How best to attenuate the exponential barrier

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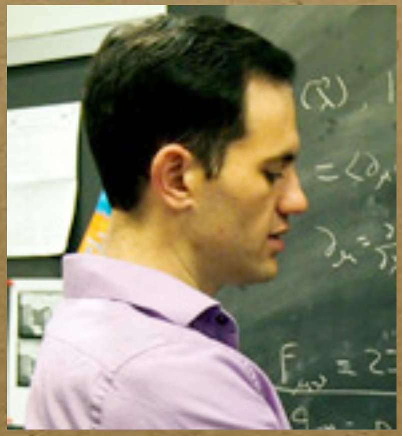
Simon's Meeting: September 4, 2014



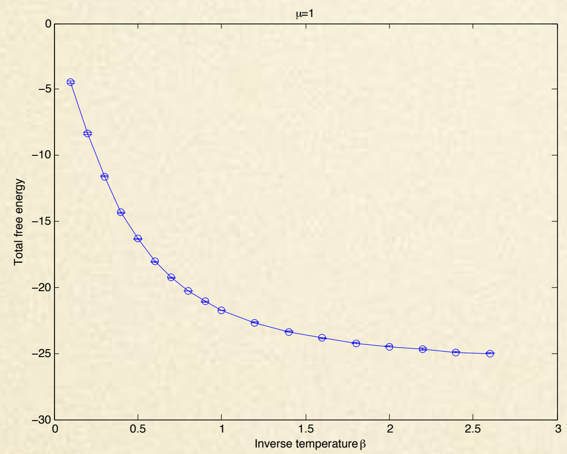
Our group works on simulating strongly correlated systems. We are currently attacking the Hubbard model as a stepping stone toward more sophisticated models.

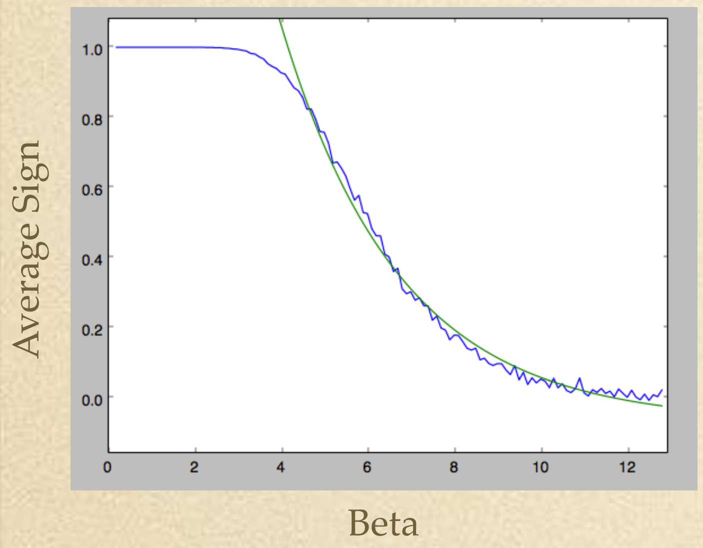
Finite T

DQMC

METTS

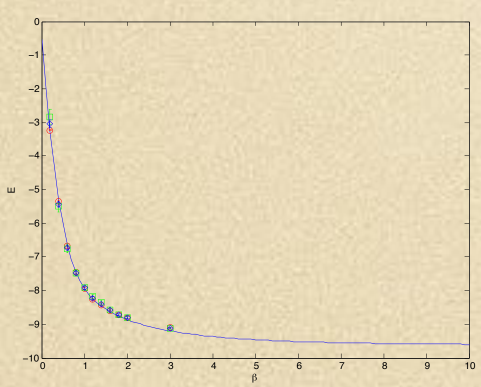
PIMC

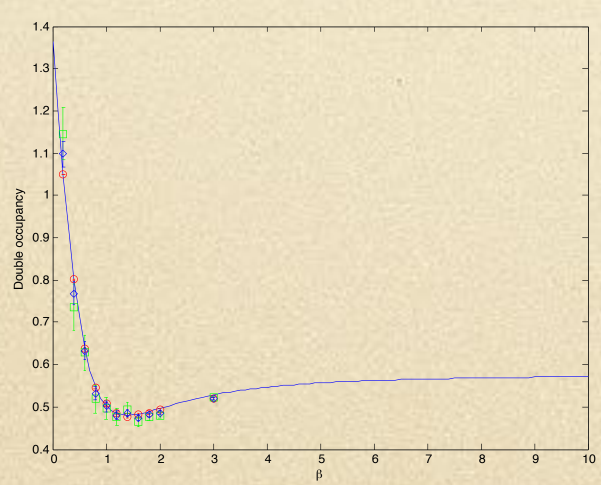




FT PMC

FT VMC

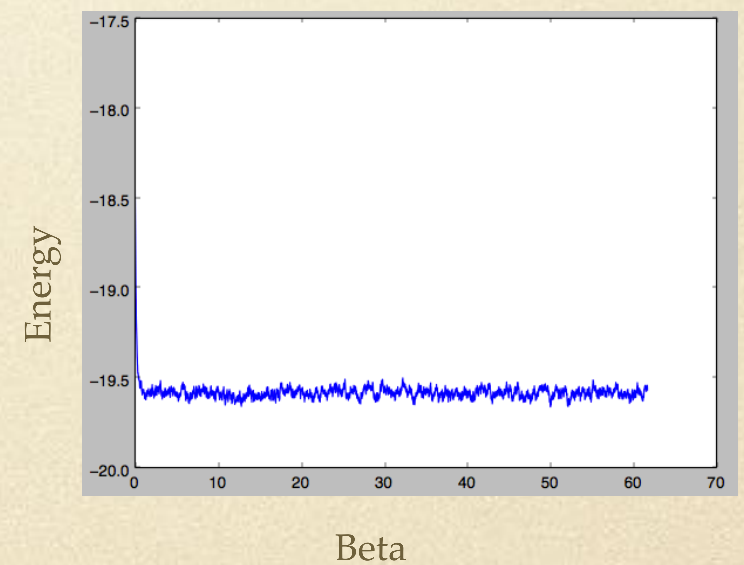


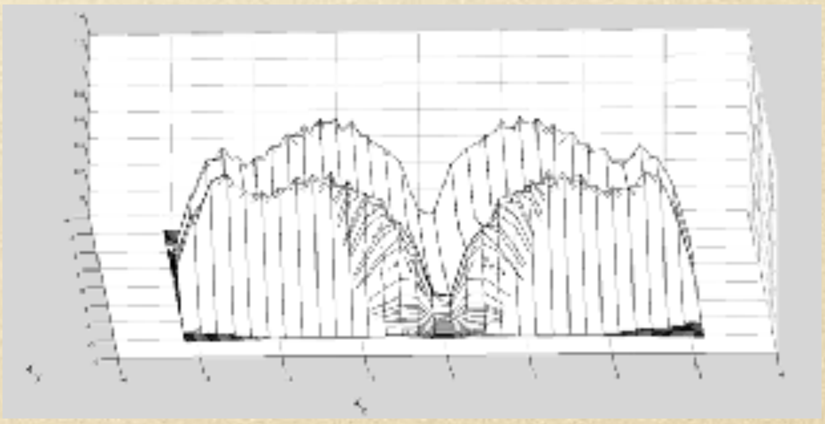


Ground State

VMC

DMRG
PEPS
TN
AFQMC
DMC
FCIQMC





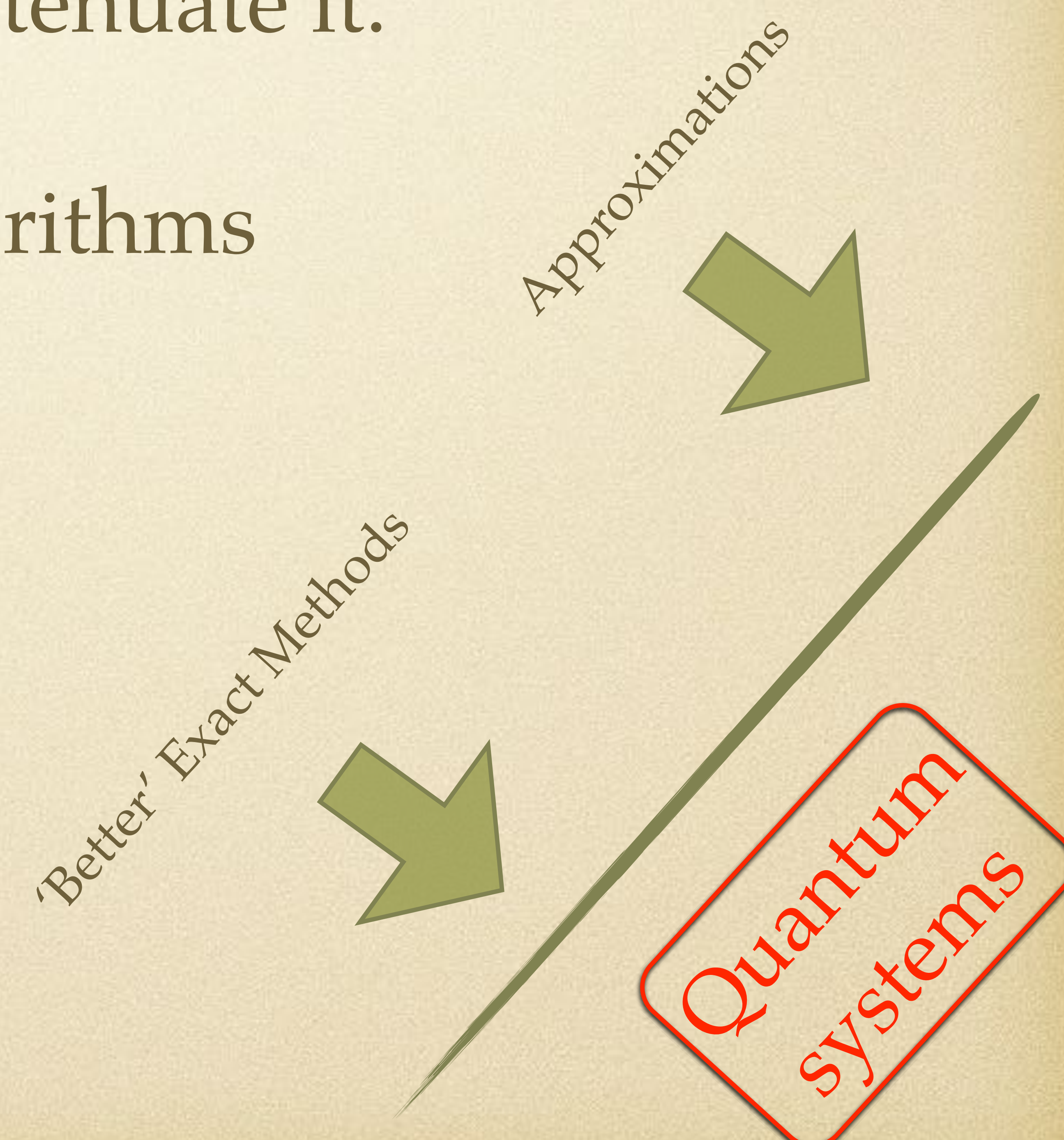
An Exponential Problem

There's an exponential wall to simulating quantum systems.

A (only slightly) biased view on the state of the art to attenuate it.

With a few new algorithms

- Partial Node FCIQMC
- Release FCIQMC
- Release + FN MPS
- Efficient Multi-MPS
- SEMPS



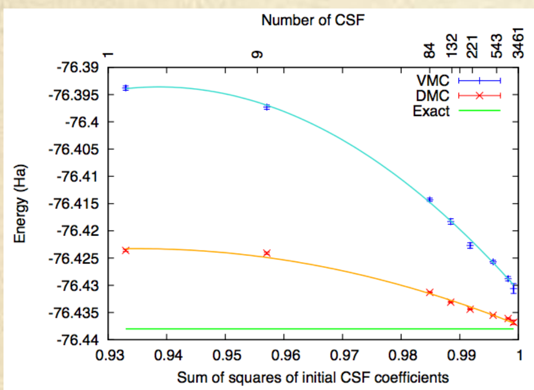
Variational

Approach I: Just write down the wave-function

Exponential number of terms

- Multislater -Jastrow++

$$|\Psi\rangle = \exp[-J(R)] \sum_k \alpha_k \det M_{\uparrow,k} \det M_{\downarrow,k}$$



exponential number of determinants

No sign problem but "bond-dimension" problem.

- PEPS or Huse-Elser or MERA

- Multi-non-orthogonal SD + symmetry projection

- MPS

Optimize without quantum numbers and project afterwards gains non-trivial energy. On triangular lattice, ~10%

- **Multi-MPS**

exponential in width

Multi-MPS

$$\alpha|\Psi_{MPS1}\rangle + \beta|\Psi_{MPS2}\rangle + \gamma|\Psi_{MPS3}\rangle$$

How do we choose the MPS

Optimize?

Faster approach to get reasonable states...

Exact: $\{|\Psi_{MPS}\rangle, H|\Psi_{MPS}\rangle, H^2|\Psi_{MPS}\rangle, \ldots\}$

Approx: $\{|\Psi_{MPS}\rangle, PH|\Psi_{MPS}\rangle, PHPH|\Psi_{MPS}\rangle, \ldots\}$

Better: Let $H=h_1+h_2+h_3+h_4+h_5$

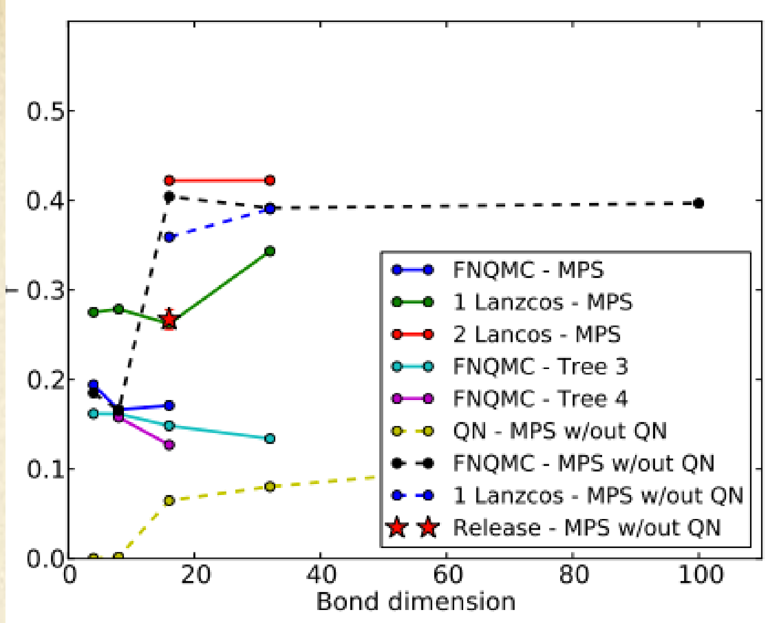
$$\{|\Psi_{MPS}\rangle, h_i|\Psi_{MPS}\rangle, h_i h_j|\Psi_{MPS}\rangle, \ldots\}$$

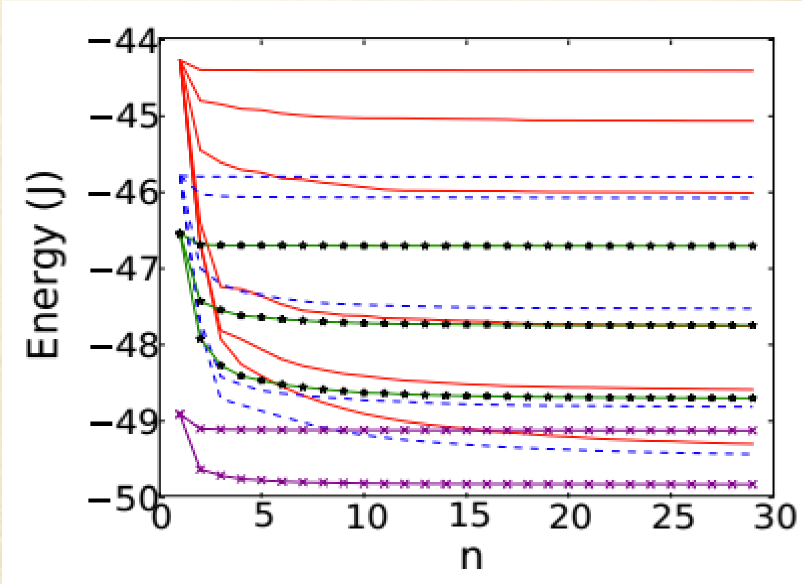
4x8 Hubbard Model:

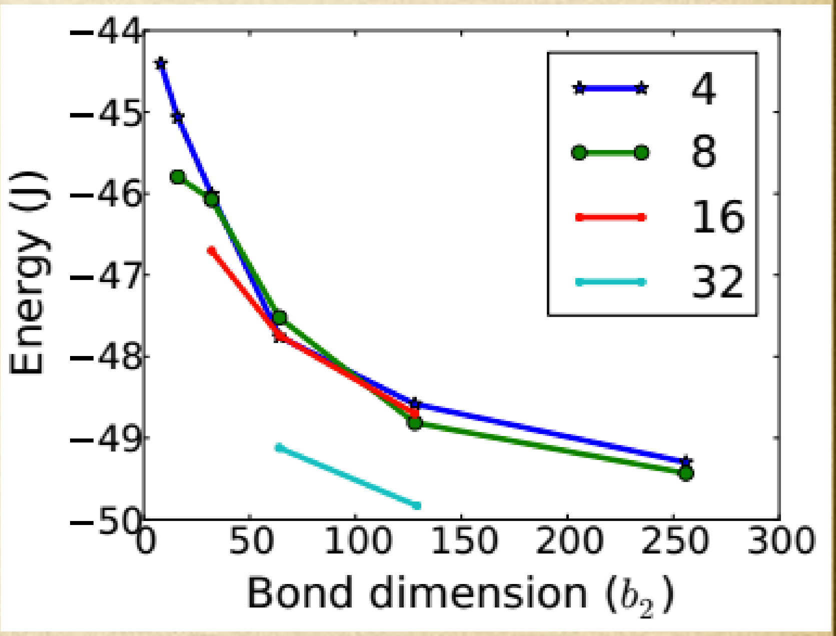
5 MPO's of size 6

1 MPO of size 18

For n=3, factor of 2000x faster!





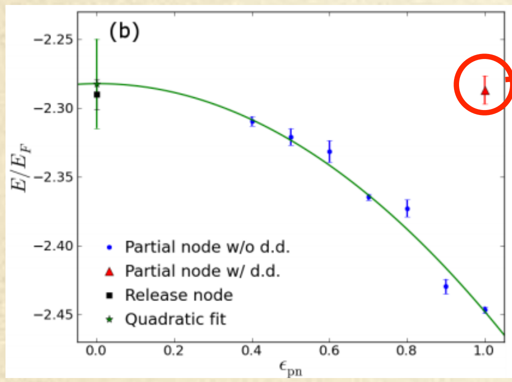


Variational ++

- Fixed Node: A (stochastic) sample of the w.f.

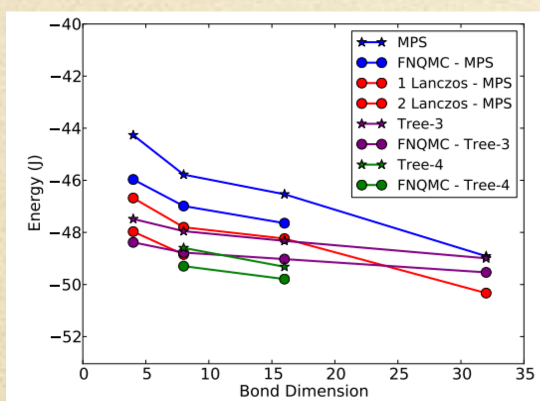
Two recent `improvements':

Fixed node for less-local Hamiltonians



10^6 connections

Fixed node on tensor networks



- Constrained Path:

Shiwei: Determinants

Garnet: MPS

Sample

Approach II: Sample

Sign Problem - Efficiency as $\exp[-\beta\Delta E]$

- PQMC + Annihilation

  Brings up Delta E

  - Kalos
  - + initiator: Ali Alavi

- AFQMC Free projection

Sample ++

Approach II: Sample

Sign Problem - Efficiency as $\exp[-\beta\Delta E]$

- PQMC + Annihilation

Brings up Delta E

Kalos

+ initiator: Ali Alavi

- AFQMC Free projection

- SEMPS

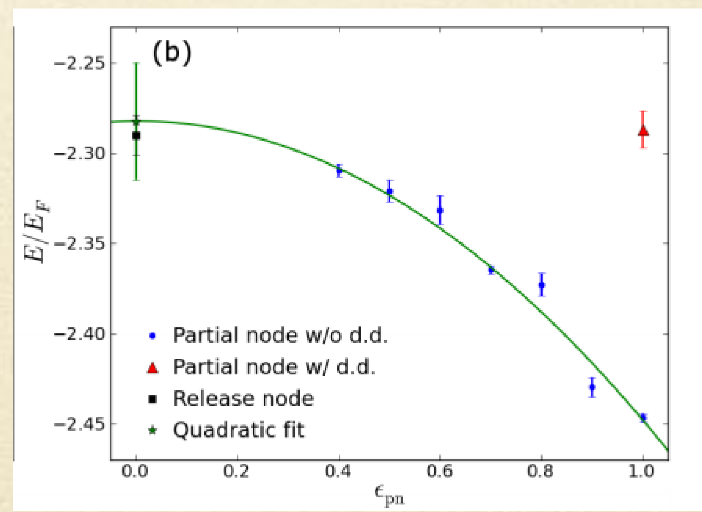
- AFQMC release

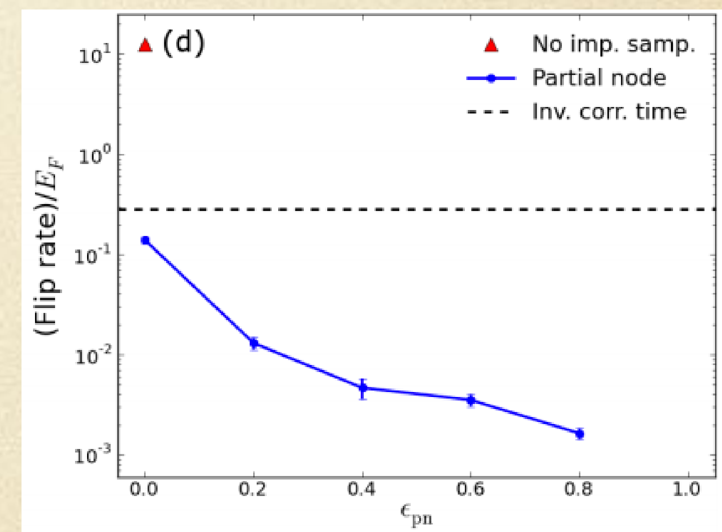
- Partial Node FCIQMC

Importance Sample +

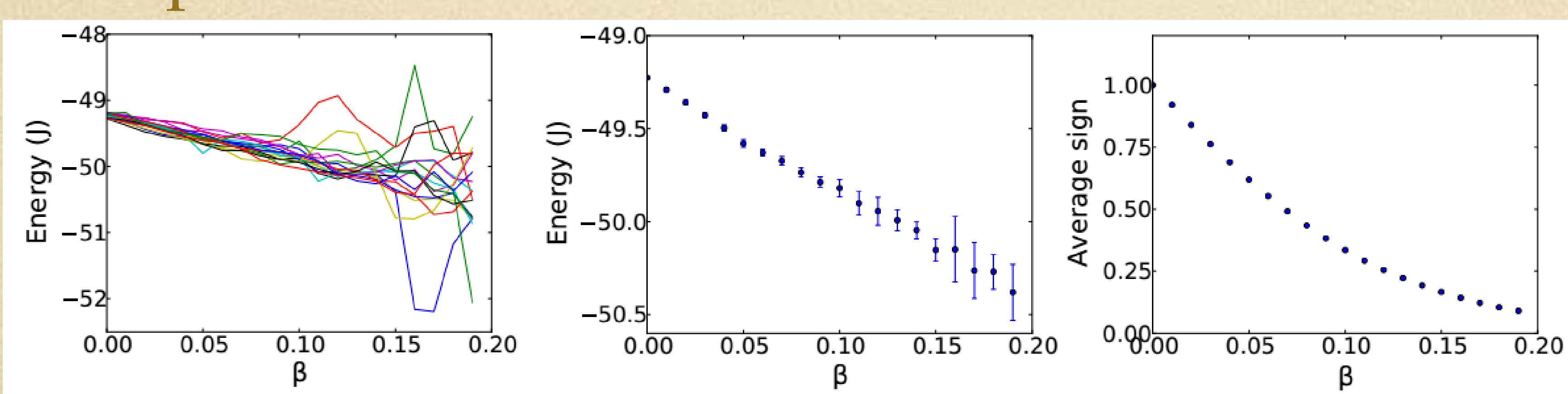
Partial Fixed-Node +

Annihilation

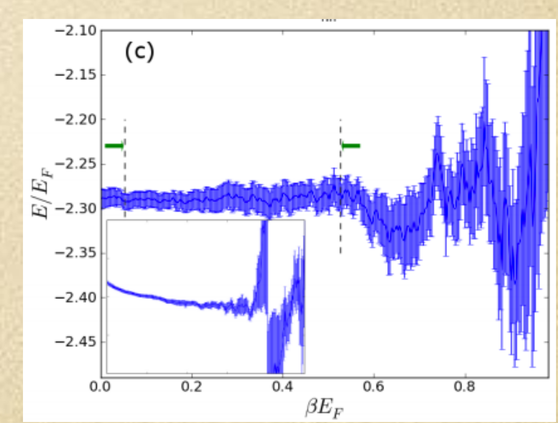




- Sample from Tensor Networks + Annihilation



- RFCIQMC



Approach II: Sample

Sign Problem - Efficiency as $\exp[-\beta\Delta E]$

Sample ++

- Annihilation + QMC

  Brings up Delta E

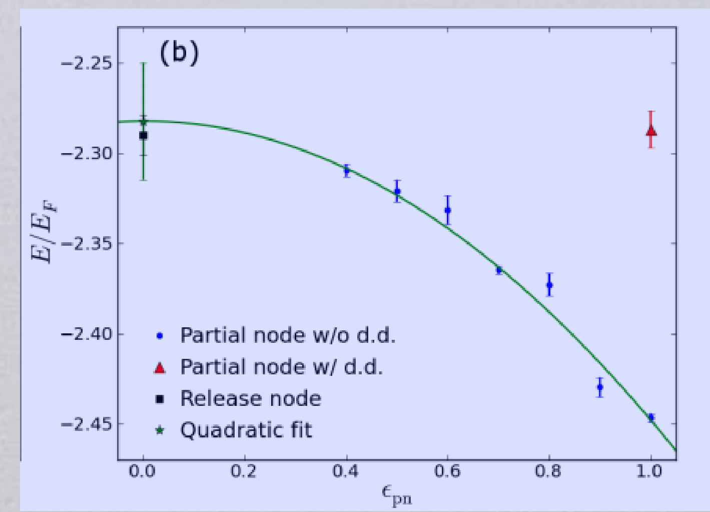
  - Kalos
  - + initiator: Ali Alavi

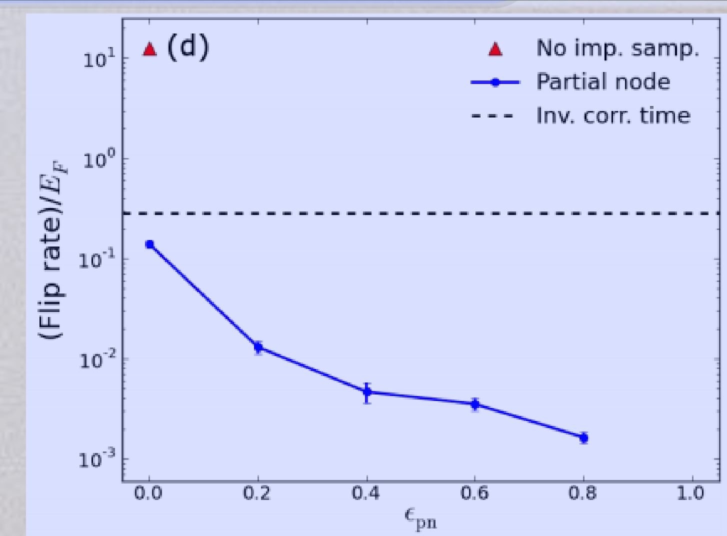
- AFQMC Free projection
- SEMPS
- AFQMC release
- Partial Node FCIQMC

  Importance Sample +

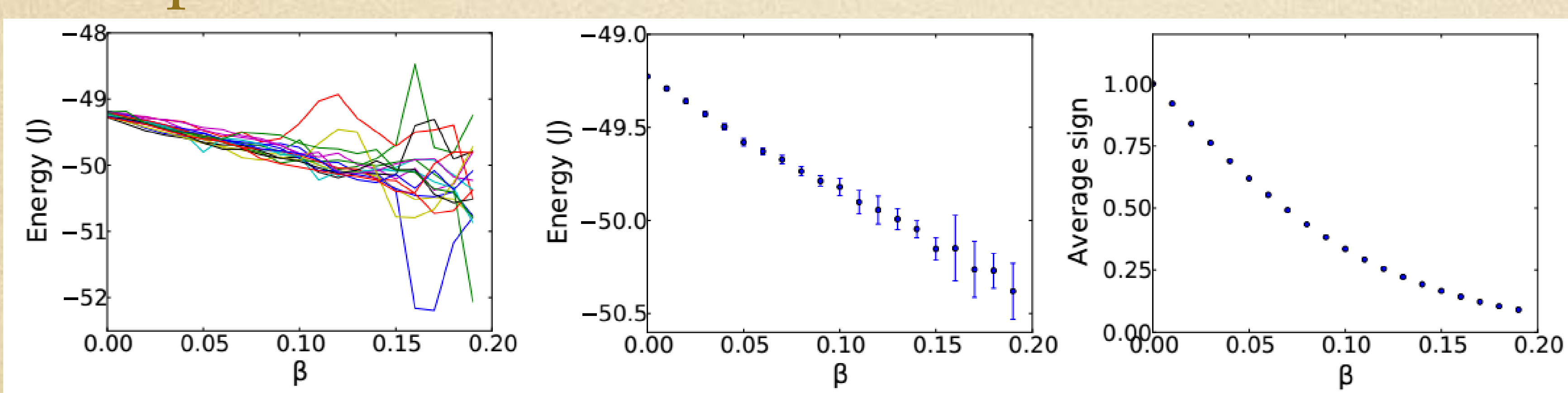
  Partial Fixed-Node +

  Annihilation





- Sample from Tensor Networks + Annihilation



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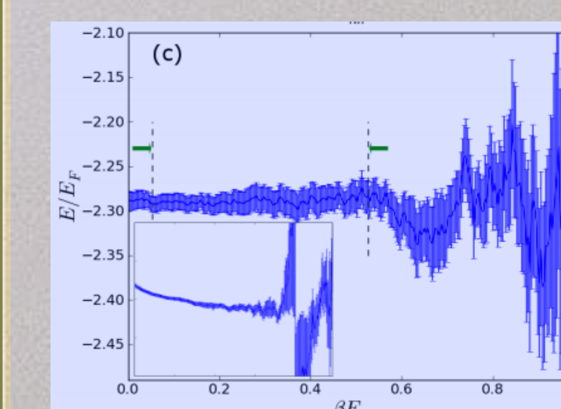


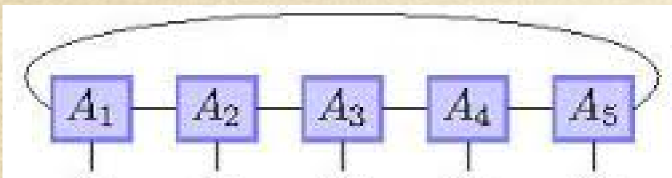
QMC: A Sign Problem

DMRG: A bond dimension problem.

Our goal is to write down an algorithm that has both a sign problem and a bond dimension problem.

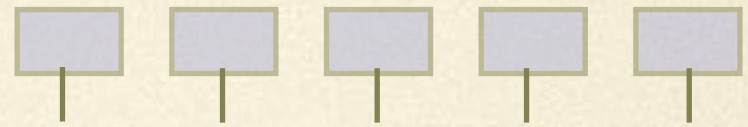
The worst of both worlds!

MPS



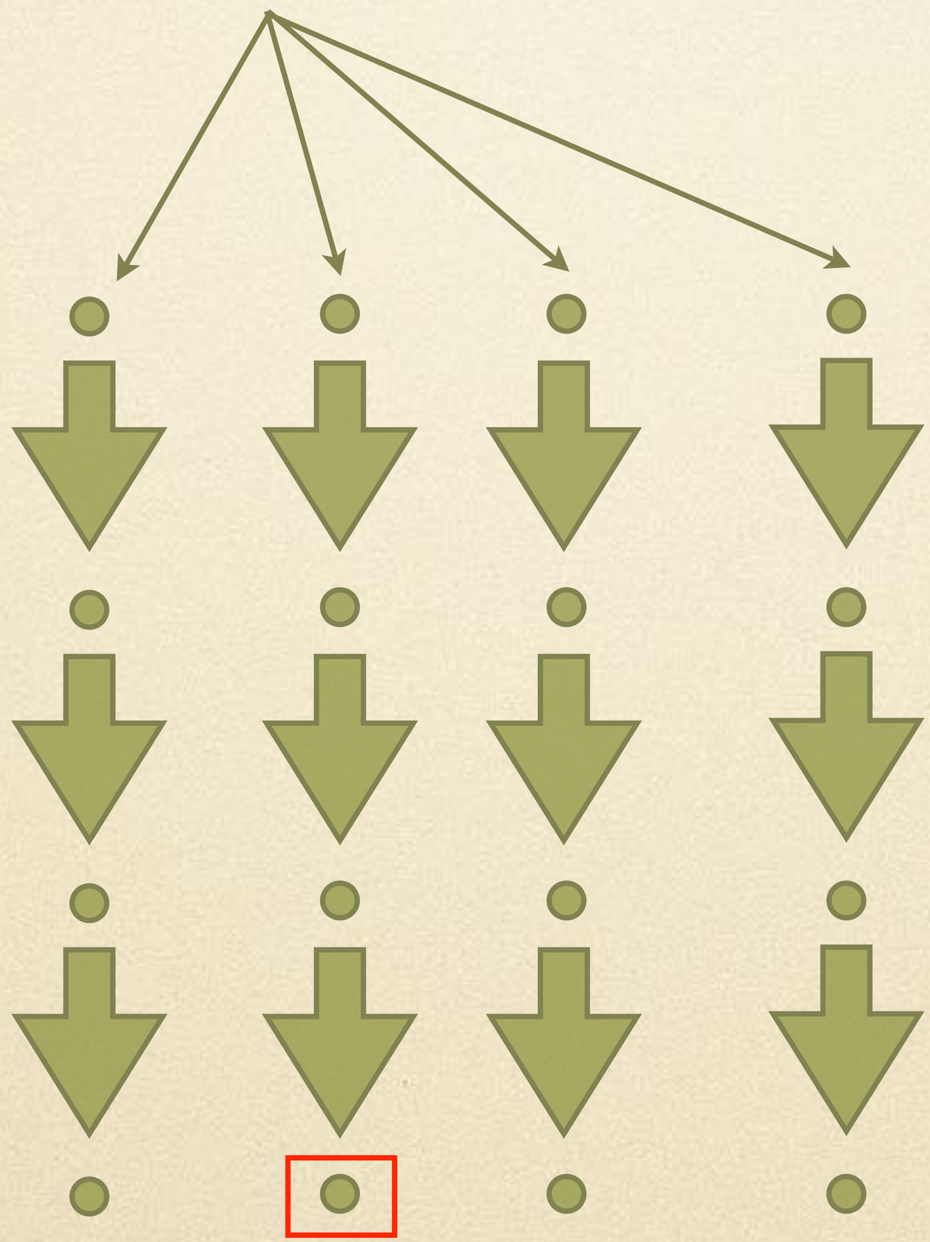
$=\sum$

Product states



Sample $|\langle MPS_1|C\rangle|^2$

weight $\boxed{\dfrac{1}{\langle MPS_1|C\rangle}}$



Bond dimension 1

Imaginary Time Evolve

Bond dimension small

Imaginary Time Evolve

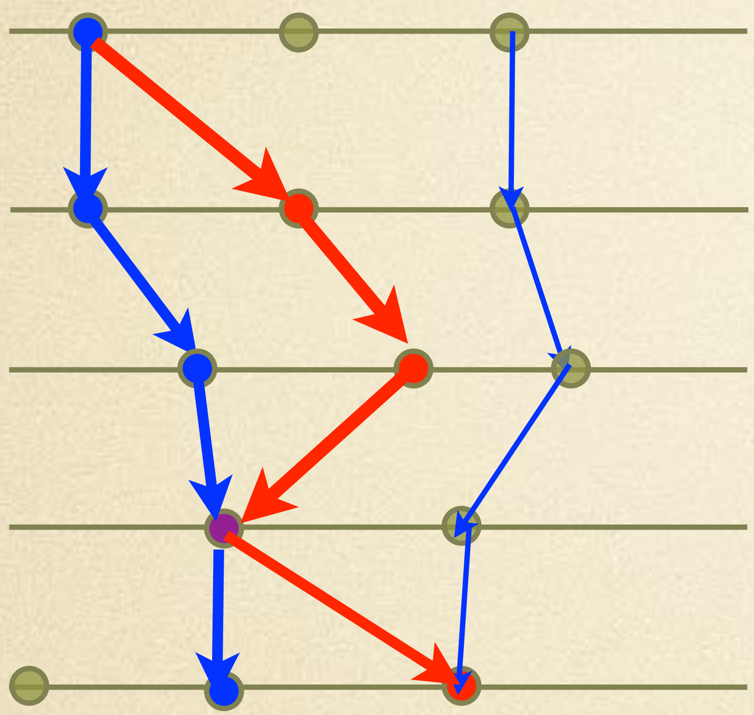
Bond dimension bigger

Imaginary Time Evolve

Energy: $$\frac{\sum_i \langle \boxed{\Psi_i} | H | \Psi_T \rangle \boxed{w_i}}{\sum_i \boxed{w_i}}$$

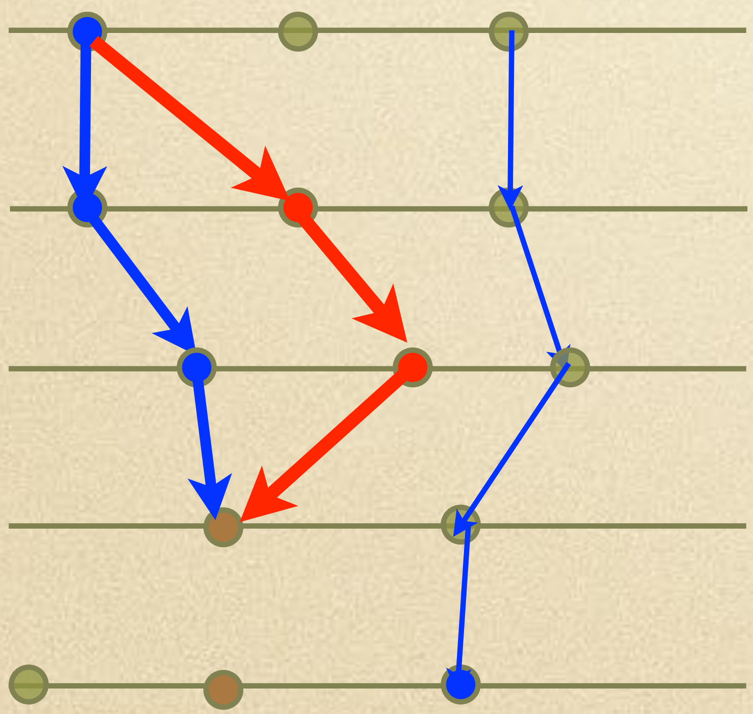
Annihilation

Without

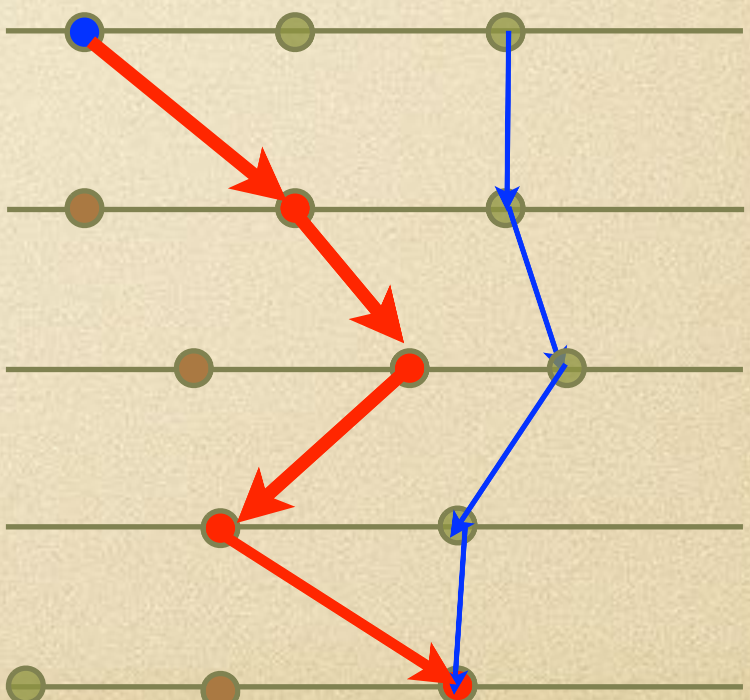


- Annihilation helps because paths of different signs cancel.
- Annihilation fails because you can't keep enough walkers to get cancellation of all paths.

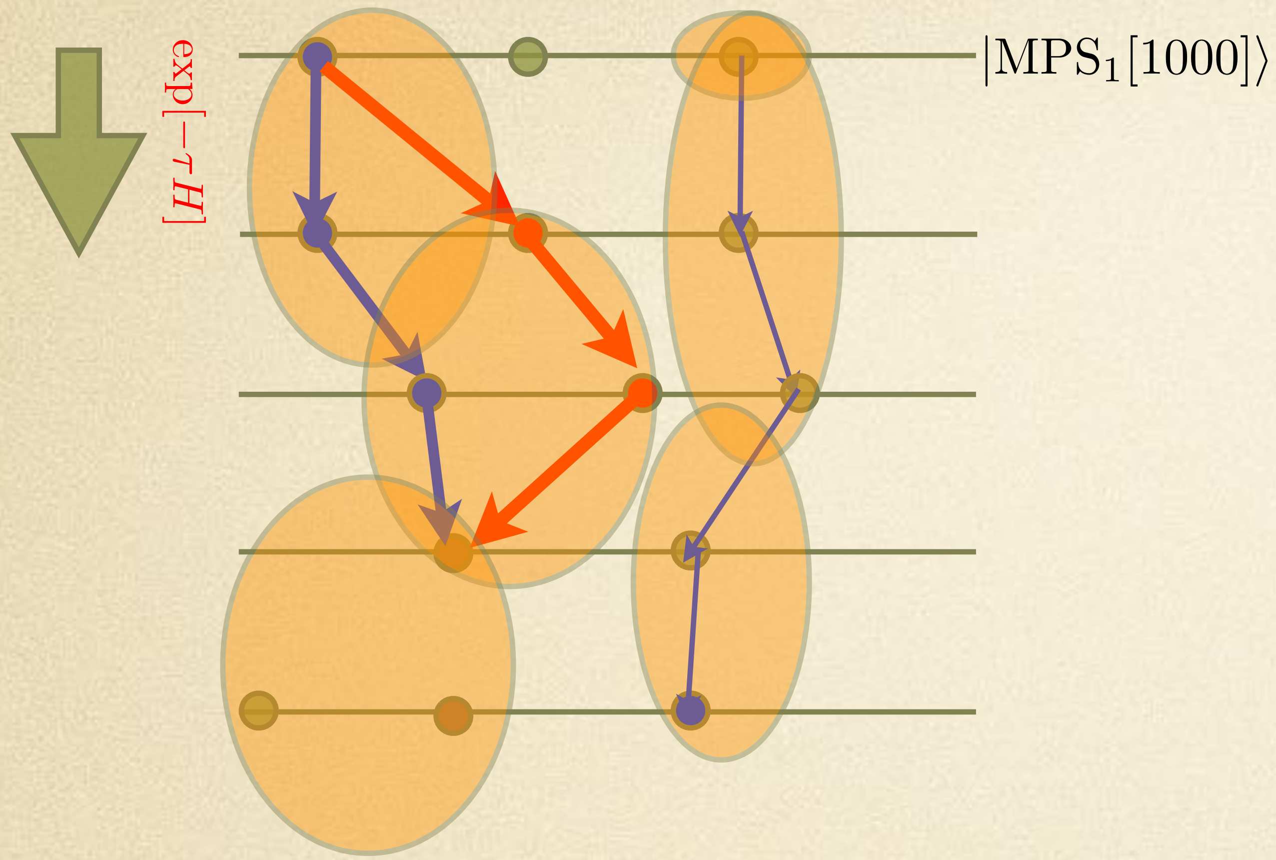
With



With but too few walkers

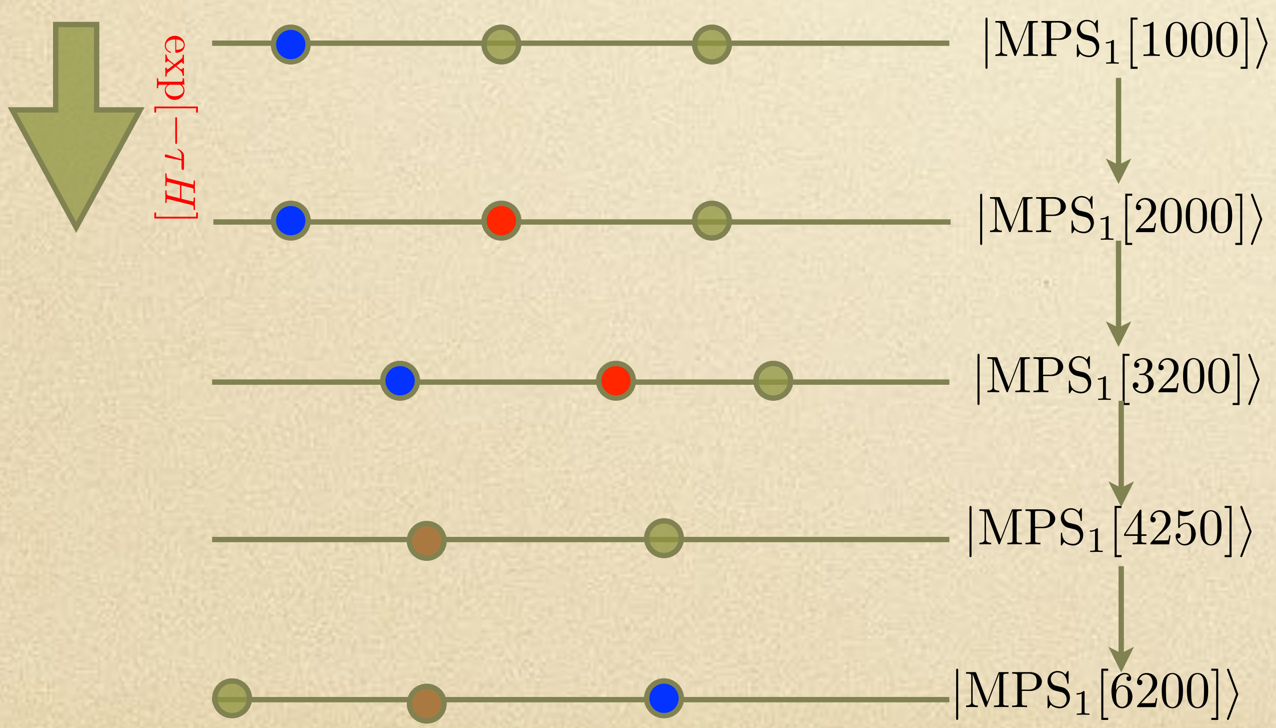


We'd really like perfect annihilation through all these paths.



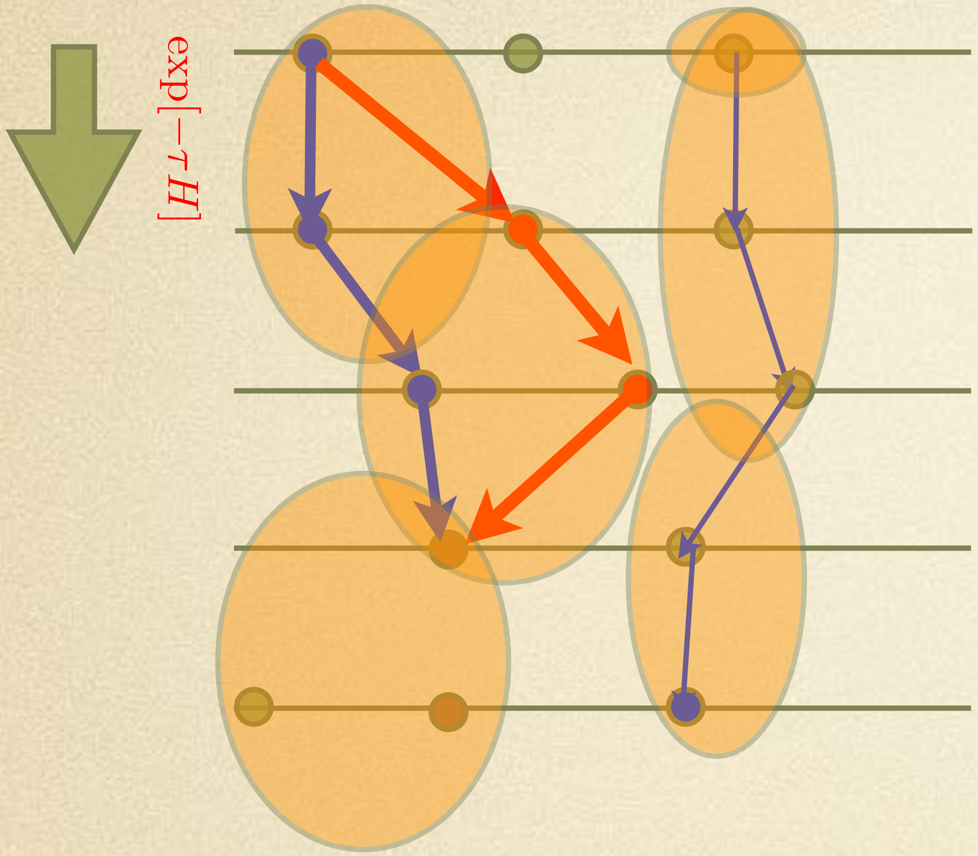
How can we do this?

We'd really like effectively higher bond dimension.



How can we do this?

We'd really like perfect annihilation through all these paths.



Sample | weight

$|MPS_1\rangle \approx |D_1\rangle + |D_3\rangle + |D_{20}\rangle + \ldots$ $\quad |\langle MPS_1|C\rangle|^2$ $\boxed{\dfrac{1}{\langle MPS_1|C\rangle}}$

$\exp[-\tau H]|D_1\rangle + \exp[-\tau H]|D_3\rangle + \exp[-\tau H]|D_{20}\rangle + \ldots$

Represented 'exactly' by MPS of small bond-dimension.

You run out of bond-dimension much slower.

You're already starting at the best MPS you can get for your bond dimension. You're guaranteed to be better.

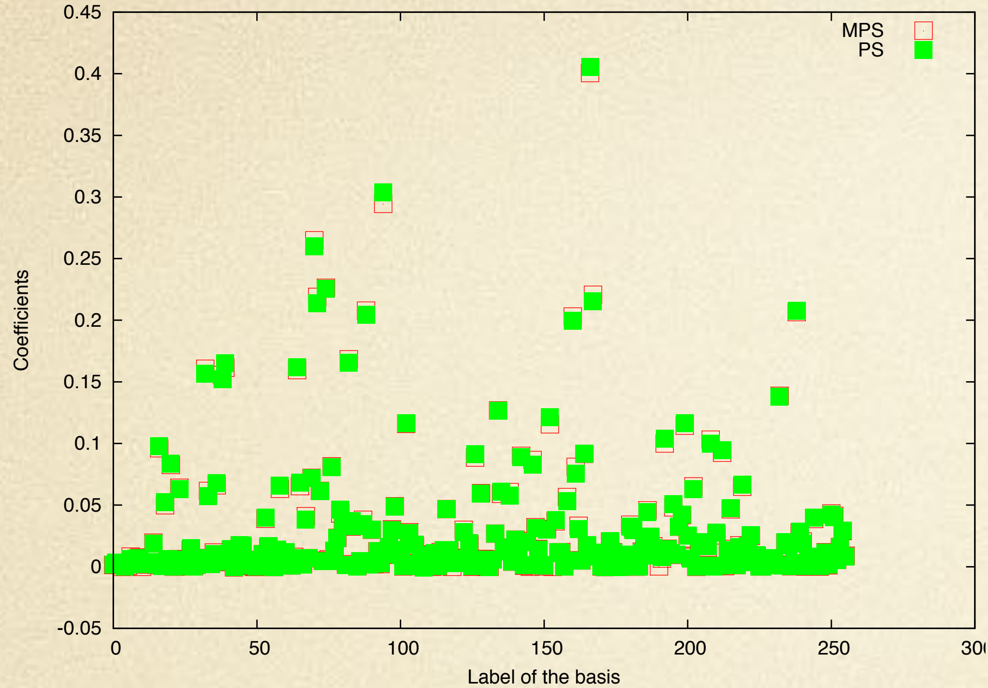
Massively Parallel

You do have a bond-dimension problem.

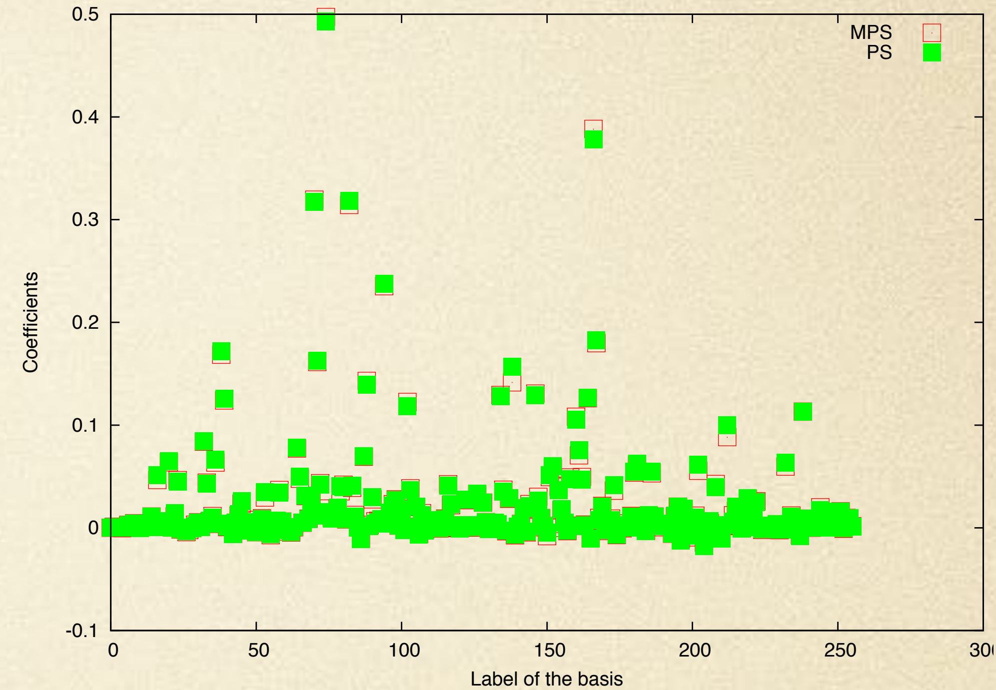
If $\mathrm{Sign}(\langle MPS_1|C\rangle) \neq \mathrm{Sign}(\langle \Psi_0|C\rangle)$, you have a weak sign problem.

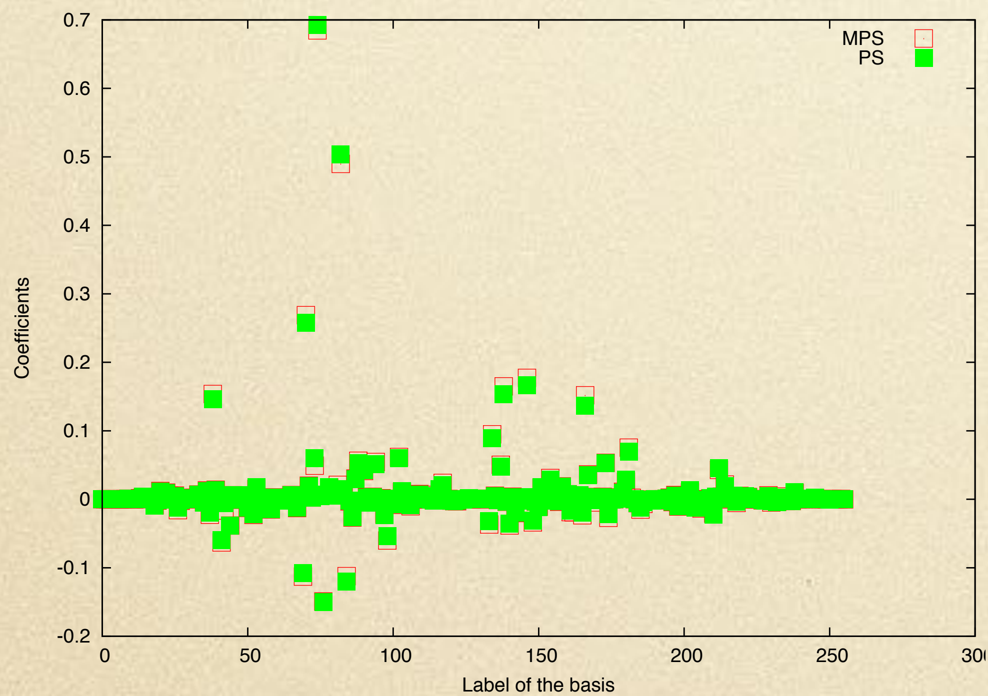
Proof of Principle

$\beta = 0.08$



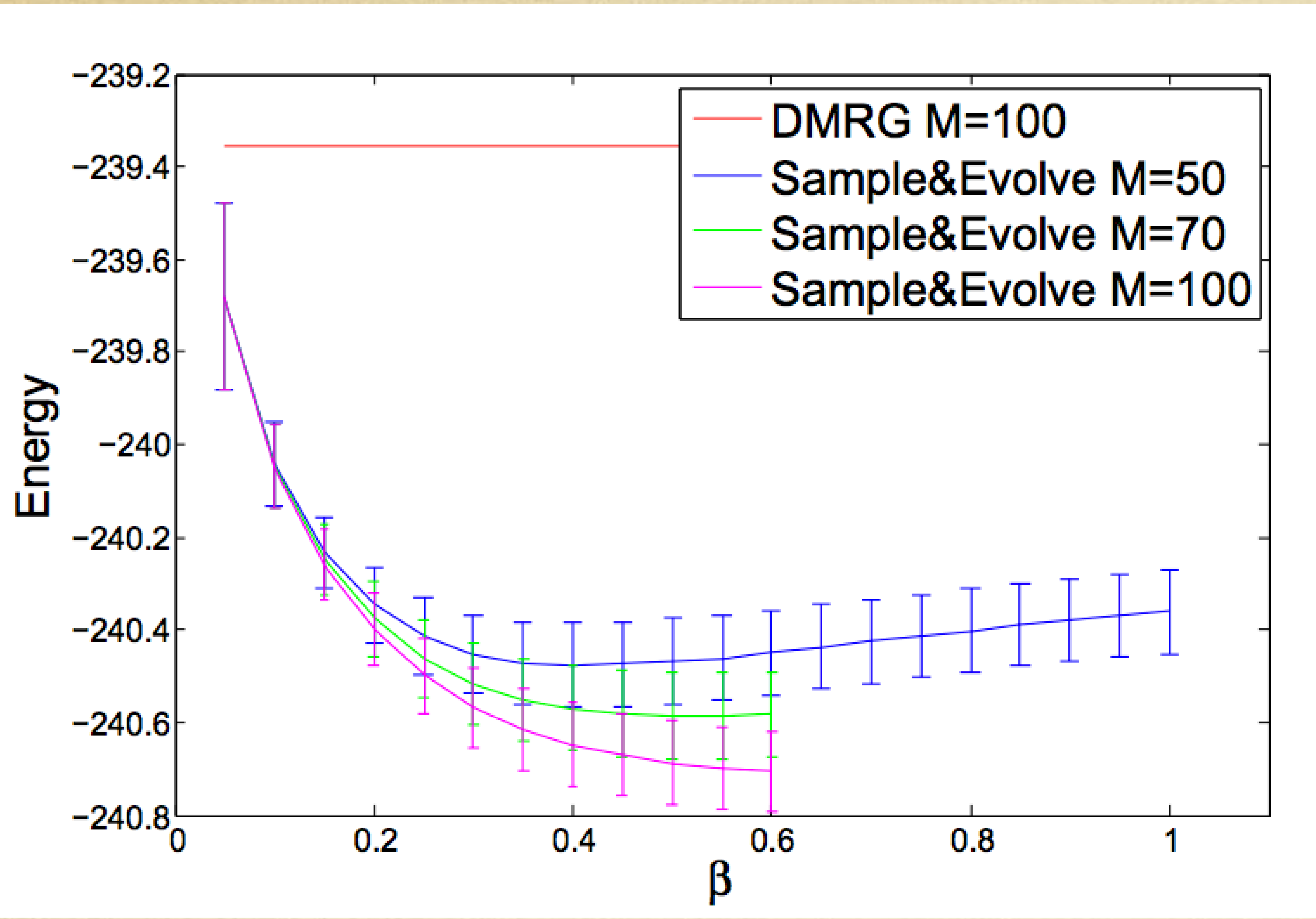
$\beta = 4.0$





Random MPS (M=8),

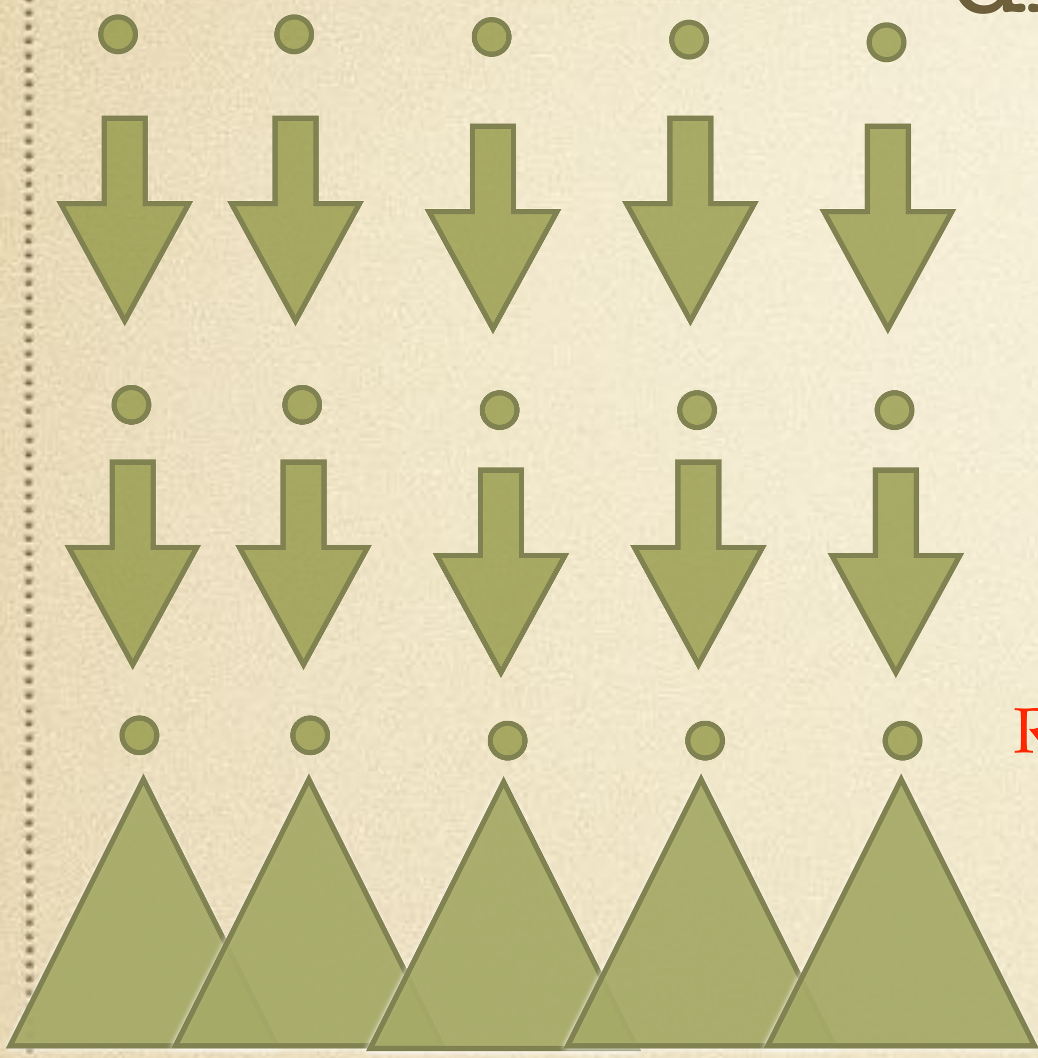
Proof of Principle



4 x 32 hubbard model

What to do when you run out of bond dimension?

SEMPS MC



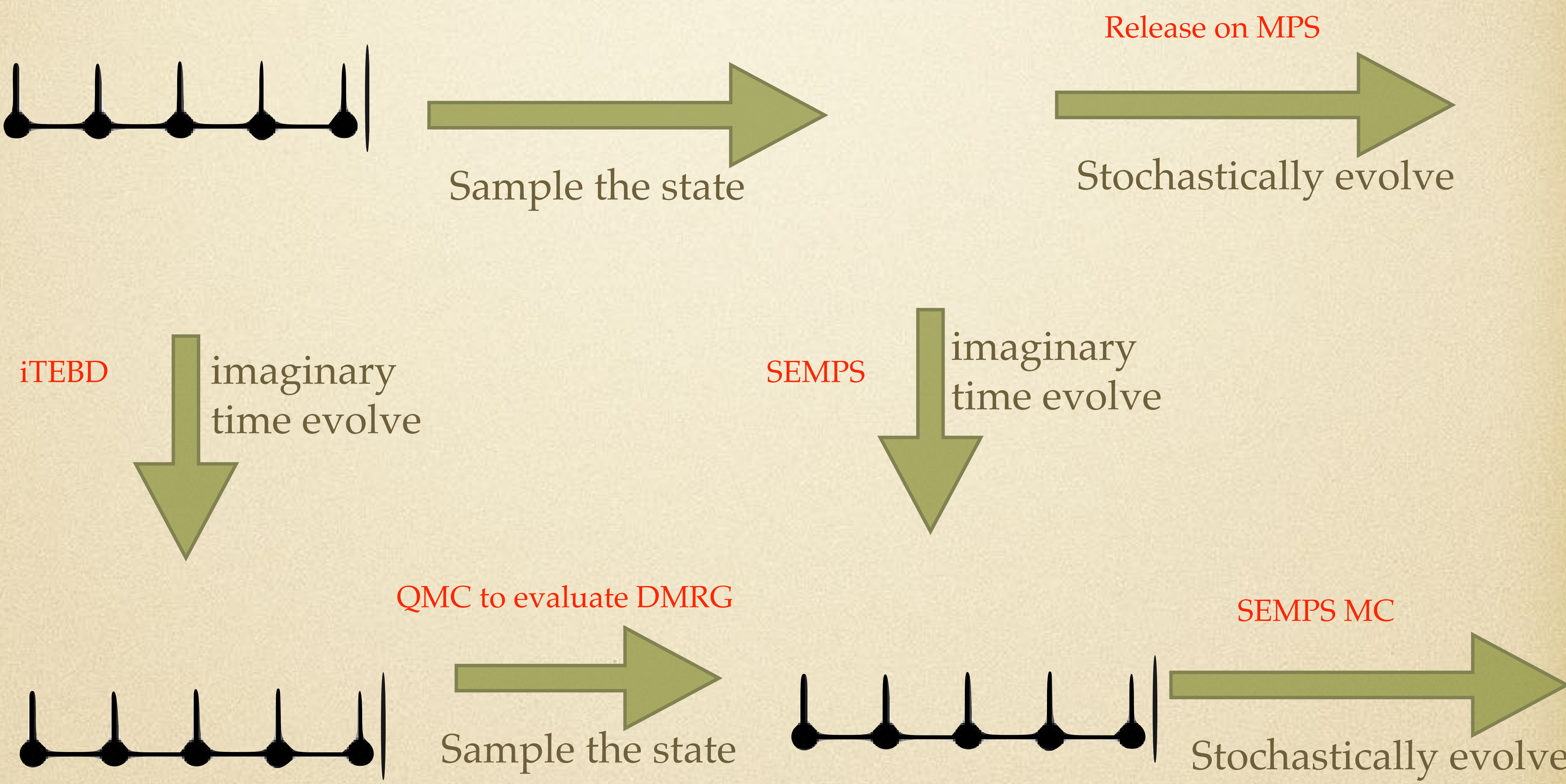
Resample here

Cone annihilation

Exact annihilation

A much smaller sign problem.

The best (or worst) of both worlds: SEMPS



Conclusions

DRMG+QMC gives us powerful new algorithms including

- Multi-MPS
- SEMPS
- Fixed-Node w/ MPS
- Release w/ MPS

<u>Pareto-Optimal:</u>

Multi-MPS SEMPS

Partial Node FCIQMC on Multi-MPS or Multi-Slater Jastrow

Release of CP AFQMC + SEMPS