Optimisation of Complex Integration Contours at Higher Order

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Outline

Introduction

Deformed Contours

Lefschetz Thimbles provide a systematic and successful approach towards the sign problem using deformed contours. Why would one consider other deformed manifolds?

Thimbles

- Thimbles are manifolds, but no closed form expression.
- Many thimbles might be needed.
- Residual sign problem, global sign problem.
- Relatively large numerical cost.

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- Many thimbles might be needed.
- Residual sign problem, global sign problem.
- Relatively large numerical cost.
- One can do better.

Related approach: (Mori, Kashiwa, Ohnishi 17; Alexandru, Bedaque, Lamm, Lawrence 18...).

General Integration Contours

Given N real integration variables, complexify the 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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For $N > 1$ these dimensions do not agree.

There is a *huge freedom* in choosing the integration contour.
No unique solution to the problem.

Strategy: Pick *a simple* integration cycle obeying $Im(S_{eff}) \approx C$ that can be evaluated with *low computational cost*.

Contour Deformation for d-Dimensional Bose Gas with $\mu \neq 0$

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 theory can be written as:

$$S = \frac{1}{\lambda\alpha^2}\sum_{\vec{r}}\left(\Phi^*_{\vec{r}}\Phi_{\vec{r}} + (\Phi^*_{\vec{r}}\Phi_{\vec{r}})^2 - \alpha\sum_{\nu=0}^{d-1}\left(\Phi^*_{\vec{r}}\Phi_{\vec{r}+\hat{\nu}}e^{-\mu\delta_{\nu,0}} + \Phi^*_{\vec{r}+\hat{\nu}}\Phi_{\vec{r}}e^{\mu\delta_{\nu,0}}\right)\right)$$

For an undeformed contour there is a sign problem:

$$\mathrm{Im}(S) = \frac{2\sinh\mu}{\lambda\alpha}\sum_{\vec{r}}\mathrm{Im}\left(\Phi^*_{\vec{r}}\Phi_{\vec{r}+\hat{0}}\right)$$

Complexify the (complex) field as:

$$\Phi_{\vec{r}} \to \Phi_{\vec{r}} = \phi_{\vec{r}} + i\psi_{\vec{r}}\,, \qquad \Phi^*_{\vec{r}} \to \bar{\Phi}_{\vec{r}} \equiv \phi^*_{\vec{r}} + i\psi^*_{\vec{r}}$$

$\bar{\Phi}_{\vec{r}}$ is the complex conjugate of $\Phi_{\vec{r}}$ only for the undeformed contour: $\psi^*_{\vec{r}} = 0$.

Defining a Contour

We look for a deformed contour by specifying $\psi_{\vec{r}} = \psi_{\vec{r}}\{\phi_{\vec{s}}\}$.
The term inducing the sign problem is proportional to the *small parameter* $0 \leq \alpha \leq \frac{1}{2d}$.

Hence, we define $\psi_{\vec{r}} = \sum_{n=1}^{\infty} \alpha^n \psi_{\vec{r}}^{(n)}$.

Expanding $\mathsf{Im}(S)$ to lowest order in α gives:

$$\mathsf{Re}\left(\sum_{\vec{r}} \phi_{\vec{r}}^{*}\left(\left(1+2|\phi_{\vec{r}}|^2\right)\psi_{\vec{r}}^{(1)} - i\,\mathsf{sinh}\,\mu\,\phi_{\vec{r}+\hat{0}}\right)\right) = 0$$

Many (continuous) solutions exist. A simple choice,

$$\psi_{\vec{r}}^{(1)} = i\,\mathsf{sinh}\,\mu\frac{\phi_{\vec{r}+\hat{0}}}{1+2|\phi_{\vec{r}}|^2} + i\phi_{\vec{r}} f_{\vec{r}}^{(1)}$$

with $f_{\vec{r}}^{(1)}$ an *arbitrary real function*.

Defining a Contour at the First Order

How to choose $f_{\vec{r}}$?

Simplicity, computational cost, reduction of sign problem.

Particular choices

$f^{(1)}_{\vec{r}} = 0$: Simplest ("contour 1").

$f^{(1)}_{\vec{r}} = -\frac{\sinh \mu}{1+2|\phi_{\vec{r}}|^2}$: Approximate continuity gives small $\psi^{(1)}_{\vec{r}}$, $\psi^{(2)}_{\vec{r}}$.

$f^{(1)}_{\vec{r}} = +\frac{\sinh \mu}{1+2|\phi_{\vec{r}}|^2}$: Some higher order terms vanish.

More generally ($a \in \mathbb{R}$, $a = 0, \pm 1$ above): $\psi^{(1)}_{\vec{r}} = i \sinh \mu \frac{a\phi_{\vec{r}} + \phi_{\vec{r}+\hat{0}}}{1+2|\phi_{\vec{r}}|^2}$.

We are forced to consider an ansatz even within the first order of a systematic expansion approach.

Generalize to "first order ansatz" ($a_i, b_i \in \mathbb{R}$, $b_i \geq 0$):

$$\psi_{\vec{r}} = i \sinh \mu \frac{a_1 \phi_{\vec{r}} + a_2 \phi_{\vec{r}+\hat{0}}}{1 + b_1 |\phi_{\vec{r}}|^2 + b_2 |\phi_{\vec{r}+\hat{0}}|^2}$$

Defining a Contour at the Second Order

Plugging the first order expression (not the general ansatz) to the action gives at the second order (defined $d_{\vec{r}} \equiv 1 + 2|\phi_{\vec{r}}|^2$):

$$\mathrm{Re}\left(\sum_{\vec{r}} \phi^*_{\vec{r}} \left(\psi^{(2)}_{\vec{r}} d_{\vec{r}} - i \cosh\mu\left(\sinh\mu \frac{\phi_{\vec{r}+2\hat{0}}}{d_{\vec{r}+\hat{0}}} + \phi_{\vec{r}+\hat{0}}\left(f^{(1)}_{\vec{r}+\hat{0}} - f^{(1)}_{\vec{r}}\right)\right) - i s_{\vec{r}}\right)\right) = 0$$

where we defined the contribution of the non-$\hat{0}$ links,

$$s_{\vec{r}} \equiv \sum_{\nu=1}^{d-1} \left(\sinh\mu\left(\frac{\phi_{\vec{r}+\hat{0}+\hat{\nu}}}{d_{\vec{r}+\hat{\nu}}} + \frac{\phi_{\vec{r}+\hat{0}-\hat{\nu}}}{d_{\vec{r}-\hat{\nu}}}\right) + \phi_{\vec{r}+\hat{\nu}} f^{(1)}_{\vec{r}+\hat{\nu}} + \phi_{\vec{r}-\hat{\nu}} f^{(1)}_{\vec{r}-\hat{\nu}}\right)$$

A possible solution to this equation is,

$$\psi^{(2)}_{\vec{r}} = \frac{i}{d_{\vec{r}}}\left(\cosh\mu\left(\sinh\mu \frac{\phi_{\vec{r}+2\hat{0}}}{d_{\vec{r}+\hat{0}}} + \phi_{\vec{r}+\hat{0}}\left(f^{(1)}_{\vec{r}+\hat{0}} - f^{(1)}_{\vec{r}}\right)\right) + s_{\vec{r}}\right) + i\phi_{\vec{r}} f^{(2)}_{\vec{r}}$$

Again, the solution depends on an arbitrary real function.

Second Order Ansatz

Generalize the second order expression to:

$$\psi_{\vec{r}} = \frac{i}{1 + b_1 \left|\phi_{\vec{r}}\right|^2 + b_2 \left|\phi_{\vec{r}+\hat{0}}\right|^2} \Bigg(a_1 \phi_{\vec{r}} + a_2 \phi_{\vec{r}+\hat{0}} + \\ + \frac{a_3 \phi_{\vec{r}} + a_4 \phi_{\vec{r}+\hat{0}} + a_5 \phi_{\vec{r}+2\hat{0}}}{1 + b_3 \left|\phi_{\vec{r}}\right|^2 + b_4 \left|\phi_{\vec{r}+\hat{0}}\right|^2 + b_5 \left|\phi_{\vec{r}+2\hat{0}}\right|^2} + \\ + \sum_{\nu=1}^{d-1} \Bigg(\frac{a_6 \phi_{\vec{r}} + a_7 \phi_{\vec{r}+\hat{0}} + a_8 \phi_{\vec{r}+\hat{0}+\hat{\nu}}}{1 + b_6 \left|\phi_{\vec{r}}\right|^2 + b_7 \left|\phi_{\vec{r}+\hat{0}}\right|^2 + b_8 \left|\phi_{\vec{r}+\hat{0}+\hat{\nu}}\right|^2} + \left(+\hat{\nu} \to -\hat{\nu}\right) \Bigg) \Bigg)$$

- First line: First order ansatz.
- Second line: Addition to second order ansatz for $d = 1$.
- Third line: Second order contribution from non-$\hat{0}$ links.

Some Fine Points

Fixing Ansatz Parameters – Problems

The ansatz includes 16 parameters: $a_1, ..., a_8, b_1, ..., b_8$.
How to find their values?

Problems for optimising the mean phase

- Erratic behaviour as a function of the parameters.
- Many local maxima.
- In 16-dim. space the volume near maxima tends to zero.
- Optimisation on a large lattice takes time.

Fixing Ansatz Parameters – Solutions

Strategy

- Start at non-generic point:
  - For small μ, around the 1^{st} or 2^{nd} order contours.
  - For large μ, around the values for slightly smaller μ.
- Find large local maximum, not the global one.
- Optimise on a small lattice. Fine tune on a larger one.
- Optimise first the 4 parameters of the 1^{st} order ansatz.
  Then, the 6 parameters of the second order ansatz at $1d$.
  Then, (for the same α) the 4 parameters at the given d.
  Fine tune all parameters.
- Optimise for $d = 1$. Fine tune for $d > 1$.
- Add randomness to the optimisation.

Interpreting the Expansion

The expansion is in *powers of* $\alpha = \frac{1}{2d+m^2}$.

Interpretations

- *Expansion around infinite mass*.
- *Expansion around infinite d*: May seem wrong, since each lattice point contributes to the sign problem from all its links, $d\alpha \approx 1$. But only $\hat{0}$ links contribute at the first order. *Expectation* (for a fixed number of lattice points):
  - Fixing α: Smaller d theories behave better.
  - Fixing m: Larger d theories behave better.
- *Expansion in order of neighbours*.

Ansätze or higher orders?

What is more important for reducing the sign problem, going to higher orders or generalizing to ansätze with more parameters?

Both approaches have drawbacks

- Higher order expressions become *complicated*, even if we take the simplest variant in which we set all the $f_{\vec{r}}^{(n)} = 0$.
- Complicated ansätze include many free parameters and it can become challenging to find their optimal value.

Expectation: More general ansätze

- In deriving the expansions we ignored the *Jacobian*.
- Expansion is actually in αe^{μ} (for $\mu > 0$). It would break down for large μ.

The Jacobian

Consider for simplicity the $d = 1$ case at first order:
The dependence of ψ_r on ϕ_r and ϕ_{r+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_r and B_r are known 2×2 matrices (of $\mathbf{Re}(\phi_r)$ and $\mathbf{Im}(\phi_r)$).

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.

Otherwise, the cost would be $O(L^4)$ per sweep.

Resolving the Problems with the Jacobian

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

Problem: While for $d = 1$ this concerns a single lattice point, for general d there are $L^{\frac{d-1}{d}}$ such points (on a cubic lattice). This is enough to cause a significant sign problem.

Other resolutions proposed in paper I. All have problems.

Instead, consider again, for simplicity, 1d first order contribution to $\mathsf{Im}(S)$ from the points $r = 1$ and $r = L$:

$$\begin{aligned} 0 &= \mathsf{Re}\left(\phi_1^*\left(d_1\psi_1^{(1)} - i\sinh\mu\,\phi_2\right) + \left(\phi_L^*\left(d_L\psi_L^{(1)} - i\sinh\mu\,\phi_1\right)\right)\right. \\ &= \mathsf{Re}\left(\phi_1^*\left(d_1\psi_1^{(1)} - i\sinh\mu\,(\phi_2 - \phi_L)\right) + \phi_L^* d_L\psi_L^{(1)}\right) \end{aligned}$$

Solution:

$$\begin{aligned} \psi_L^{(1)} &= i\phi_L f_L^{(1)} \\ \psi_1^{(1)} &= i\sinh\mu\frac{\phi_2 - \phi_L}{1 + 2|\phi_1|^2} + i\phi_1 f_1^{(1)} \end{aligned}$$

Simulation Results

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In the following simulation results are presented.

The vevs of the density, $\langle n \rangle = \frac{\partial_\mu \ln(Z)}{V}$ and action density, $\frac{\langle S \rangle}{V}$, are used as examples of observable.

The main focus is on the mean phase, $\left\langle e^{i \operatorname{Im}(S_{eff})} \right\rangle_{\operatorname{Re}(S_{eff})}$ as a measure of the sign problem.

The change of variables was implemented ab initio and Jacobians from the change of variables were included in S_{eff}.

All runs were performed with 300,000 sweeps and with $\lambda = 1$.

Silver Blaze

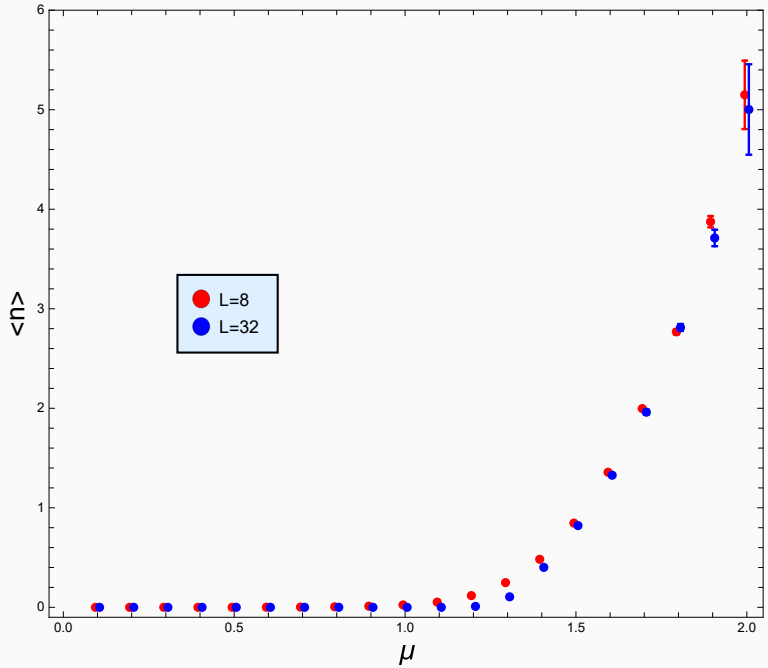
First order simple contour for $d = 1$, $m = 1$.

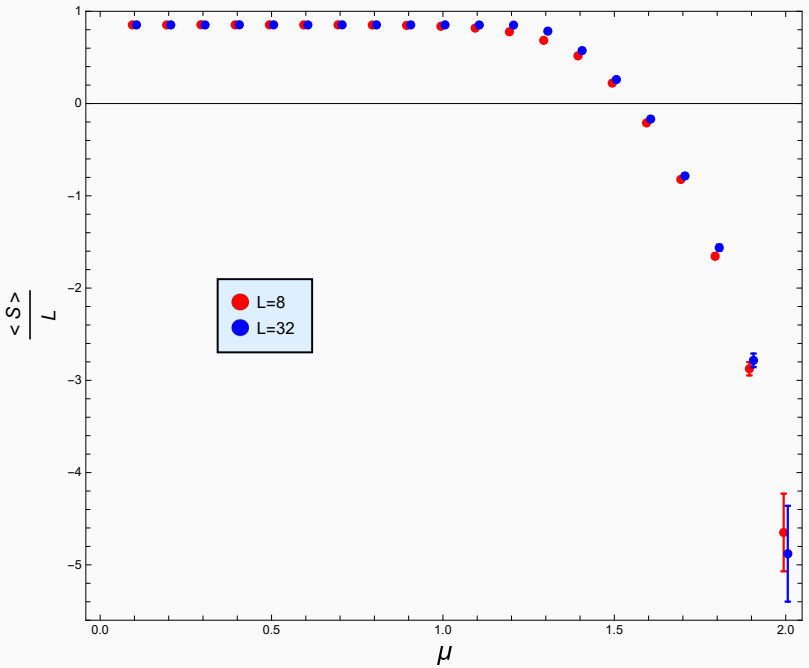
Left: The density as a function of μ for $L = 8$, $L = 32$.

Right: The action density as a function of μ for $L = 8$, $L = 32$.

Points are horizontally separated for clarity.

At $\mu = 2$ the mean phase is 0.003 for $L = 8$ and is consistent with zero for $L = 32$.

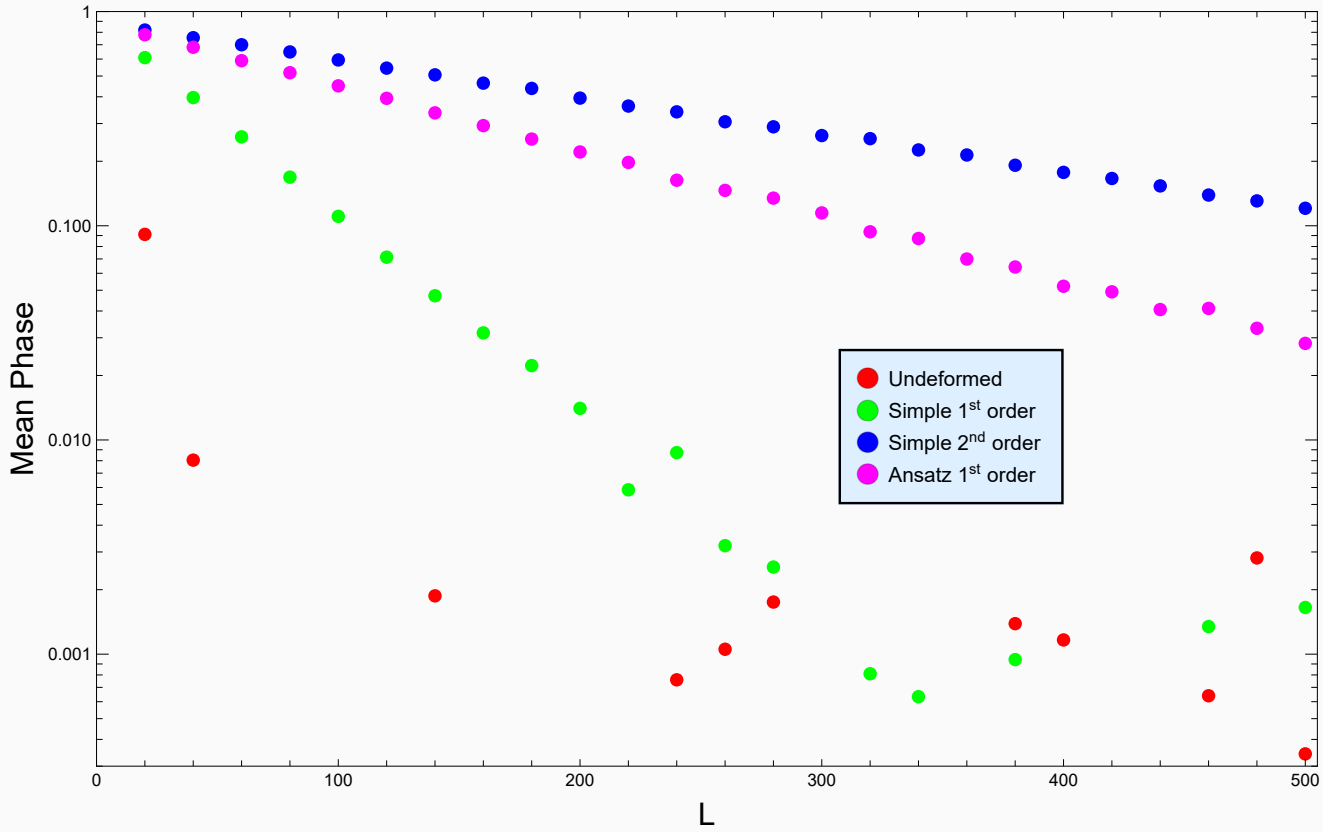




The Mean Phase as a Function of Lattice Size

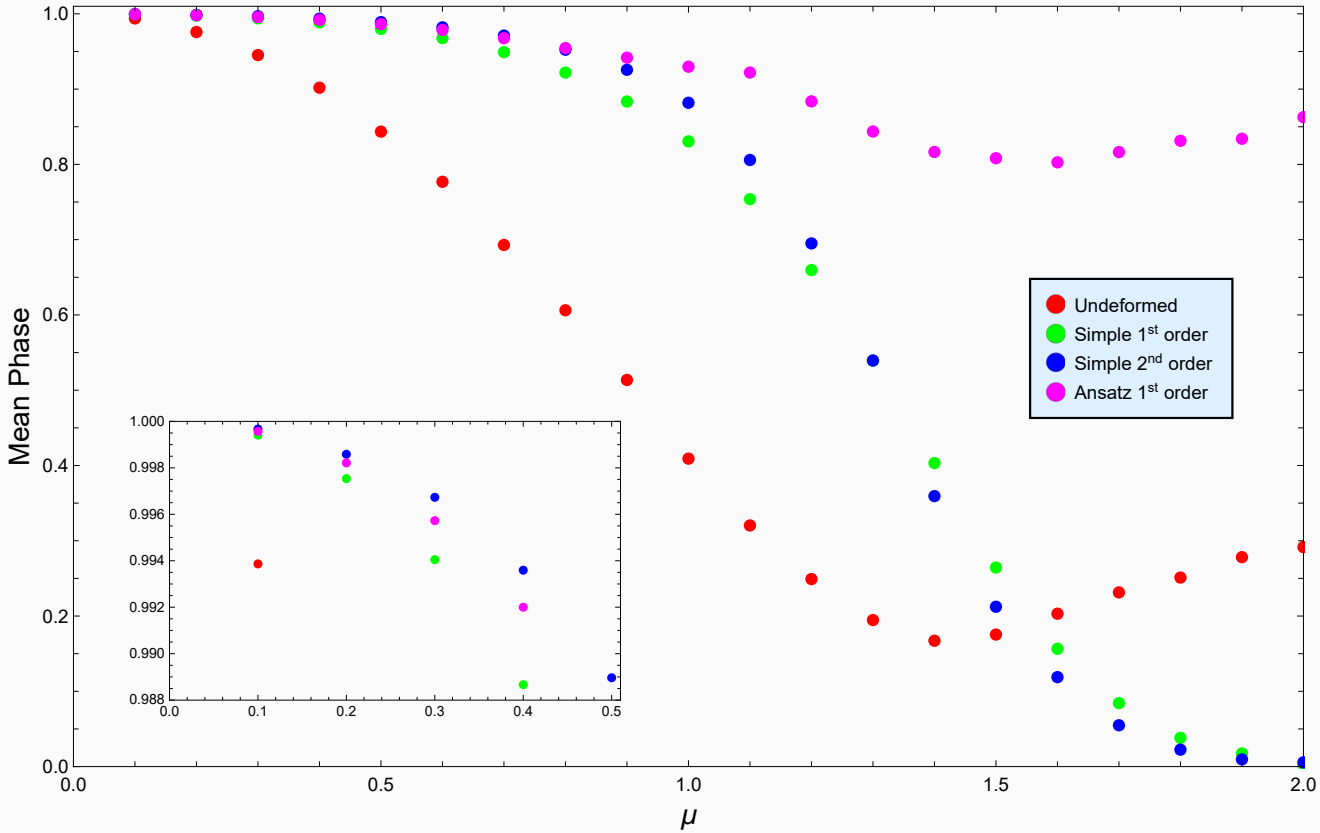
Various contours, for $d = 1$ with $m = \mu = 1$.

Exponential decay up to the onset of the sign problem.



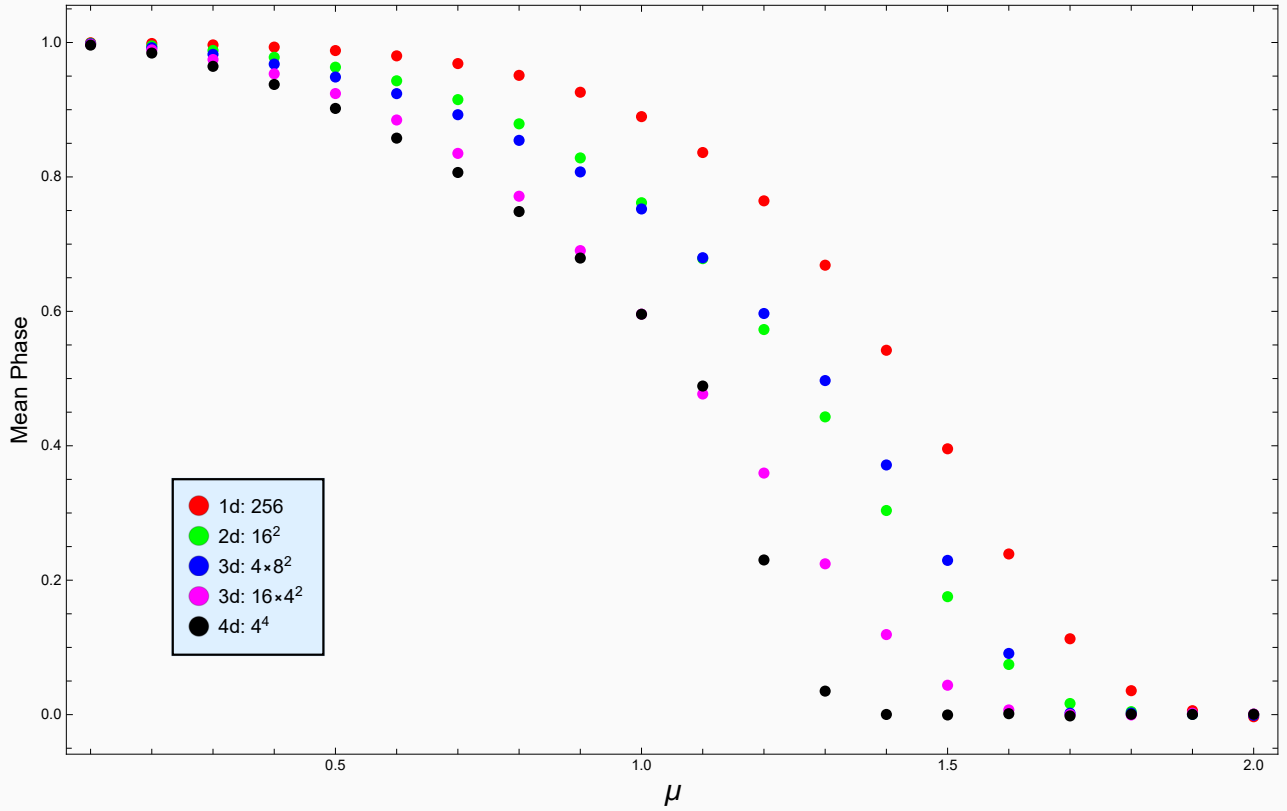
The Mean Phase as a Function of μ for $d = 1$, $L = 8$

The simple second order contour wins for small μ but as the expansion becomes unreliable the first order ansatz wins.



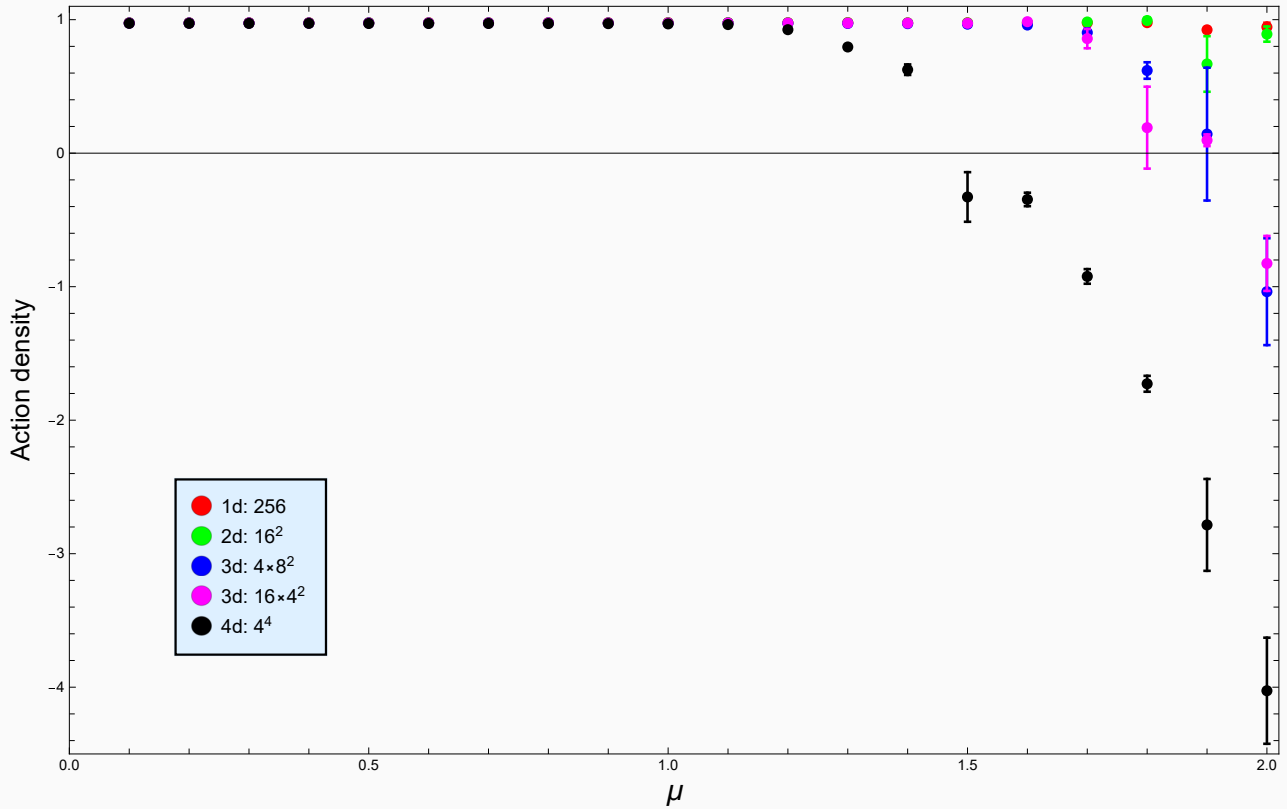
Comparing Different Dimensions

Simple 1^{st} order contours.
For fixed value of $\alpha = \frac{1}{9}$ ($m = 1$ for $d = 4$, $m = \sqrt{7}$ for $d = 1$) and 256 lattice sites the phase factor is larger for smaller d (although the result depends also on the geometry).



Comparing Different Dimensions – Observables

The action as a function of μ for the same contours.
Silver Blaze to higher μ values (since m is larger) for lower d.
Appearance of large error bars is correlated with the drop of the mean phase.

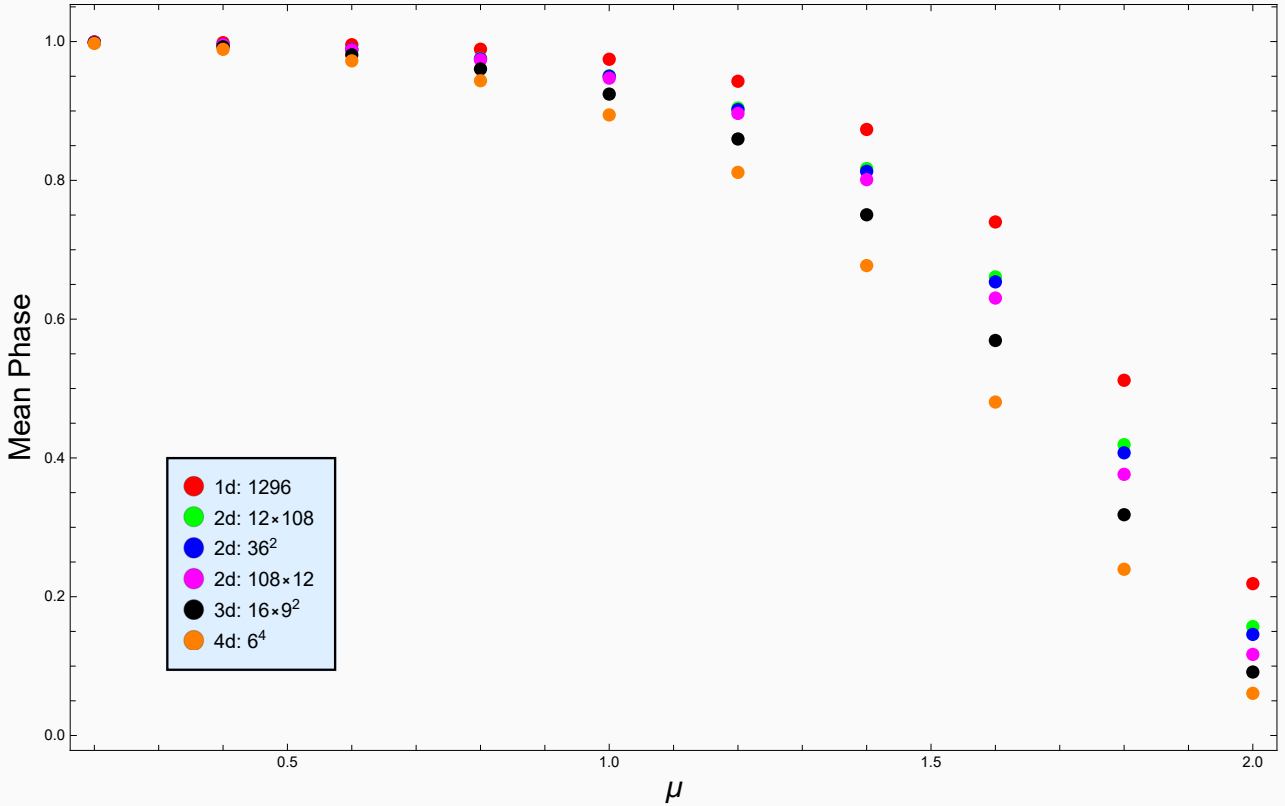


Comparing Different Dimensions – Another Example ($\alpha = \frac{1}{20}$)

With larger lattices the influence of the boundary is reduced.

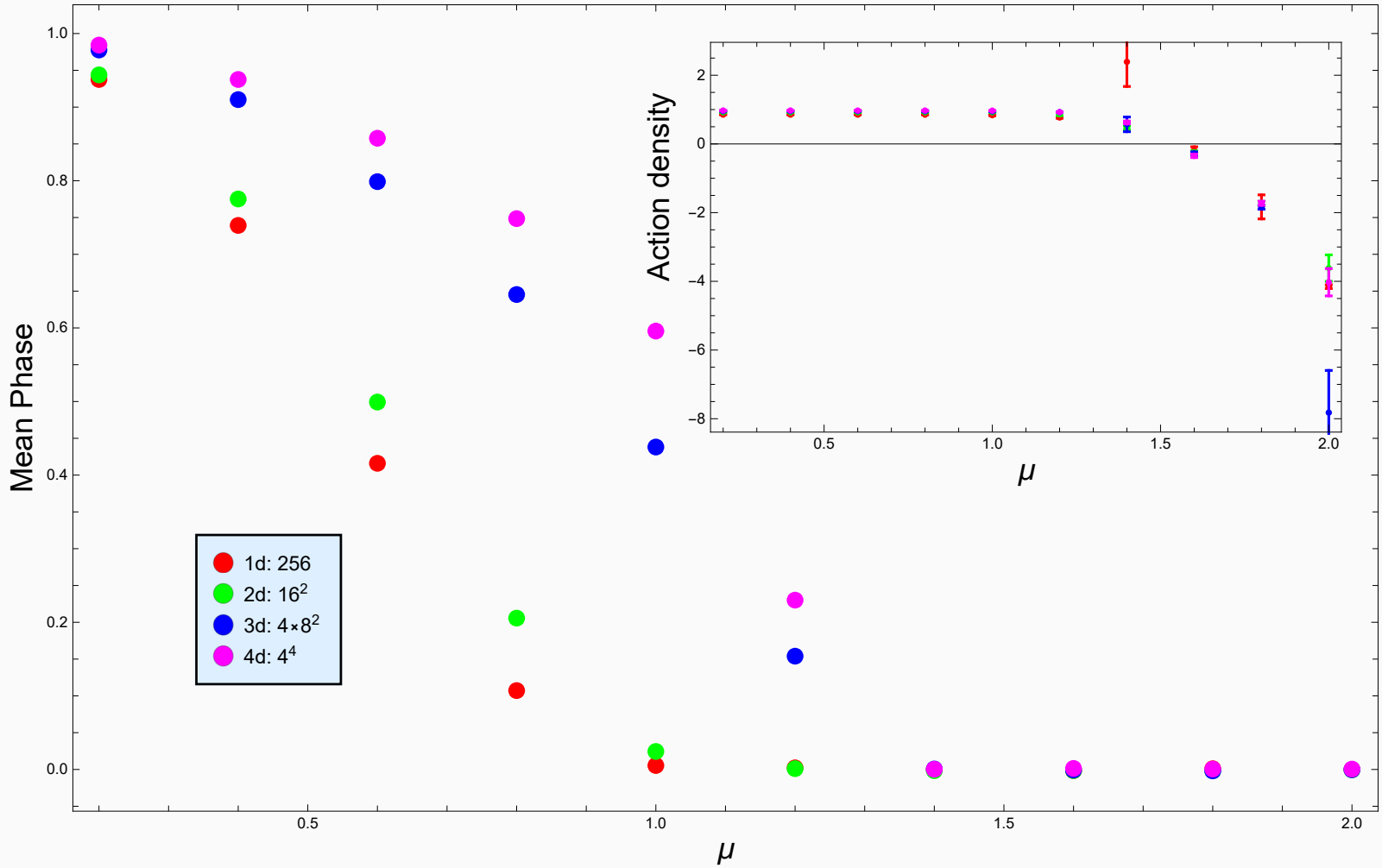
Smaller d behave better.

For $d = 2$ shorter temporal lattices behave better.



Comparing Different Dimensions – Fixed $m = 1$

Action behaves the same. Sign problem stronger for smaller d.
Results seem to be reliable way after the phase goes to zero.



Summary and Outlook

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Contour deformation is a good approach for the sign problem.

Address the source of the sign problem (nearest $\hat{0}$ neighbour).

An efficient computational method with a determinant that can be evaluated with complexity $O(V)$ for arbitrary d.

Understand the limitations of various expansions.

Consider different expansions for different parameters regimes.
Consider different expansions for different observables.

Use ansätze.

Second order ansatz ($d = 1$): phase above zero at least up to $L = 5,000$. Reliable results at least up to $L = 25,000$.

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

THANK YOU