# Minimally entangled typical thermal states of fermions in DMRG++

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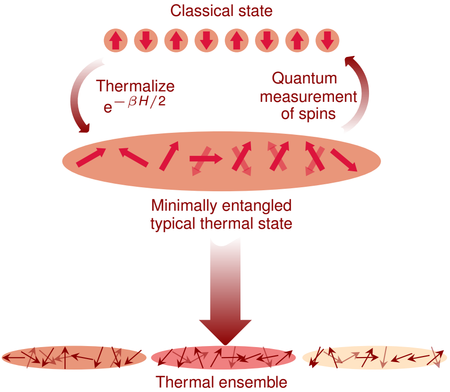



Adapted from Schollwöck, 2009

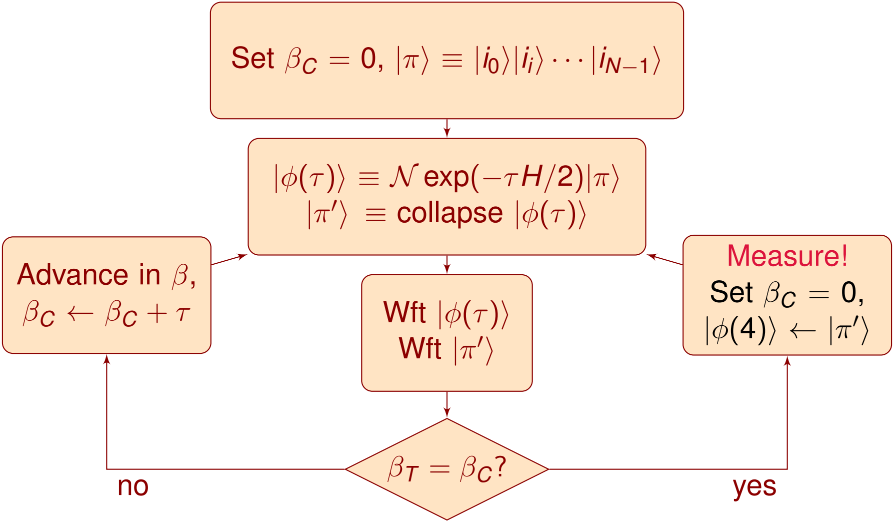
# Krylov-space Imaginary Time Evolution

Alvarez, 2013

G. Alvarez, Production of minimally entangled typical thermal states with the Krylov-space approach,
Phys. Rev. B 87, 245130, (2013)

http://arxiv.org/abs/1307.8034

# The Krylov-space Recipe



# We use Krylov-space Time Evolution

Tridiagonalize $H = V^\dagger T V$ starting Lanczos with $|\phi\rangle$.
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Finally,* compute the evolution with

$$\exp(\alpha H)|\phi\rangle_i = \sum_{k,k',k'',j} V^*_{i,k} S^\dagger_{k,k'} \exp(\alpha d_{k'}) S_{k',k''} V_{j,k''} |\phi\rangle_j$$

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* This is within a DMRG method, so don't forget to target the appropriate states. For an implementation, see Alvarez et al., 2011.

# The "Collapse" Step and Ergodicity

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$$\underset{\text{CPS}}{|\pi\rangle} \xrightarrow[\beta]{\text{evolve}} \frac{e^{-\beta H_0/2}|\pi\rangle}{\langle\pi|e^{-\beta H_0}|\pi\rangle} \underset{\text{natural basis}}{\overset{\text{collapse}}{\Longrightarrow}} |\pi'\rangle$$

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When collapsing into the natural basis, $|\pi'\rangle$ does not depend on $\mu$!

Therefore, observables don't depend on $\mu$, and we get incorrect results.

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One collapses in a random basis $|\alpha_i\rangle = \sum_{\eta_i} M_{\alpha_i,\eta_i}|\eta_i\rangle$

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$$|\phi(\tau)\rangle = \sum_{\alpha_L,\alpha_i,\alpha_R} A_{\alpha_L,\alpha_i,\alpha_R} \sum_{\eta_i} M_{\alpha_i,\eta_i}|\alpha_L\rangle|\eta_i\rangle|\alpha_R\rangle \equiv \sum_{\eta_i} |\bar{\pi}(\eta_i)\rangle,$$

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The new state $\mathcal{N}\bar{\pi}(\eta_i)$ is collapsed with probability

$$p(\eta_i) = ||\bar{\pi}(\eta_i)\rangle||^2$$

# The “Collapse” Step and Ergodicity

To avoid ergodicity problems in METTS,

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To avoid ergodicity problems in METTS,

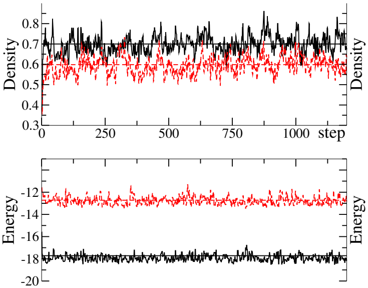
we collapse into a random basis.

Local symmetries are not preserved anymore.

For example, one uses the grand canonical ensemble.

# Accuracy and Convergence

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} V_i n_{i,\sigma},$$



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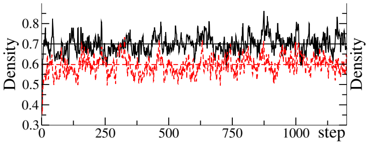
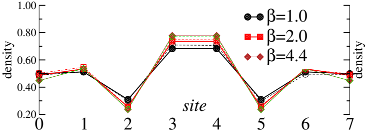
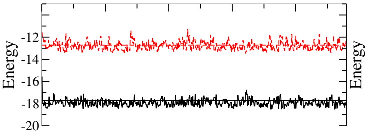
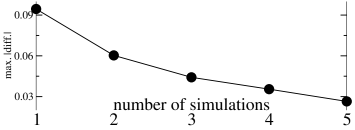


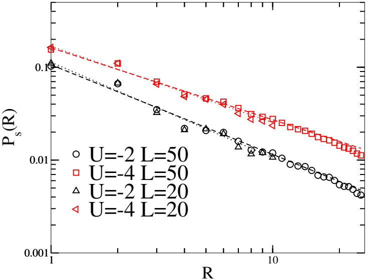



# Hubbard Chain at $T > 0$

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \mu \hat{N}$$




Hubbard chain with length $L$ (as indicated) for $T = 0$.

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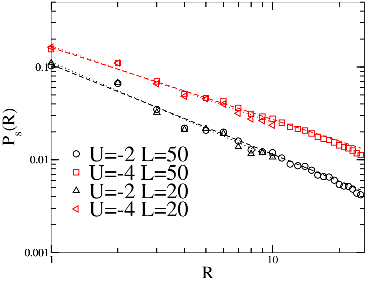


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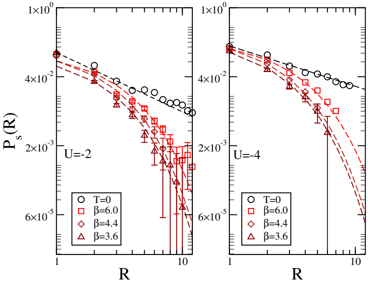


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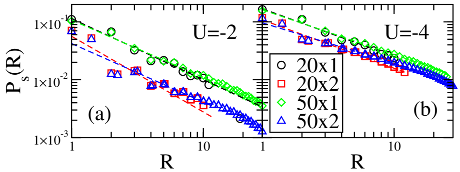

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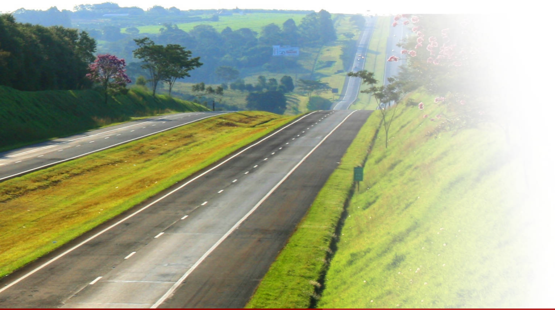

# The Road Ahead: Our Strategic Vision

- Make tons of improvements to our codebase
- Implement parallel DMRG
  Stoudenmire and White, 2013
- Work towards 2D DMRG
- Develop a matrix product states code
- Stay at the vanguard of renormalization methods

Corboz and Vidal, 2009, Evenbly and Vidal, 2009, Koenig et al., 2009, M. Aguado, 2008
M. Rizzi, 2008, Pfeifer et al., 2009, Vidal, 2008, Barthel et al., 2009, Kraus et al., 2010

# Summary

- PRB Paper:
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This talk is at `https://web.ornl.gov/~gz1/talks/`

# Credit Line


## Thanks to:

K. Al-Hassanieh, E. Dagotto, L. Dias da Silva, P. Kent, T. Maier, S. Manmana, E. Stoudenmire, J. Rincón, M. Summers, S. R. White.

## Credit Line

This work was supported by the Center for Nanophase Materials Sciences, sponsored by the Scientific User Facilities Division, Basic Energy Sciences, U.S. Department of Energy, under contract with UT-Battelle. This research used resources of the National Center for Computational Sciences, as well as the OIC at Oak Ridge National Laboratory. G.A. acknowledges support from the DOE Early Career Research Program. Thanks to U.S. DEPARTMENT OF ENERGY | Office of Science

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# Colophon

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