Combining QMC and Tensor Networks as a route toward predictive computing

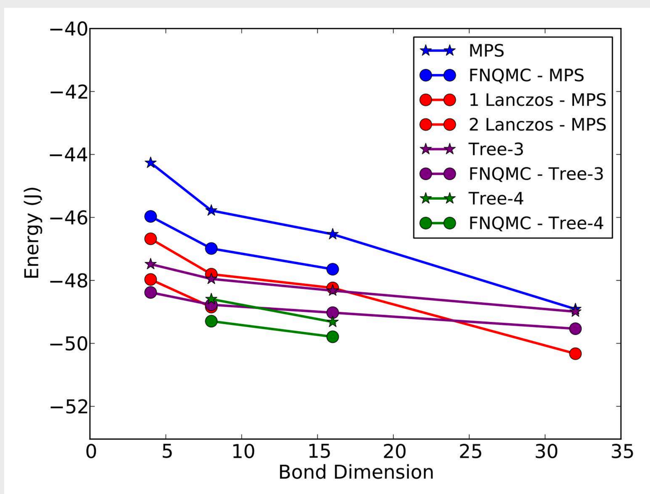
Bryan Clark (with Hitesh Changlani)
University of Illinois at Urbana Champaign
Arxiv: 1404.2296

Abstract

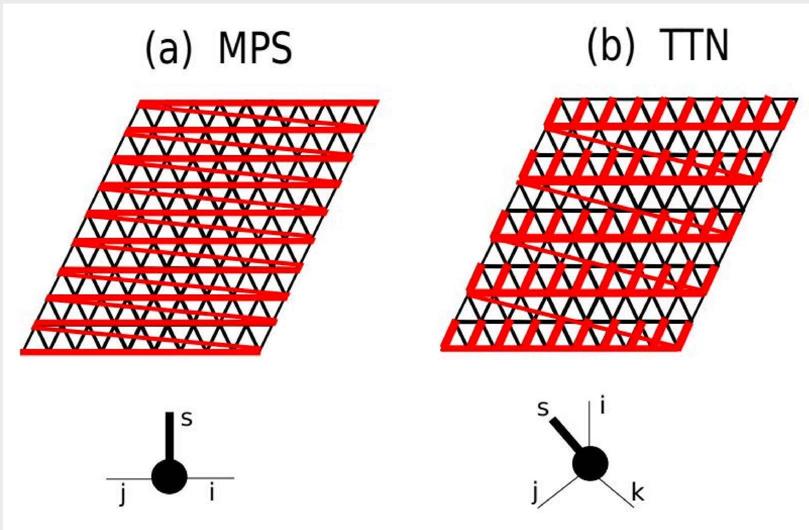
We apply a series of projection techniques on top of tensor networks to compute energies of ground state wave functions with higher accuracy than tensor networks alone with minimal additional cost. We consider both matrix product states as well as tree tensor networks in this work. Building on top of these approaches, we apply fixed-node quantum Monte Carlo, Lanczos steps, and exact projection. We demonstrate these improvements for the triangular lattice Heisenberg model, where we capture up to 57% of the remaining energy not captured by the tensor network alone. We conclude by discussing further ways to improve our approach.

QMC + Tensor Networks

The short summary



Wave functions



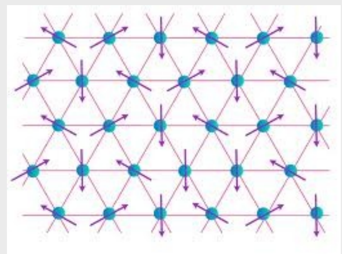
Tensor Networks

- Matrix product states
- Tree tensor networks: TTN have physical indices at the nodes of the tree. They can capture significant local entanglement structure missed by MPS. In our tests, they capture 30-40% of the energy missed by MPS for the same bond dimension!

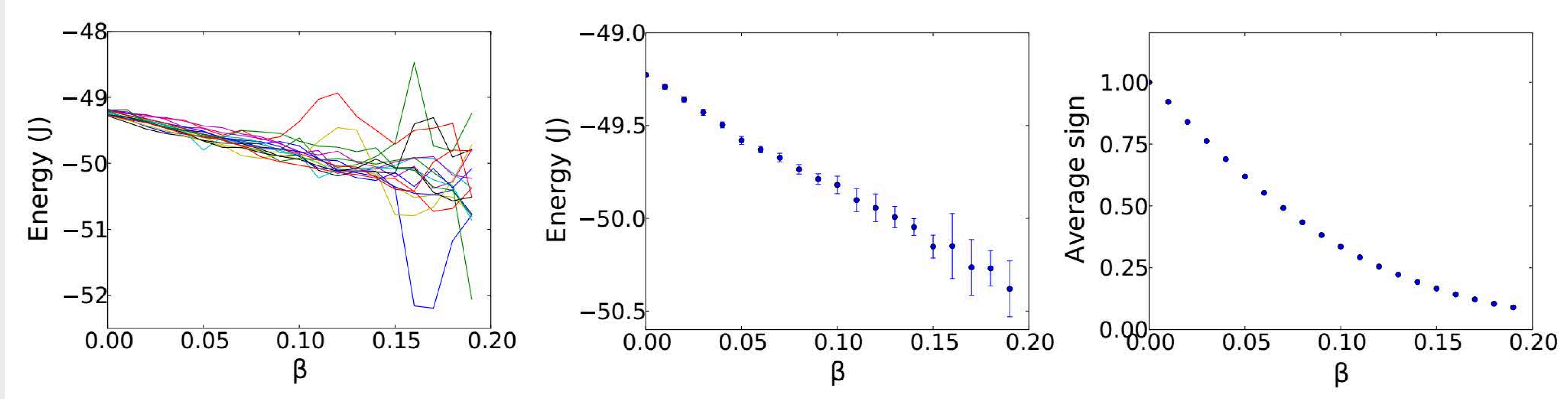
Test System

- Heisenberg Model on a Triangular Lattice
- 10 x 10 lattice
- open boundary conditions

$$H = \sum_{\langle i,j \rangle} S_i \cdot S_j$$



Methods



Exact (Stochastic) Projection $|\Psi_0\rangle = \exp[-\beta H]|\Psi_T\rangle$

Ψ_T

- Sample R with probability $|\Psi_T(R)|^2$
- Apply $G(R \to R') = (I - \tau H(R,R'))\dfrac{\Psi(R')}{\Psi(R)}$
- Compute Observables

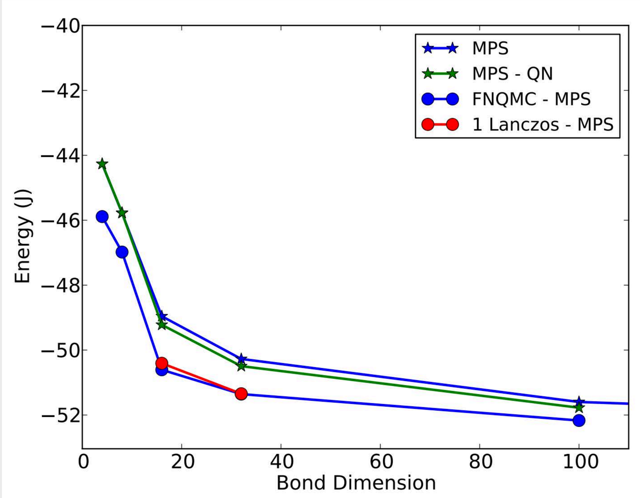
Cost: $O(D^\alpha)$ per Monte Carlo step

Ψ_0

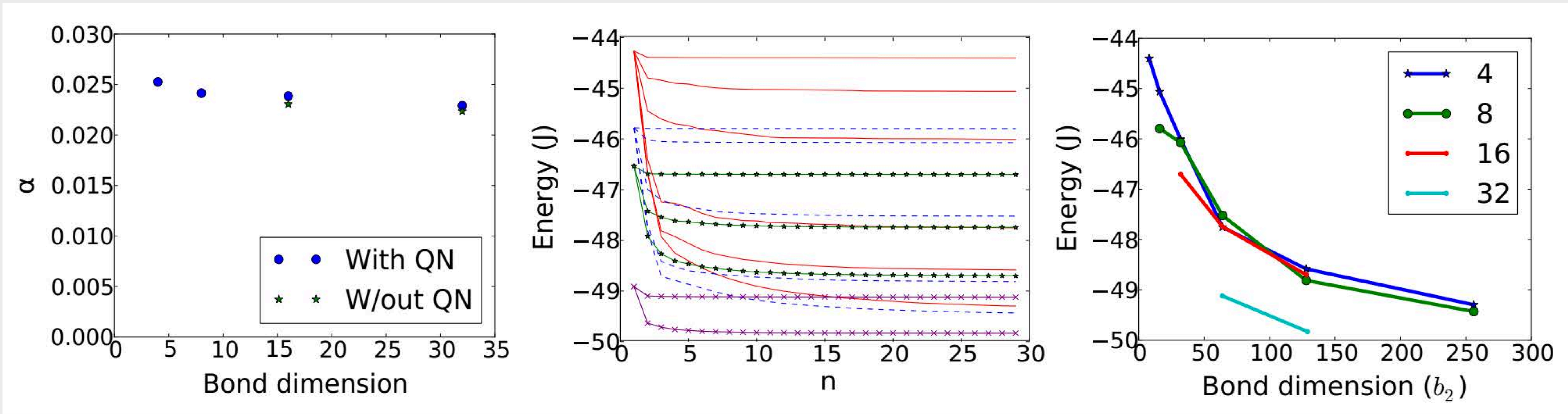
Fixed Node $\boxed{H} \to \boxed{H_{\mathrm{FN}}[\Psi_T]}$

Bad sign problem
Exact

No sign problem
Approximate
Upper Bound



Lanczos++



Basis: $\{|\Psi\rangle, H|\Psi\rangle, H^2|\Psi\rangle, H^3|\Psi\rangle, H^4|\Psi\rangle, \ldots\}$

Solve: $H|\Psi\rangle = ES|\Psi\rangle$ in this basis

Exactly: 3 basis elements

Approximately: 30 basis elements

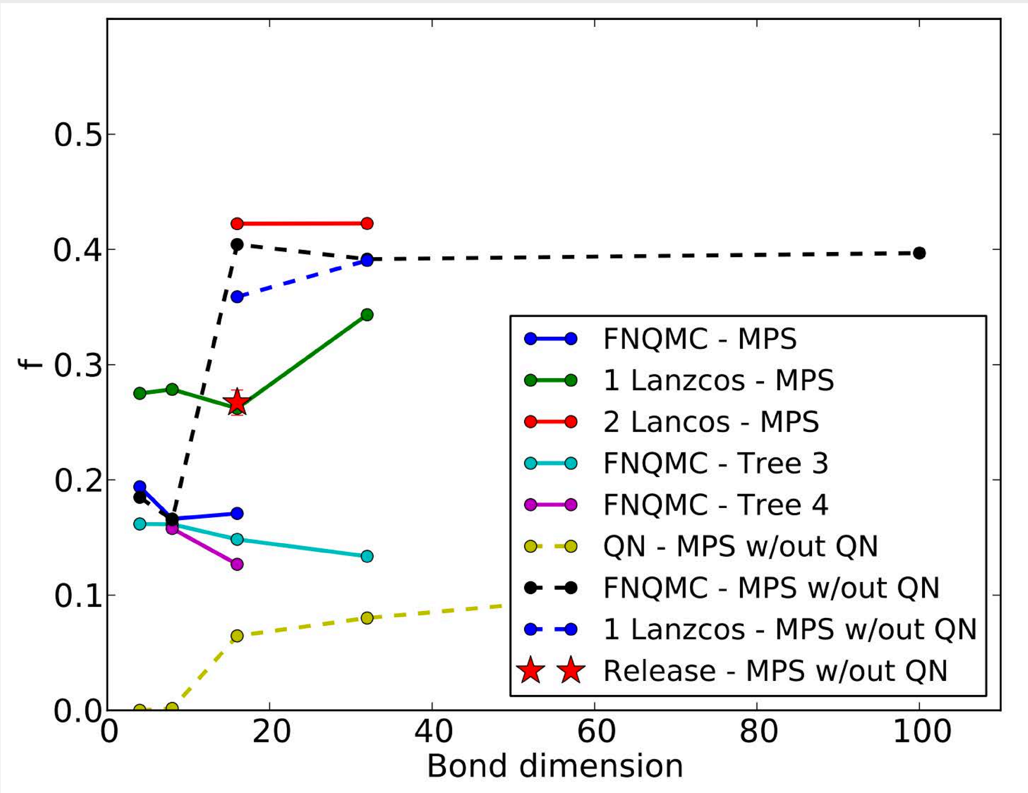
Ways to (exactly) compute basis

- MPS/MPO Formalism
- Quantum Monte Carlo
- Hybrid QMC/MPO

Way to (approximately) compute basis

- Apply $H|\Psi\rangle$ via MPO
- Truncate to smaller bond dimension b2
- Iterate

Results



Conclusions

These 4 approaches allow us to push beyond what is possible with tensor networks alone. We believe future applications using PEPS and other tensor networks will show even more significant gains.

Exact (Stochastic) Projection

Fixed Node

Exact Lanczos (3 basis elements)

Approximate Lanczos (30 basis elements)

References

1. S. Sorella, Phys. Rev. B 64, 024512 (2001)
2. E. Heeb and T. Rice, Physik B Condensed Matter 90, 73 (1993).
3. H. J. M. van Bemmel et al., Phys. Rev. Lett. 72, 2442 (1994)
4. H. J. M. van Bemmel et al., Phys. Rev. Lett. 72, 2442 (1994)
5. The ITensor library is a freely available code developed and maintained on http://itensor.org/index.html.
6. D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. 45, 566 (1980)
7. M. Kolodrubetz and B. K. Clark, Phys. Rev. B 86, 075109 (2012).
8. E. Stoudenmire and S. R. White, New Journal of Physics 12, 055026 (2010).
9. A. W. Sandvik and G. Vidal, Phys. Rev. Lett. 99, 220602 (2007)
10. U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005)
11. M. d. C. de Jongh, J. Van Leeuwen, and W. Van Saarloos, Physical Review B 62, 14844 (2000)

Acknowledgements

We acknowledge support from grant DOE, SciDAC FG02-12ER46875. Computation was done on Blue Waters (award number ACI 1238993) and TauB. We thank Cyrus Umrigar for discussions and critical reading of the manuscript, Katie Hyatt and Michael Kolodrubetz for useful conversations and Miles Stoudenmire for help with ITensor.