


New Finite Temperature Methods for Strongly Correlated Systems

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Telluride

Stochastic Methods in Electronic Structure Theory

Caveats

Not ab-initio

Simplified models

(some even in 1D)

~~Stochastic~~ **Methods** in ~~Electronic Structure~~ **Theory**

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Stochastic Methods in ~~Electronic Structure~~ Theory

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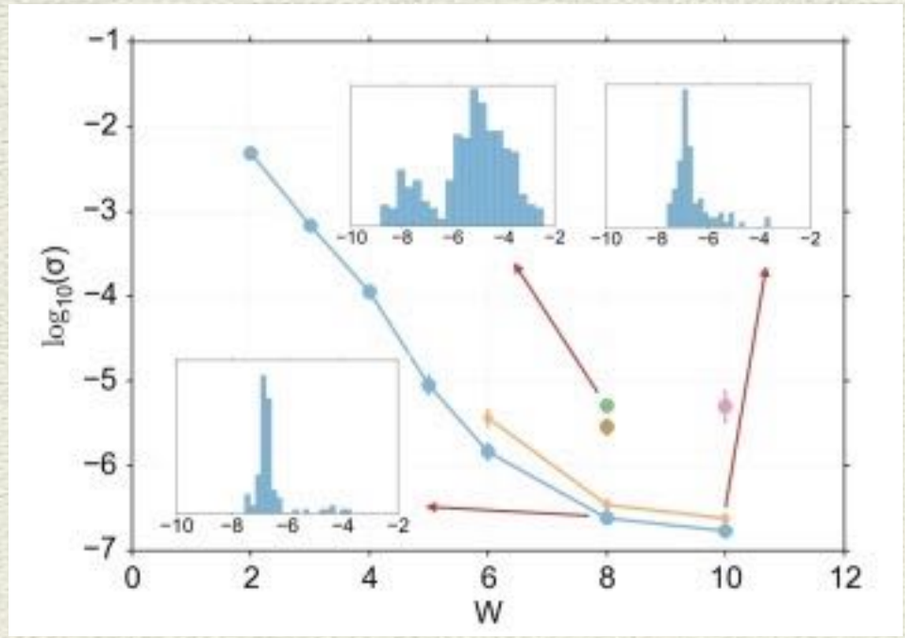
Stochastic Methods *probably useful*
in Electronic Structure Theory

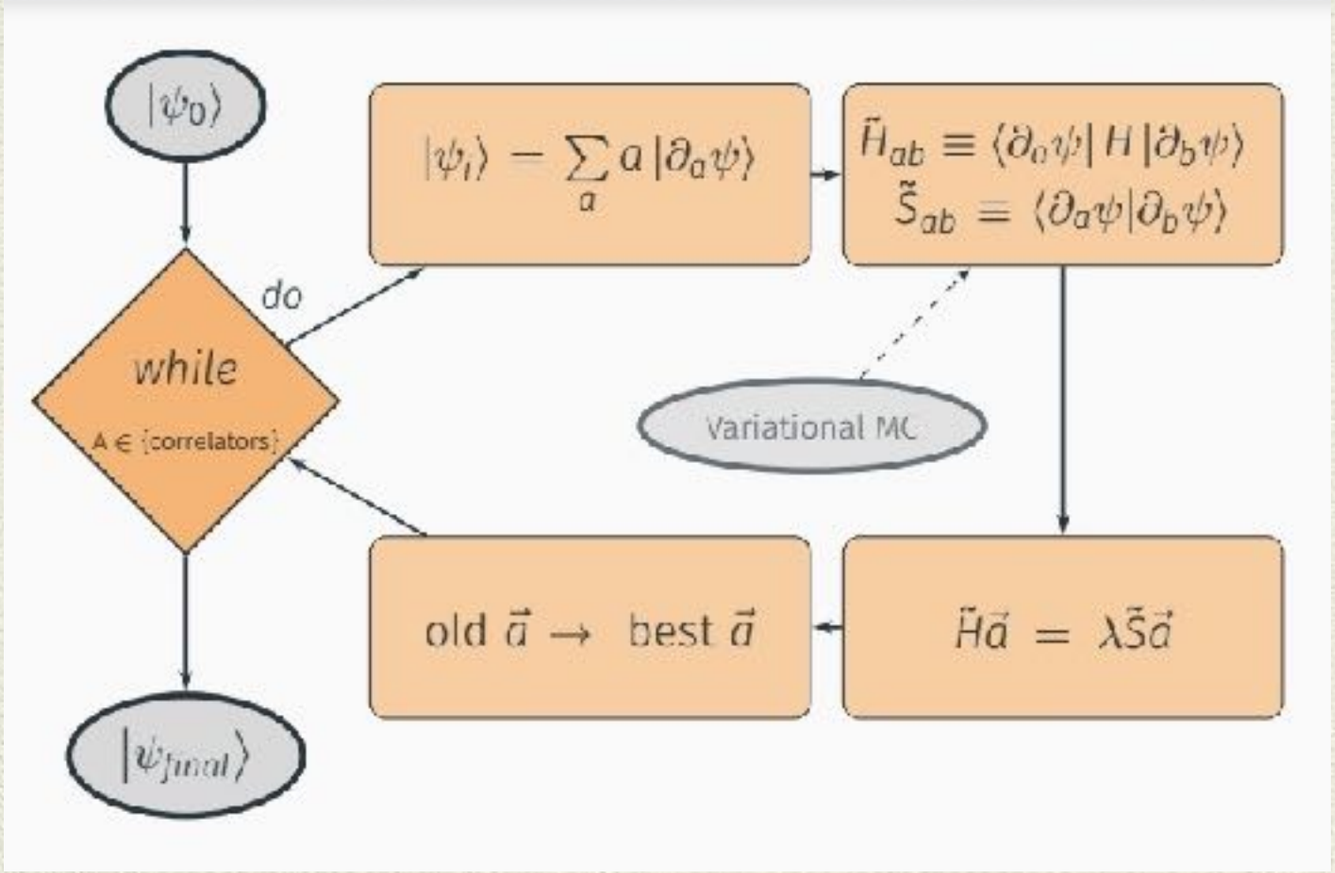
Advertisement **Finding highly excited states…..** 2^{100}

Many Body Localization

One-dimension

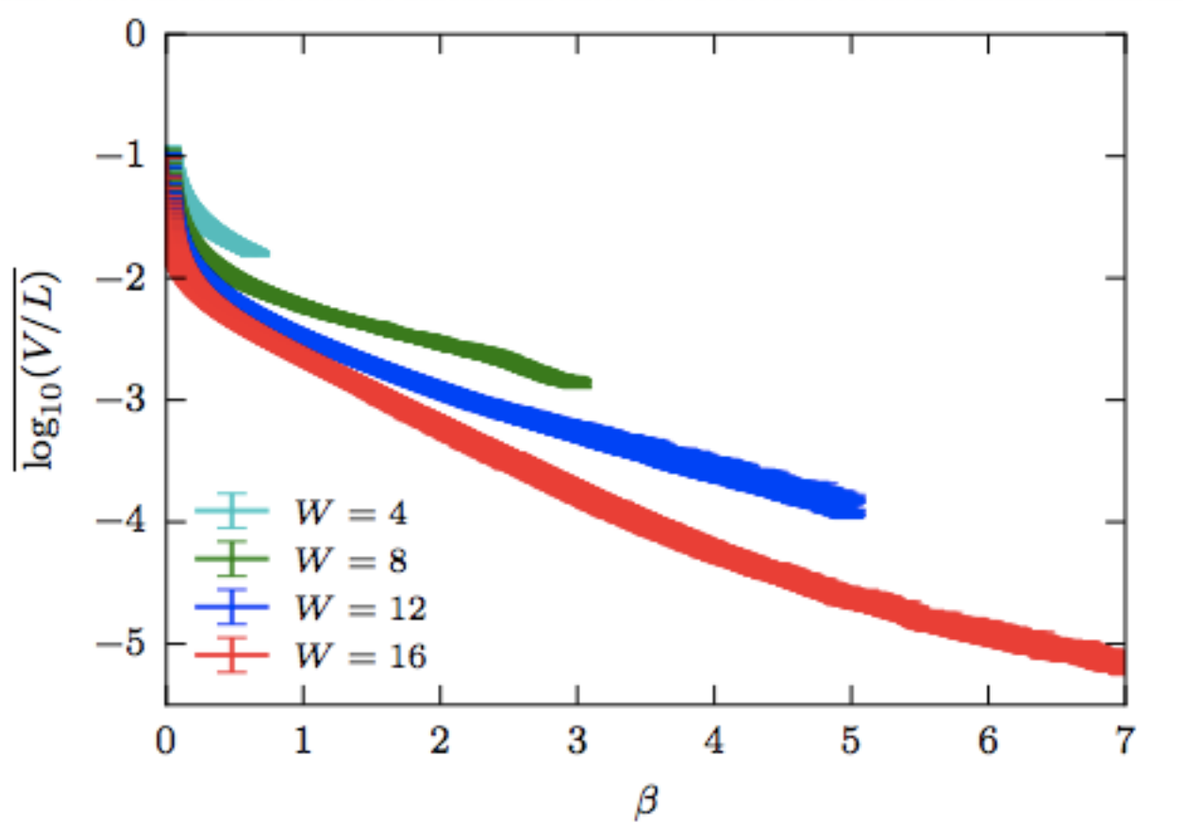
Interaction + Disorder (W)





with:
Xiongjie Yu,
Benjamin Corregea
David Pekker

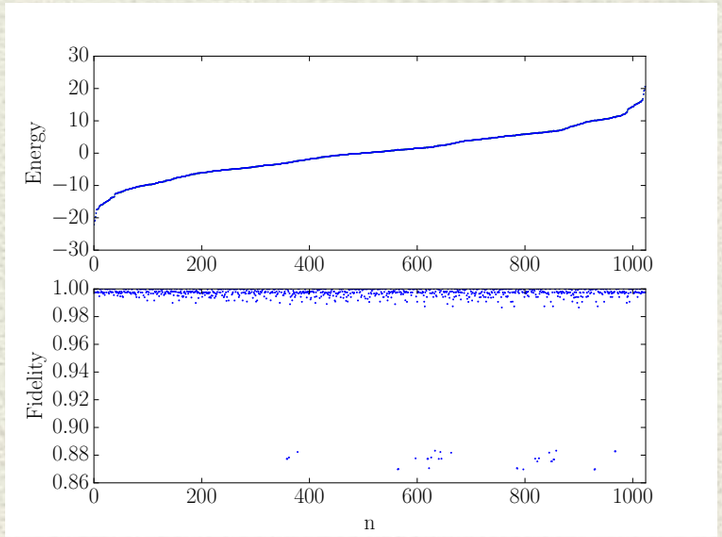
Finding chunks of spectrum…

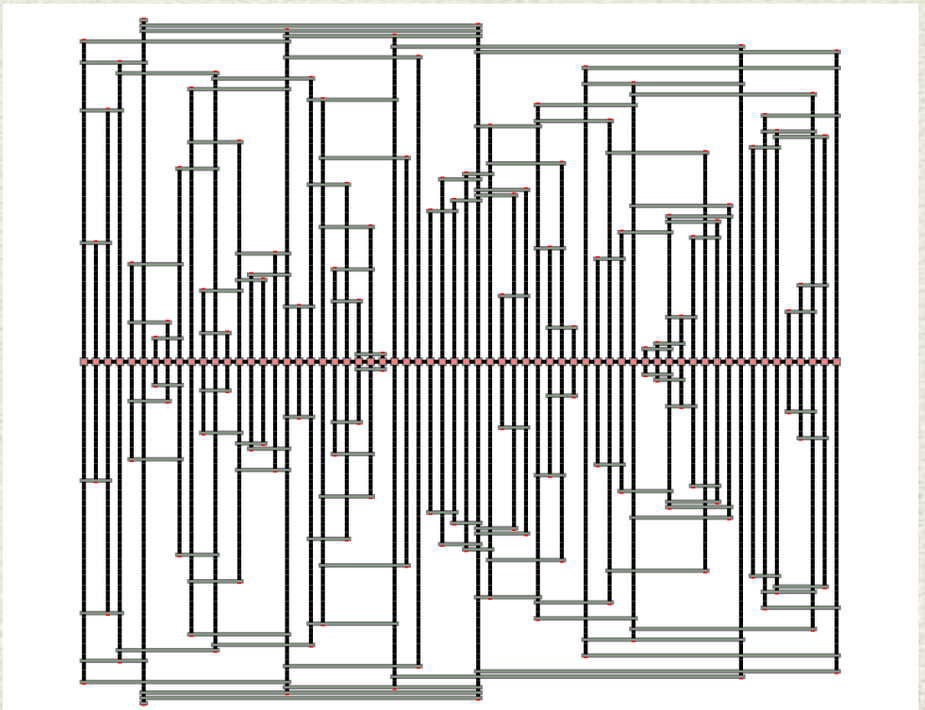


Many Body Localization

One-dimension

Interaction + Disorder (W)





with:

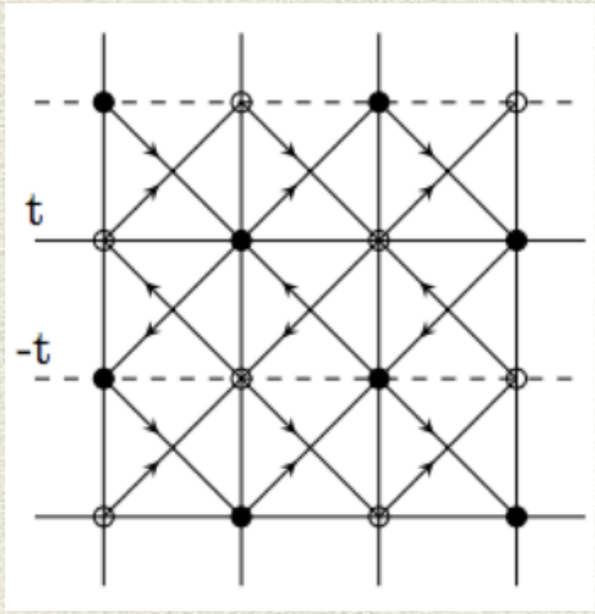
Xiongjie Yu,

David Pekker

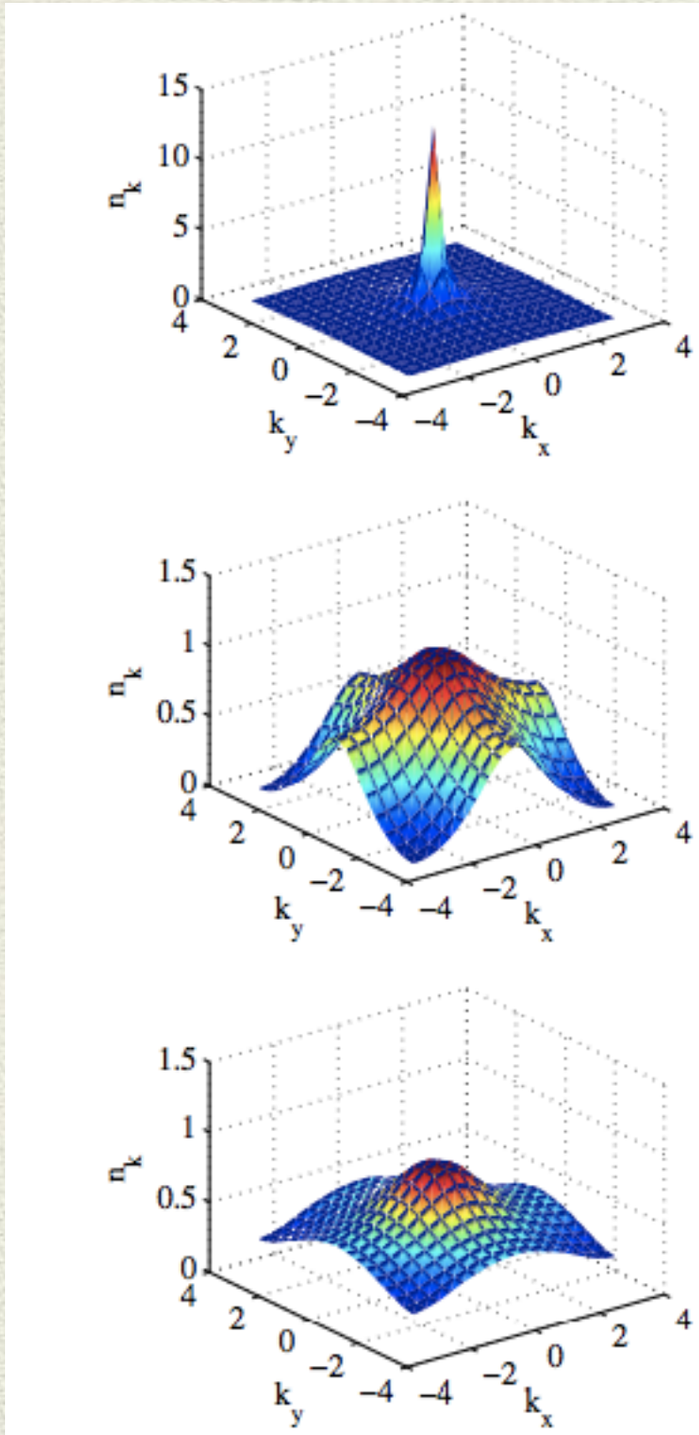
Bosonic Wave-Functions: Beyond Jastrows

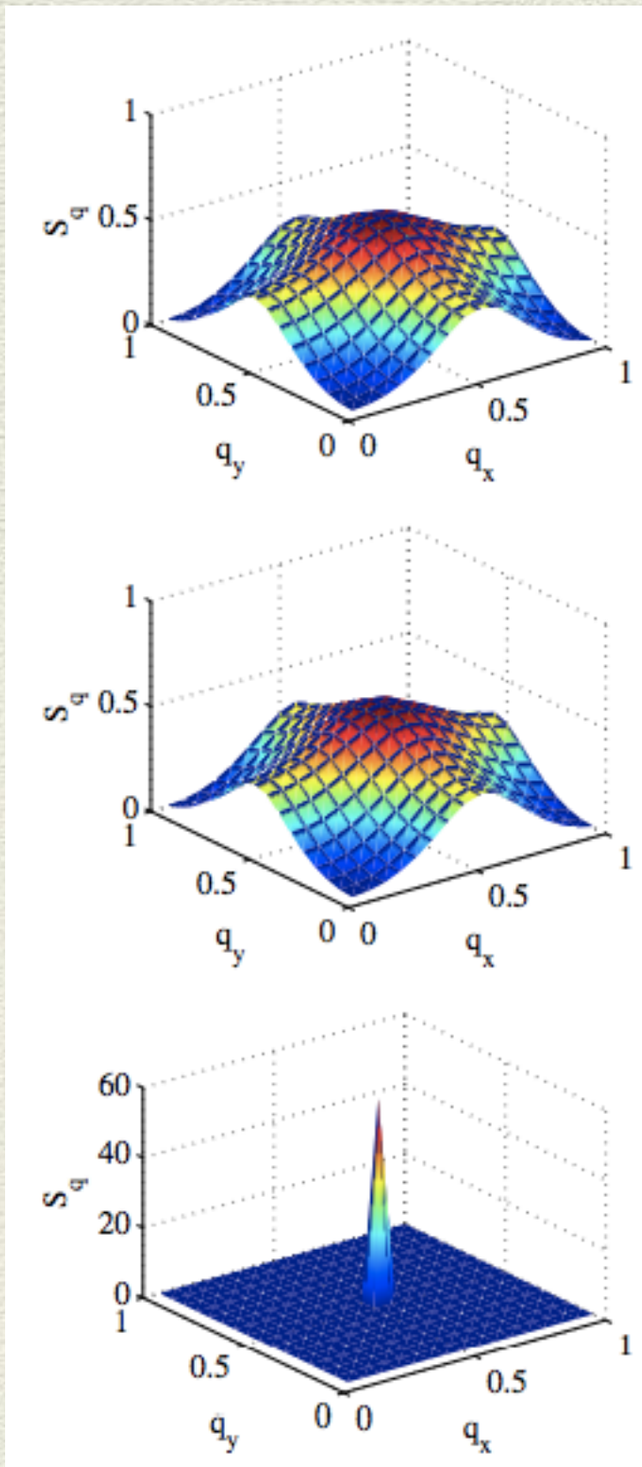
with:

Hassan Shapourian



$$H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i \sum_{\langle\langle ik \rangle\rangle} \Delta_{ik} c_i^\dagger c_k + \sum_i m_i c_i^\dagger c_i$$





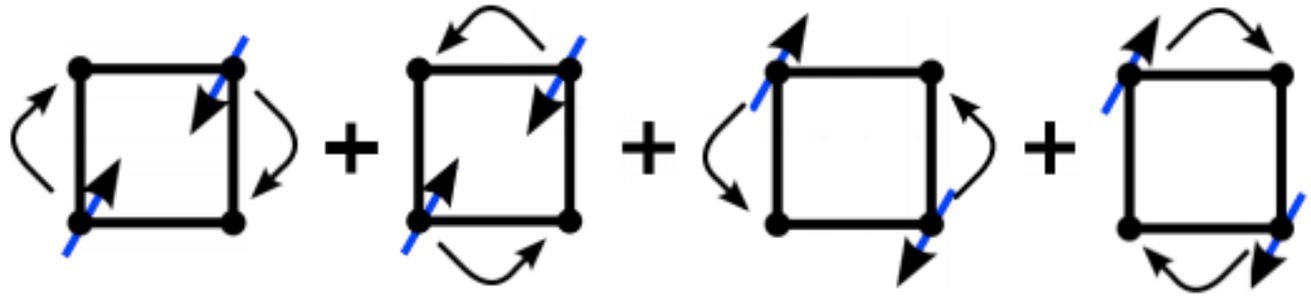
$$\Psi(\{\mathbf{r}_i\}) = \det{}_1(\{\mathbf{r}_i\}) \times \det{}_2(\{\mathbf{r}_i\})$$

Strange Metals

ok…some actual electrons

with:
Katie Hyatt
Matthew Fisher

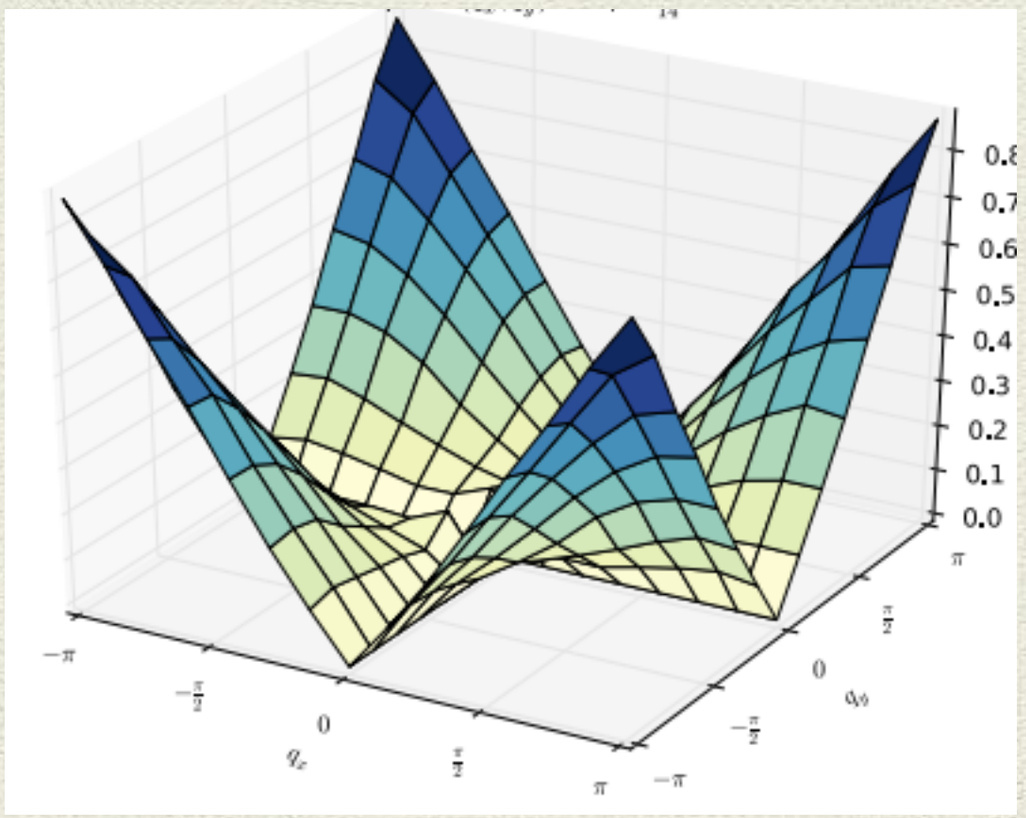
$$\hat{H} = K \sum_{\mathbf{r}} c^{\dagger}_{\mathbf{r}\uparrow} c_{\mathbf{r}+\hat{\mathbf{x}},\uparrow} c^{\dagger}_{\mathbf{r}+\hat{\mathbf{x}}+\hat{\mathbf{y}},\downarrow} c_{\mathbf{r}+\hat{\mathbf{y}},\downarrow} + \uparrow \leftrightarrow \downarrow + \text{h.c.}$$



No sign problem

Done with reputation +DMC

Worse forward walking + population bias I've ever seen.



Done with advertisment

Ground State Methods

Variational Monte Carlo

Variational Error

Fixed-Node Diffusion Monte Carlo

`Better' Variational Error

Diffusion Monte Carlo

Statistical Error

Finite Temperature Methods

Variational Density Matrices (VDM)

Variational Error

Restricted Path Integral Monte Carlo

`Better' Variational Error

Path Integral Monte Carlo

Statistical Error

In this talk, we will consider the question: *What are the some algorithms to compute finite temperature properties of fermionic, strongly correlated systems?*

We will discuss three algorithms:

- VAFT <—> A new (*implicit*) Variational Density Matrix
- RPIMC with (morally) the new VDM as the restriction
- Variational Finite T PI

Variational Density Matrices

Choose a class of trial density matrices $\rho[\beta, \vec{\alpha}]$

Select the one with the lowest free energy.

This optimization is not straightforward.

Choice 1

Compute Free Energy by thermodynamic integration.

Need all $\rho(\tau)$ for $0 < \tau < \beta$

How are you going to optimize this?

Choice 2

Use a Monte Carlo move to swap between density matrices and measure time at each spot.

Trial Density Matrices

$$\rho(R^*, R)$$

$$\rho(R^*, R) = \det[\exp[-k(r_i^* - r_j)^2]]$$

Free fermion density matrix

$$k = 1/(4\lambda\tau)$$
$$\tau = 1/T$$

Outer product of wave-functions

$$\rho(R^*, R) = \langle R^* | \left(\sum_{i,j} \alpha_{ij} |\Psi_i\rangle\langle\Psi_j| \right) |R\rangle$$

Ground state

$$\rho(R^*, R) = \langle R^* | \Psi_0 \rangle \langle \Psi_0 | R \rangle$$

eigenstates

$$\rho(R^*, R) = \langle R^* | \left(\sum_i \exp[-\tau E_i] |\Psi_i\rangle\langle\Psi_i| \right) |R\rangle$$

$$\rho(R^*, R) = \langle R^* | \left(\sum_i \exp[-\tau E_i] |\Psi_i\rangle\langle\Psi_i| \right) |R\rangle$$

This is the right answer and an appealing start for an approximation.

Just need to

Guess a wave-function for each excitation

Guess an energy for each excitation

(but at least we have experience in wave-functions)

$$\rho(R^*, R) = \langle R^* | \left(\sum_i \exp[-\tau E_i] |\Psi_i\rangle\langle\Psi_i| \right) |R\rangle$$

This is the right answer and an appealing start for an approximation.

Just need to

Guess a wave-function for each excitation

many excitations, hard per excitation, hard to sum…

Guess an energy for each excitation

(but at least we have experience in wave-functions)

$$\rho(R^*, R) = \langle R^* | \left(\sum_i \exp[-\tau E_i] |\Psi_i\rangle\langle\Psi_i| \right) |R\rangle$$

This is the right answer and an appealing start for an approximation.

Just need to

Guess a wave-function for each excitation

Guess an energy for each excitation

(but at least we have experience in wave-functions)

Write the right answer and approximate is a good approach.

Need a different representation of the right answer.

A Different Representation

(Sneakily) an exponential sum of outer products that we can compute with.

VAFT

Input: Variational Manifold of wave-functions

Output: Approximate samples from a variational many-body density matrix.

High level approach: Write down a Markov chain (*not metropolis)* which samples configurations from the many body density matrix.

Discover you can't do the Markov chain.

Write down a new Markov chain which hopefully has a stationary distribution close to the actual one.

Notice that this is also sampling from some many-body density matrix.

A Markov chain whose fixed point probability distribution is the diagonal of the finite temperature many-body density matrix.

$|R\rangle$

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

$|R'\rangle \rightarrow |R\rangle$

Proof: Two slice PIMC with an exact action of inverse temperature $\beta/2$.

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

Proof by PIMC

Typical PIMC: move R, move R′, move R, move R′, …

Atypical PIMC 1: move R a lot, move R′ a lot, move R a lot, ….

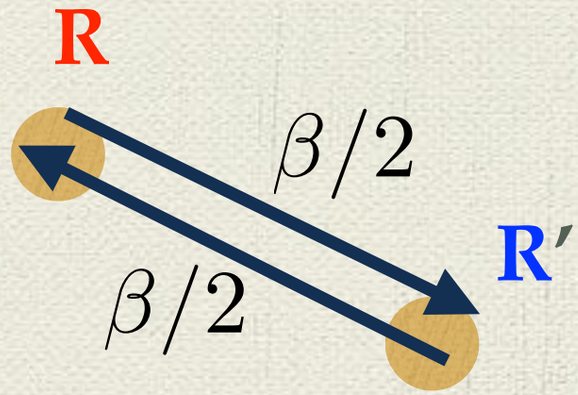
Atypical PIMC 2:

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

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

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

….



A Markov chain whose fixed point probability distribution is the diagonal of the finite temperature many-body density matrix.

$|R\rangle$

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

How?

$|R'\rangle \rightarrow |R\rangle$

Sample using VMC

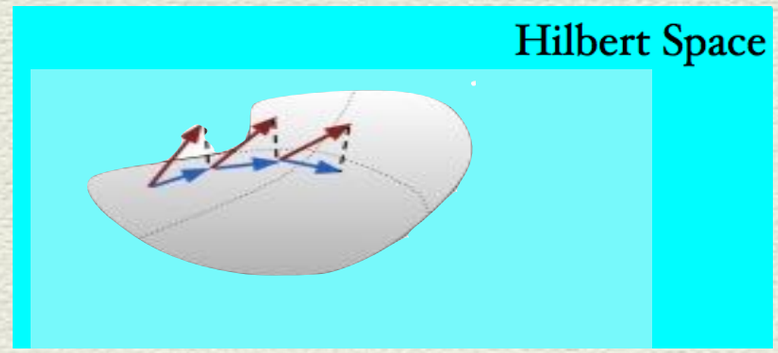
Select $|R'\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$

Imaginary time evolution of arbitrary variational wave-functions

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

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

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

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

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

Q: Is the approximation a variational density matrix?

Yes…implicitly (at least for a fixed β)

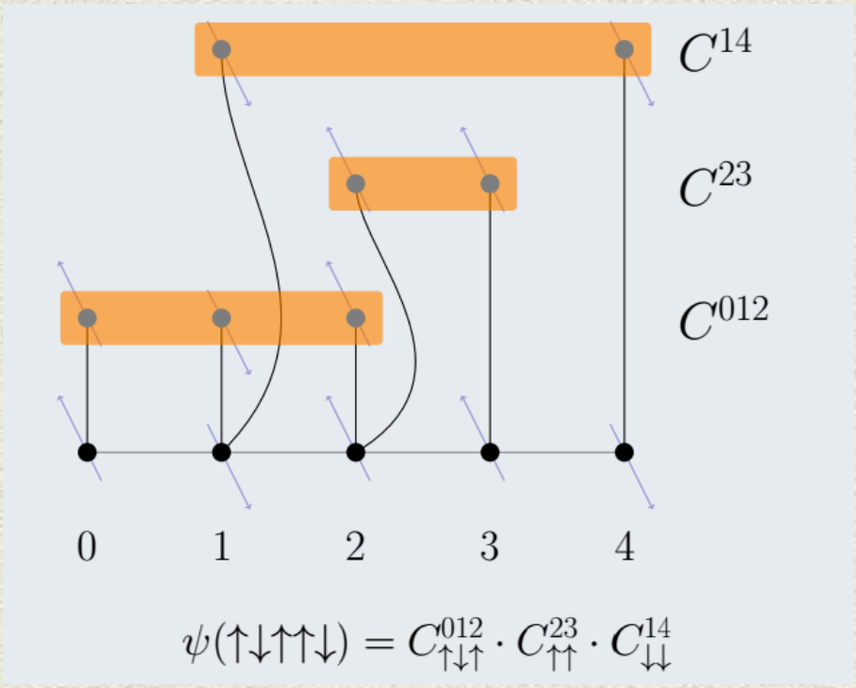
$$\sum_c \frac{|\tilde{\Psi}[\beta/2;c]\rangle\langle\tilde{\Psi}[\beta/2;c]|}{\langle\tilde{\Psi}[\beta/2;c]|\tilde{\Psi}[\beta/2;c]\rangle}\tilde{p}(c)$$

Ideal $\widetilde{p}(c) = \dfrac{\langle c|e^{-\beta' H}|c\rangle}{Tr(e^{-\beta' H})}$

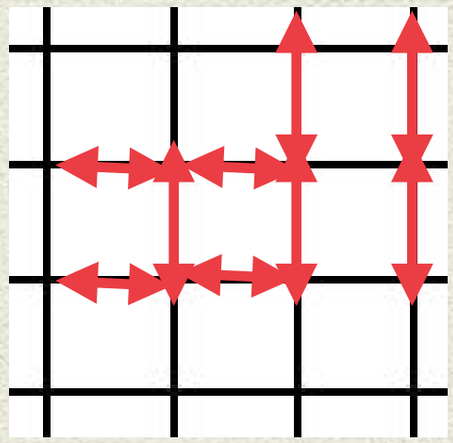
Reality $\tilde{p}$ is defined implicitly by the markov chain

A prototypical variational wave-function: Essentially a fancy Jastrow

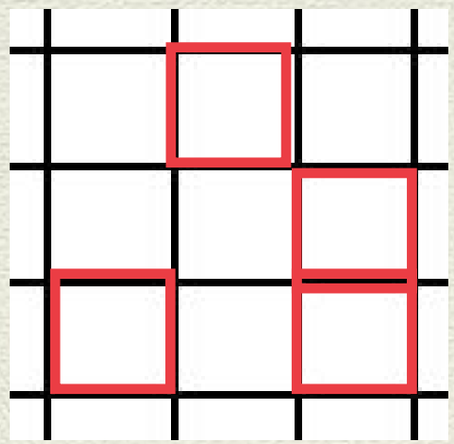
Huse-Elser States (aka correlated product states, entangled plaquette states, graph tensor networks states, …)



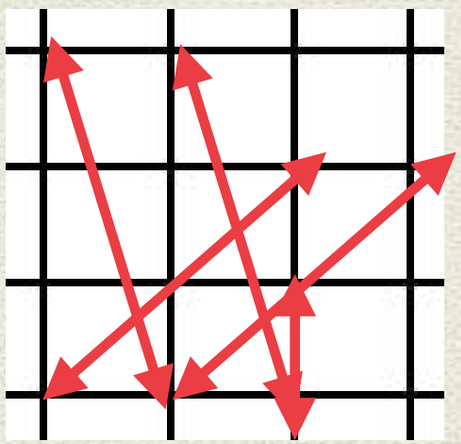
Can choose different patterns.



nn pairs



plaquettes

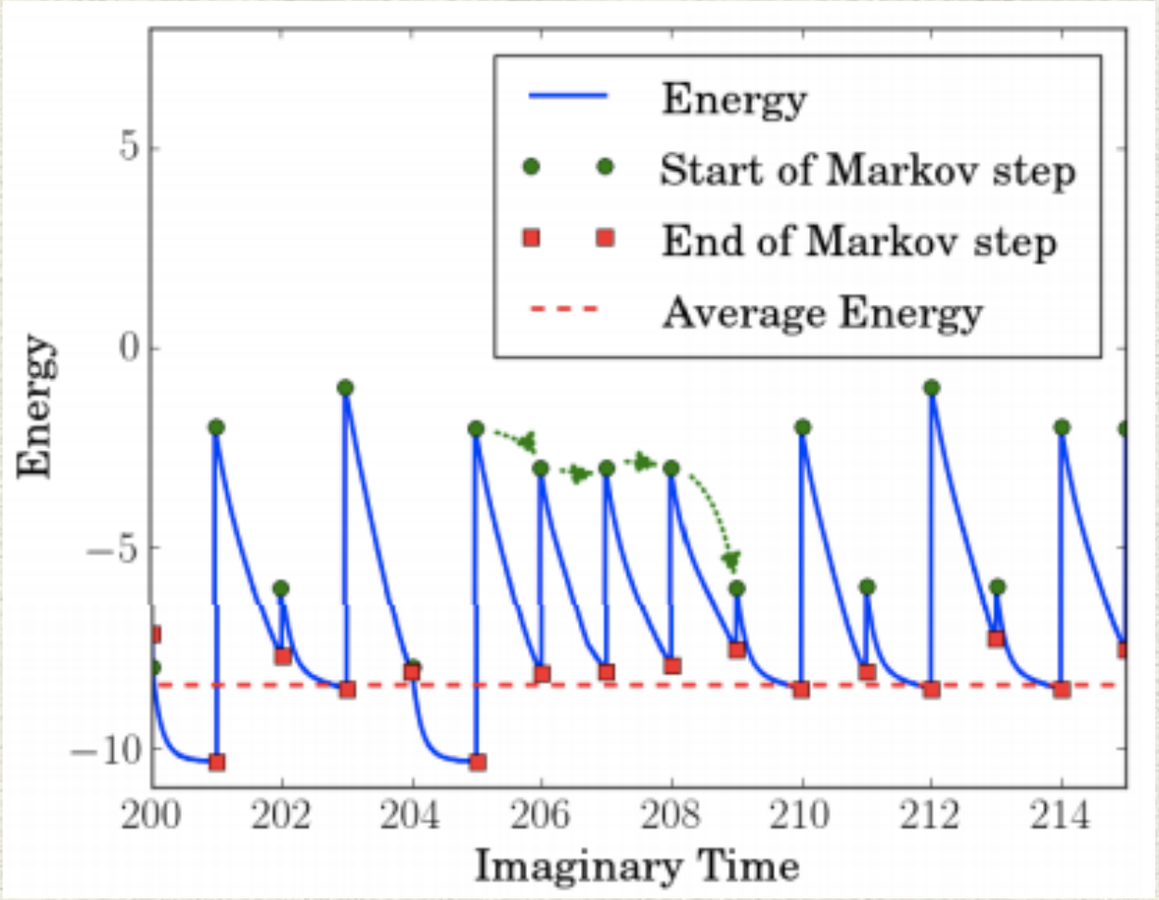


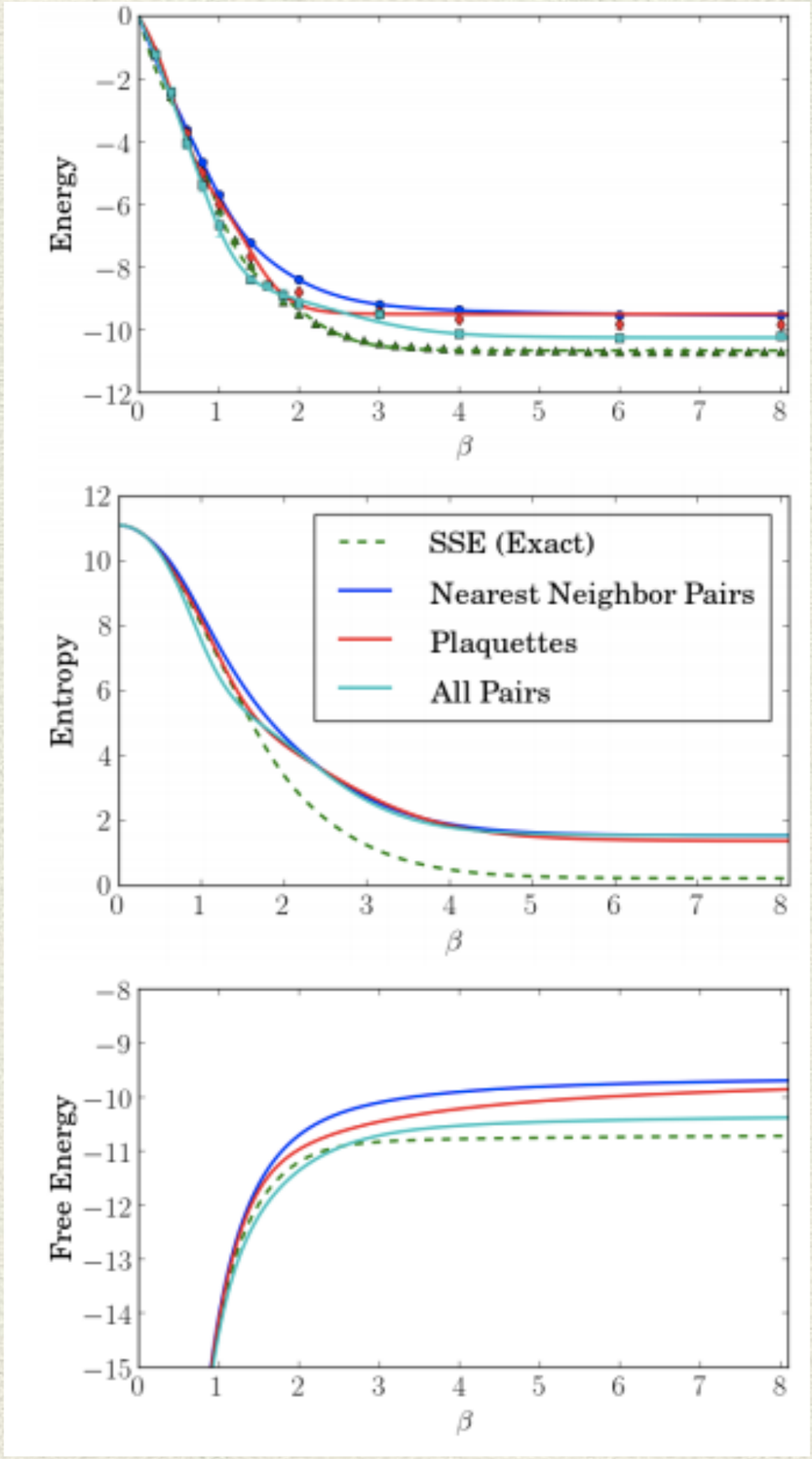
all pairs

A prototypical Hamiltonian: **Heisenberg Model**

$$H = \sum_{\langle ij \rangle} \sigma_i \cdot \sigma_j$$

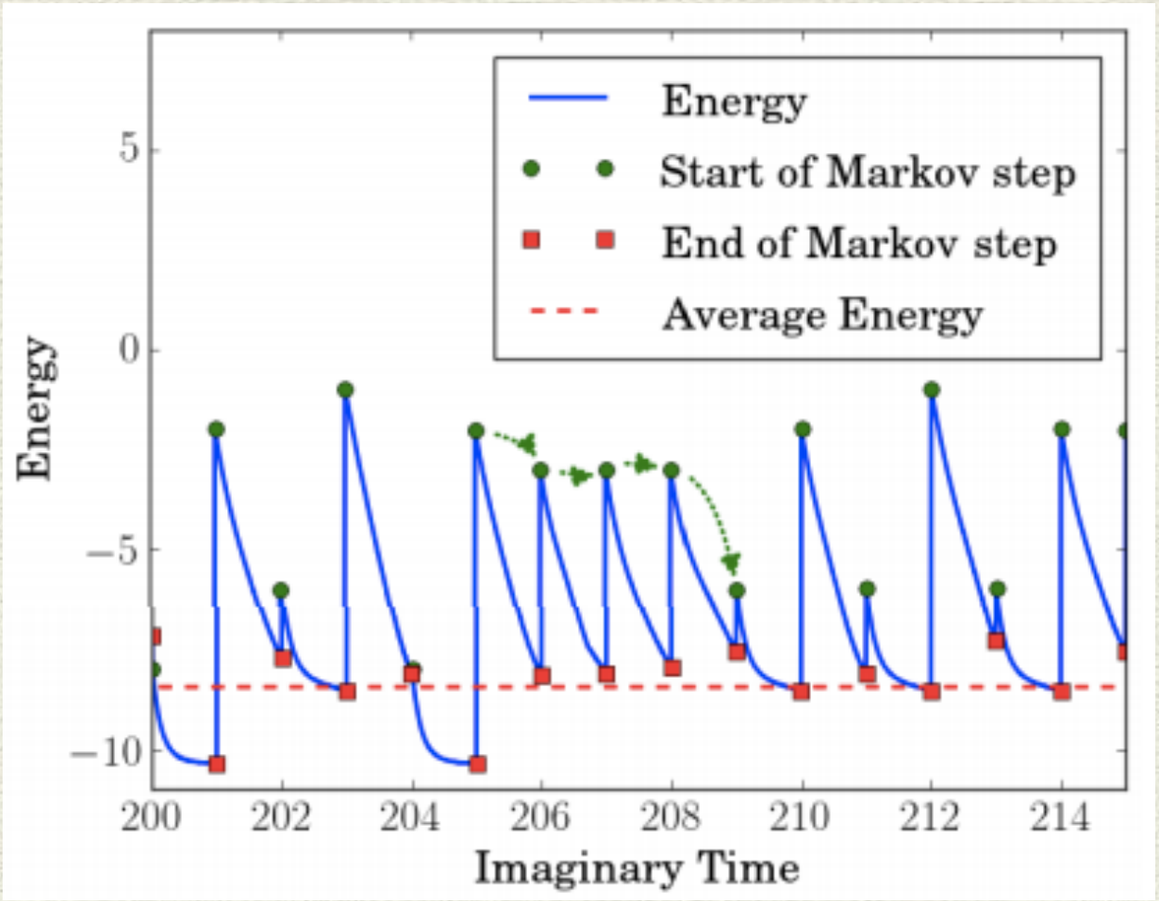
On a bipartite lattice can do exactly with SSE to compare new method against.

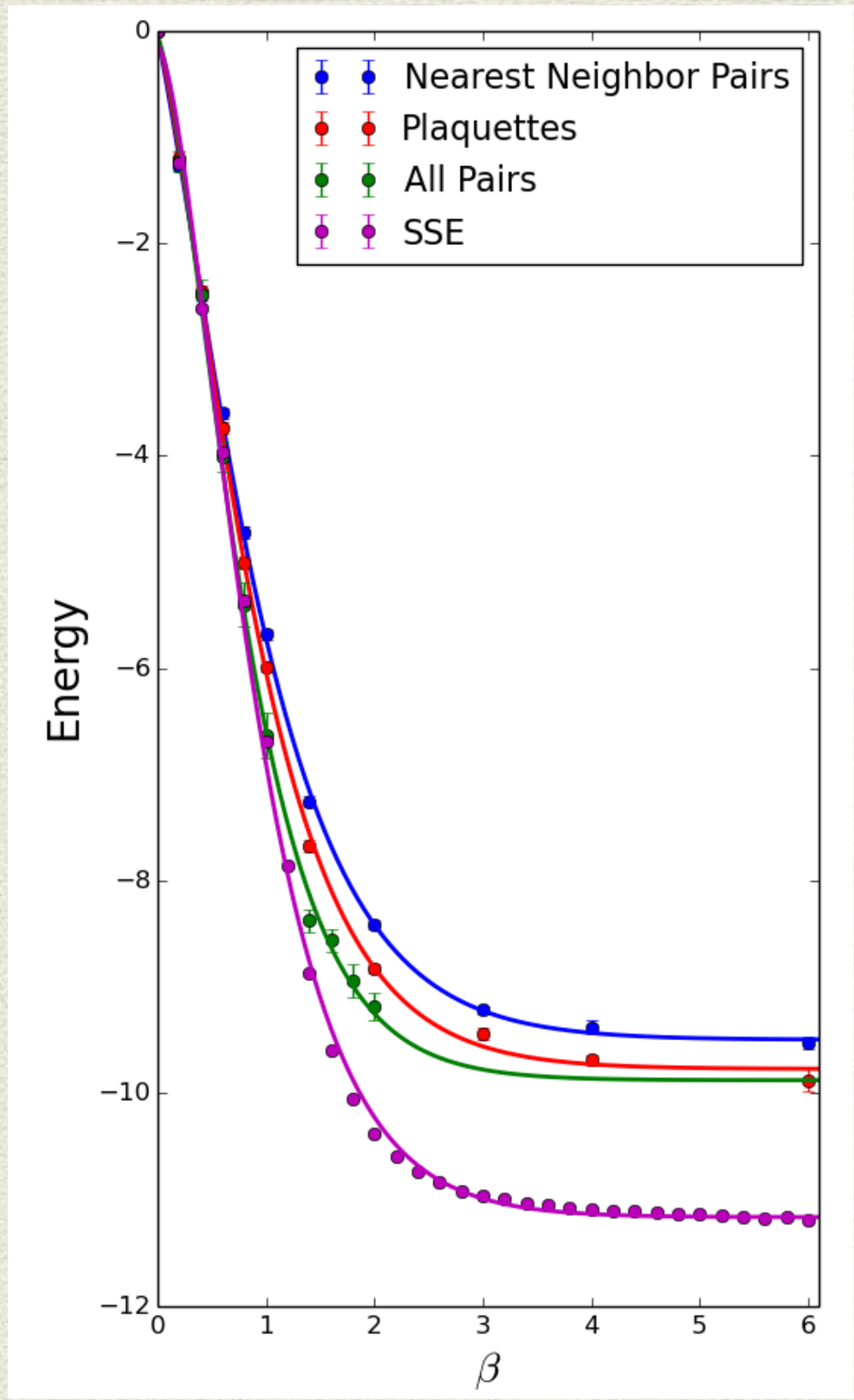




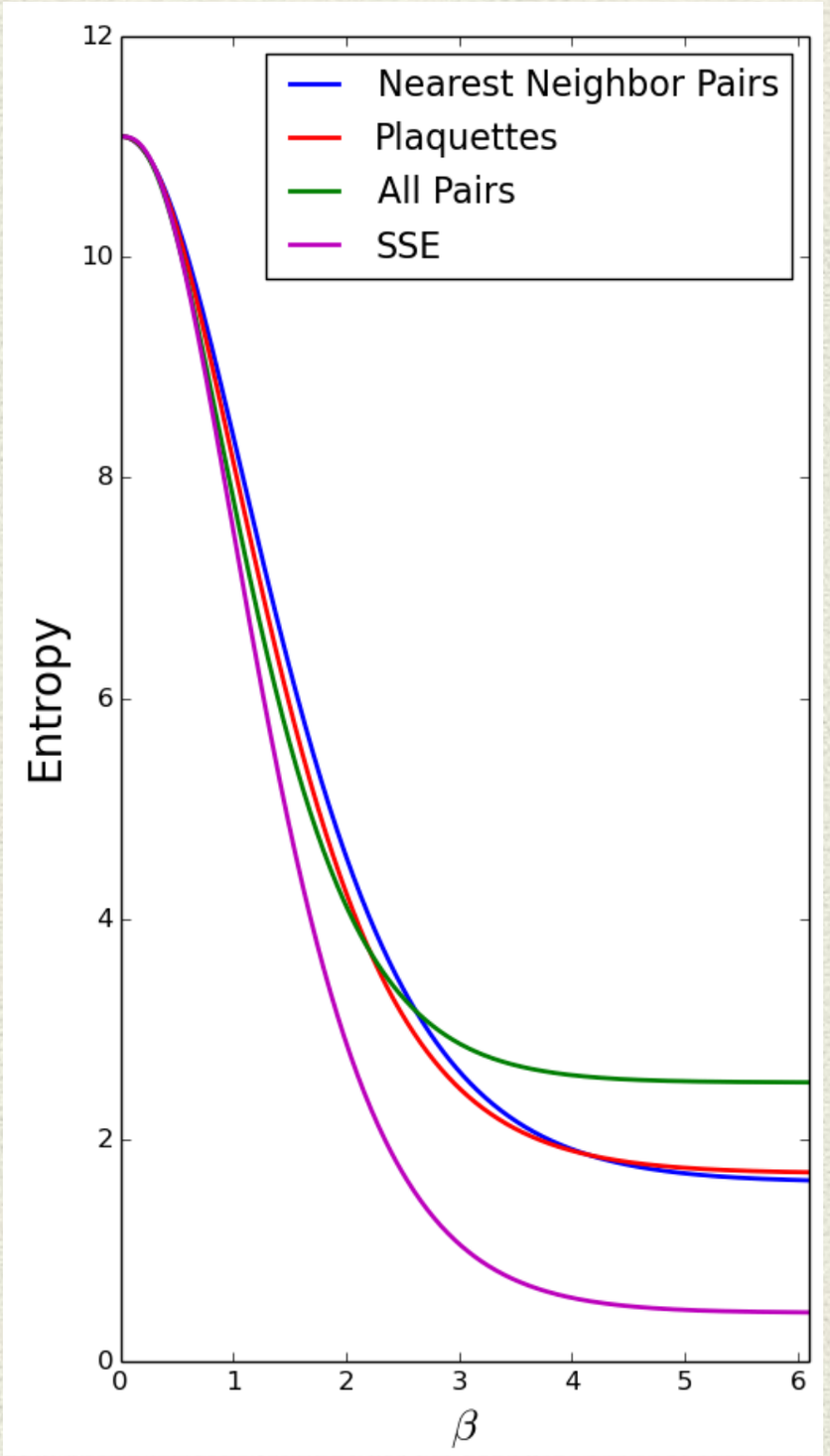
Via thermodynamic integration
Free energy variational principle
Gives best variational manifold*

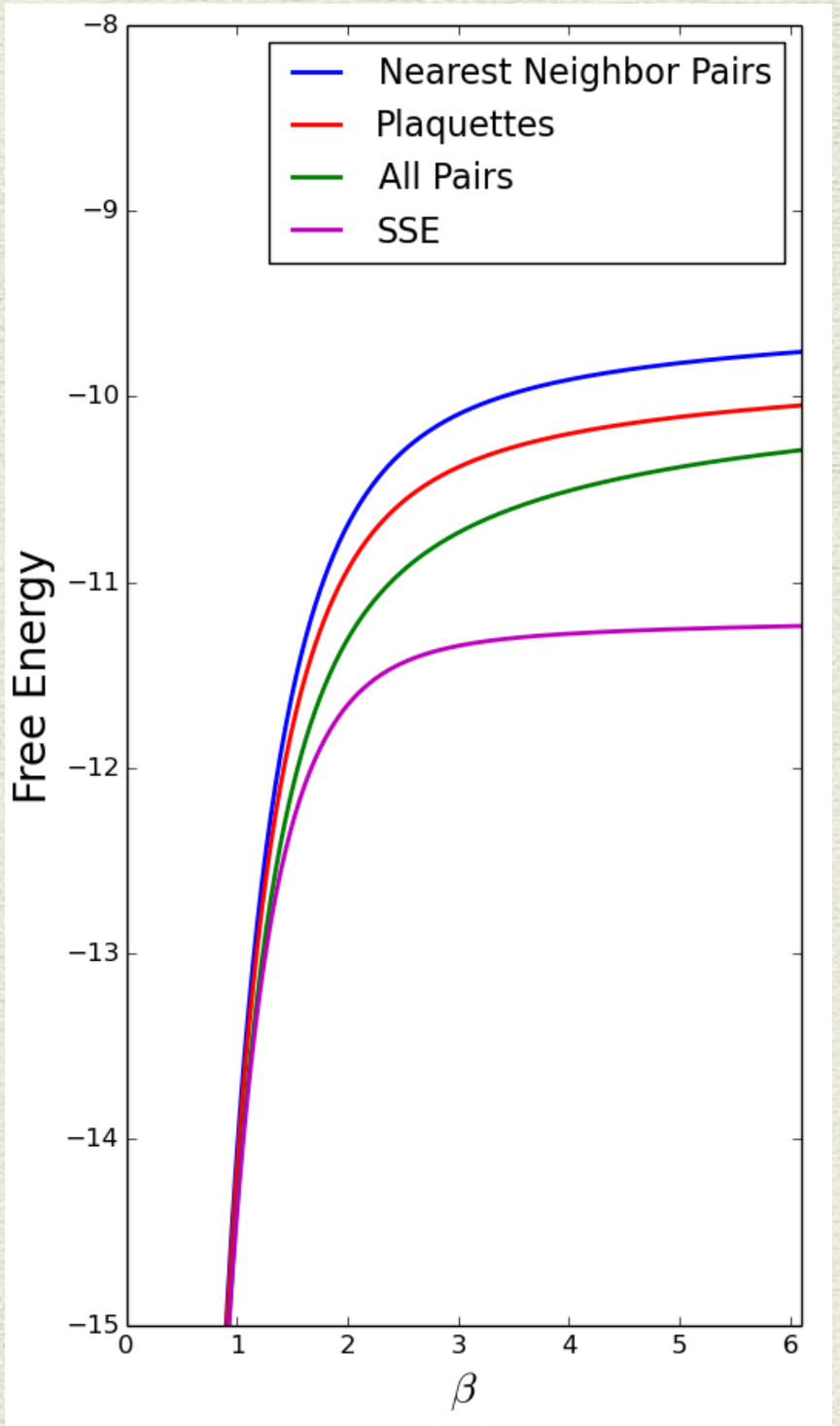
*Free energy of "all DM"





4 x 4 bipartite Heisenberg



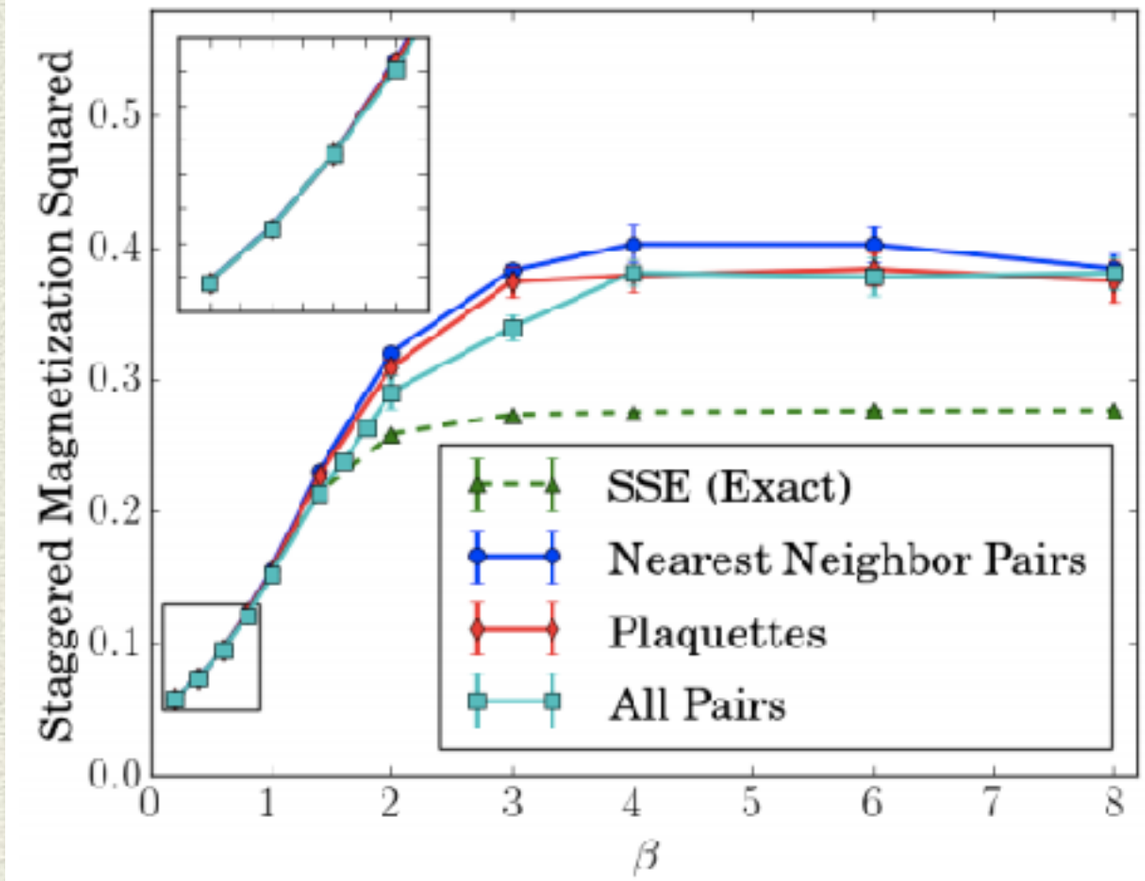


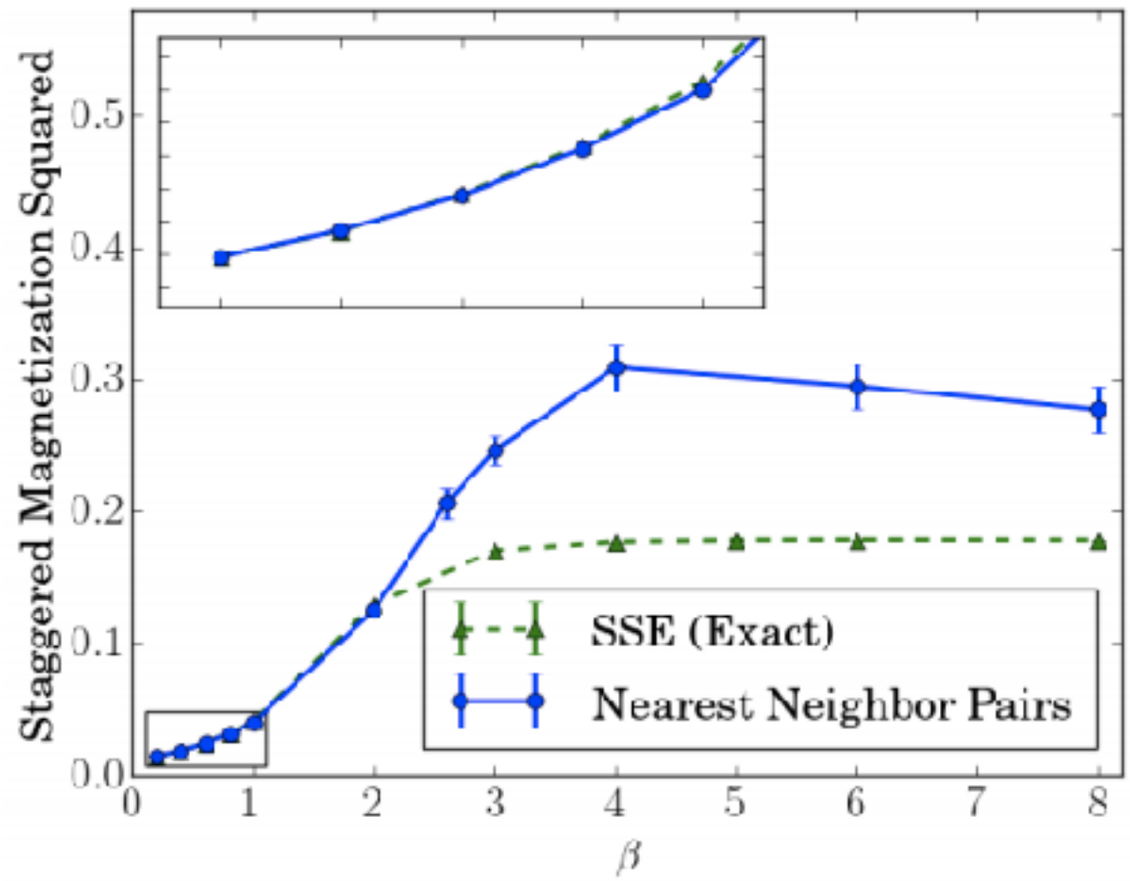
Warning: Minor subtle point on the thermodynamic integration.

via thermodynamic integration

Free energy variational principle (tells you which variational manifolds are 'better')

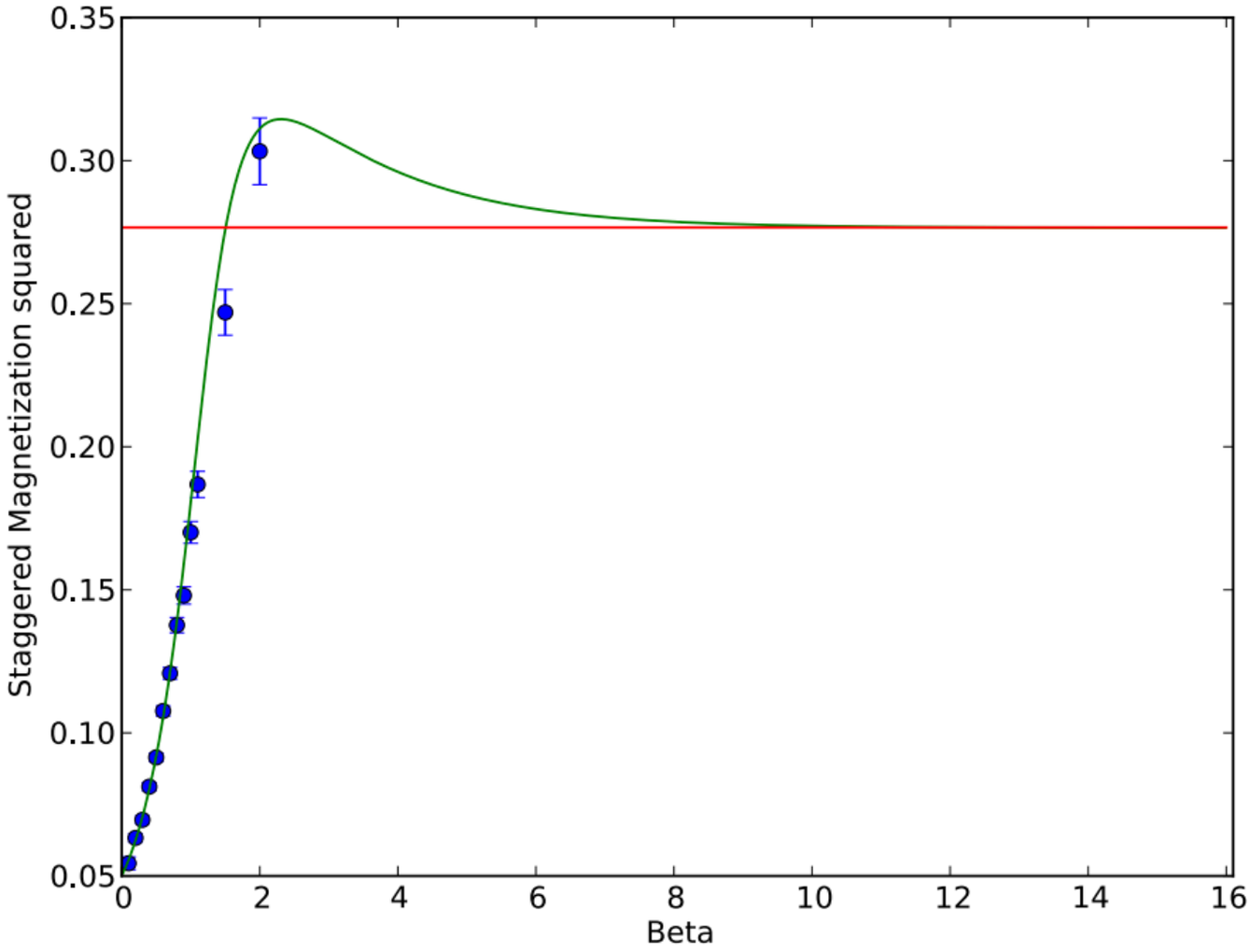
Can compute arbitrary properties of the "variational density matrix."





We have versions of this with projector Monte Carlo
(sign problem but you can beat it down with FCIQMC)

Dift?



A better (in some ways) DMQMC

Also developing fixed-phase AFQMC version

Advantages…

No `optimization'

Exact when variational ansatz gets sophisticated enough.

Probably a better density matrix.

No stochasticity or sign problem

Consistent approach for all temperatures.

Disadvantages..

Variational Error

Slow….

Question (*not answered yet*): How does VAFT compare to RPIMC with simple trial density matrix.

Finite Temperature Methods

Variational Density Matrices (VDM)

Variational Error

not explicitly representable

Can this be used?

Restricted Path Integral Monte Carlo

`Better' Variational Error

Path Integral Monte Carlo

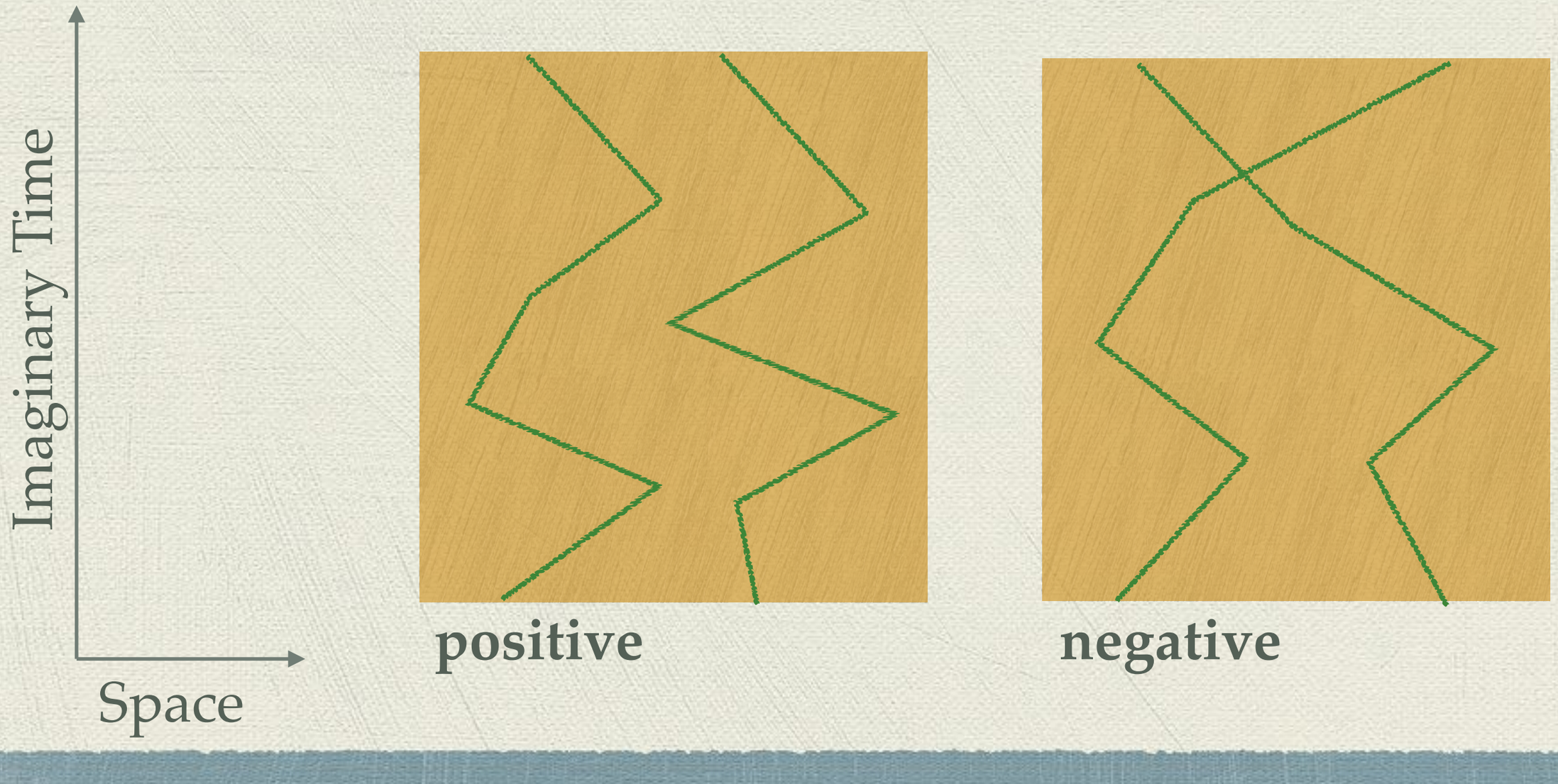
Statistical Error

Path Integrals for Fermions (without approximations)

$$\rho_F(R^*, R; \beta') = \frac{1}{N!} \sum_{\pi} (-1)^{\pi} \int_{R^*}^{\pi(R)} dR_t \exp[-S(R(t)]$$

Sample all paths + permutations

Odd permutations count negative

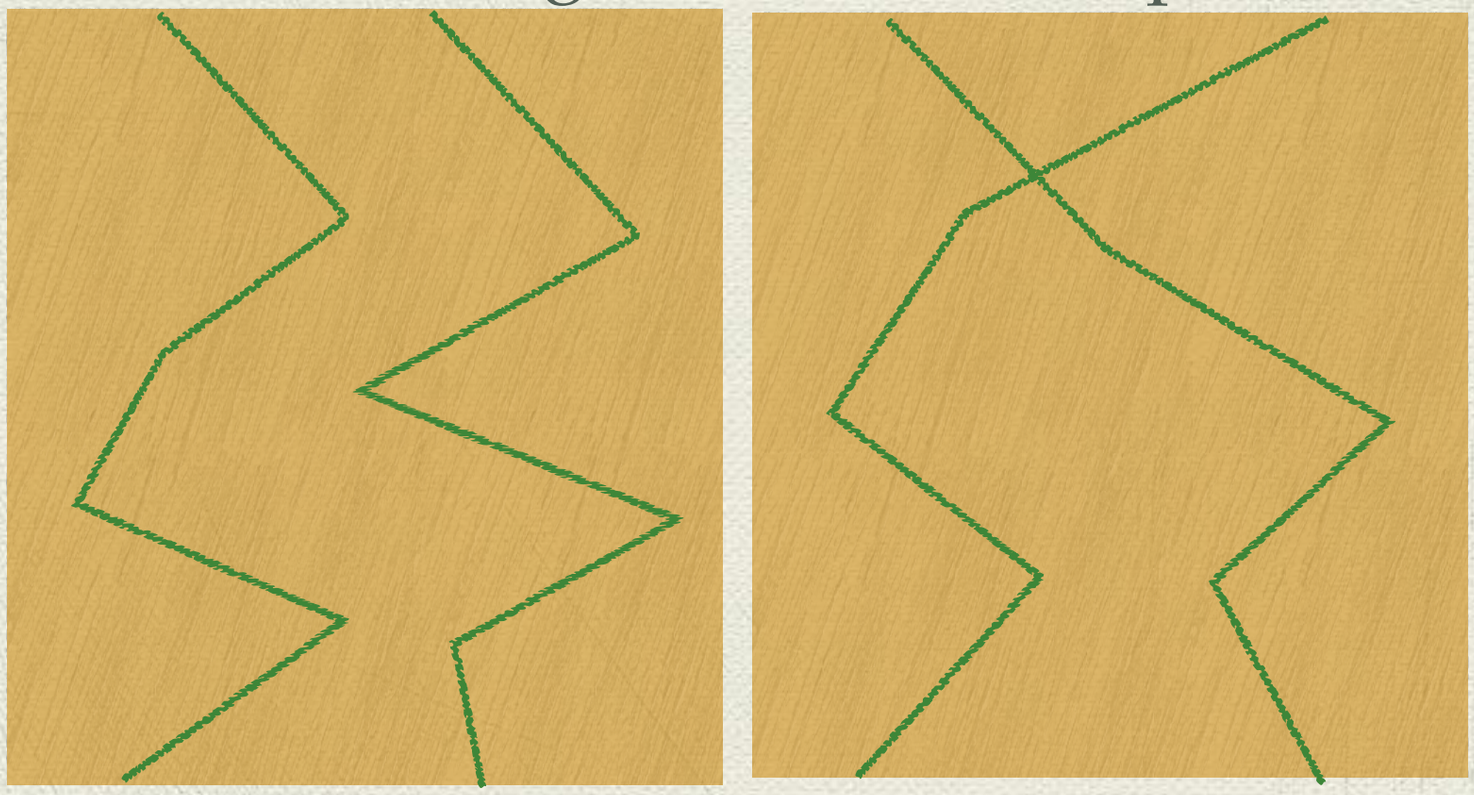


Path Integrals for Fermions (with approximations)

Restricted Path Integral Monte Carlo

$$\rho_F(R^*, R; \beta') = \frac{1}{N!} \sum_{\pi} (-1)^{\pi} \int_{\rho_F(R^*, R; \beta')} dR_t \exp[-S(R(t)]$$

Removes all negative and some positive



Restricted Path Integral Monte Carlo needs to know for R*, R if

$$\rho(R^*, R) \equiv \langle R^* | \exp[-k\tau H] | R \rangle > 0$$

Typical Approach

Pick some variational density matrix (*free fermions*)

$$\rho_T(R^*, R; k\tau) > 0$$

Improved Approach

Pick some class of variational density matrices

$$\{\rho_T(\tau)\}$$

Optimize over them

Optimization is hard :(

Writing down compact density matrices is hard :(

Q: Can we mirror VAFT?

Write the right answer and approximate is a good approach.

Q: Can we mirror VAFT?

Write the right answer and approximate is a good approach.

$$\rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0$$

If we could just evaluate this matrix element, we would be done.

(of course, then we wouldn't have to do PIMC then)

Q: Can we mirror VAFT?

Write the right answer and approximate is a good approach.

$$\rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0$$

If we could just evaluate this matrix element, we would be done.

(of course, then we wouldn't have to do PIMC then)

So, we want to approximate it.

$$\rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0$$

This highlighted region is a wave-function.

We just need to have a wave-function $|\Psi_{R^*,\tau}\rangle$ for every (R^*, τ)

Then we can do $\langle \Psi_{R^*,\tau} | R \rangle$

This naively looks worse then a wave-function per excitation

just generate it variationally.

Not quite the same density matrix

Also breaks time symmetry (data still coming but probably not a problem)

Finite Temperature Methods

Variational Density Matrices (VDM)

Variational Error

Restricted Path Integral Monte Carlo

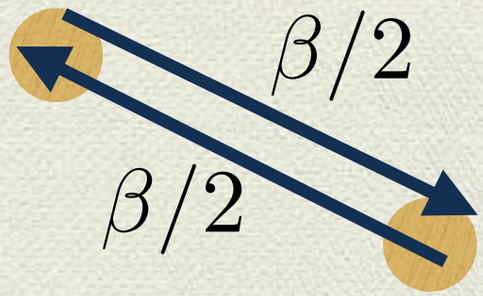
`Better' Variational Error

Path Integral Monte Carlo

Statistical Error

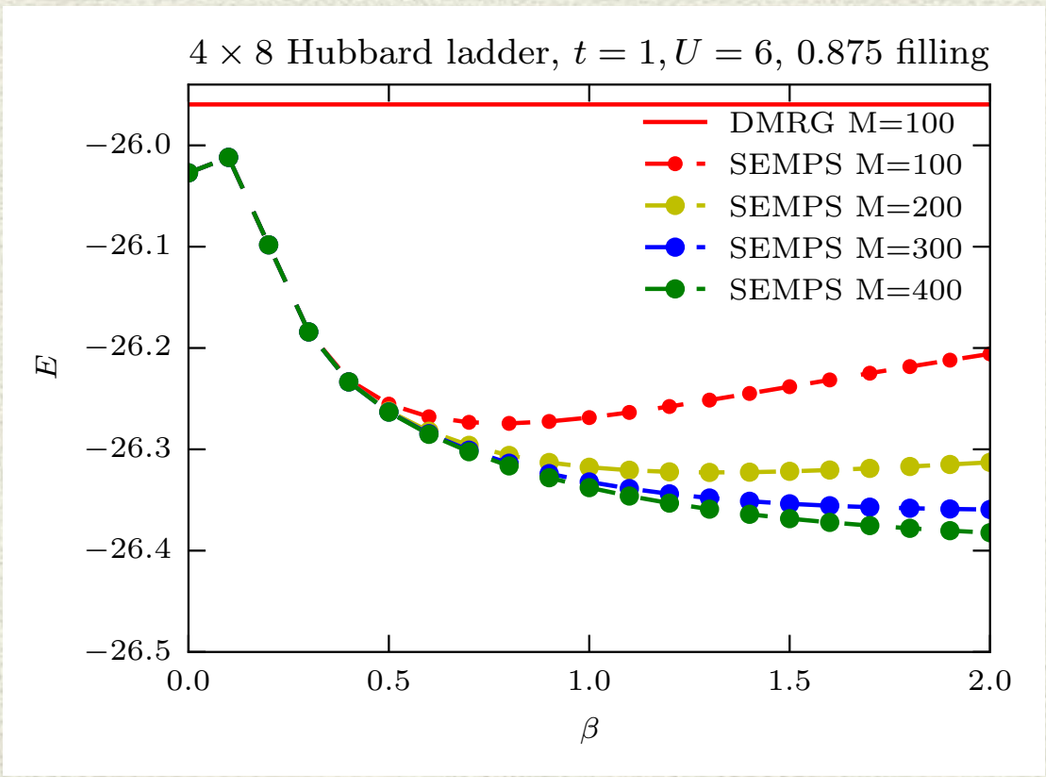
Do any of these ideas help us here?

Do any of these ideas help us in PIMC?



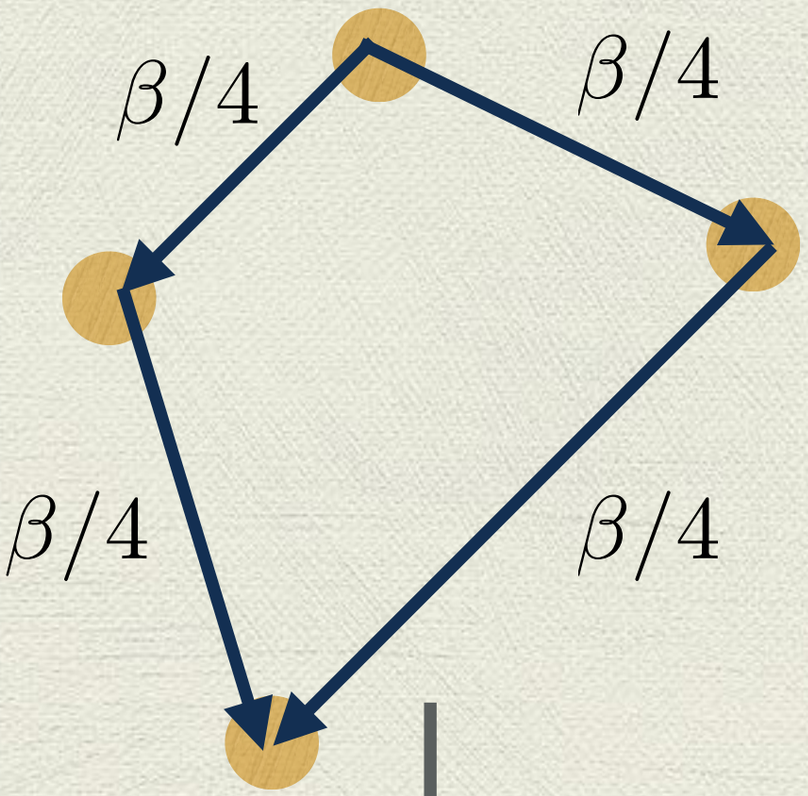
If my propagation to $\beta/2$ is exact then so is this.

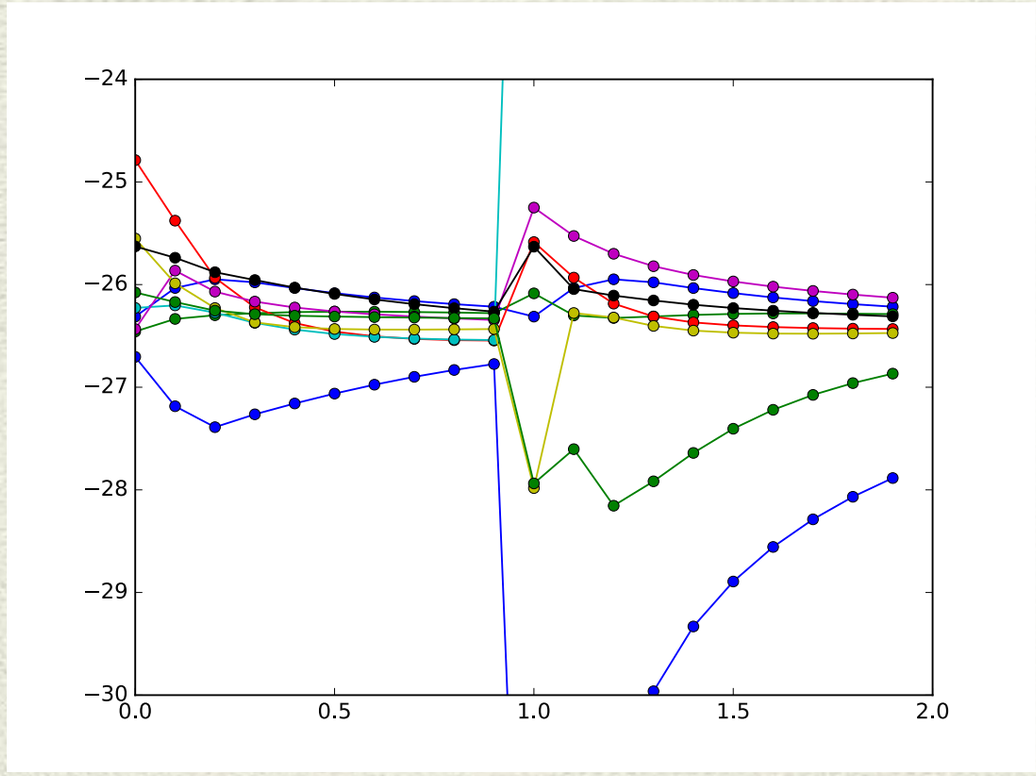
But my propagation probably isn't exact that far



Do any of these ideas help us in PIMC?

Yes!



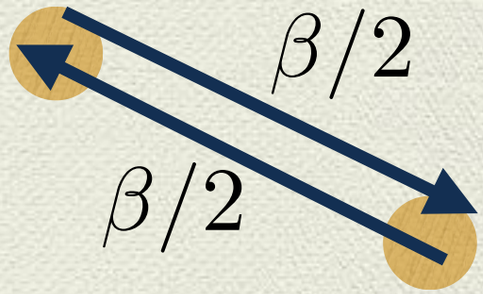


exact annihilation **exact annihilation** **exact annihilation** **exact annihilation**

Removes all sign-incoherent paths which start from R and go beta of 1.

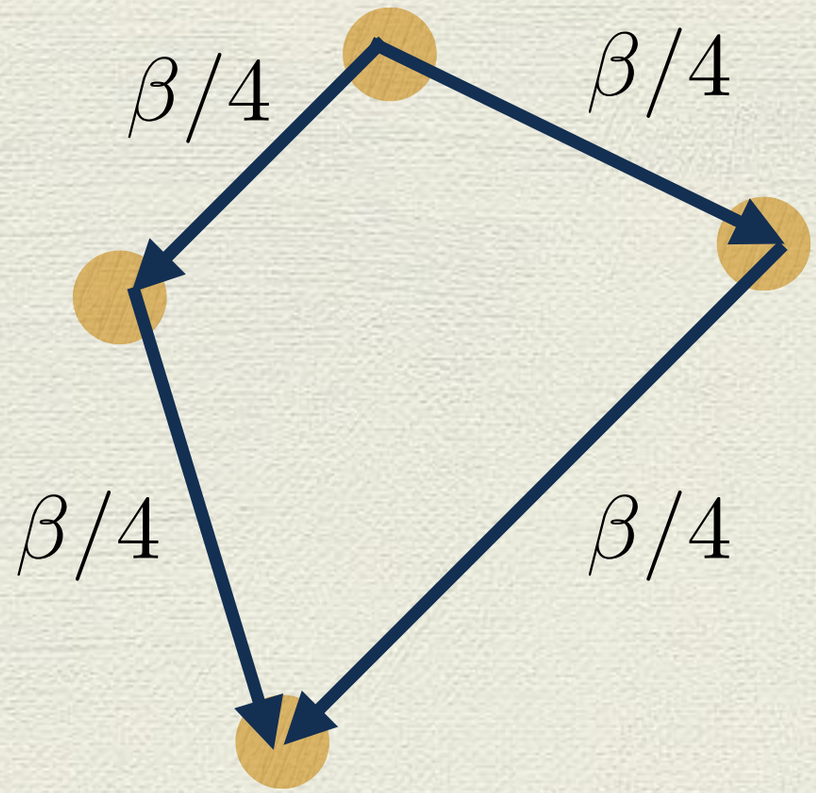
Attenuates the sign problem…

An alternative approximation



If my propagation to $\beta/2$ is not exact then this is VAFT.

An alternative approximation



Two Slices — **Many Slices**

Worse Sign Problem →

← Variational Error

Where do you want to sit at fixed computer time?

Finite Temperature Methods

Variational Density Matrices (VDM)

Variational Approximate Path Integrals

Path Integral Monte Carlo

Statistical Error

Restricted Path Integral Monte Carlo

`Better' Variational Error

Q: Can you combined restricted with this better density matrices?

In principle, it should be possible.

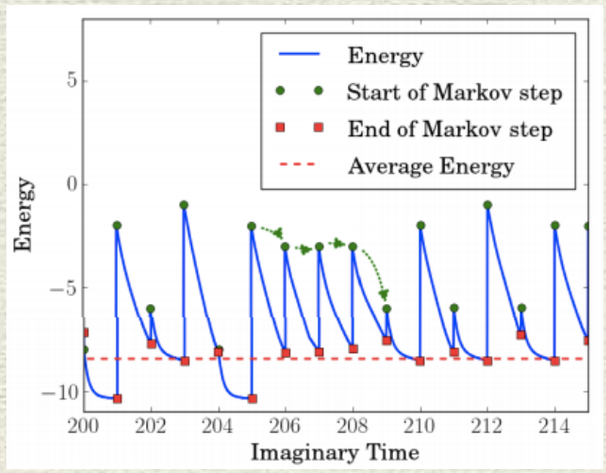
In practice their is a nodal error I don't know how to deal with.

Conclusion…

An implicit variational density matrix (VAFT)

Eats class of variational ansatz

Return Finite Temperature Properties



Can (morally) use this for RPIMC

$$\rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0$$

New approach combining variational and PIMC