Optimisation of Complex Integration Contours

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Outline

Introduction

Lefschetz Thimbles

Lefschetz Thimbles provide a systematic and successful approach towards the sign problem. But:

Problems with thimbles

- Thimbles are manifolds, but no closed form expression.
- Many thimbles might be needed.
- Residual sign problem, global sign problem.
- *Expensive checks* for verifying that the data is on the thimble (however (Alexandru et al. 16)).

General Integration Contours

As with thimbles, complexify the N integration variables and look for a real N dim submanifold of the complex N dim space.

For $N = 1$ the condition $Im(S) = C$ defines the thimble.
With more variables we look for N dim real manifold embedded in $2N$ dim real space, but the requirement $Im(S) = C$ leads to a $2N - 1$ dim object.
For $N > 1$ these dimensions do not agree.

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We don't care if the integration cycle is a thimble
(also (Mori, Kashiwa, Ohnishi 17; Alexandru, Bedaque, Lamm, Lawrence 18)).

Strategy: Pick *a simple* integration cycle obeying the equation $Im(S) = C$ at least approximately that can be evaluated with *low computational cost*.

Deforming Contours

Let $z_k = x_k + iy_k$ $(k = 1..N)$ be the complexified variables.

We have to solve one equation, $Im(S(x_k, y_k)) = C$, in N variables, e.g., we could find $y_k(x_m)$ to define an N dim integration manifold. How hard can it be?

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Restrictions on solutions

- $y_k(x_m)$ must have proper boundary conditions (C is fixed).
- $y_k(x_m)$ must be continuous for Cauchy's theorem to hold.
- $y_k(x_m)$ are allowed to approach infinity, but only as long as the integral of the action remains well defined.
- If S is has singular points, those should be avoided while deforming the contour.

Simplicity and Other Criteria for Choosing a Contour

- Explicit expression for the cycle:
  avoid expensive verifications.
- As local as possible: reduces numerical cost.
- Use variables that *do not lead to expensive Jacobians*.
- Include the phase of coming from the Jacobian ab initio.
- Trade accuracy of $Im(S) = C$ for simplicity if possible.
- Respect the symmetries of the theory if possible,
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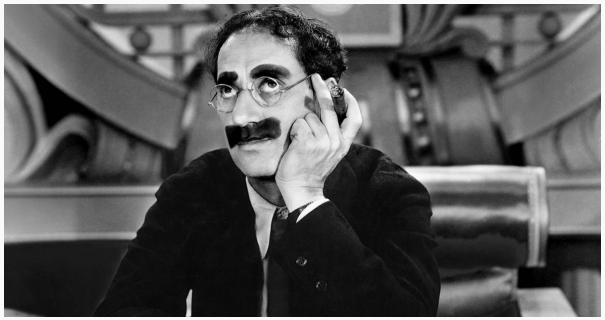

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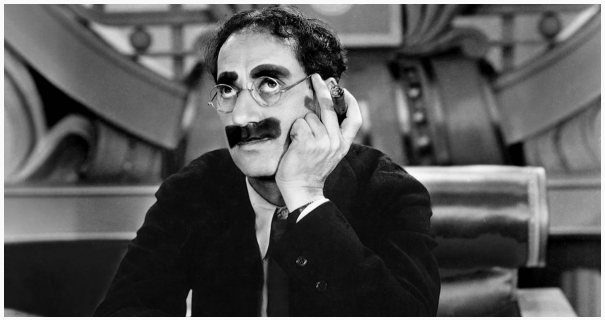

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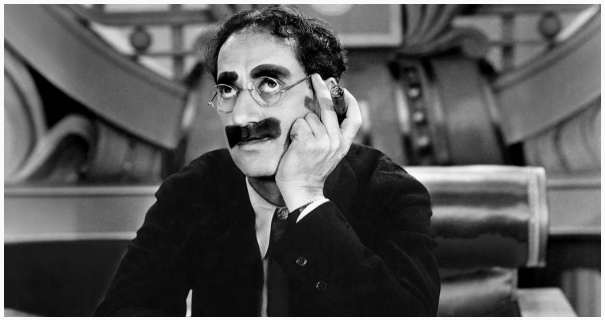

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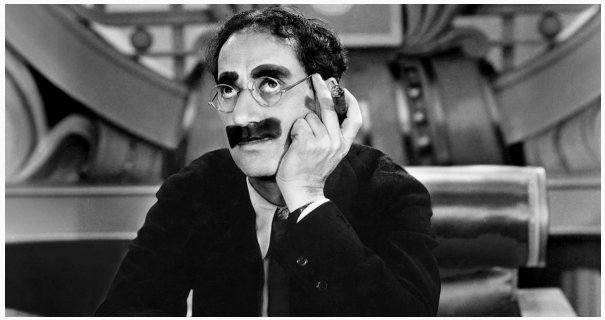

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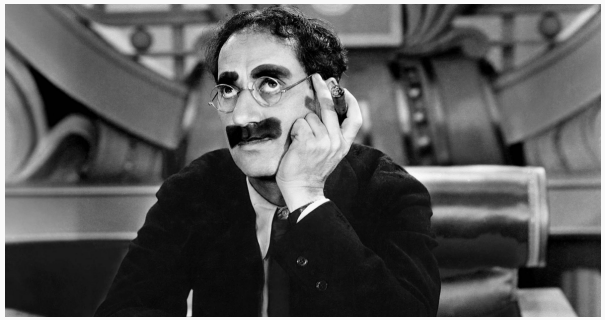

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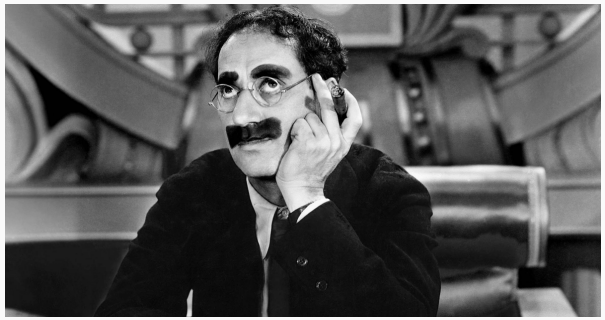

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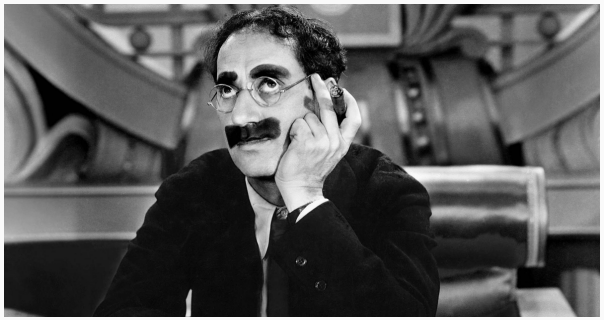

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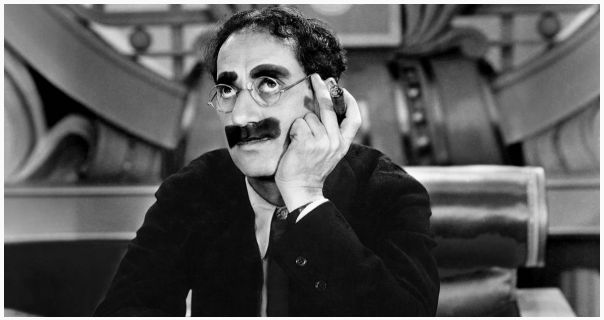

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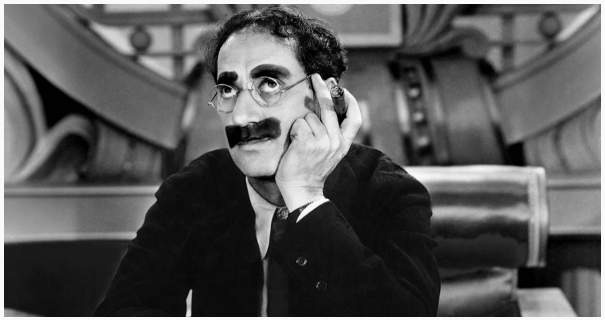

The Model: $d = 1$ Bose Gas

The Bose Gas at Finite Chemical Potential

Consider Bose gas with μ: A theory of a single complex scalar. Define $\alpha \equiv \frac{1}{2d+m^2}$. In lattice units the $d = 1$ theory is:

$$S = \frac{1}{\lambda\alpha^2} \sum_{k=1}^{L} \left(\varphi_k^* \varphi_k + (\varphi_k^* \varphi_k)^2 - \alpha \left(\varphi_k^* e^{-\mu} \varphi_{k+1} + \varphi_{k+1}^* e^{\mu} \varphi_k \right) \right)$$

For an undeformed contour:

$$\mathrm{Im}(S) = \frac{2 \sinh \mu}{\lambda\alpha} \sum_{k=1}^{L} \mathrm{Im} \left(\varphi_k^* \varphi_{k+1} \right)$$

Complexify the complex field as: $\varphi_k \to \phi_k + i\psi_k$, $\varphi_k^* \to \phi_k^* + i\psi_k^*$ (ϕ_k, ψ_k are complex fields) and we have to define $\psi_k = \psi_k(\phi_m)$ in order to get back to the correct number of d.o.f's.

Defining a Contour

Substitute the complexified coordinates in the action:

$$\mathrm{Im}(S) = \frac{2}{\lambda\alpha^2}\,\mathrm{Re}\sum_{k=1}^{L}\Big(\phi_k^*\psi_k\big(1+2\phi_k^*\phi_k-2\psi_k^*\psi_k\big)\Big)$$
$$-\alpha\cosh\mu\big(\phi_k^*\psi_{k+1}+\phi_{k+1}^*\psi_k\big)-i\alpha\sinh\mu\big(\phi_k^*\phi_{k+1}-\psi_k^*\psi_{k+1}\big)\Big)$$

Attempt to solve without summation in order to obtain local translationally invariant expressions:

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Next, $\psi_k^{(2)} = \dfrac{i\sinh\mu\cosh\mu}{\big(1+2\phi_k^*\phi_k\big)\big(1+2\phi_{k+1}^*\phi_{k+1}\big)}\phi_{k+2}$.

The expansion in *powers of* α looks like an expansion in the *order of neighbours*.

A More General Ansatz for the Contours

By rearranging the sums one can obtained other expressions, e.g., expressions in which ψ_k depends on ϕ_{k-1} or even on $\phi_{k\pm1}$.

It is important to avoid expressions of the latter form, since it would lead to an increased computational complexity in the evaluation of the Jacobian.

The Jacobian was not considered in defining ψ_k.
Instead, we generalize the form of ψ_k to the *ansatz*:

$$\psi_k = \frac{i\alpha \sinh \mu}{1 + 2b_0\phi_k^*\phi_k + 2b_1\phi_{k+1}^*\phi_{k+1}}\left(a_0\phi_k + a_1\phi_{k+1}\right)$$

This generalization respects the $U(1)$ symmetry of the action.
The parameters can be complex, but we keep them real.
In the original expression $a_0 = b_1 = 0$, $a_1 = b_0 = 1$.

The Jacobian

The dependence of ψ_k on ϕ_k and ϕ_{k+1} implies that the Jacobian takes the form:

$$J = \det \begin{pmatrix} A_1 & B_1 & 0 & 0 & \dots \\ 0 & A_2 & B_2 & 0 & \dots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & A_{L-1} & B_{L-1} \\ B_L & 0 & \dots & 0 & A_L \end{pmatrix}$$

Here, A_k and B_k are known 2×2 matrices.

Without the B_L the Jacobian would have been given by a product of L determinants of size 2×2. Thus, the update of the Jacobian would have been $O(1)$ per site, or $O(L)$ per sweep.

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The simplest solution: *Don't allow dependencw of ψ_L on ϕ_1.*

Simulation Results

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In the following we present simulation results.
We concentrate on the vev of the action density as an example of an observable.
In the thermodynamical limit $\frac{\langle S \rangle}{N}$ should approach a constant.

We also present the mean phase obtained in the simulations, as a measure of the sign problem.

Simulations were run with different lattice sizes for a fixed value of the parameters: $m = \mu = \lambda = 1$.

The change of variables was implemented ab initio and Jacobians from the change of variables were included.
We used 3×10^5 configurations in each run.

The Contours Used

We compare several contours:

Contour 0 is the one without complexification. We expect to see the sign problem there.

Contour 1 is the one obtain by substituting the obtained $\psi^{(1)}$.

Contour 5f is obtained by fitting on a small lattice the 4 parameters in the presented ansatz in a way that maximizes the mean phase.

Contours 1 and 2 are other specific choices within the ansatz.

Contour 5 is a more general ansatz, which is not one-sided and is therefore slow.

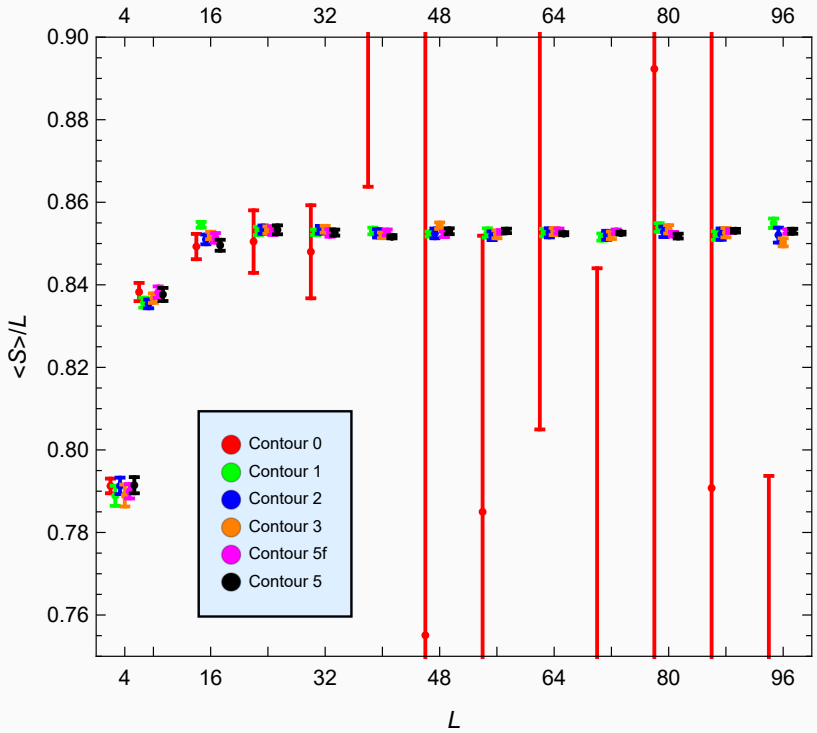
The Action

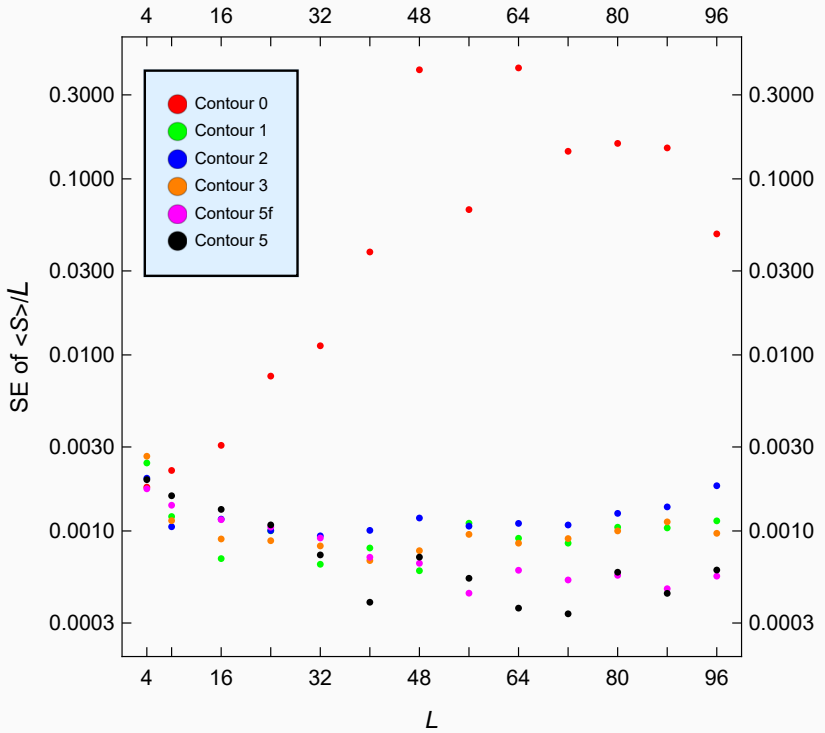
Left: The action density as a function of lattice size.

Right: The standard error in the evaluation of the action.

The various contours are color marked.

Points are horizontally separated for clarity.

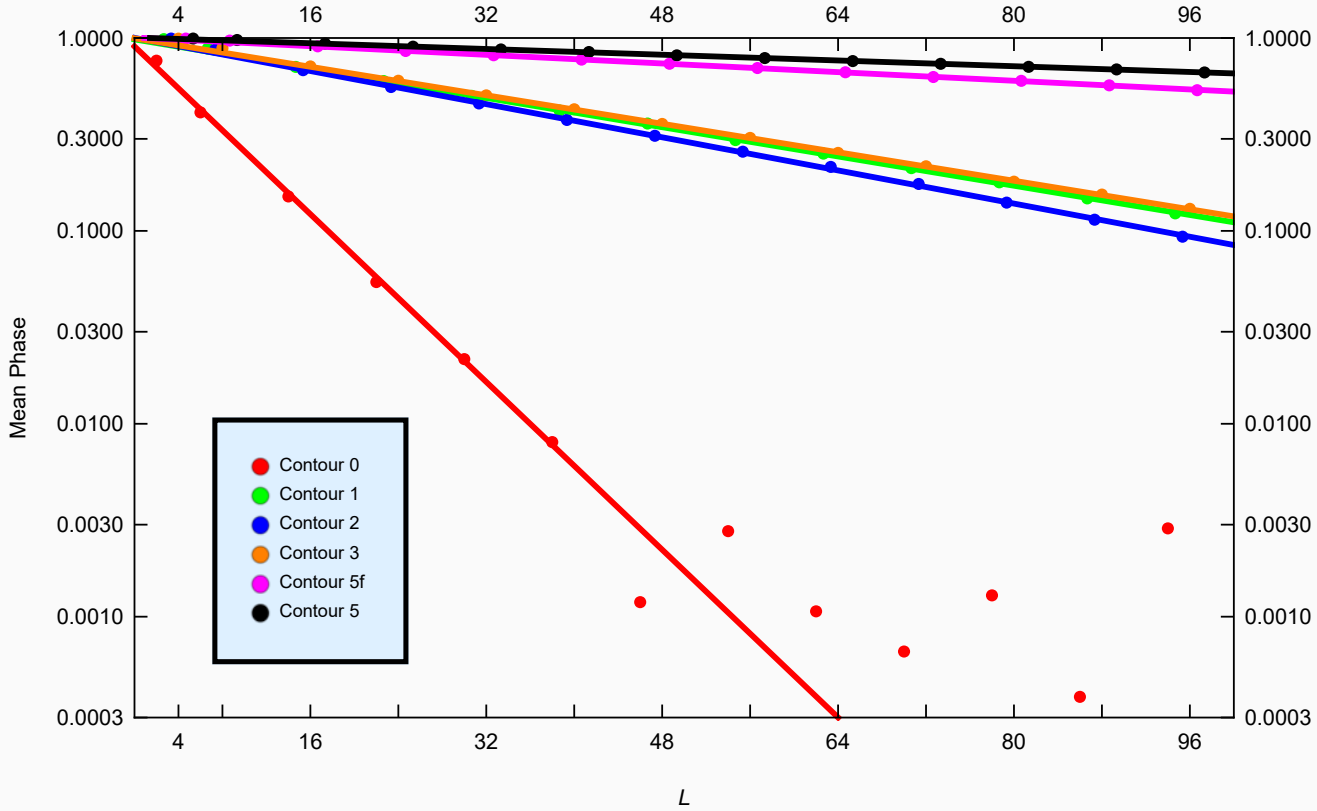




The Mean Phase

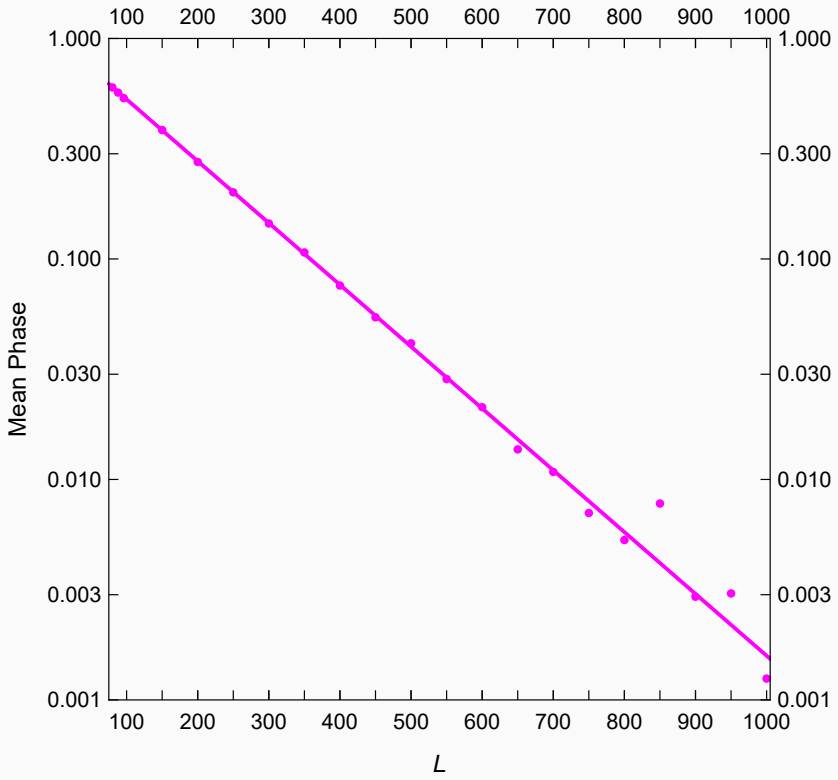
The mean phase as a function of lattice size.
The various contours are color marked (and separated).

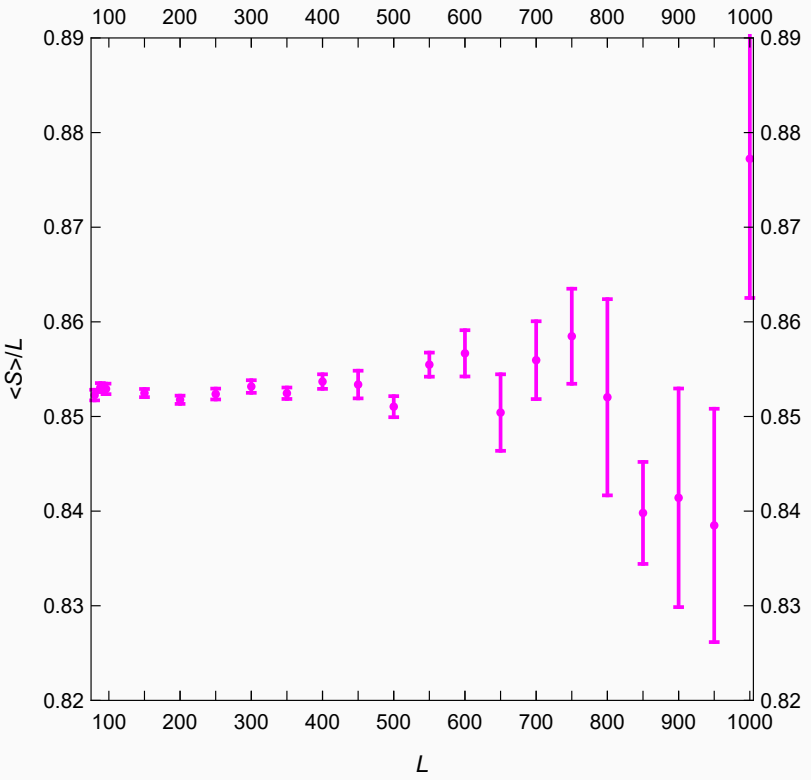
Exponential decay up to the onset of the sign problem.



Larger Lattices With Contour 5f

Examine the action and the mean phase as a function of lattice size for contour 5f on larger lattices.





Summary and Outlook

Summary of Presented Results

A simple method can address a complicated question.

Address the actual source of the sign problem
(nearest neighbour terms).

An efficient computational method with a determinant that can be evaluated with complexity $O(N)$.
This relies on the (block) upper triangular form of the Jacobian matrix (with one point having a different form for the contour).
The longest run ($L = 1000$) took 20 minutes on a laptop.

Summary and Outlook

In progress

- Examine behaviour with varying μ.
- Examine in higher dimensions.
  A lexicographic ordering of lattice points with the time coordinate as the most important one, leads to an upper triangular Jacobian matrix when we only change the form of the contours on a $d-1$ dim surface.
- An ansatz based on the form of the second order contribution (next to nearest neighbour).

Next: Apply to other systems, including to ones with fermions.

THANK YOU