Lefschetz Thimble Quantum Monte Carlo for Spin Systems

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1. Path Integral Quantum Monte Carlo

- Algorithm to simulate quantum systems in thermal equilibrium classically and find expectations of observables
- Write out time-discretized path integral of the partition function

$$\mathcal{Z} = \mathrm{Tr}\{e^{-\beta H}\} = \sum_{n_0,\cdots,n_{T-1}} \prod_{k=0}^{T-1} \langle n_{k+1}|e^{-\beta H/T}|n_k\rangle$$

- Run Monte Carlo, sampling paths according to their amplitudes
- Often written with an "action": $\mathcal{Z} = \sum_{n_0,\cdots,n_{T-1}} e^{-\beta\mathcal{S}[\{n_i\}]}$

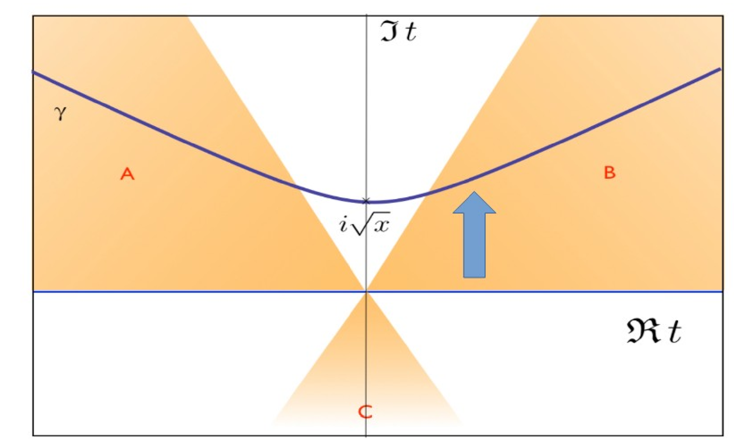
2. The Sign Problem

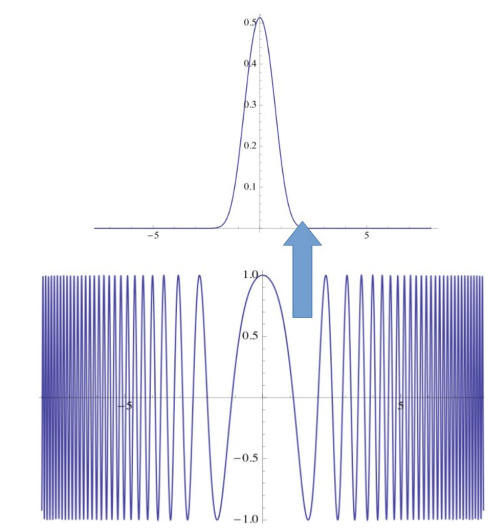
- What if $\mathcal{S}$ isn't real?
- Solution: Reweighting
- Relative error in expected phase grows exponentially with β and particle number
  - This exponential scaling is the **sign problem**
- Basis dependent, but solving generically is NP-hard
- Still can solve/mitigate in special cases

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

3. Lefschetz Thimble Monte Carlo (LTMC)

- For continuous path integrals (i.e. position, momentum), we can deform the contours as we like
- Deform from original integration contour onto Lefschetz thimbles – multi-dimensional stationary phase contours with no sign problem
- Associated numerical techniques: Lefschetz thimble Monte Carlo, generalized thimble method (GTMMC)





arXiv: 1512.08039

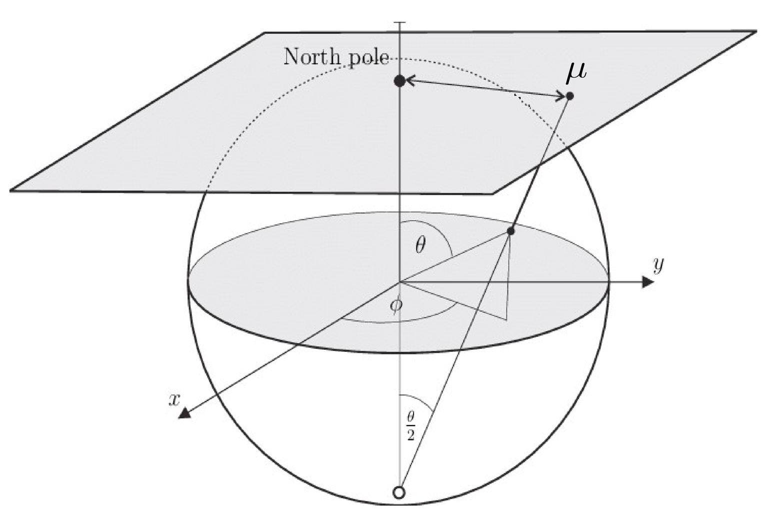
4. Spin Coherent States

- LTMC works for continuous resolutions of the identity, but not for discrete ones like spin
- Need to rewrite spin states with continuous variables
- Solution: Spin coherent states
  - Define as $|\mu\rangle = \frac{1}{(1+|\mu|^2)^S}\exp(\mu S_-)|+S_z\rangle$ for spin S system, complex number μ
  - Resolves the identity: $I = \frac{2S+1}{\pi}\int \frac{d\mathrm{Re}(\mu)\, d\mathrm{Im}(\mu)}{(1+|\mu|^2)^2}|\mu\rangle\langle\mu|$
- Path integral (SCSPI): Letting x and y be the real and imaginary parts of the spin coherent state we integrate over, and $H^{cl}(x,y) \equiv \langle x+iy|H|x+iy\rangle$, then

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

$$\mathcal{S}[x,y] = \int_0^\beta d\tau \left(2iS\frac{\dot{y}x - \dot{x}y}{1+x^2+y^2} + H^{cl}(x,y)\right)$$

- Introduces sign problem into partition function



Acknowledgments

The research of T.C.M. was partially supported by the National Institute of Standards and Technology (NIST) Summer Undergraduate Research Fellowship (SURF) program in the Information Technology Lab (ITL). J.B. acknowledges support by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Department of Energy Computational Science Graduate Fellowship (award No. DE-SC0019323).

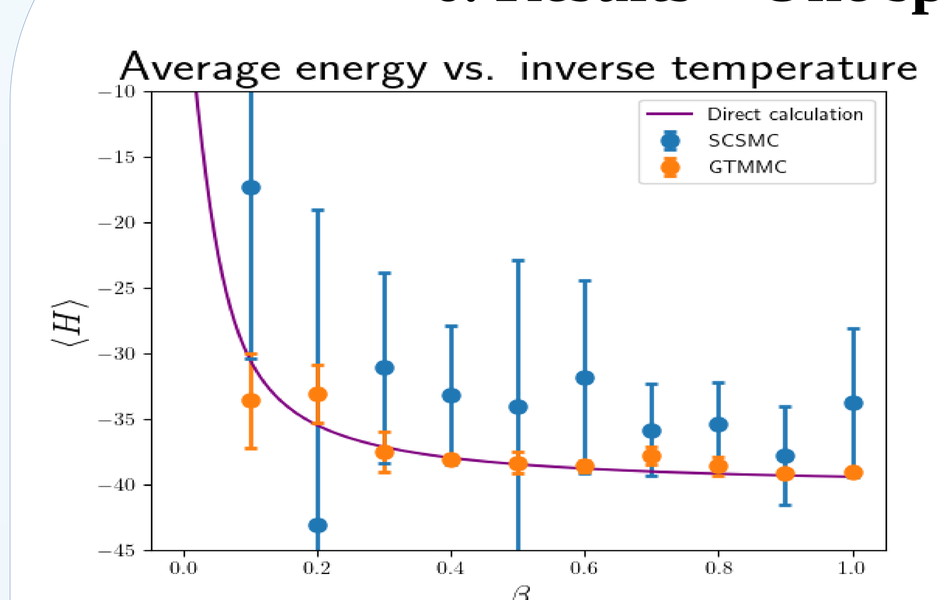
5. Our Setup

- We choose to deal with high-spin systems as SCSPI has less error for high spins
- Two tests:
  - Can LTMC overcome the sign problem the SCSPI introduces?
  - How about for a system with an actual sign problem?
- First test: Spin-40 particle with $H = J_y$
  - Originally no sign problem
  - Sign problem comes from SCSPI completely
- Second test: 3 spin-10 particles with frustrated spin triplet Hamiltonian

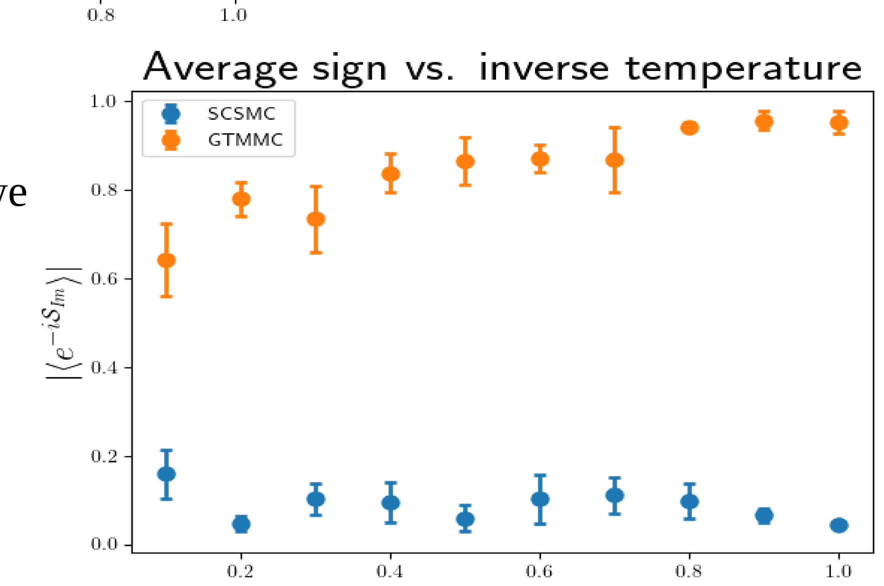
$$H = J_{x1}J_{x2} + J_{x1}J_{x3} + J_{x2}J_{x3} + J_{z1}J_{z2} + J_{z1}J_{z3} + J_{z2}J_{z3}$$

  - Severe sign problem

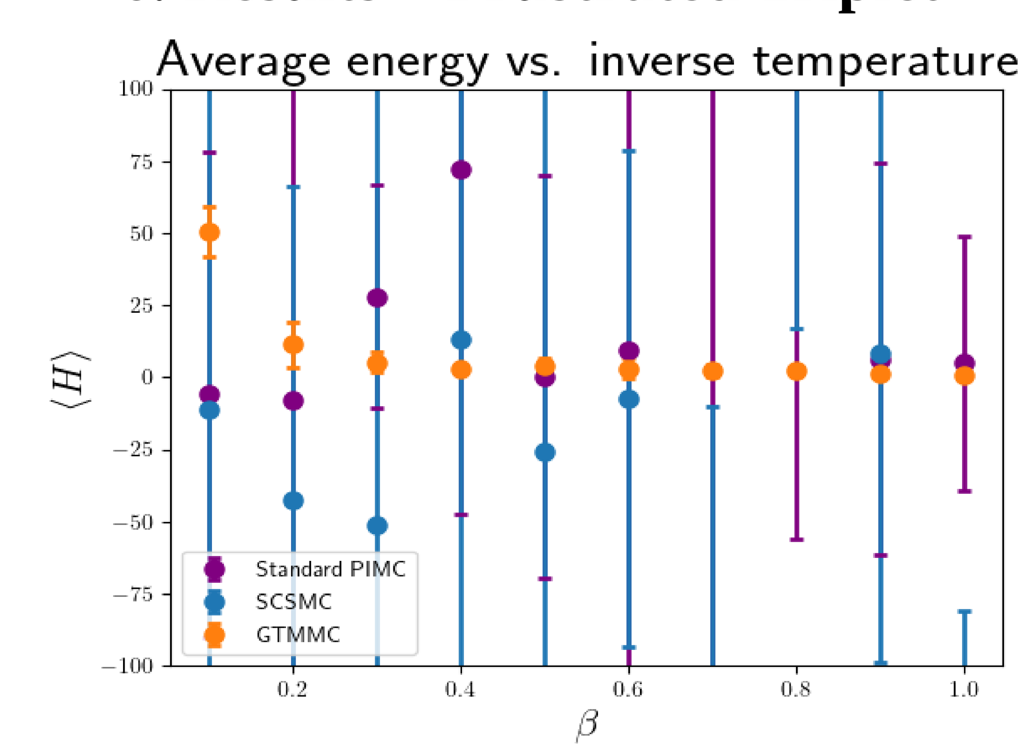
6. Results – One spin case

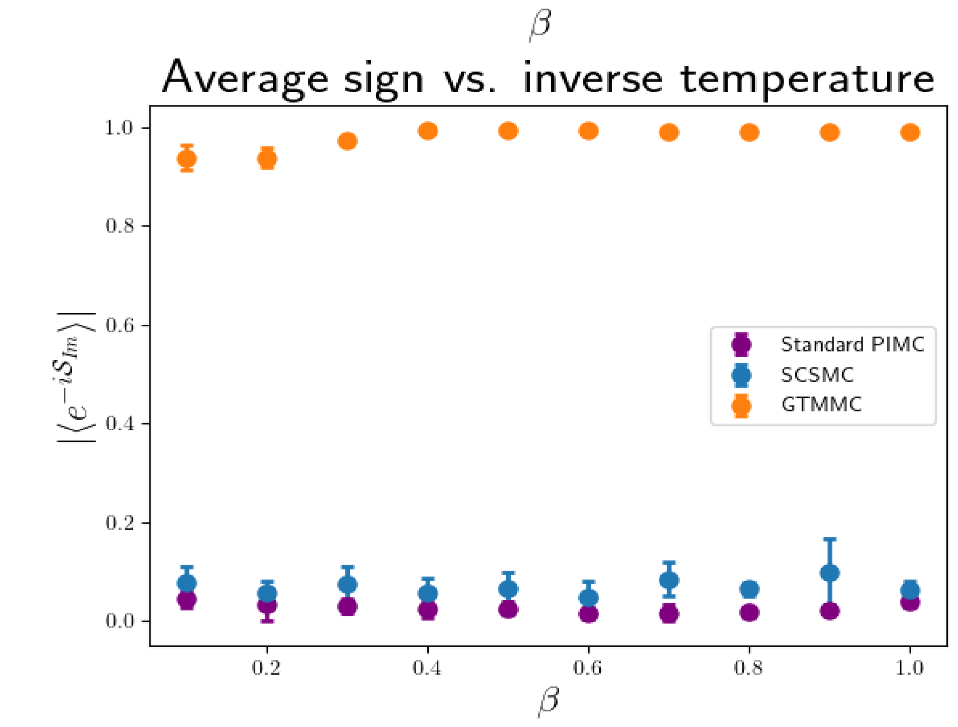


- Average sign is the metric we use to evaluate the severity of the sign problem – the higher it is, the less severe the sign problem is



6. Results – Frustrated Triplet





7. Conclusions

- LTMC can be applied effectively to simulate spin systems via spin coherent states
  - LTMC can overcome the sign problem induced by the SCSPI and proceed to mitigate the original sign problem
- Further considerations:
  - How does this method perform at lower spins?
  - What exactly is the complexity of this algorithm?