Lefschetz Thimble Quantum Monte Carlo for Spin Systems

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Overview

The Sign Problem: Numerical instabilities due to oscillations in Boltzmann weights

Lefschetz Thimble Methods: Mitigation strategies involving deforming integration contours onto cycles of stationary phase

Quantum Mechanics

Quantum states – Complex vectors

$$|\psi\rangle \in \mathbb{C}^n$$

- For spin, n is finite

The Hamiltonian Operator H

Thermal equilibrium

- Partition Function: $\mathcal{Z} = \mathrm{Tr}\{e^{-\beta H}\}$
- Expectation: $\langle O \rangle = \dfrac{\mathrm{Tr}\{Oe^{-\beta H}\}}{\mathcal{Z}}$

This is all Linear Algebra!

$$\beta \propto \frac{1}{\text{Temperature}}$$

Path Integrals

Assume $I = \int dx\, f(x)|x\rangle\langle x|$.
Then,

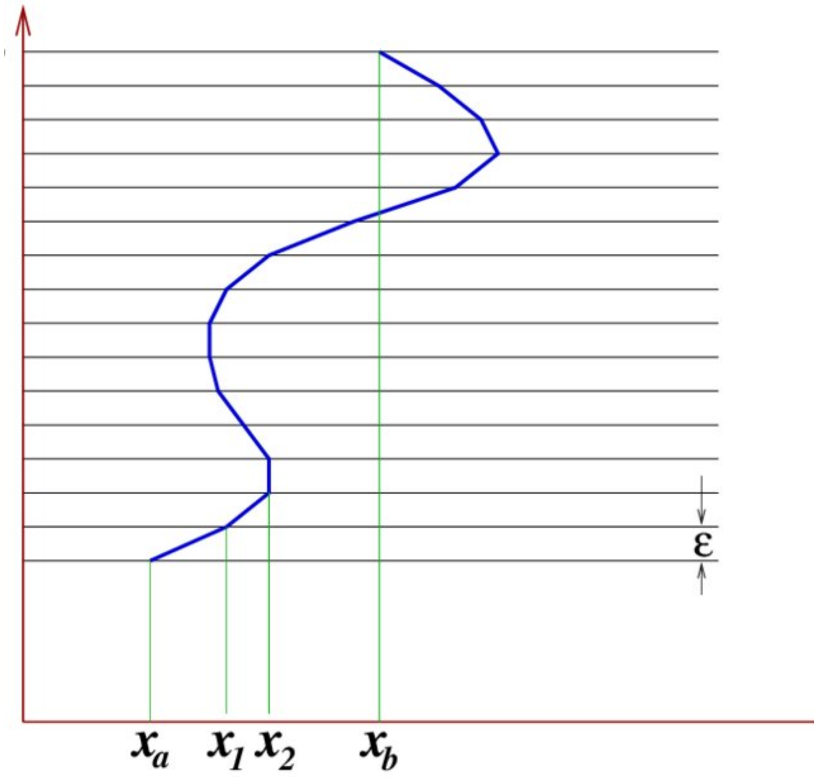
$$\mathcal{Z} = \int \prod_{k=0}^{T-1} \left(f(x_k)dx_k\right) \left(\prod_{k=0}^{T-1} \langle x_{k+1}|e^{-\beta H/T}|x_k\rangle \right)$$

Now, define $\prod_{k=0}^{T-1} \langle x_{k+1}|e^{-\beta H/T}|x_k\rangle \equiv e^{-\beta \boxed{S[\{x_i\}]}}$

The Action

$$\mathcal{Z} = \oint \mathcal{D}x e^{-\beta S[x]}$$

Quantum → Classical



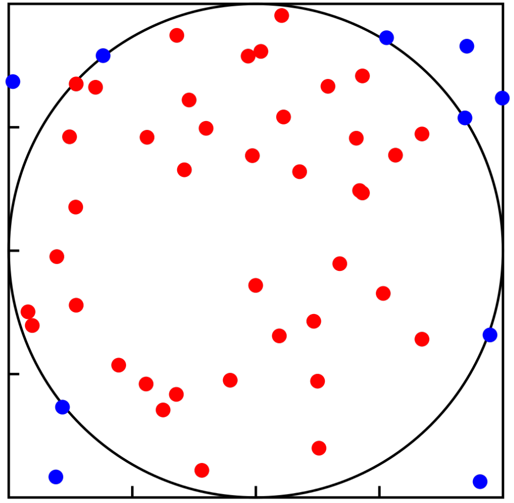
Monte Carlo Simulations

Random sampling for calculations

Metropolis-Hastings

- Given function f, samples with proportional probability
- 2 step process:
  - Generate next point in step randomly according to $g(x'|x_k)$
  - Accept with probability $A(x', x_k)$
    - Else, $x_{k+1} = x_k$

$$\langle O \rangle \approx \langle O \rangle_{M.C.} = \frac{1}{N} \sum_i O(x_i)$$



Metropolis et al., doi: 10.1063/1.1699114; Hastings, doi: 10.2307/2334940

The Sign Problem

How do you sample if $S[x] \notin \mathbb{R}$?

$$\mathcal{Z} = \oint \mathcal{D}\varphi e^{-\beta S[\varphi]}$$

The answer: **Reweighting**

$$\langle O \rangle = \frac{1}{\mathcal{Z}} \oint \mathcal{D}\varphi O e^{-\beta S[\varphi]}$$

If $\mathrm{Im} S$ fluctuates a lot, we're in trouble

Solving generically is **NP-hard**

$$= \frac{1}{\mathcal{Z}} \oint \mathcal{D}\varphi O e^{-i\beta \mathrm{Im} S[\varphi]} e^{-\beta \mathrm{Re} S[\varphi]}$$

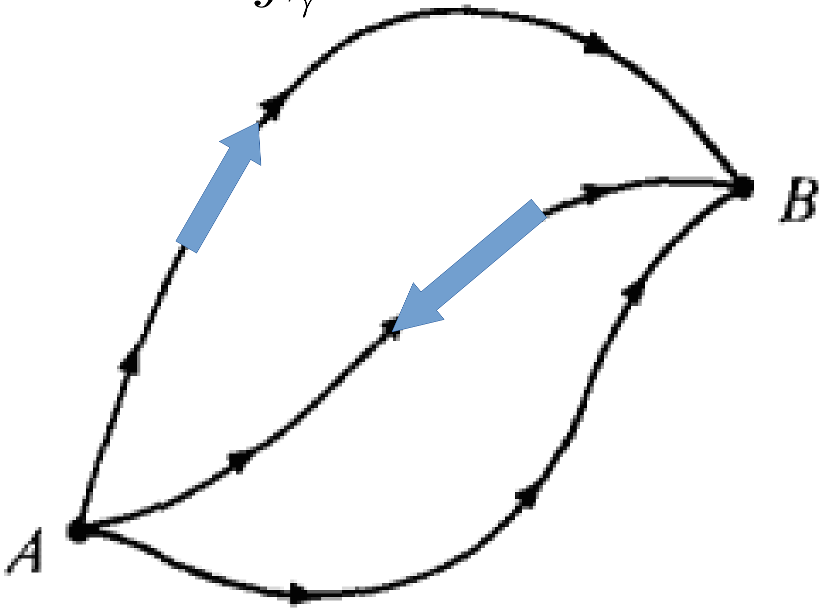
$$= \frac{\langle O e^{-i\beta \mathrm{Im} S} \rangle_{\mathrm{Re}}}{\mathcal{Z}}$$

Cauchy's Theorem

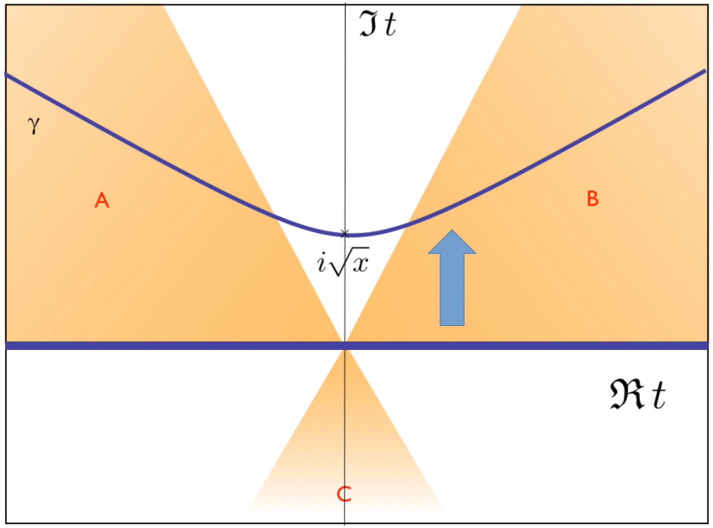
"If f is analytic in a simply connected region R, then for any closed curve γ completely in the region, $\oint_\gamma f(z)dz = 0$*."*

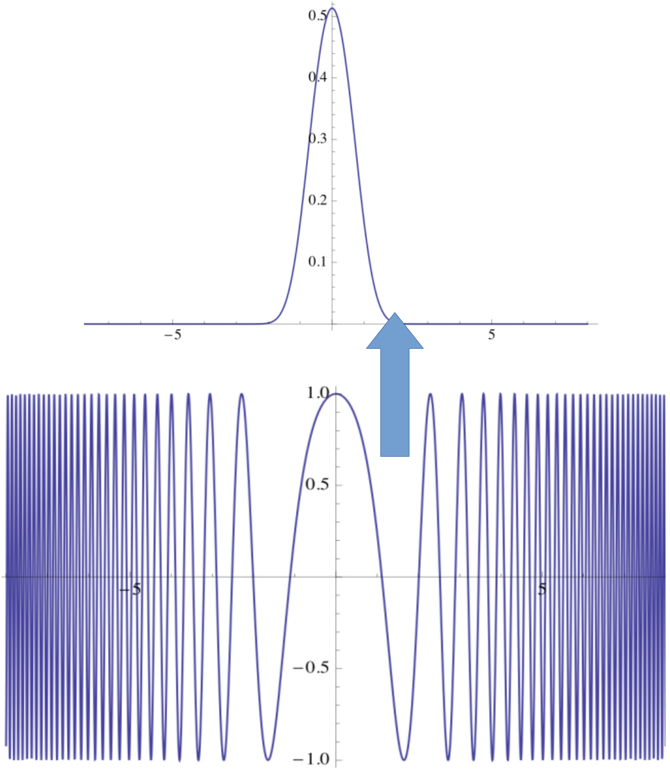
Path independence

Contour deformation
Higher dimensions



Lefschetz Thimbles





Known to help in HEP!

Pham, doi: 10.1090/pspum/040.2; Witten, arXiv:1001.2933; Alexandru et al., arXiv: 2007.05436

Spin Coherent States

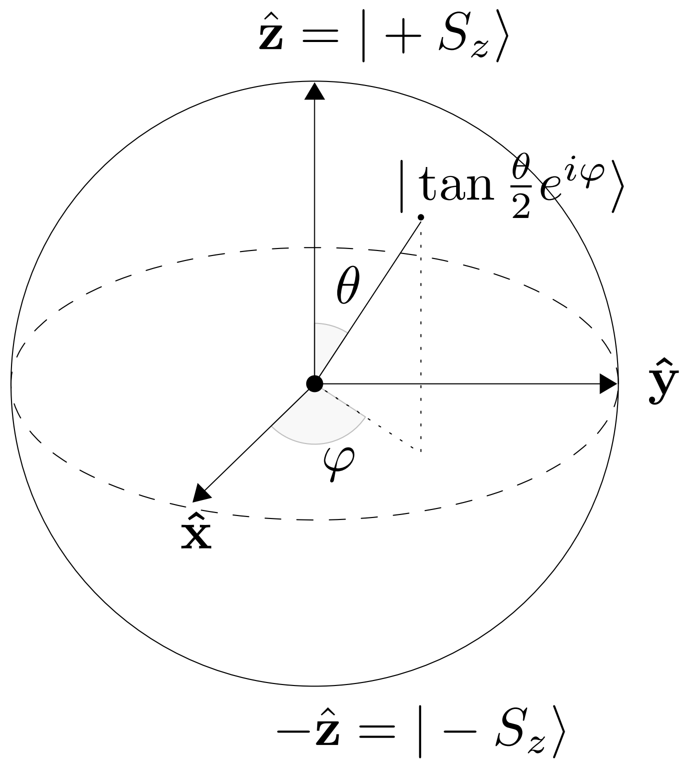
One big problem: Spin states are discrete!

Need to make continuous

The answer: Spin coherent states

Closest to classical spin possible

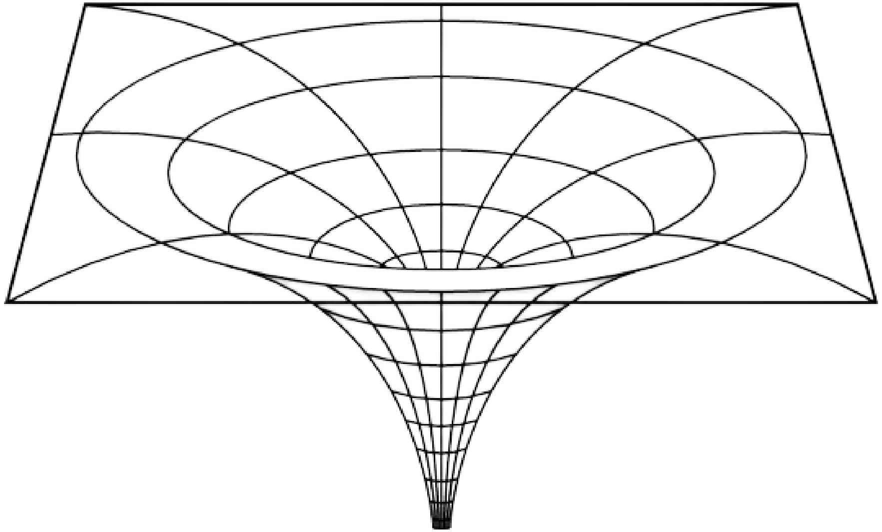
Can resolve the identity

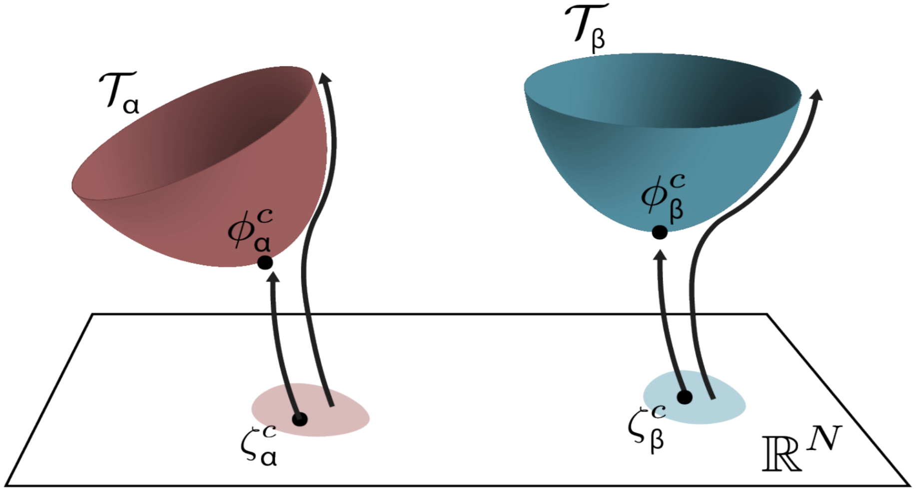


Radcliffe, doi: 10.1088/0305-4470/4/3/009

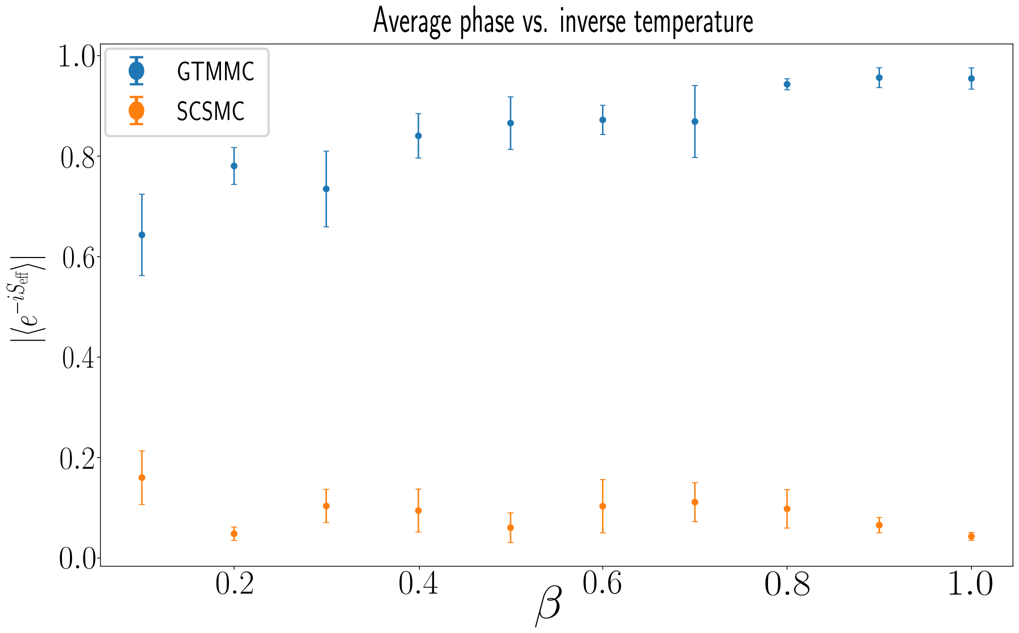
Our Results

- Challenges:
  - Singularities
  - Trapping

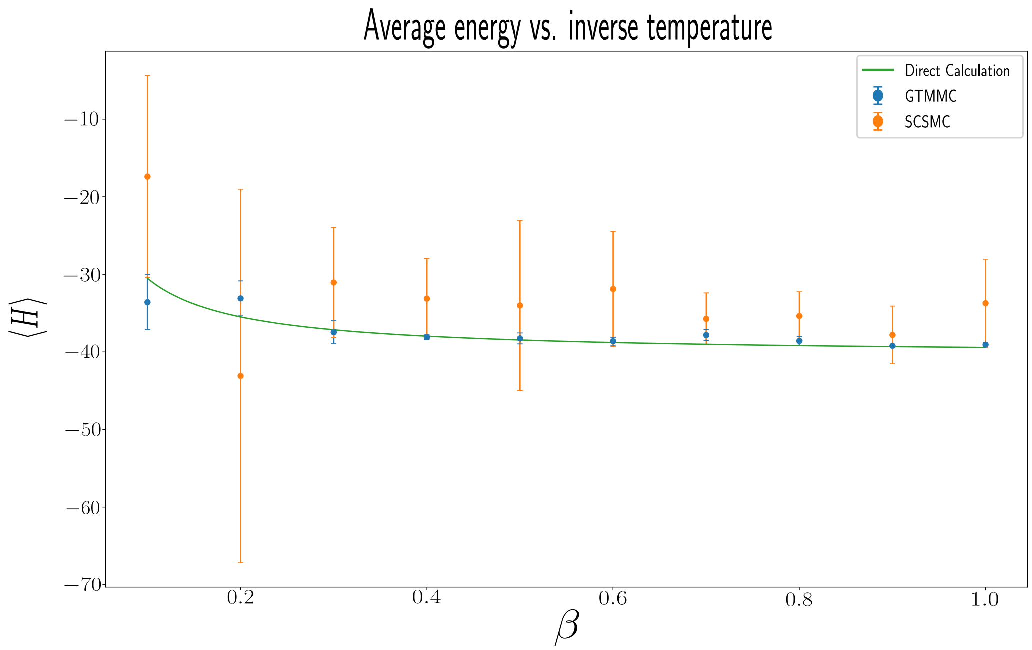




Our Results



Still, the results are encouraging!



Future Directions

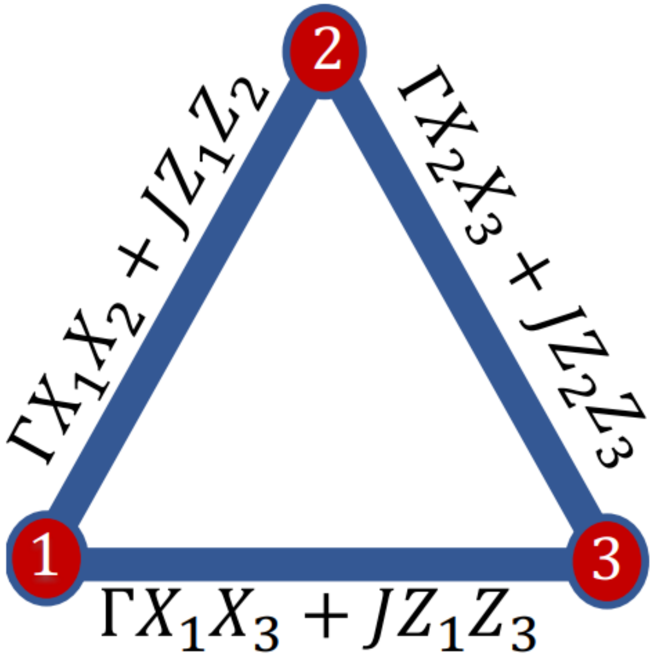
So far, just **proof of concept**

Multi-spin systems

Actual sign problems

- Frustrated triplet

Mitigate, not solve



Thank you for listening!

Any Questions?

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Backup Slides

Path Integral Quantum Monte Carlo

How about expectations?

$$\langle O \rangle = \frac{1}{\mathcal{Z}} \oint \mathcal{D}x O(x(0)) e^{-\beta S[x]} \qquad O(x(0)) \equiv \langle x(0)|O|x(0)\rangle$$

Note: Not right for off-diagonal O in discrete limit!

We can run Monte Carlo to sample w.r.t. $e^{-\beta S[x]}$!