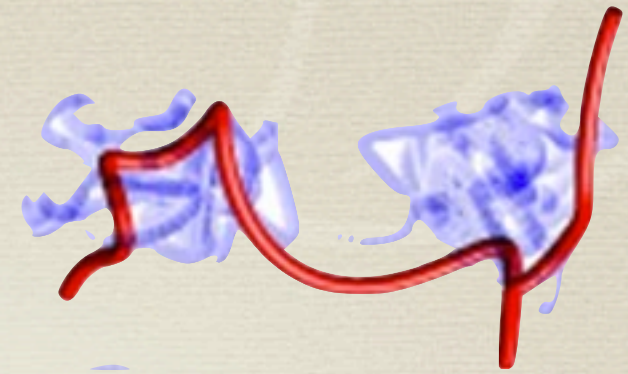
ALGORITHMS FOR FINITE TEMPERATURE QMC

Bryan Clark
Station Q

QMC INT Conference: June 12, 2013

Current de-facto standard for
fermions at finite temperature
Restricted Path Integral Monte Carlo!



* see PIMC++

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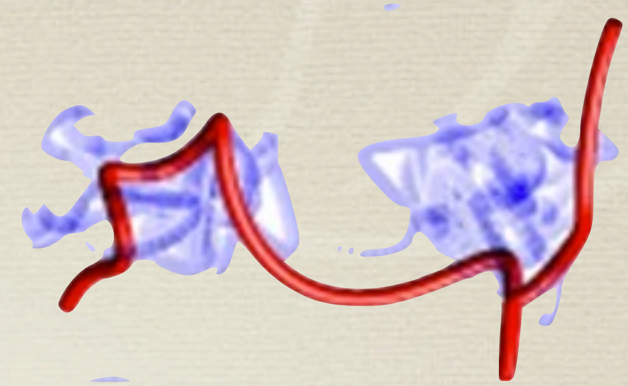
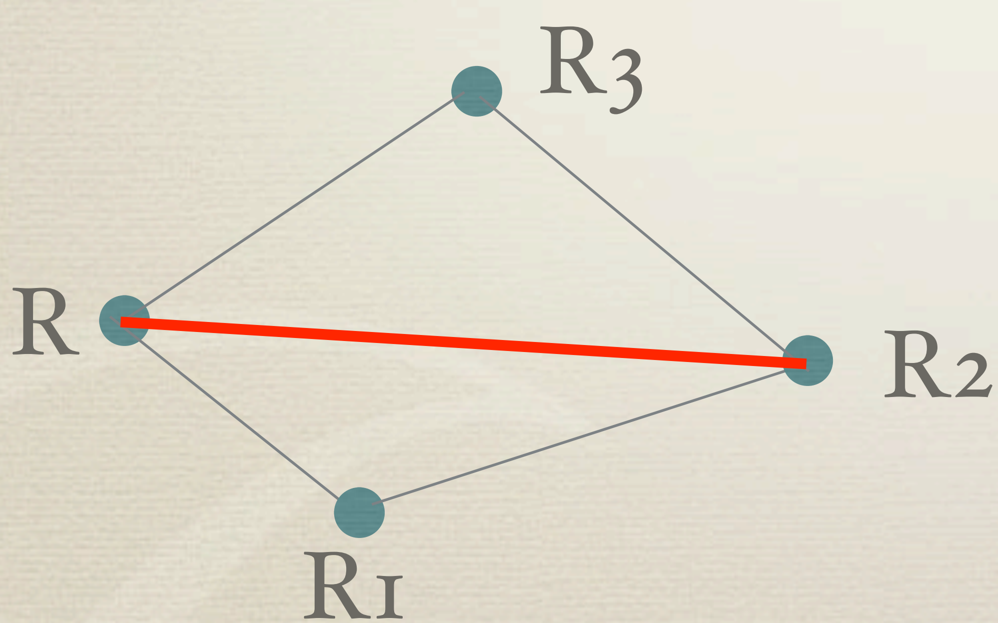


* see PIMC++

RPIMC is a black box that (approximately) gives out samples R with probability $\rho(R,R) = \langle R|\exp[-\beta H]|R\rangle$

1. Pick bead i at random

2. Move it to spot R_i^{new} with probability $\frac{\langle R_{i-1}|\exp[-\tau H]|R_i^{\text{new}}\rangle\langle R_i^{\text{new}}|\exp[-\tau H]|R_{i+1}\rangle}{\langle R_{i-1}|\exp[-\tau H]|R_i\rangle\langle R_i|\exp[-\tau H]|R_{i+1}\rangle}$



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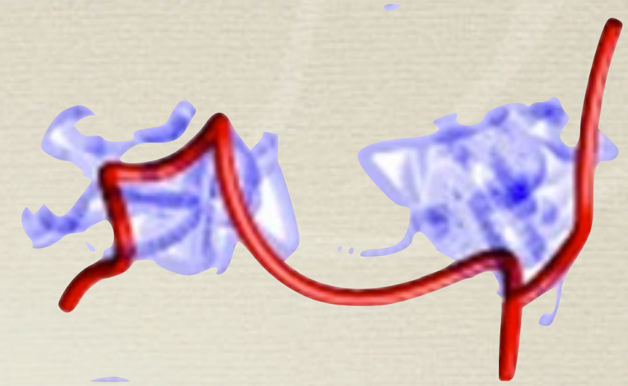

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But there are some problems...

1992

Ceperley - 1996

We think that the Path Integral Monte Carlo method is a very powerful method ; and there are many challenges

1. Clearly much work needs to be done in figuring out what we should use as nodes since the restriction is the only uncontrolled approximation. Free-particle

2. We need ways to get to lower temperatures. One of

Current de-facto standard for fermions at finite temperature

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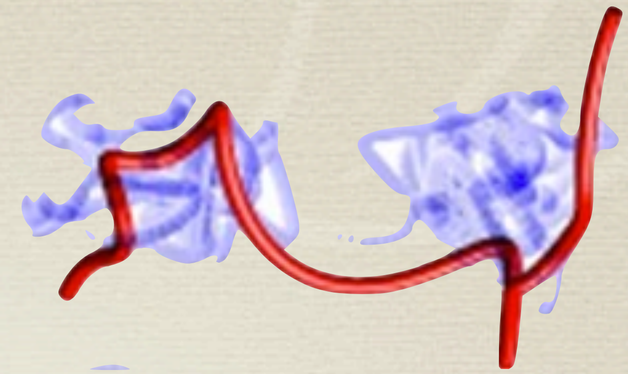

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But there are some problems...

Militzer - 2012

Problem 2: **More accurate nodes** needed at low temperature.

Problem 3: Acceptance ratio of **reference point moves** decreases at low temperature. Low sampling efficiency.
Hydrogen: $T > 0.1 \times T_{fermi}$

Current de-facto standard for fermions at finite temperature

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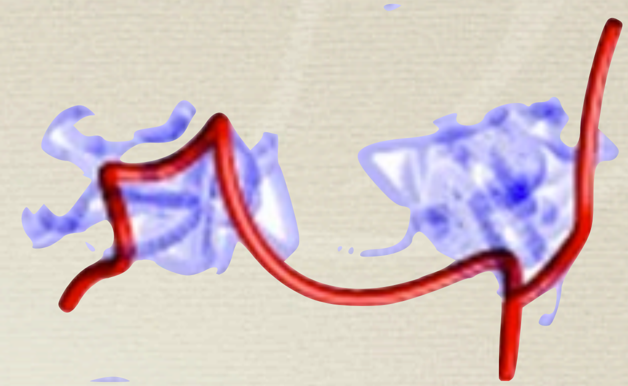

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But there are some problems...

Need to guess a trial many body density matrix

(seems harder then guessing a trial wave-function)

Ergodicity at low temperature

The Solution: Stop using Path Integral Monte Carlo

What else could we use then?

ground state

- Projector QMC??
- Variational Monte Carlo??
- Fixed Node Diffusion Monte Carlo??

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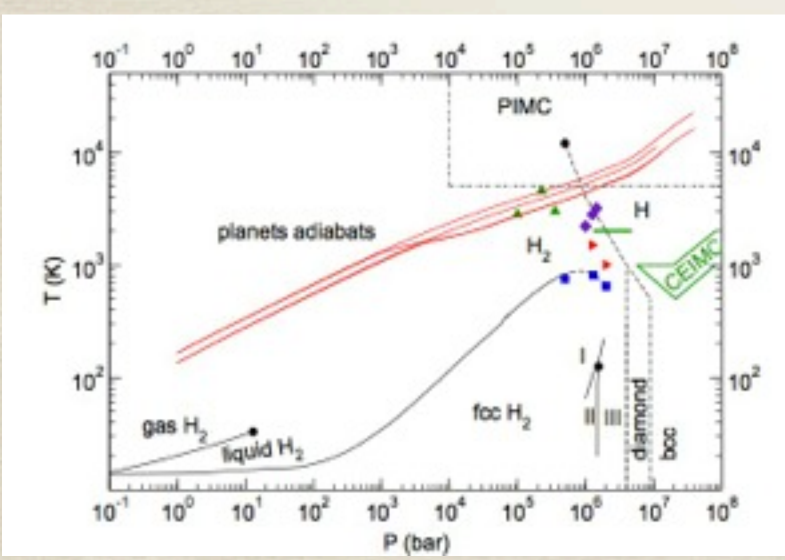
CEIMC?

Finite temperature protons - ground state fermions

Invented because PIMC gets stuck



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<u>Today's goal</u> (a work in progress):

Show you new algorithms we've been developing for finite temperature calculations based on projector QMC.

The Solution: Stop using Path Integral Monte Carlo

What else could we use then?

finite temperature

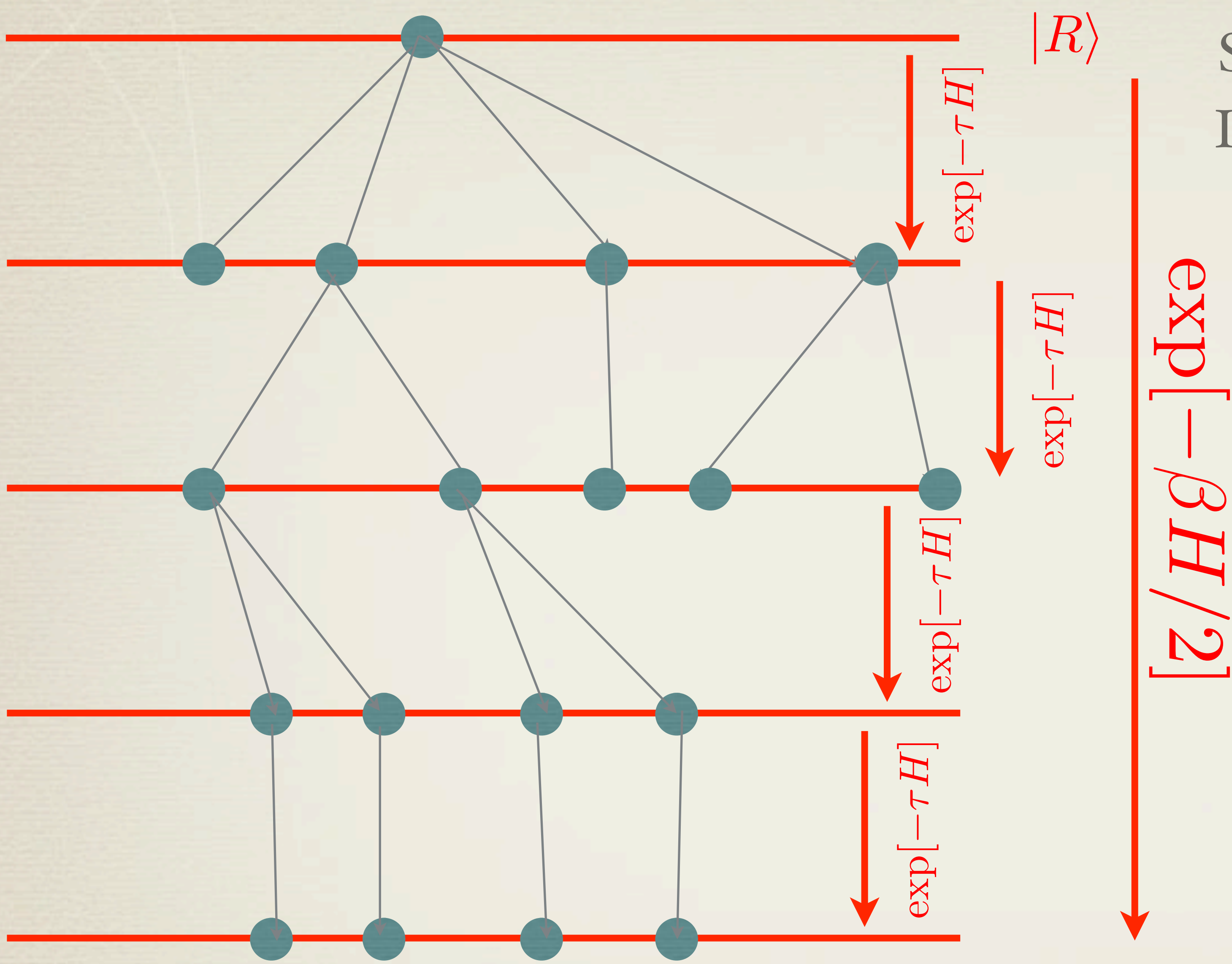
- Projector QMC?? **Part I**
- Variational Monte Carlo?? **Part II**
- Fixed Node Diffusion Monte Carlo?? **Part III**

<u>Today's goal</u> (a work in progress):

Show you new algorithms we've been developing for finite temperature calculations based on projector QMC.

Part I: Projector QMC at Finite T

Projector QMC

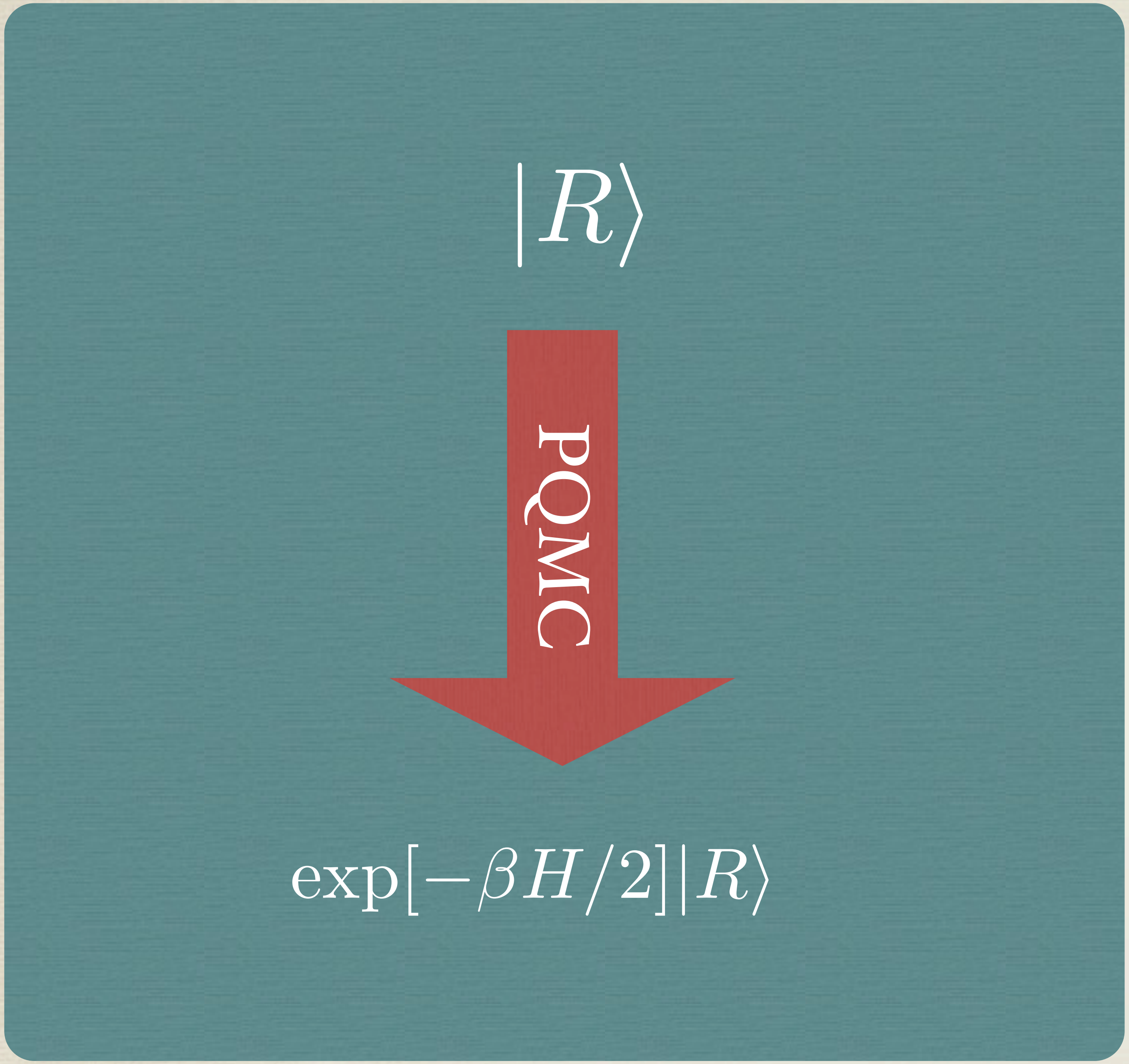


Samples $\exp[-\beta H/2]|R\rangle$

In the limit of large beta: Samples $|\Psi_0\rangle$

3n dimensional space

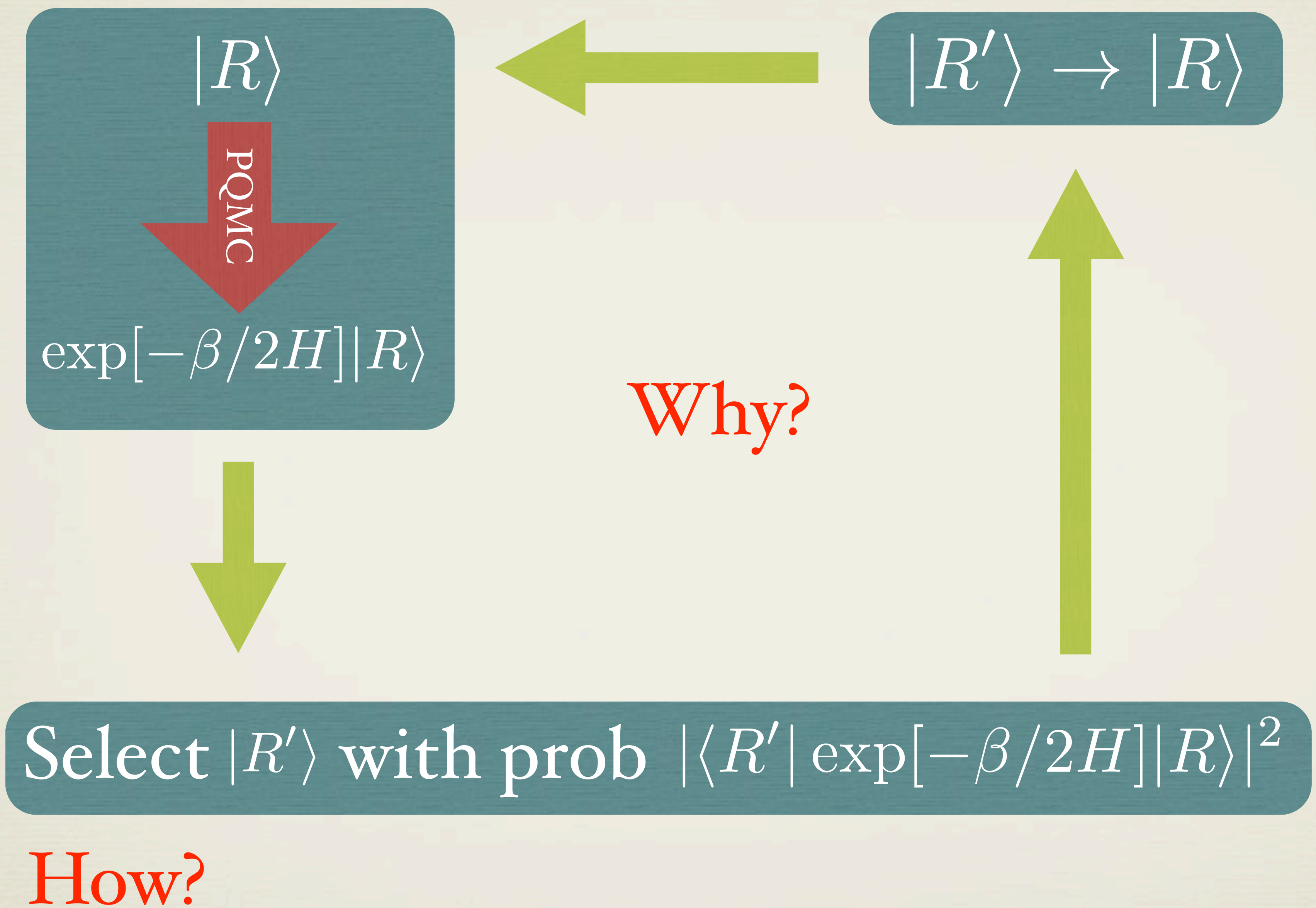
Projector QMC



Samples $\exp[-\beta H/2]|R\rangle$

In the limit of large beta: Samples $|\Psi_0\rangle$

FT Projector QMC

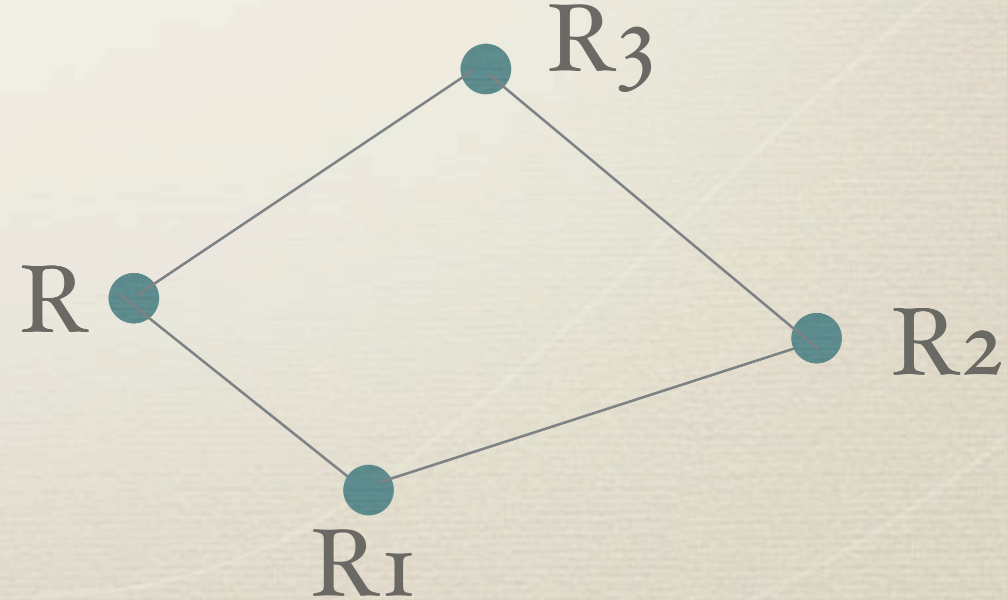


Also used by METTS

Why? - Proof via PIMC

1. Pick bead i at random

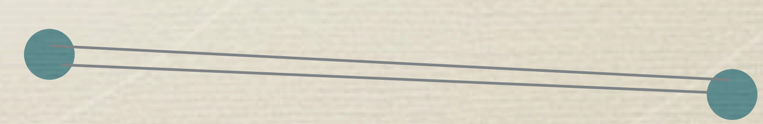
2. Move it to spot $R_i^{\rm new}$ with probability $\frac{\langle R_{i-1}|\exp[-\tau H]|R_i^{\rm new}\rangle\langle R_i^{\rm new}|\exp[-\tau H]|R_{i+1}\rangle}{\langle R_{i-1}|\exp[-\tau H]|R_i\rangle\langle R_i|\exp[-\tau H]|R_{i+1}\rangle}$



Why? - Proof via PIMC

1. Pick bead i at random

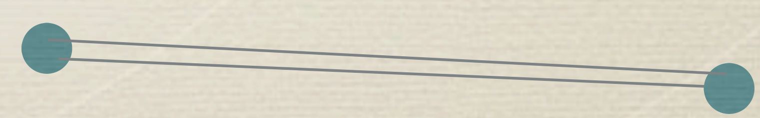
2. Move it to spot R_i^{new} with probability $\frac{|\langle R_{i-1}| \exp[-\beta H/2] |R_i^{new}\rangle|^2}{|\langle R_{i-1}| \exp[-\beta H/2] |R_i\rangle|^2}$



Why? - Proof via PIMC

1. Move bead 0 it to spot R_0^{new} with probability $\frac{|\langle R_1|\exp[-\beta H/2]|R_0^{new}\rangle|^2}{|\langle R_1|\exp[-\beta H/2]|R_0\rangle|^2}$

2. Move bead 1 it to spot R_1^{new} with probability $\frac{|\langle R_0|\exp[-\beta H/2]|R_1^{new}\rangle|^2}{|\langle R_0|\exp[-\beta H/2]|R_1\rangle|^2}$



Why? - Proof via PIMC

1. Move bead 0 it to spot R_0^{new} with probability $\frac{|\langle R_1|\exp[-\beta H/2]|R_0^{new}\rangle|^2}{|\langle R_1|\exp[-\beta H/2]|R_0\rangle|^2}$ 1000000 times

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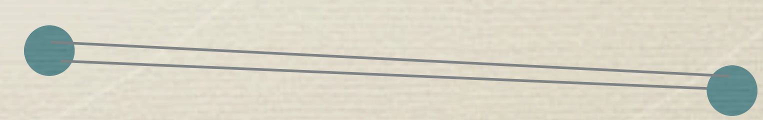

Why? - Proof via PIMC

1. Sample R_0 with probability $|\langle R_1|\exp[-\beta H/2]|R_0\rangle|^2$
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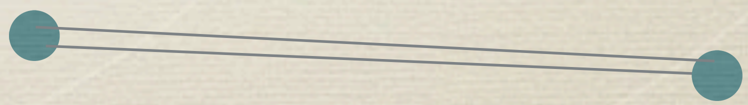

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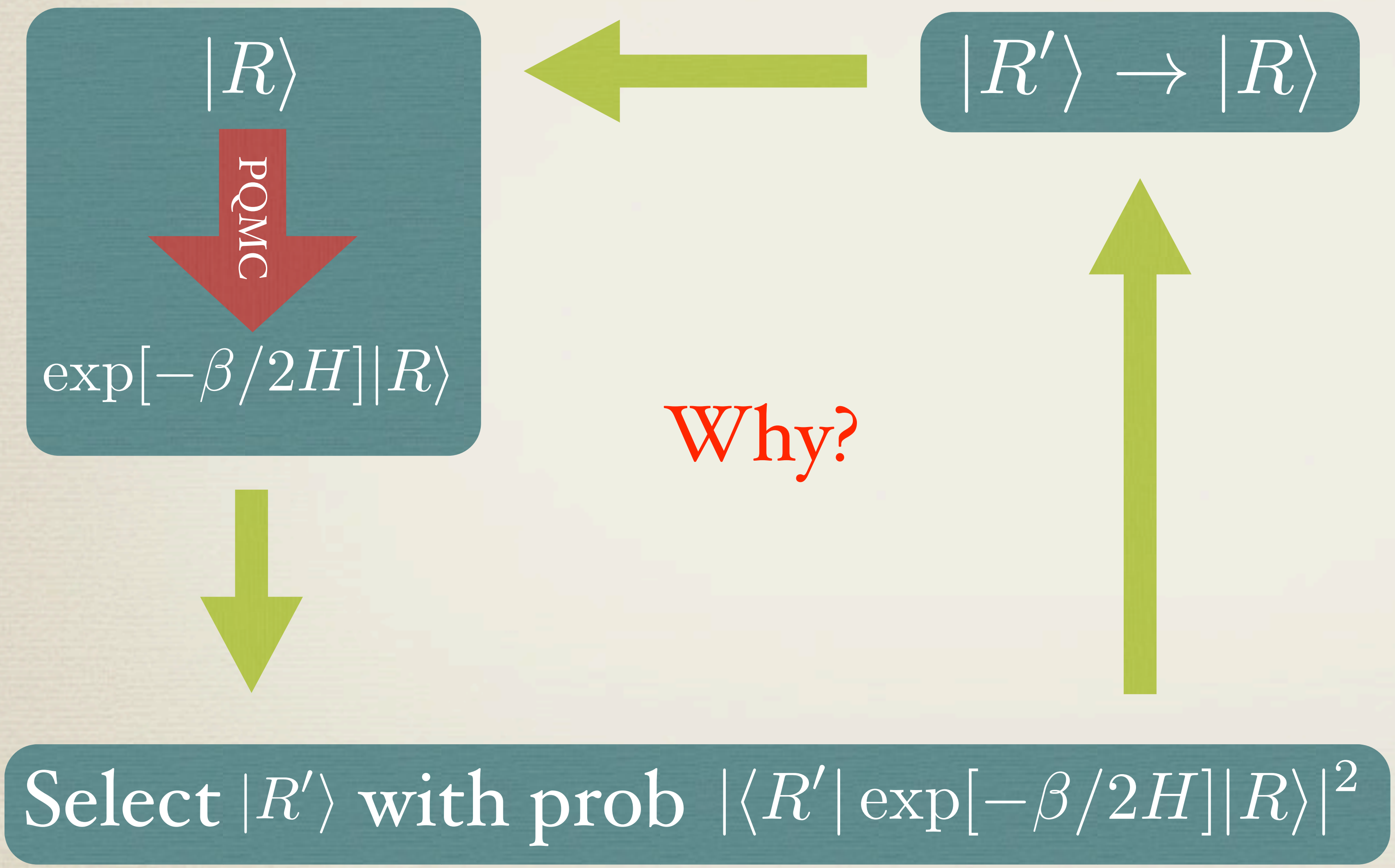
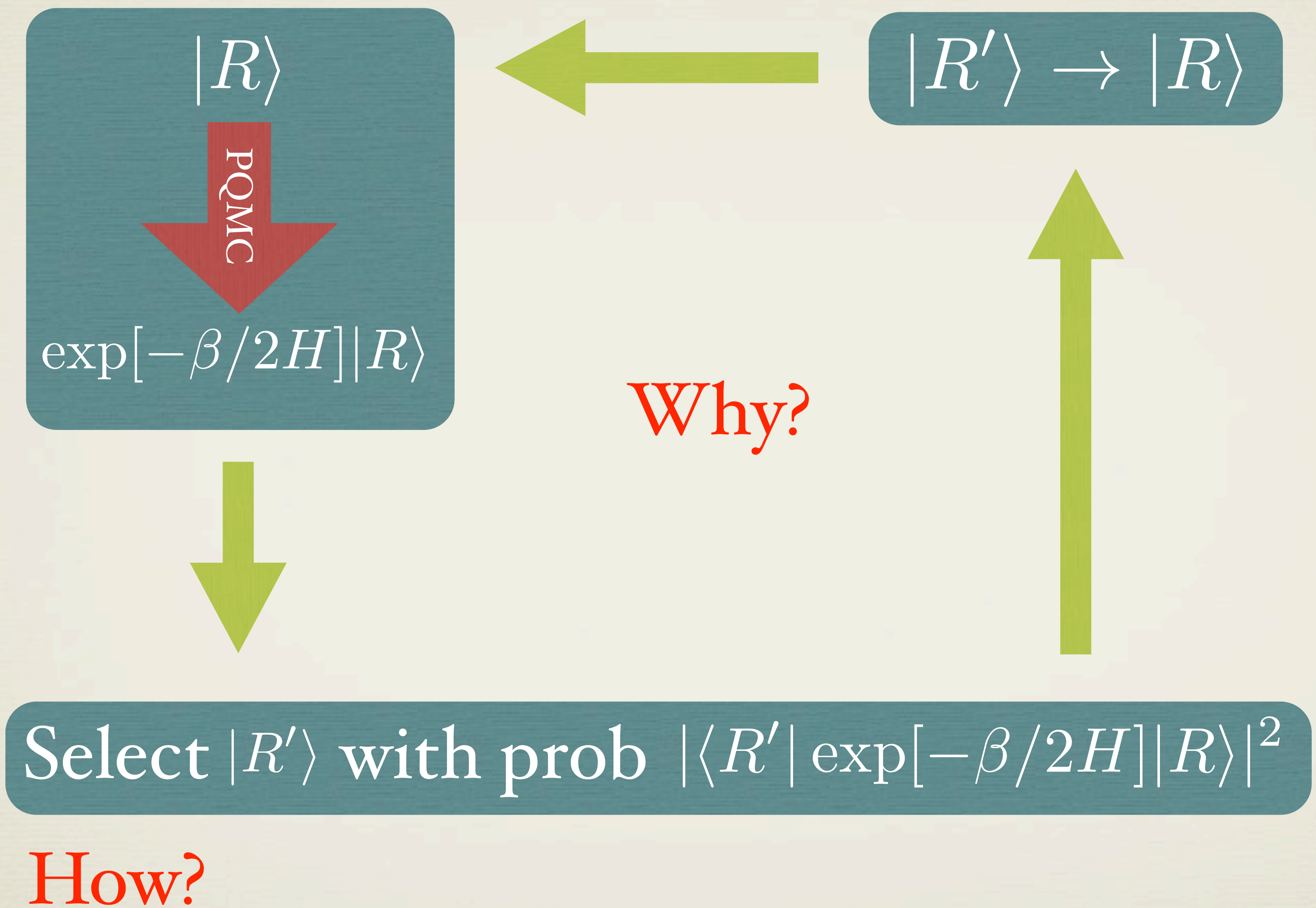


FT Projector QMC



How?

Select $|R'\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$

Option 1 Square the weight of each walker.

Option 2 Overlap of two simulations.

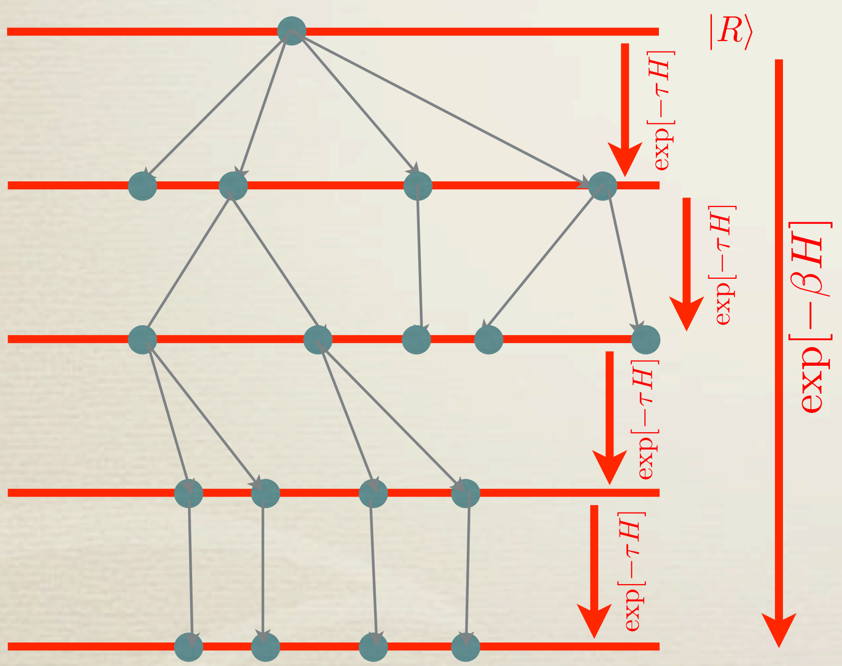
Option 3 Sample $\langle\Psi_T|R\rangle\langle R|\exp[-\beta H/2]|R'\rangle$ with importance sampling.

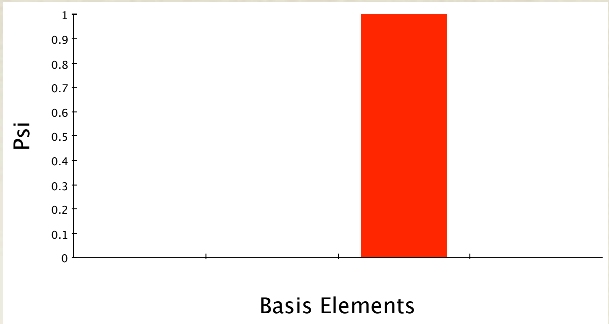
Select $|R'\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$

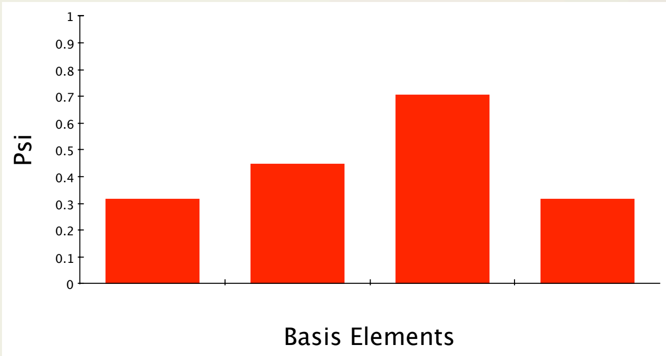
Option 1

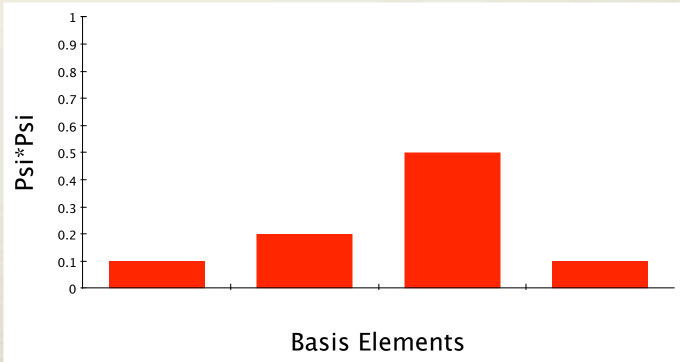
Systematically Biased...

But not too bad when FCIQMC works









A Test System

Heisenberg Model: $H = \sum_{ij} \sigma_i \cdot \sigma_j$

Locked to Sz=0 sector

4x4 model

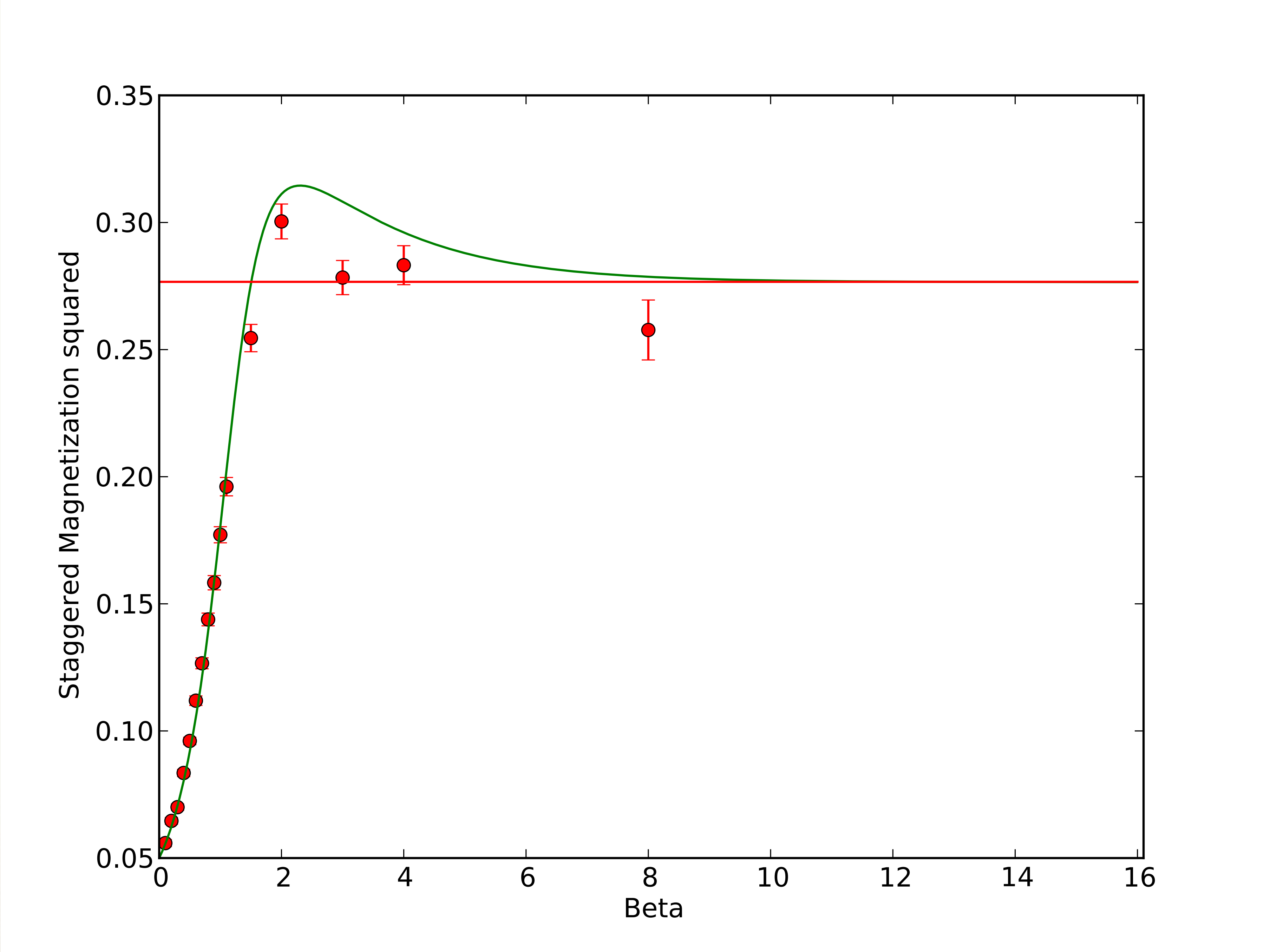
Tractable exactly

Like a fermion system (in second quantization)

No sign problem - show algorithms

Squaring a snapshot

* 1 core
* ~100,000 walkers



Select $|R'\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$

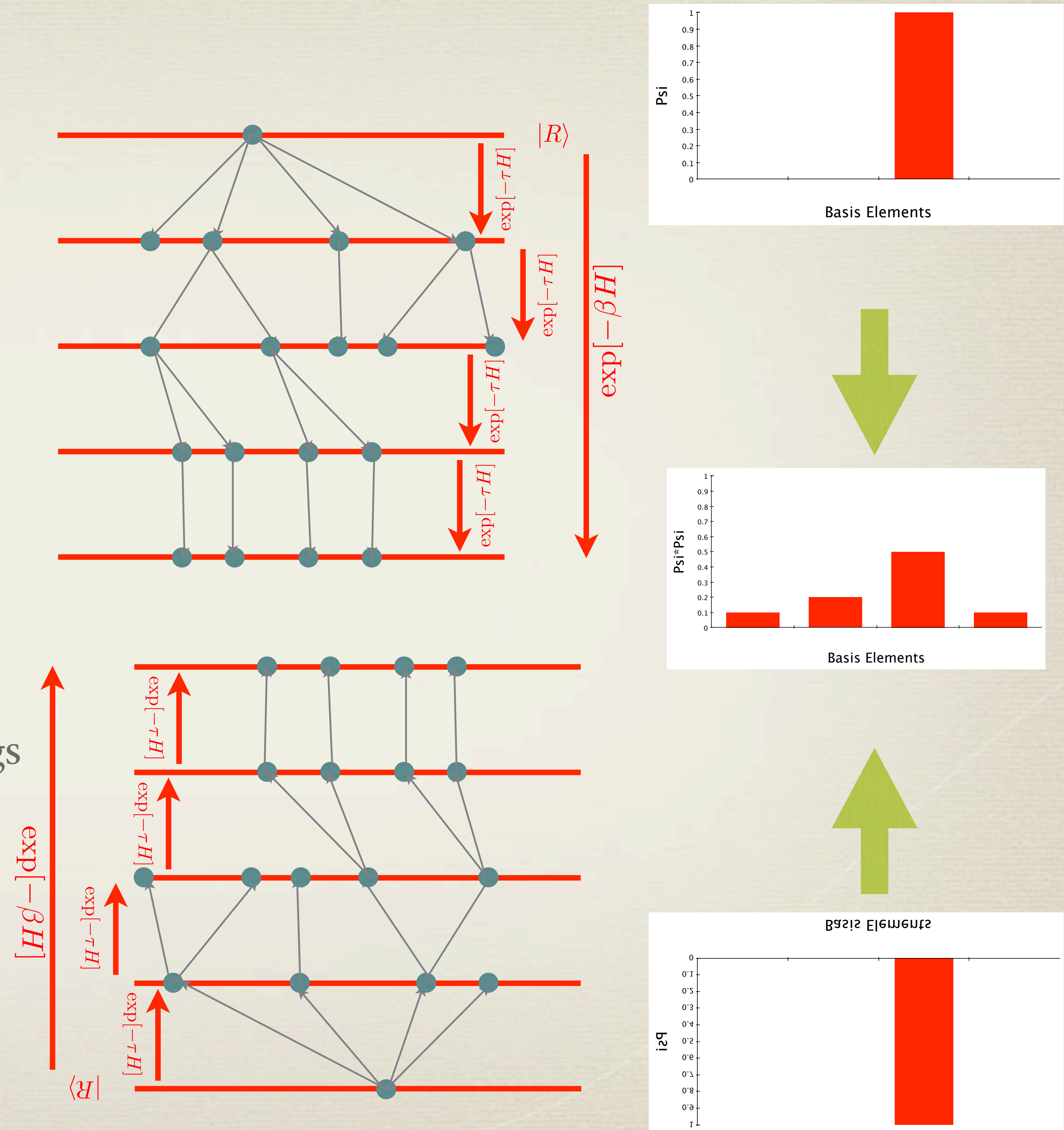
Option 2

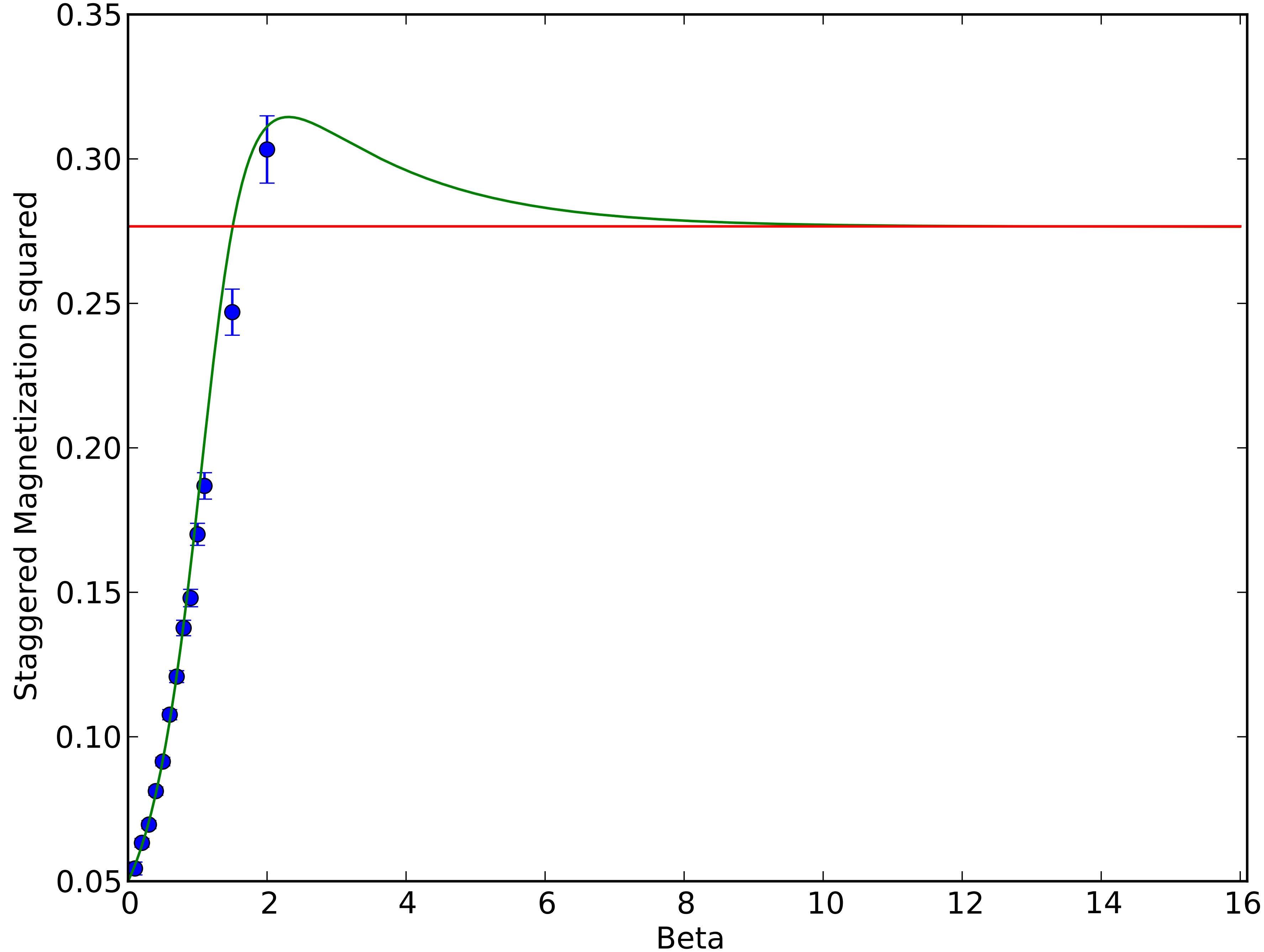
Exact but lose statistical accuracy

But not too bad when FCIQMC works

Similar ideas:

- Bilinear Sampling: Kalos, Shiwei
- DMQMC: Foulkes
- Improvements with Matt Hastings





0.35
0.30
0.25
0.20
0.15
0.10
0.05
Staggered Magnetization squared
0
2
4
6
8
10
12
14
16
Beta

Select $|R'\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$

Option 3

- Sample $\langle\Psi_T|R\rangle\langle R|\exp[-\beta H/2]|R'\rangle$ with importance sampling
- Just like diffusion Monte Carlo
- Need to choose $|\Psi_T\rangle \approx |\exp[-\beta H/2]|R'\rangle$
- `Mixed Estimator'

Q: How can we pick?
A: Later in the talk.

(maybe) correct by forward walking..

How?

Select $|R'\rangle$ with prob $|\langle R'| \exp[-\beta/2H]|R\rangle|^2$

Option 1 Square the weight of each walker.

* Systematically biased but not too bad.

Option 2 Overlap of two simulations.

* Larger statistical errors but not too bad.

Option 3 Sample $\langle \Psi_T|R\rangle\langle R| \exp[-\beta H/2]|R'\rangle$ with importance sampling.

* Mixed Estimator

(DMC) Problems

- Time step error: Removable in the lattice
- population bias? There is none here. The population bias comes from different steps having an adjusted S.
  - You can use this to fix the population bias at T=0
- "Squaring" bias / statistical problems /mixed estimator
- Sign problem: Prevents big systems

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* "Squaring" bias / statistical problems /mixed estimator
* Sign problem: Prevents big systems

Part I: Projector QMC at Finite T

The good

No ergodicity problem

No guessing trial density matrix

Annihilation attenuates sign problem

Everyone seems to like DMC more then PIMC

The bad

There's a sign problem

'Mixed estimator' problem

Part II: Variational Monte Carlo at Finite T

VMC at Finite T

$|R\rangle$

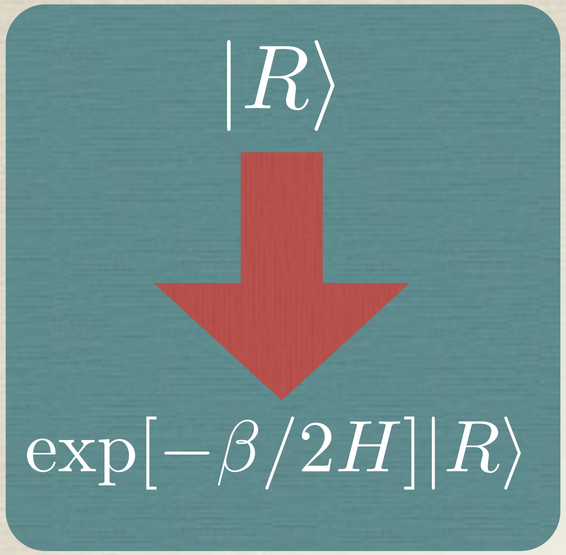
$\exp[-\beta/2H]|R\rangle$

How?

Select $|R'\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$

How?

$|R'\rangle \to |R\rangle$

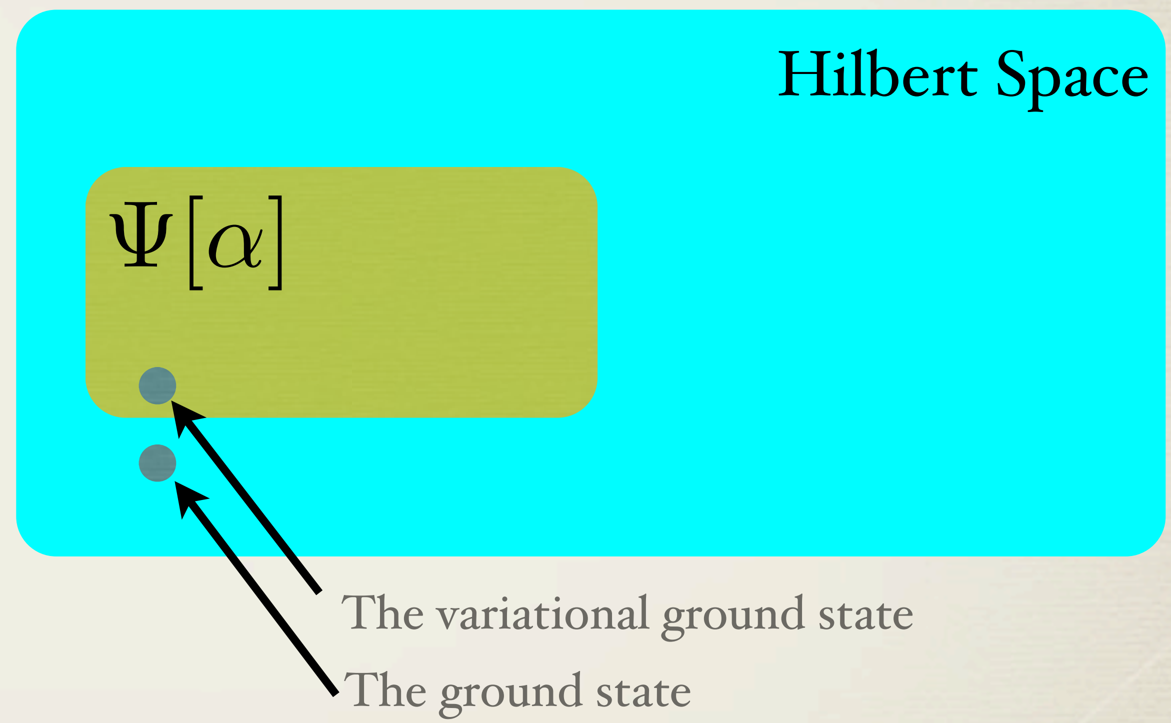


Stochastic nature in PQMC gives sign problem.

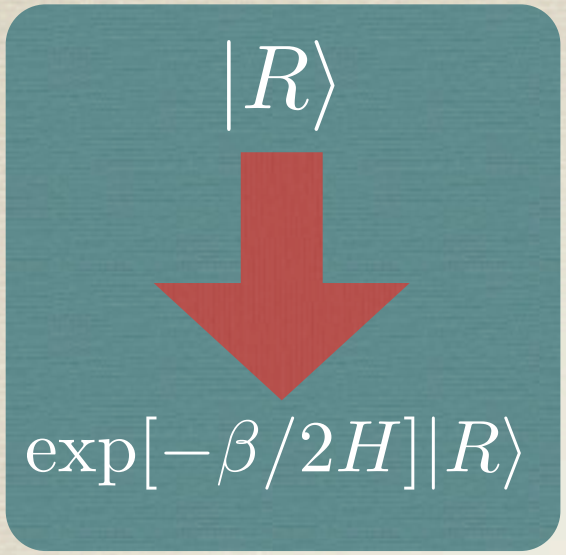
Variational Monte Carlo: Trades sign problem for variational subspace.

$\Psi[\alpha]$ could be geminals, SJ, etc.

Ground-state VMC: $\Psi[\alpha_{\text{best}}] \approx \Psi_{\text{gs}}$



Similar in spirit to METTS.



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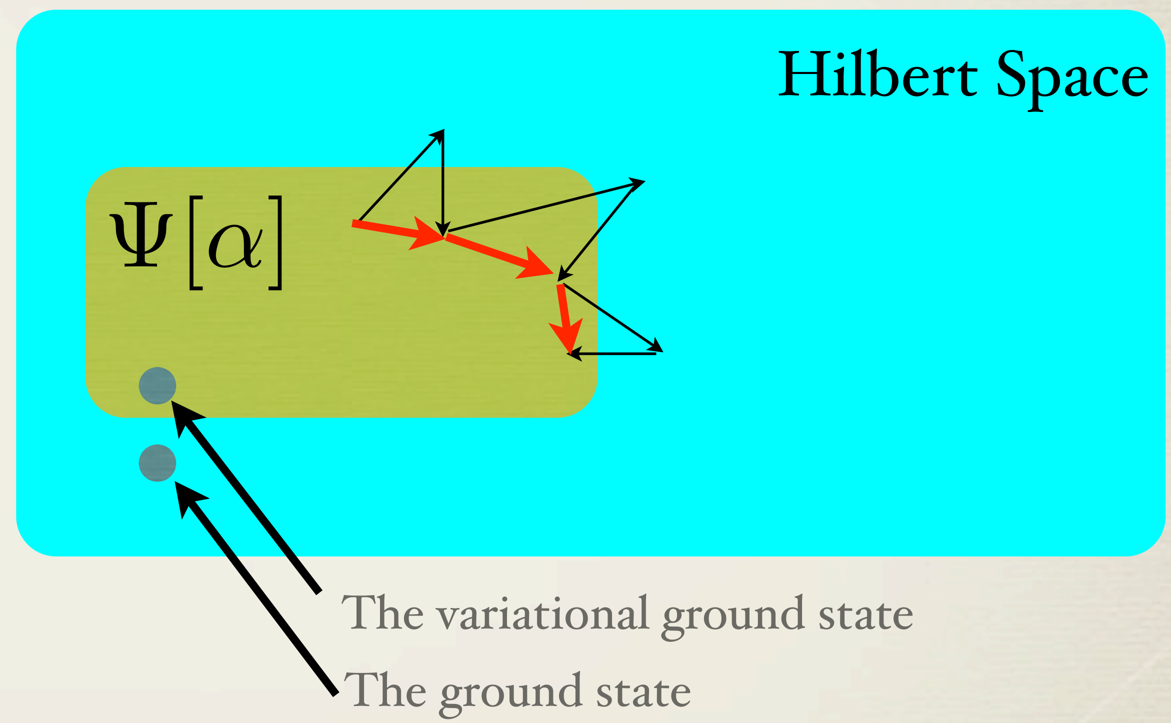

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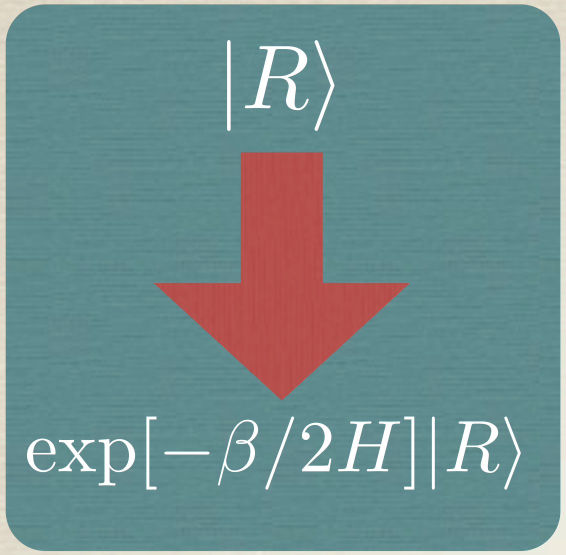

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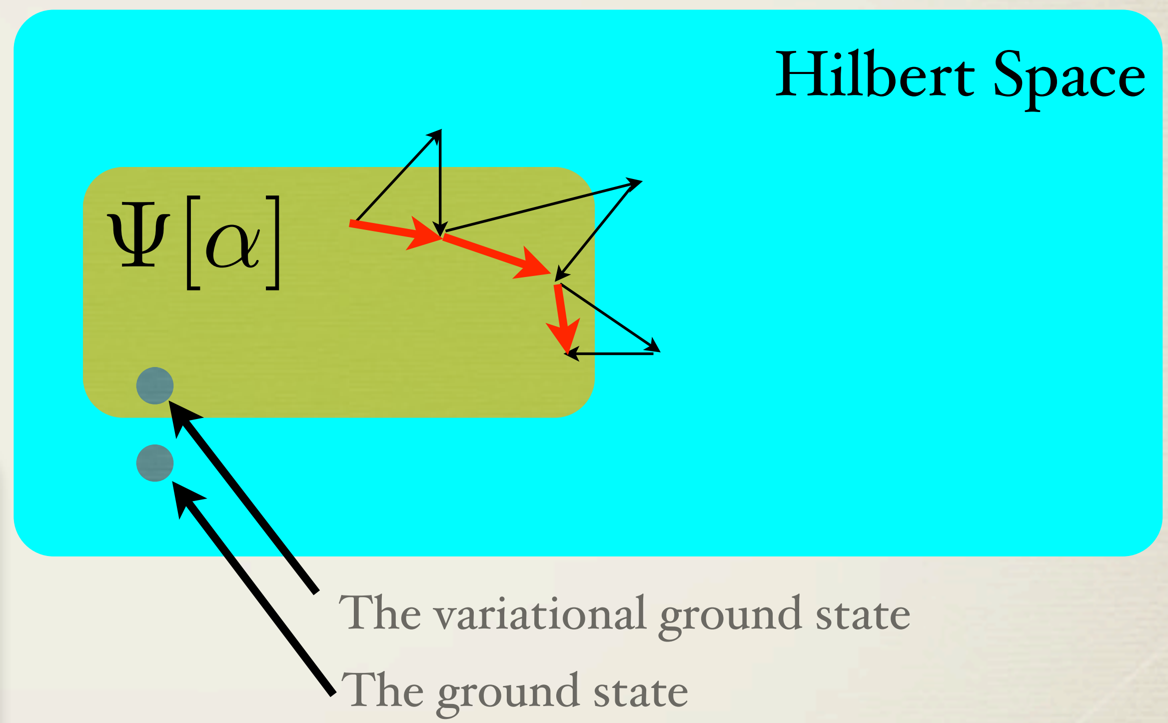
Ground-state VMC: $\Psi[\alpha_{\text{best}}] \approx \Psi_{\text{gs}}$

Want $\Psi[\beta_{\text{best}}] \approx \exp[-\beta H/2]|R\rangle$



<u>High level approach</u>

$$\exp[-\tau H]\exp[-\tau H]\exp[-\tau H]|R\rangle$$

$$P\exp[-\tau H]P\exp[-\tau H]P\exp[-\tau H]|R\rangle$$

Low level approach: Stochastic reconfiguration

Similar in spirit to METTS.

High level approach

$$\exp[-\tau H]\exp[-\tau H]\exp[-\tau H]|R\rangle$$

$$P\exp[-\tau H]P\exp[-\tau H]P\exp[-\tau H]|R\rangle$$

Low level approach: Stochastic reconfiguration

Schrodinger equation in the tangent space of local variational subspace.

Tangent space of $\Psi[\vec{\alpha}]$: $\partial\psi[\vec{\alpha}]/\partial\alpha_0, \partial\psi[\vec{\alpha}]/\partial\alpha_1, \partial\psi[\vec{\alpha}]/\partial\alpha_2, \ldots$

$$H_{ij} \equiv \langle\partial\psi[\alpha_i]|\hat{H}|\partial\psi[\alpha_j]\rangle$$

→ Run VMC on $|\Psi[\alpha]\rangle$
Measure H and S

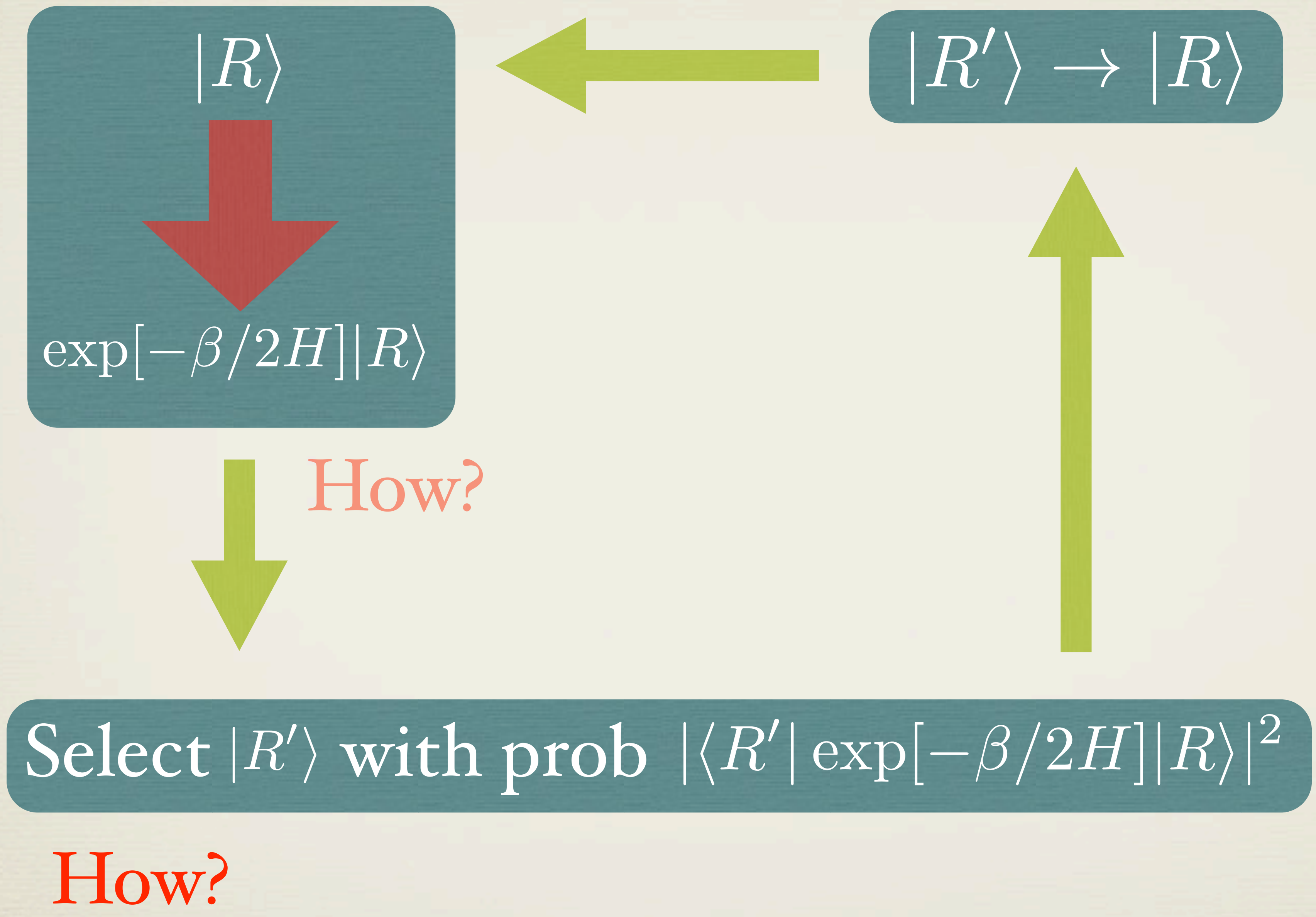
$$S_{ij} \equiv \langle\partial\psi[\alpha_i]|\partial\psi[\alpha_j]\rangle$$

$$(1-\tau HS^{-1})|\Psi[\alpha]\rangle$$

Side Note:

Option 3 If we can pick $|\Psi_T\rangle \approx |\exp[-\beta H/2]|R'\rangle$

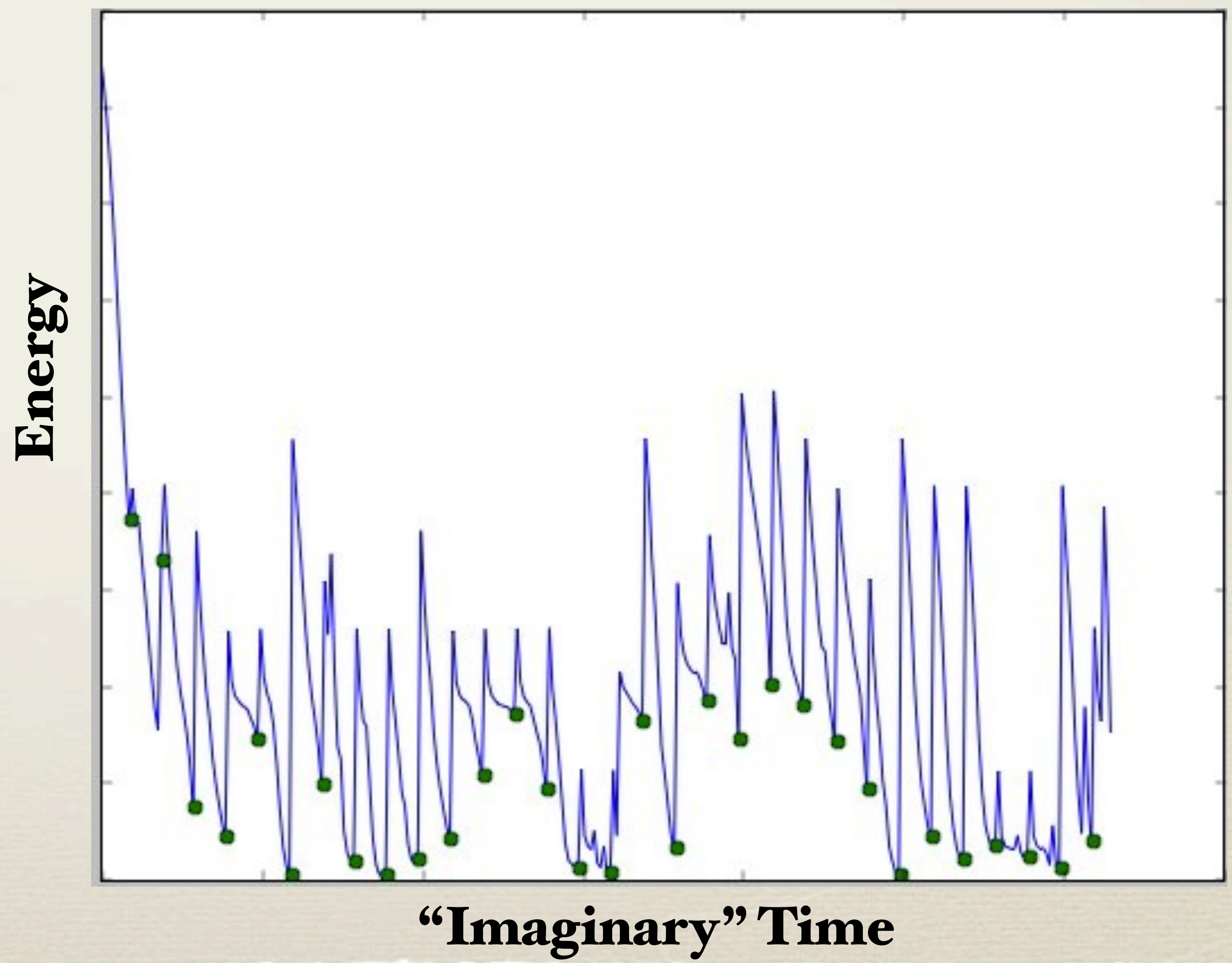
VMC at Finite T



Select $|R'\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$

We have an explicit form $\Psi[\beta] \approx \exp[-\beta H/2]\Psi[\alpha]$

Variational Monte Carlo is the black box that takes a wave function $\Psi[\beta]$ and samples R' with probability $\langle R'|\Psi[\beta]\rangle|^2$.



Two questions:

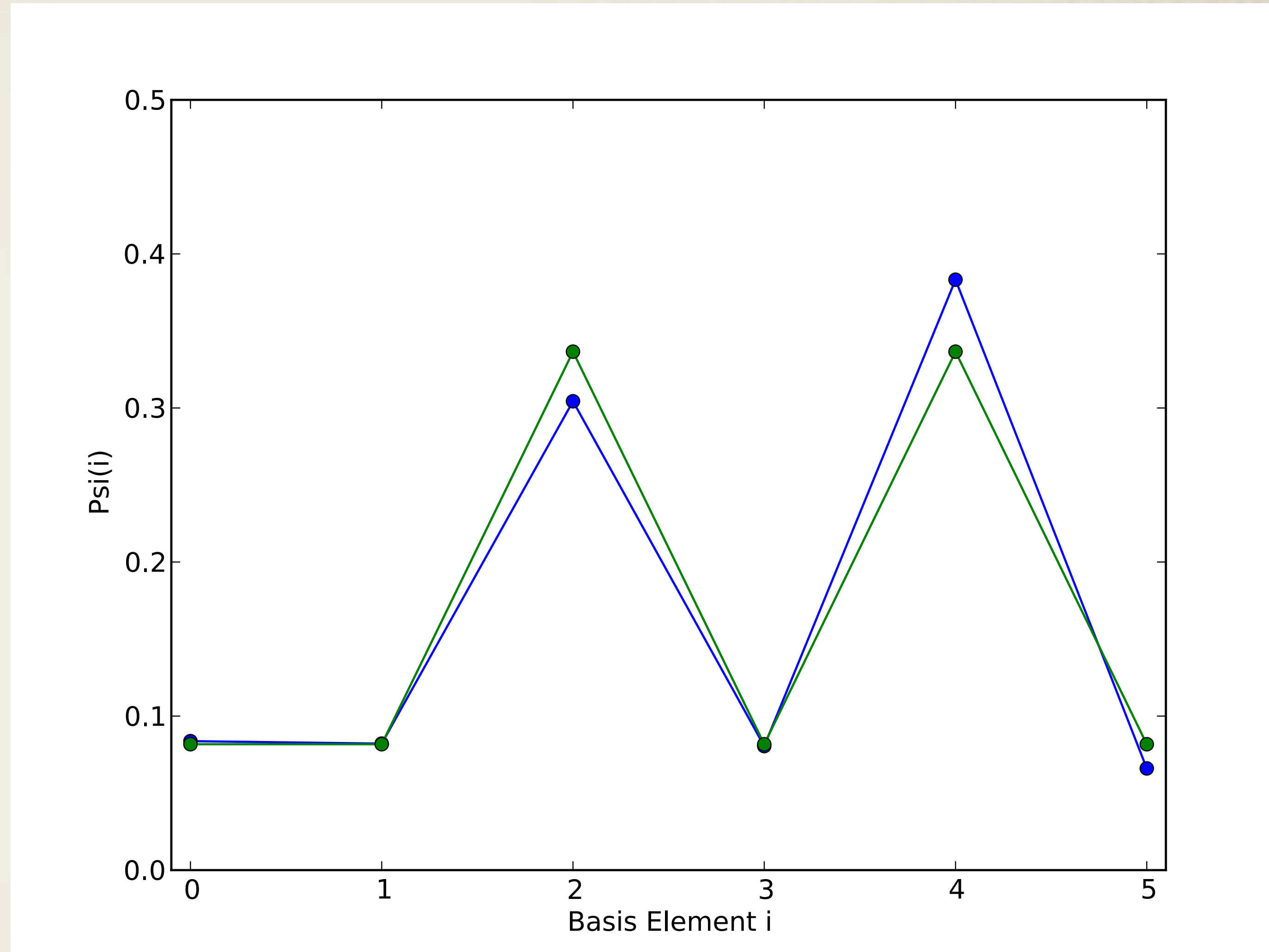
1. Both steps are done stochastically. Is this good enough?
2. How is the accuracy of the wave-function?

Surviving Stochasticity

- 4x1 Heisenberg Model
- Beta=2.0
- Complete ansatz

$\Psi[\alpha]$

Hilbert Space

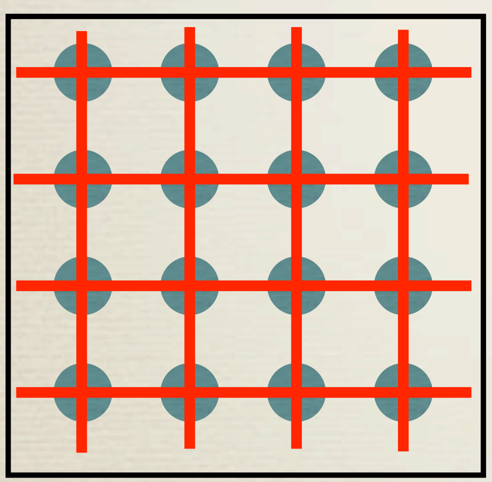


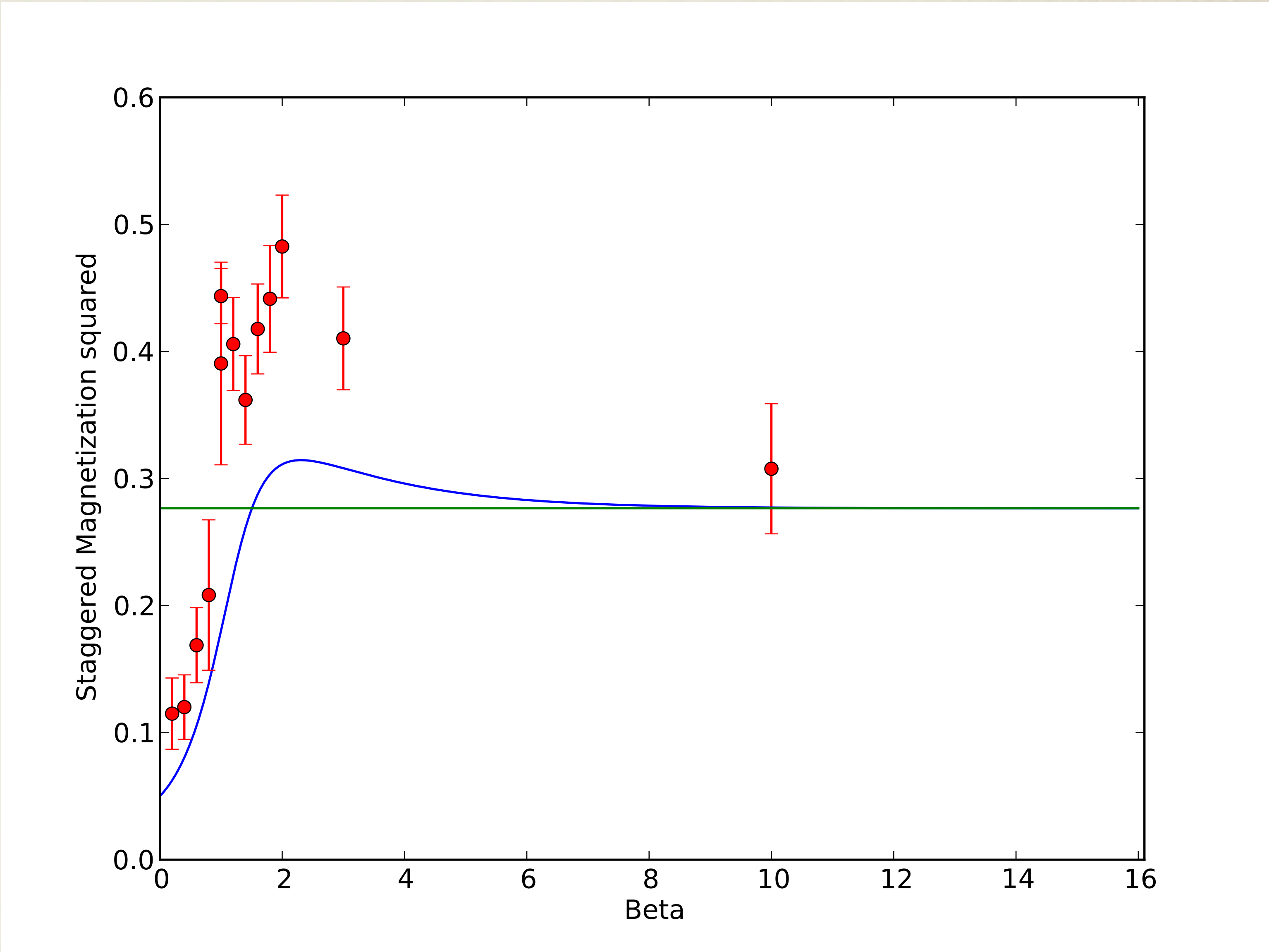
$$\Psi[\vec{c}] = \sum_{\vec{\alpha}} c_{\alpha_1\alpha_2\alpha_3\alpha_4} |\alpha_1\alpha_2\alpha_3\alpha_4\rangle$$

How good?

* 4x4 heisenberg model

Huse-Elser states



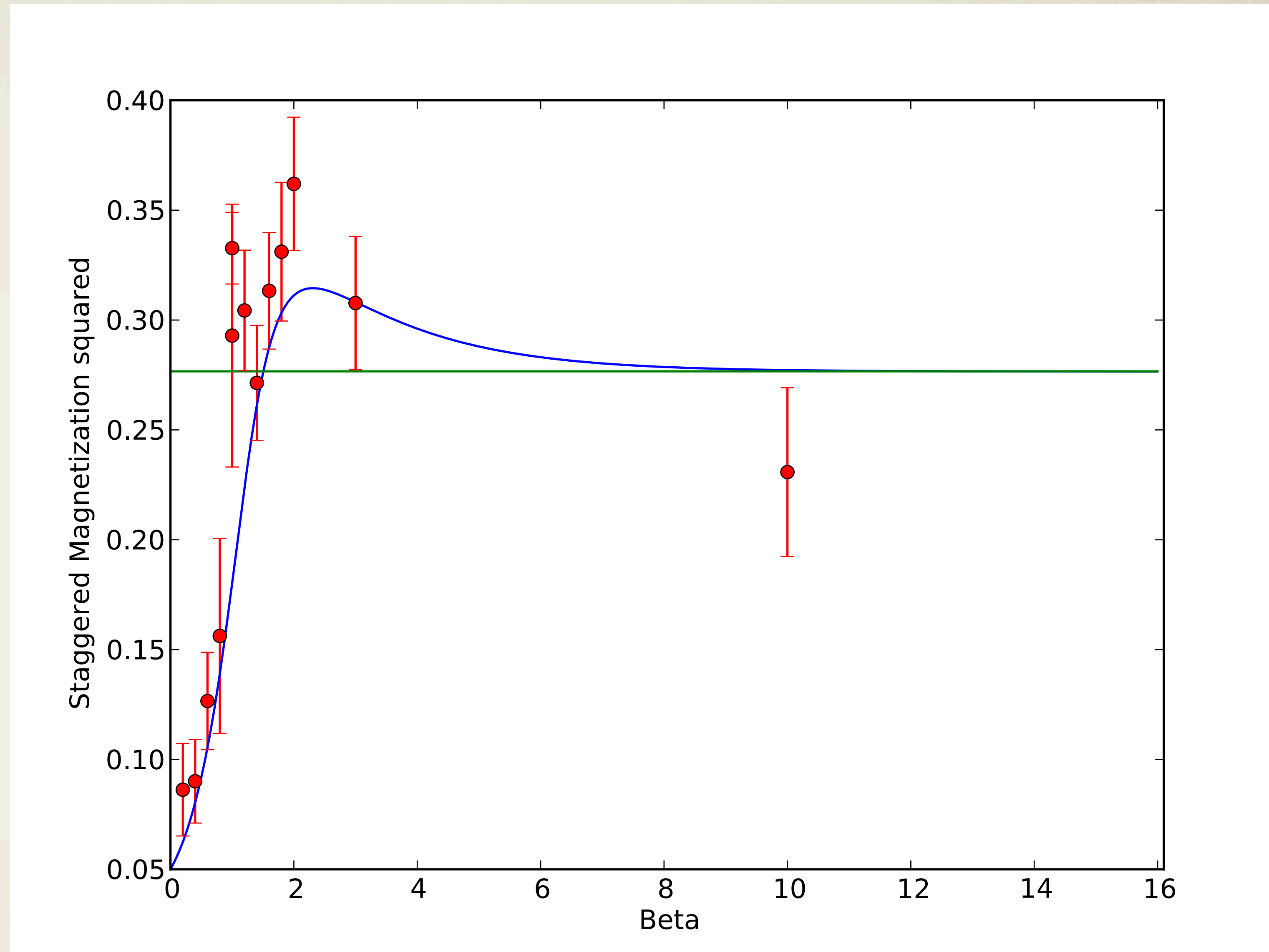


Systematically overestimated.

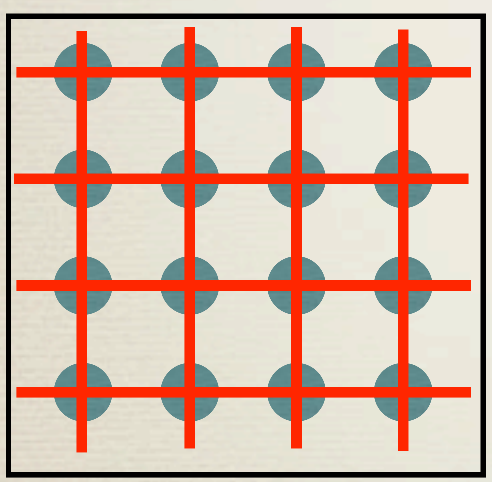
$$\Psi[\vec{c}] = \sum_{\alpha} c_{\alpha_1\alpha_2\alpha_3\alpha_4} c_{\alpha_5\alpha_6\alpha_7\alpha_8} \cdots c_{\alpha_1\alpha_5\alpha_9\alpha_{13}} |\alpha_1\alpha_2\alpha_3\alpha_4\alpha_5..\alpha_{16}\rangle$$

How good?

* 4x4 heisenberg model



Huse-Elser states



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Part II: Variational Monte Carlo at Finite T

The good

No ergodicity problem

No guessing trial density matrix

No exponential variance

The bad

Variational

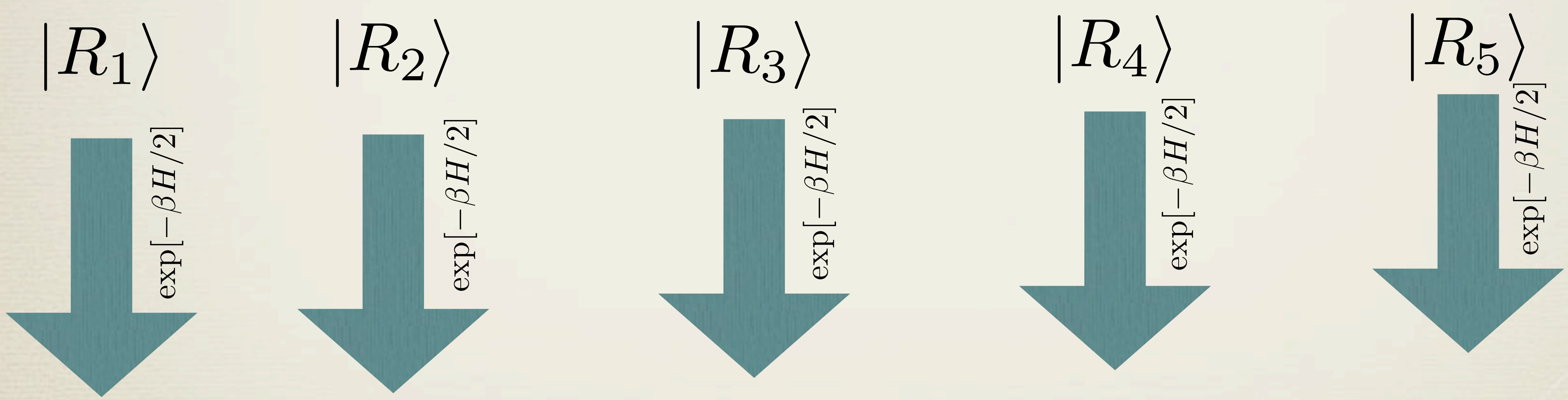
Part III: Fixed Node Projector Monte Carlo at Finite T

Can we do better?

- FT-VMC: Approximate but statistically stable.
- FT-DMC: Sign problem

The ground state answer to this problem is fixed node.

We want a finite temperature variant.



We propagate by applying $G = (1 - \tau H)$ which has a sign problem

We need to propagate by another G which gives the same result but has no sign problem.

Finite Temperature Fixed Node

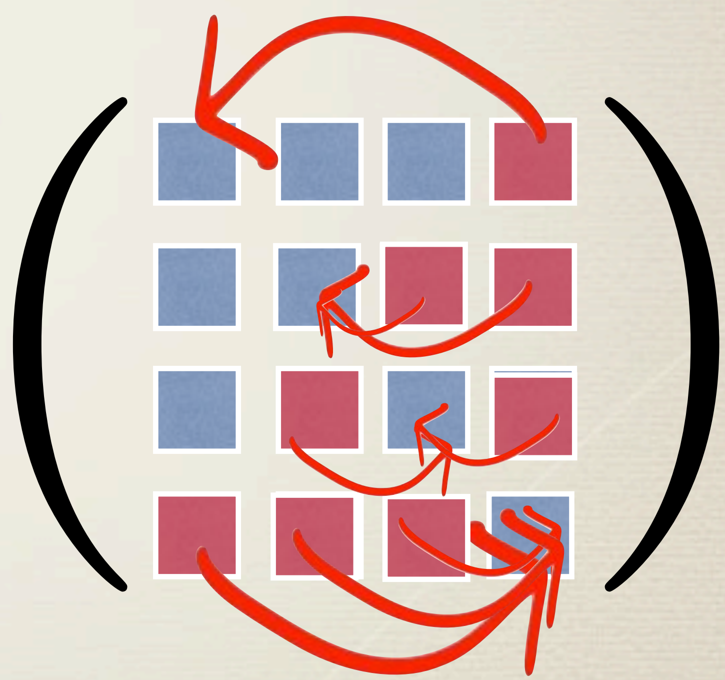
Lattice

$$\tilde{G}(R,R';k\tau) = G(R,R') \text{ if } \Psi_T(R;k\tau)\Psi_T(R';k\tau)G(R,R') > 0$$

$$\tilde{G}(R,R';k\tau) = 0 \qquad \text{ if } \Psi_T(R;k\tau)\Psi_T(R';k\tau)G(R,R') < 0$$

$$\tilde{G}(R,R;k\tau) = G(R,R) + \sum_{\text{sign violating}} \frac{\Psi_T(R';\tau)}{\Psi_T(R;\tau)} G(R,R)$$

$$\Psi_T(R;k\tau) = \langle R|\boxed{\exp[-k\tau H]|R_{\text{init}}}\rangle$$



Trial wave-function depends on where you are in the path and where you started.

In the continuum, don't cross a node defined by same trial function.

Proof

Probability you are in node j is

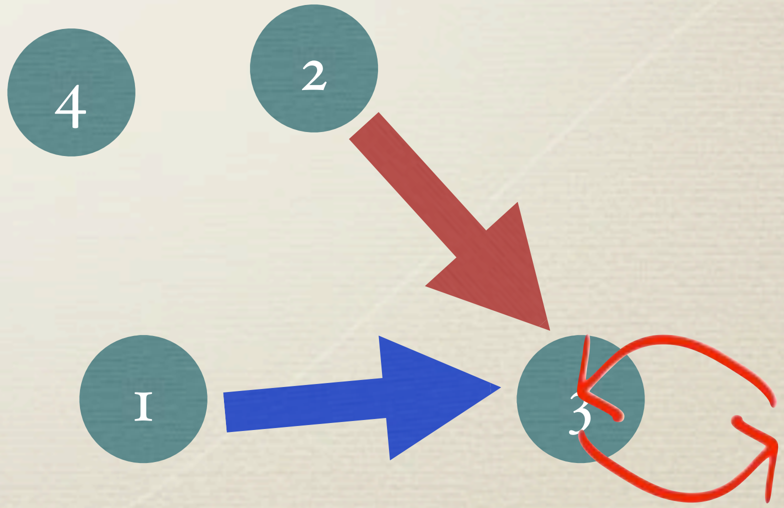
$$Pr(j;t) = \sum_i Pr(i;t-1)Pr(i \to j)$$

$$\Psi[j;t] = \sum_{i \neq j} \Psi[i;t-1]G_{ij} + \Psi[j;t-1]G_{jj}$$

$$\Psi[j;t] = \sum_{i \neq j \in \text{good}} \Psi[i;t-1]G_{ij} + \sum_{i \neq j \in \text{bad}} \Psi[i;t-1]G_{ij} + \Psi[j;t-1]G_{jj}$$

$$\Psi[j;t] = \sum_{i \neq j \in \text{good}} \Psi[i;t-1]\tilde{G}_{ij}[t-1] + \Psi[j;t-1]\tilde{G}_{jj}[t-1]$$

Let $\tilde{G}_{jj}[t-1] = \Psi[j;t-1]G_{jj} + \frac{\Psi[i;t-1]}{\Psi[j;t-1]}G_{ij}$



So far...

Projector QMC which gives you finite temperature results.

Variational MC which gives you finite temperature results.

Fixed node MC which gives you finite temperature results.

These methods may help generate imaginary time-imaginary time correlation functions.

Part III: Fixed Node Projector Monte Carlo at Finite T

The good

No ergodicity problem

No guessing trial density matrix

No exponential variance

Less variational then FT-VMC

The bad

Variational (with nodes)

Mixed estimator

Problem: Path Integral Monte Carlo has problems

The Solution: Stop using Path Integral Monte Carlo

Problem: Path Integral Monte Carlo has problems

The Solution: Stop using Path Integral Monte Carlo

But... I like Path Integral Monte Carlo

Can we fix it?

Part IV: Fix Path Integral Monte Carlo

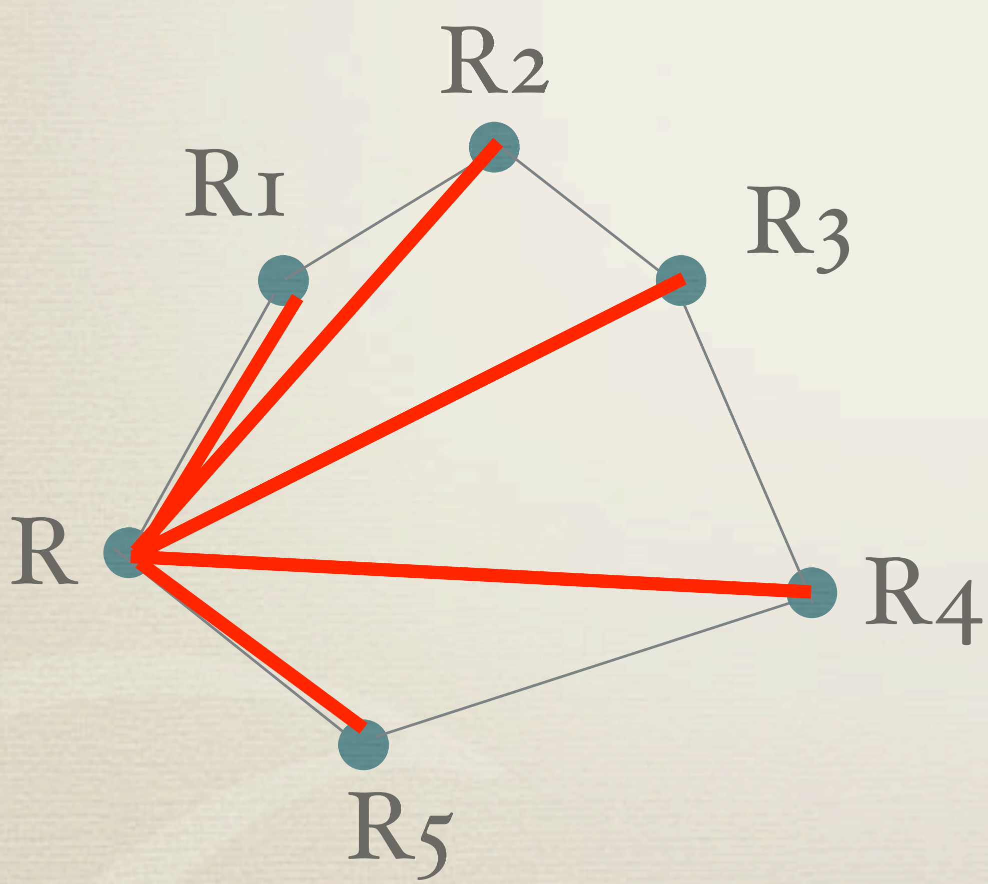
One problem: Ergodicity

Ceperley - 1996

2. We need ways to get to lower temperatures. One of

Militzer - 2012

Problem 3: Acceptance ratio of **reference point moves** decreases at low temperature. Low sampling efficiency.
Hydrogen: $T > 0.1 \times T_{fermi}$

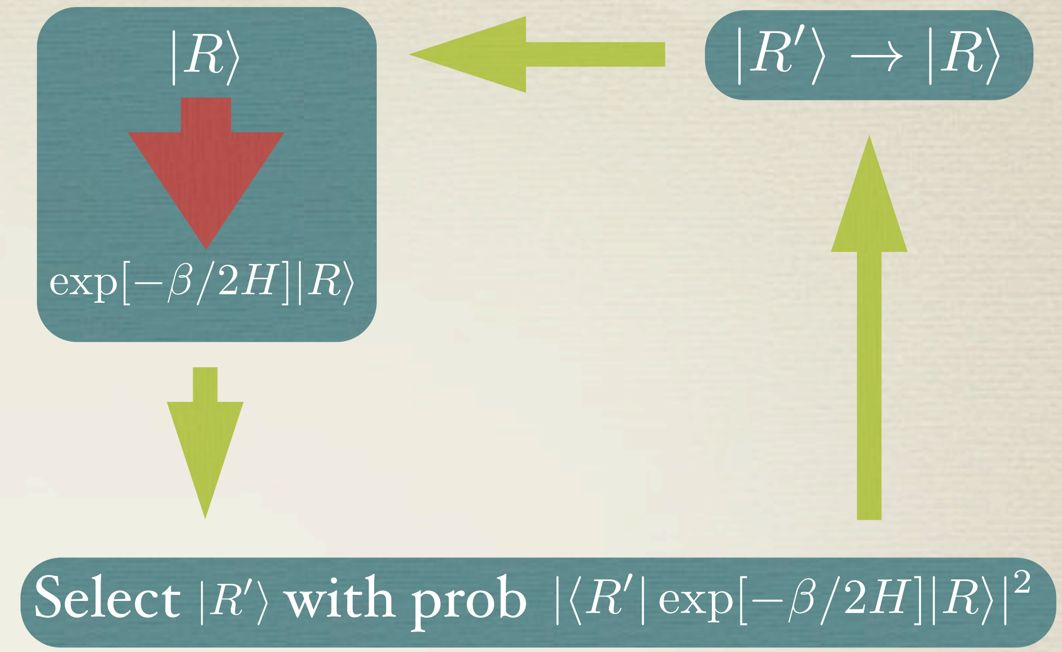


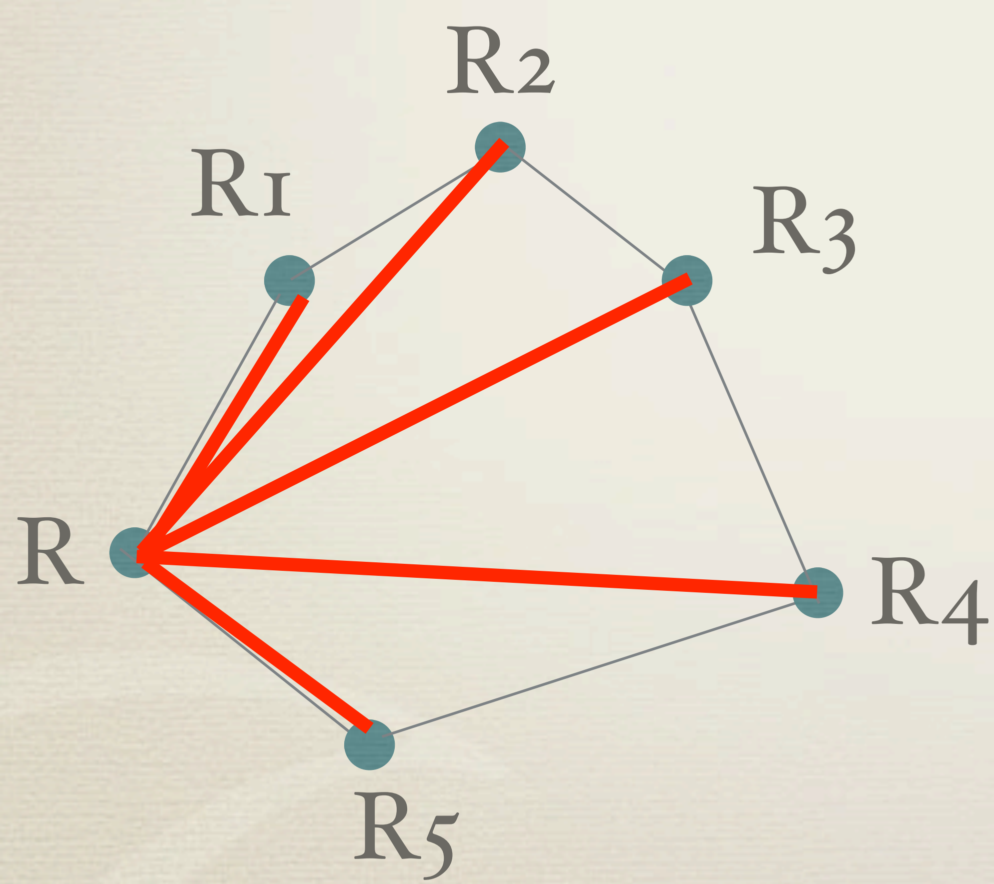
Constraints

$$\rho(R, R_1; \tau) > 0$$
$$\rho(R, R_2; 2\tau) > 0$$
$$\rho(R, R_3; 3\tau) > 0$$
$$\rho(R, R_4; 2\tau) > 0$$
$$\rho(R, R_5; \tau) > 0$$

Many constraints on R; can't move it.

One problem: Ergodicity





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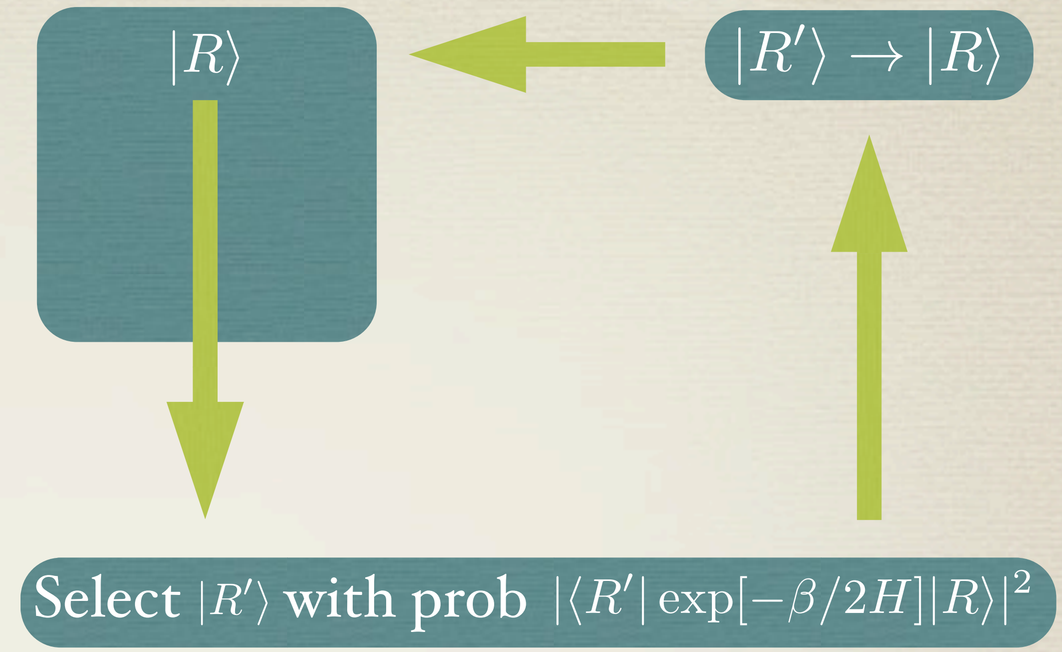
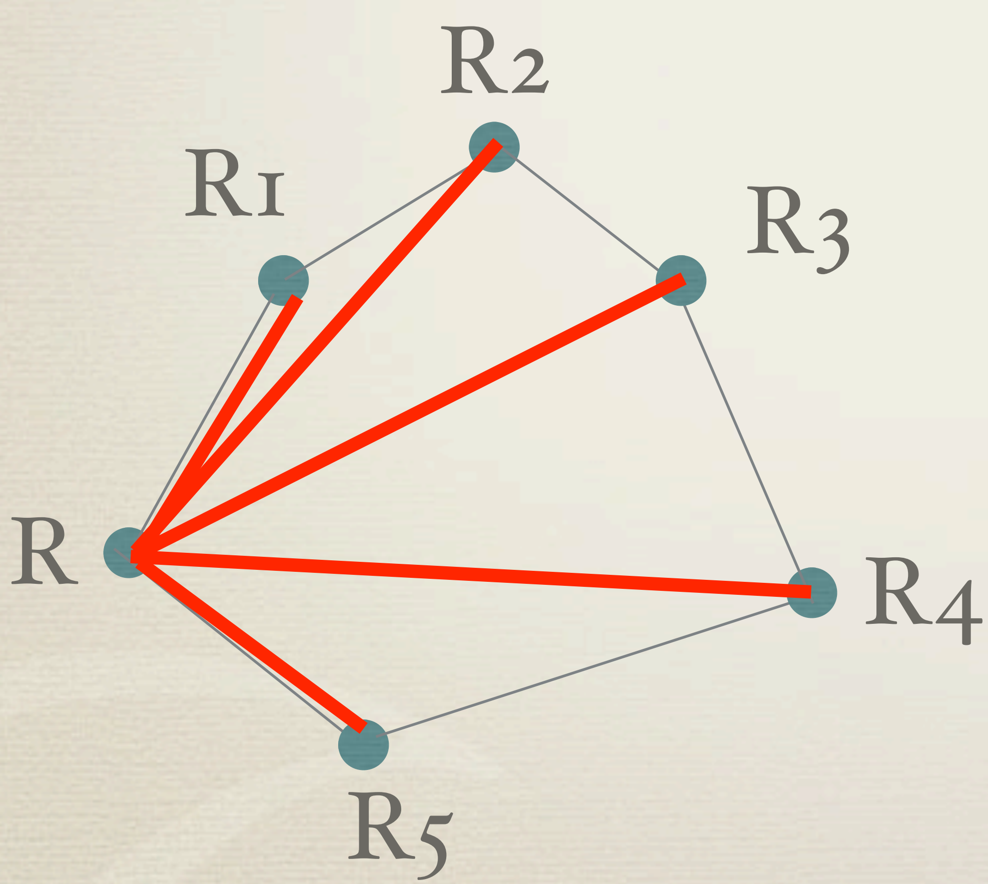
Many constraints on R; can't move it.

(Formal) Solution

1. Select R3 with probability $|\langle R_3| \exp[-\beta H/2] |R\rangle|^2$



2. R3 → R



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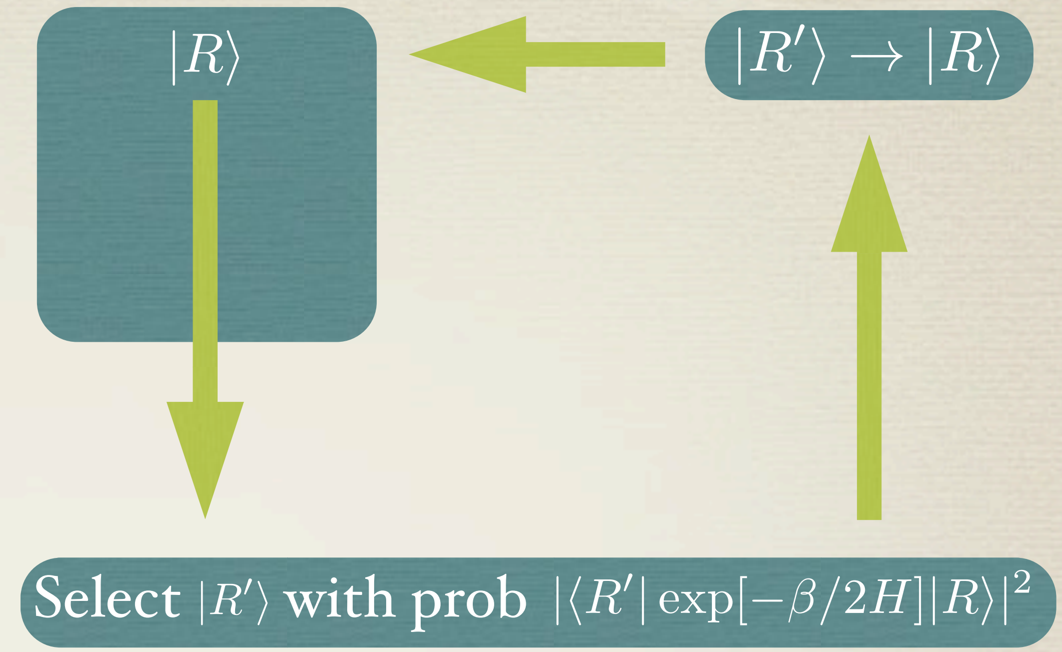
$$\rho(R, R_5; \tau) > 0$$

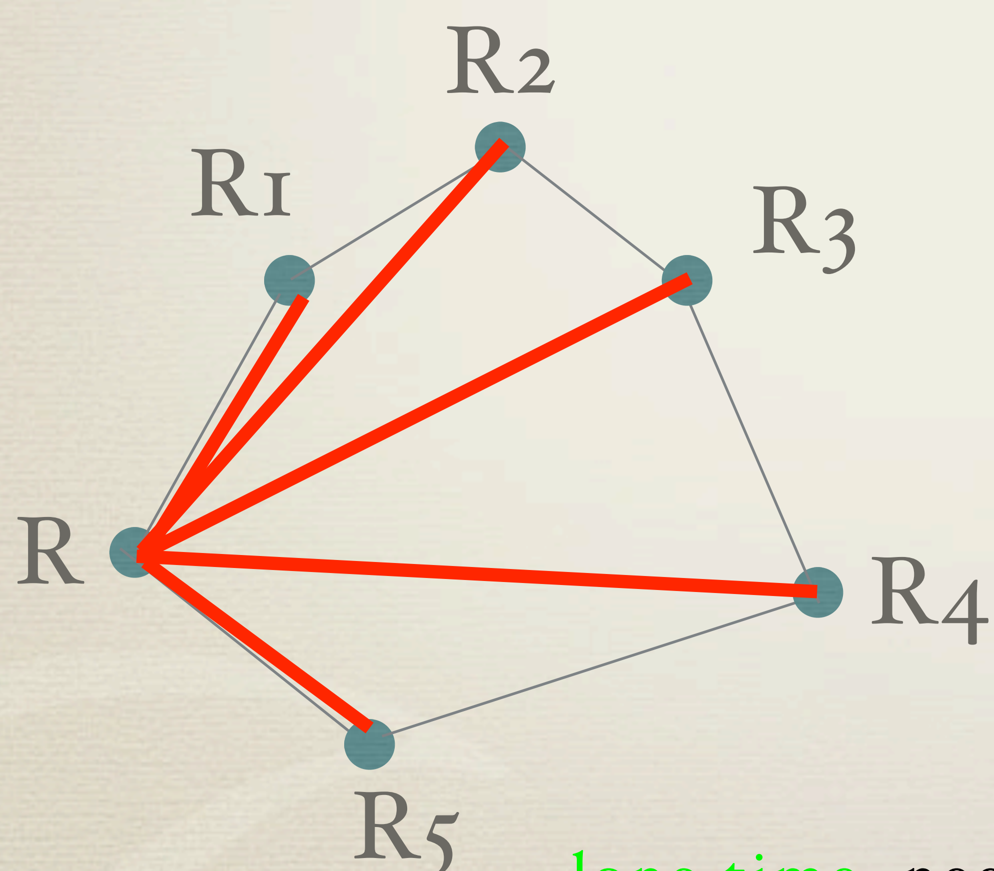
Many constraints on R; can't move it.

(Formal) Solution

1. Select R3 with probability $|\langle R_3| \exp[-\beta H/2] |R\rangle|^2$
   * Fix R
   * Run PIMC with everything else for a long time.
   * Pick R3

2. R3 → R





long time: needs to mix

Constraints

$$\rho(R, R_1; \tau) > 0$$

$$\rho(R, R_2; 2\tau) > 0$$

$$\rho(R, R_3; 3\tau) > 0$$

$$\rho(R, R_4; 2\tau) > 0$$

$$\rho(R, R_5; \tau) > 0$$

Many constraints on R; can't move it.

Another problem: nodes

1. Clearly much work needs to be done in figuring out what we should use as nodes since the restriction is the only uncontrolled approximation. Free-particle

Problem 2: **More accurate nodes** needed at low temperature.

Guessing a trial density matrix seems hard.

Optimizing a trial density matrix seems hard.

Previous attempts:

- Free fermion nodes
- Variational Density Matrix (Militzer and Pollock

A more complex way of changing the nodes is to put in backflow effects. This has been found to be very suc-

Another approach

We need to be able to evaluate whether $\langle R|\exp[-k\tau H]|R'\rangle > 0$

We've seen using VMC + stochastic reconfiguration, we start with a variational subspace $\Psi[\alpha]$ and approximately generate the wave-function $\langle R|\exp[-k\tau H]$.

This gives us a new nodal constraint for path integrals starting only with a variational subspace.

We only need to guess a variational subspace (lots of experience with this). No optimization needed! (at the level of path integrals).

Conclusions

<u>3 New Methods</u>

Finite Temperature Projector QMC

Finite Temperature VMC

Fixed Node Finite Temperature QMC

<u>2 'Improvements' to Path Integral Monte Carlo</u>

Remove ergodic problems at low T

Different nodal constraint

<u>Future</u>

Better access to imaginary time correlation functions

Applications; AFQMC version coming soon.