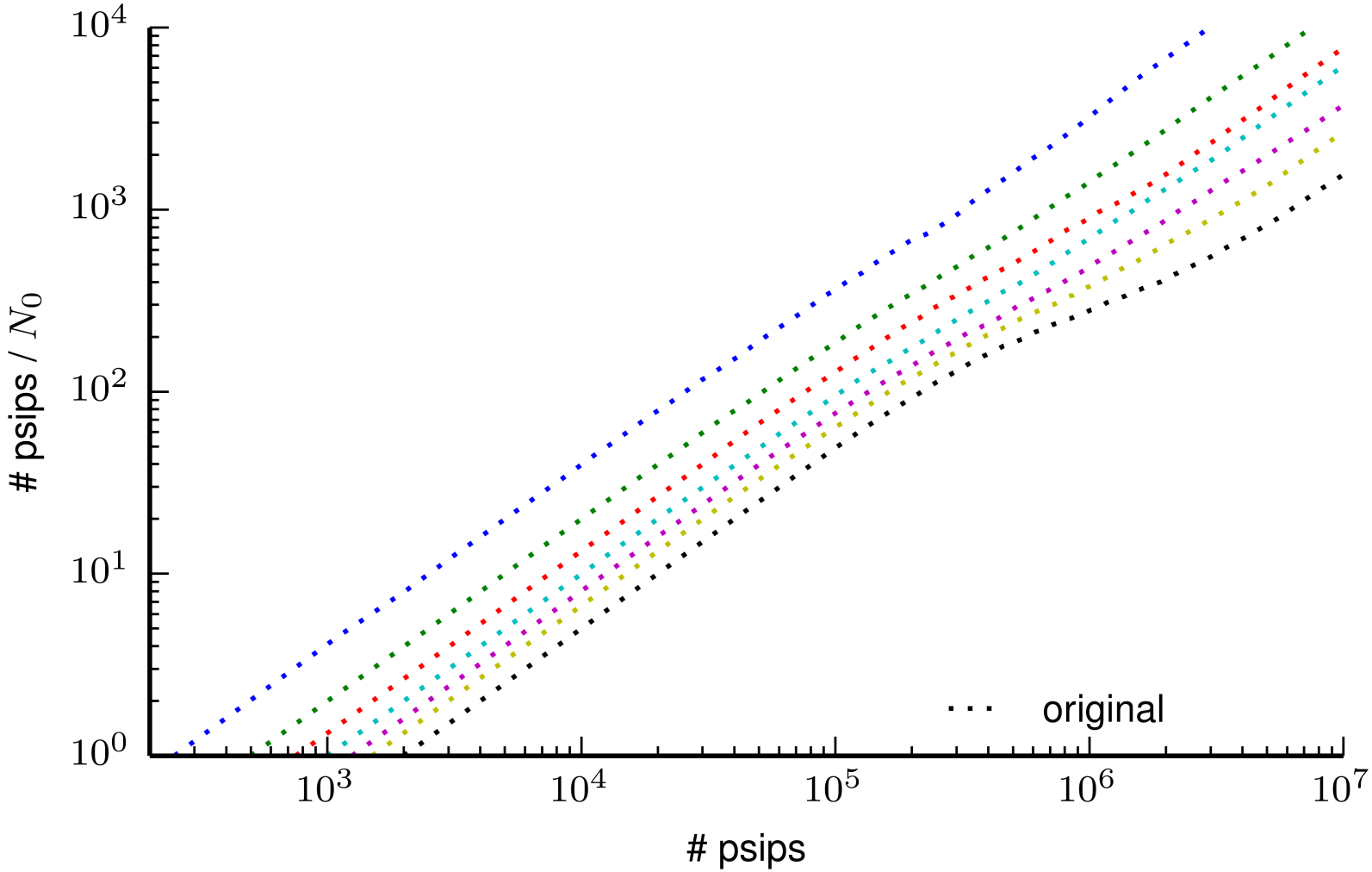
$$\Psi = e^{\hat{T}} \left|\mathrm{HF}\right\rangle; \quad \hat{T} = \sum_{ia} t_i^a \hat{c}_a^\dagger \hat{c}_i + \frac{1}{2} \sum_{ijab} t_{ij}^{ab} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_j \hat{c}_i + \cdots.$$



[5] A.J.W. Thom, PRL 105 263004 (2010)

CCMC: full non-composite clusters algorithm[6]

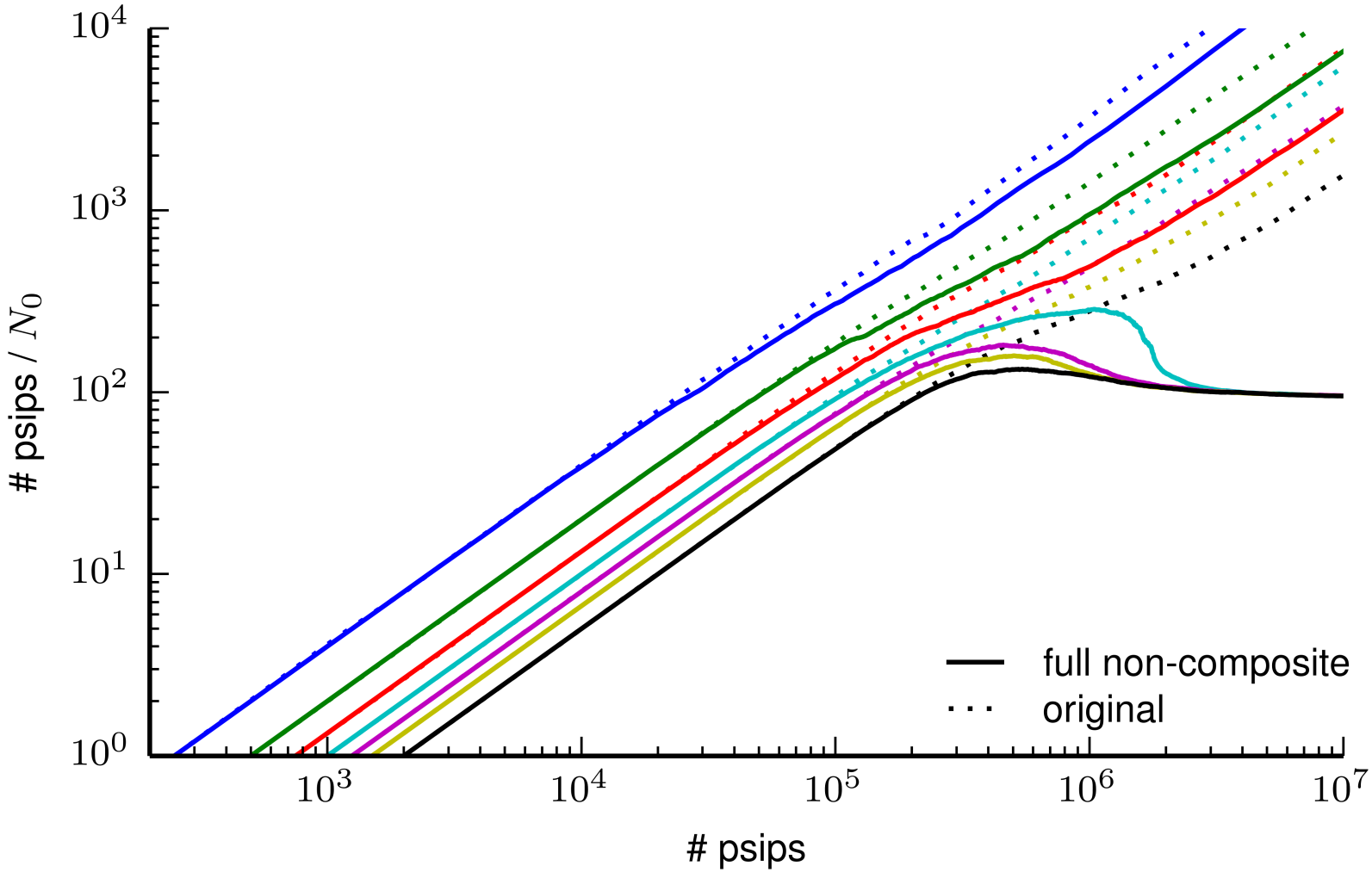
Problem—population on reference can grow slower than the rest of the space.



[6] A.J.W. Thom, W.A. Vigor

CCMC: full non-composite clusters algorithm[6]

Split cluster selection: select all occupied excitors and randomly select clusters of excitors.



[6] A.J.W. Thom, W.A. Vigor

Parallel CCMC[7]

Key difference from FCIQMC: cooperative spawning.

$$t_i^a t_j^b \rightarrow t_{ij}^{ab}$$

Need to minimise communication to ensure good performance.

[7] A.J.W. Thom

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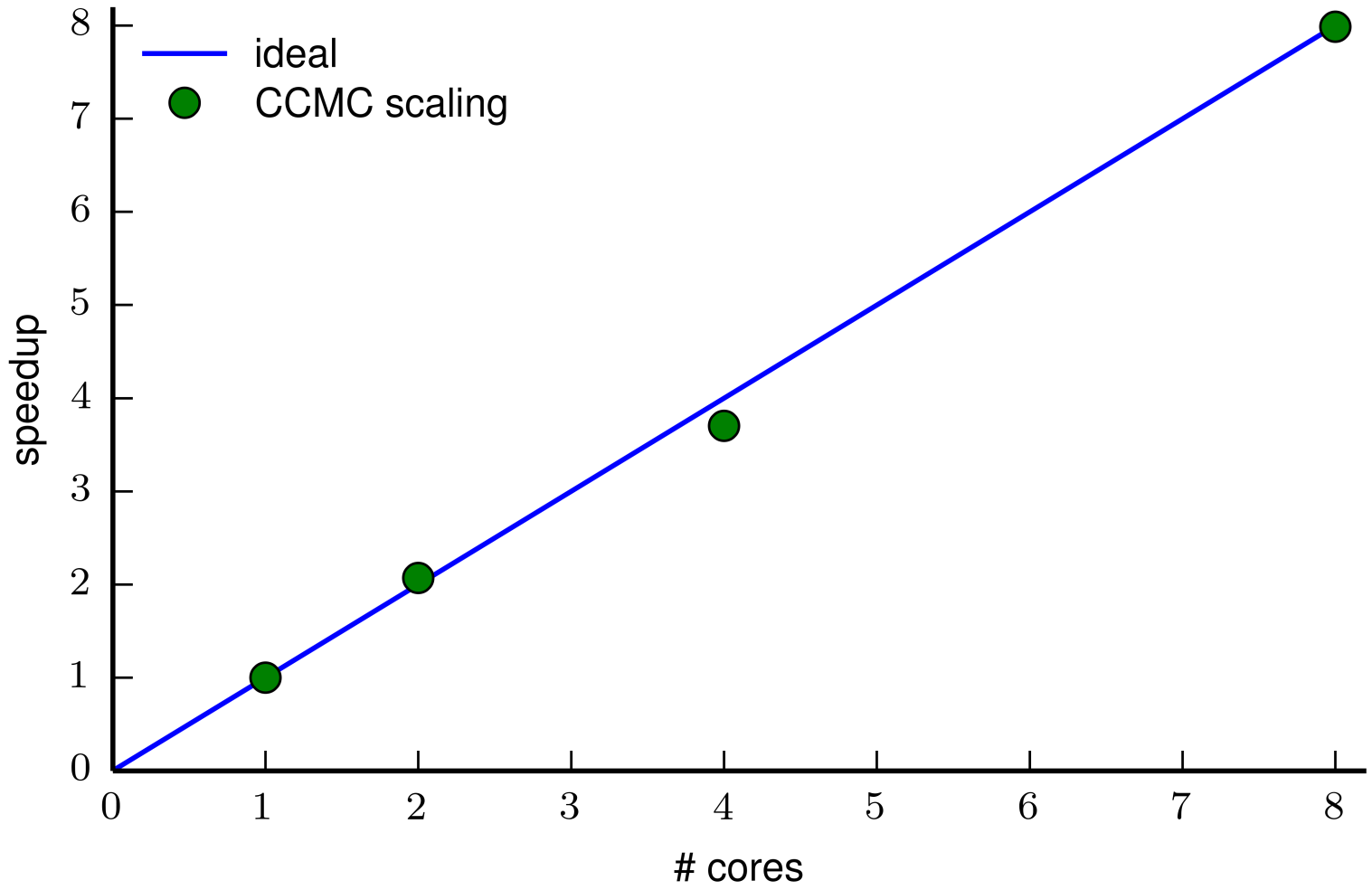
FCIQMC: $p(|D\rangle) = \text{hash}(|D\rangle) \mod N_p$

CCMC: $p(|D\rangle) = \text{hash}(|D\rangle + o(|D\rangle)) \mod N_p$

$$o(|D\rangle) = (\text{hash}(|D\rangle) + N_{\text{iter}}) \gg x$$

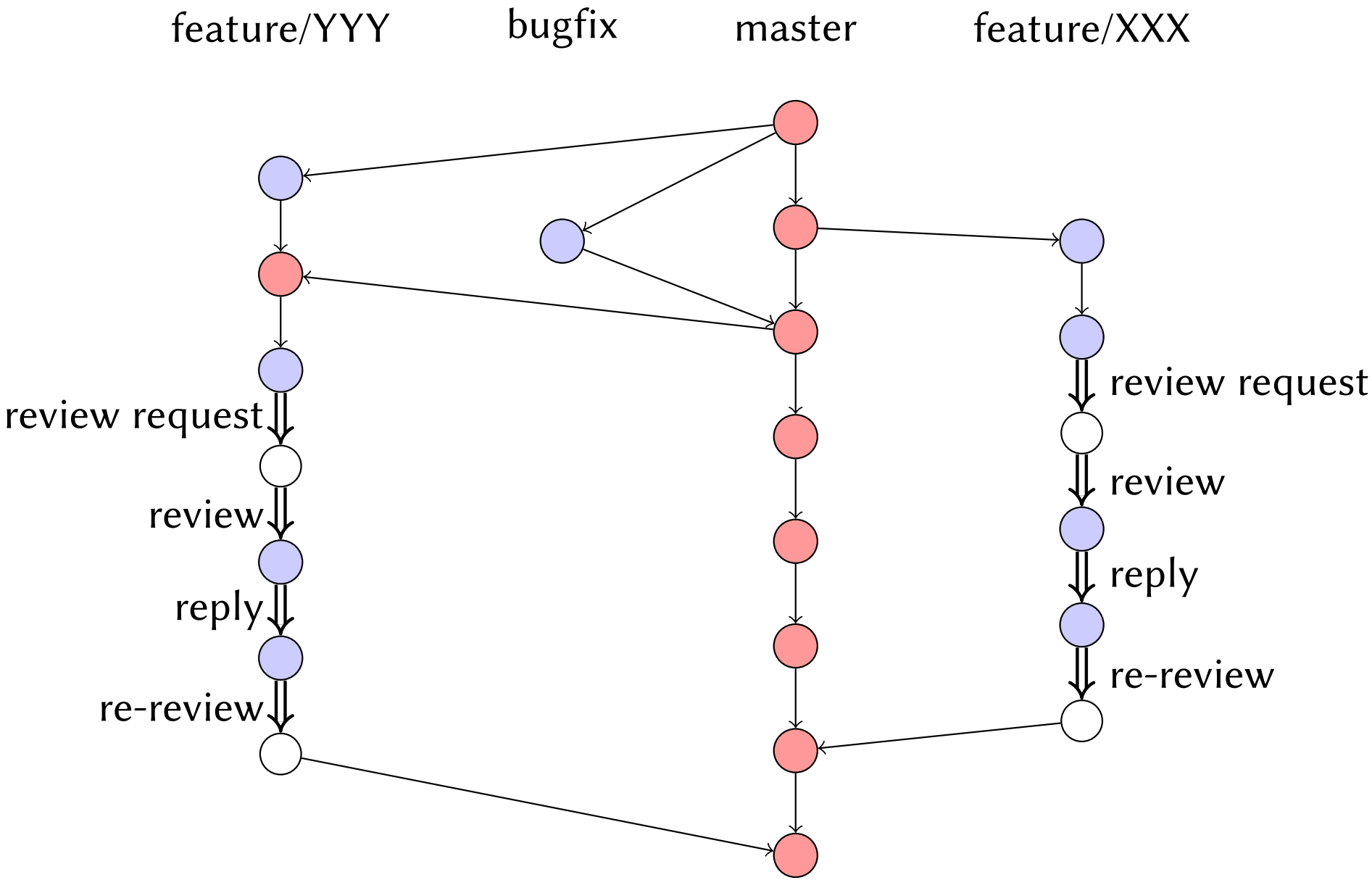
[7] A.J.W. Thom

Parallel CCMC: scaling



Outline

git-flow development model[8]

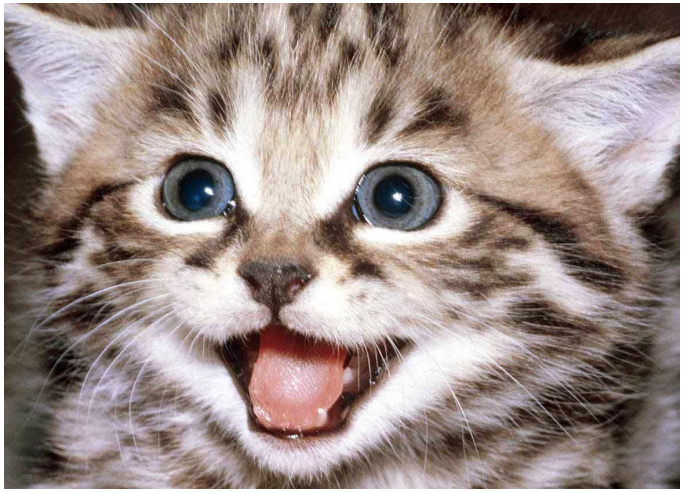


[8] A successful Git branching model, V.Driessen

Training

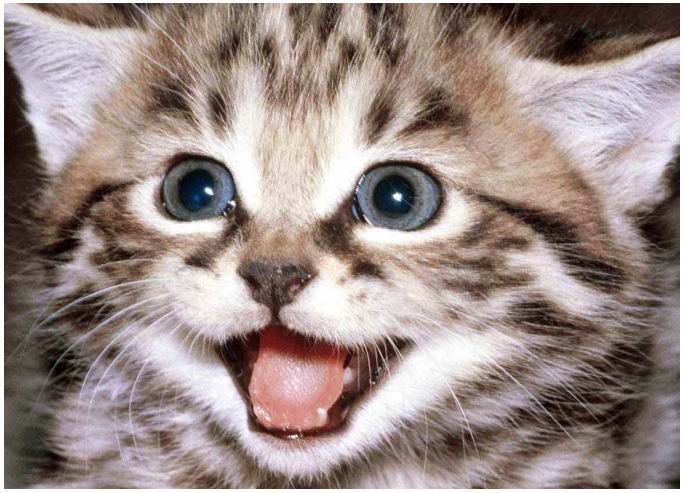
- new students
  - minimal ‘toy’ FCIQMC code
  - introductory(ish) projects
- ongoing
  - code review
  - encourage ownership
  - coding retreats
- scratch own itch
  - convert users $\rightarrow$ developers

Swings and roundabouts



well documented
fast
flexible data structures
python scientific stack
lua-based input file (coming)
easy to extend

Swings and roundabouts



well documented
fast
flexible data structures
python scientific stack
lua-based input file (coming)
easy to extend

(some) global data
complex optimised code
legacy code

Outline

Future work

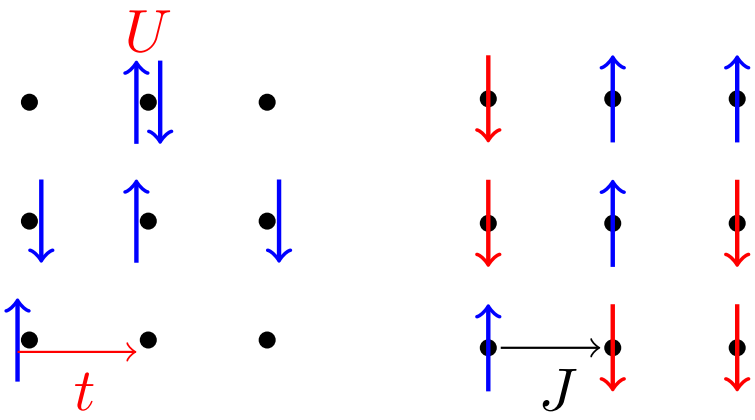
Time for consolidation

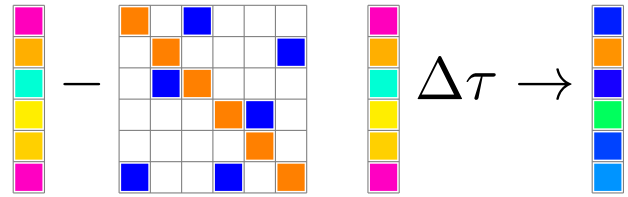
- Systematic studies on 'model' quantum chemistry problems
- Coupled cluster Monte Carlo studies
  - Hilbert spaces
  - truncation levels
- Like-for-like comparison between methods on a range of systems
  - How does the sign problem vary?
  - Run with 1D Hubbard model datasets[9]
- Fixed node approximations[10]
  - implementation
  - N_2 dissociation
- Beyond the initiator approximation
  - ...

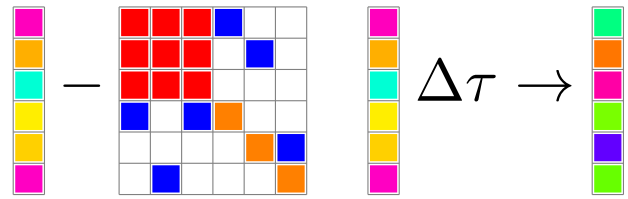
[9] DOI:10.6084/m9.figshare.1096136 and DOI:10.6084/m9.figshare.1106864, J.J. Shepherd and JSS

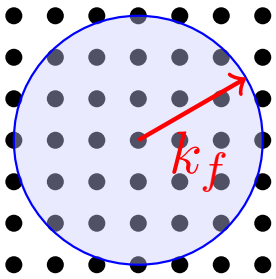
[10] Kolodrubetz, Clark, PRB 86 075109; Mukherjee, Alhassid, PRA 88, 053622; Roggero, Mukherjee, Pederiva, PRB 88, 115138

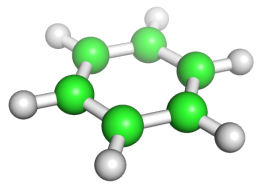
Highly Accurate N-DEterminant QMC

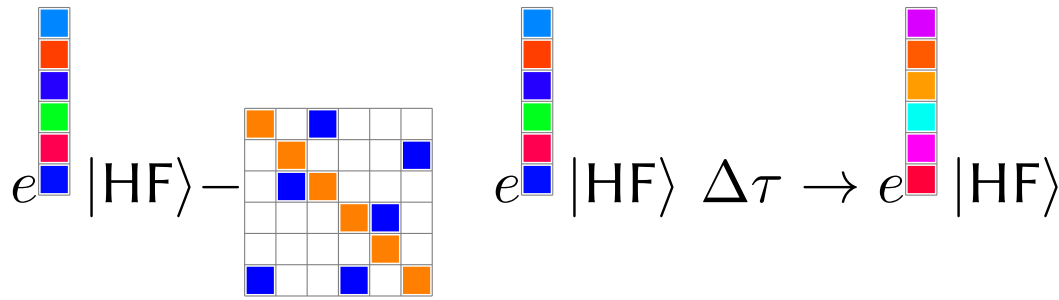






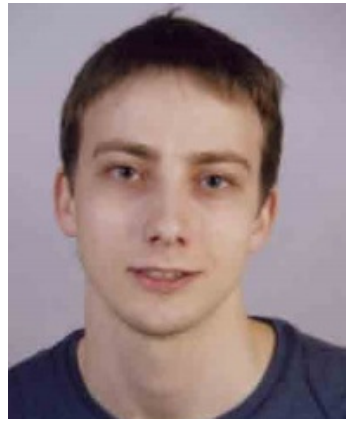






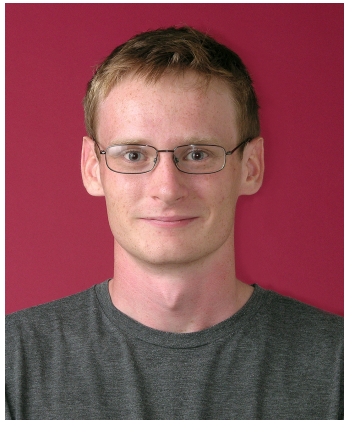
HANDE team

Alex Thom



Nick Blunt

Will Vigor



Fionn Malone

Matthew Foulkes

James Shepherd

Past contributors: Will Handley, Tom Rogers, Joe Weston.

HANDE publications

- Understanding
  - The sign problem and population dynamics in the FCIQMC method, JSS, N.S. Blunt, W.M.C. Foulkes, JCP 136 054110 (2012).
  - The effect of quantization on the FCIQMC sign problem, M.H. Kolodrubetz, JSS, B.K. Clark and W.M.C. Foulkes, JCP 138 024110 (2013).
  - Unloading the dice: Minimising biases in FCIQMC, W.A. Vigor, JSS, M.J. Bearpark, A.J.W. Thom, arXiv:1407.1753.
  - The sign problem in FCIQMC: linear and sublinear representation regimes, J.S. Shepherd, G.E. Scuseria, JSS, arXiv:1407.4800.
- Method and algorithm development
  - Density Matrix Quantum Monte Carlo, N.S. Blunt, T.W. Rogers, JSS, W.M.C. Foulkes, PRB 89 245124 (2014).
  - Improved parallel algorithms for stochastic diagonalisation, F.D. Malone, W.M.C. Foulkes, JSS, in preparation.
  - Highly scalable stochastic coupled cluster theory, JSS, W.A. Vigor, A.J.W. Thom, in preparation.
- Approach to scientific software development
  - The Highly Accurate N-DEterminant (HANDE) quantum Monte Carlo project: Open-source stochastic diagonalisation for quantum chemistry, arXiv:1407.5407.