Taylor expansions and Padé approximations for Lefschetz thimbles and beyond

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[3] Speaker

Introduction

- Goal: probe the QCD phase diagram by non-perturbative techniques. The lattice would be a natural candidate also through numerical simulations.
- Compute

$$\langle O \rangle \equiv \frac{1}{Z} \int dx^n \, O(x) \; e^{-S(x)}$$

stochastically, by sampling configurations from $P \propto e^{-S(x)}$.

However lattice QCD at finite density displays the prototype of a sign problem: S is complex $\to e^{-S(x)}$ does not define a legitimate probability distribution

- A possible workaround: complexify the dof of the theory and deform the domain of integration to remove (or mitigate) the sign problem

Lefschetz thimbles regularization (Phys. Rev. D 86 (2012) 074506, JHEP 10 (2013) 147)

1. we complexify the theory:

$$x \mapsto z = x + iy$$

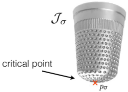
$$S(x) \mapsto S(z) = S_R(z) + iS_I(z)$$

2. we look for the critical points:

$$\partial_z S\big|_{z_\sigma} = 0$$

3. for each critical point, we define the thimble $\mathcal{J}_\sigma$ as the union of the SA paths leaving z_σ:

$$\frac{dz_i}{dt} = \frac{\partial \bar{S}}{\partial \bar{z}_i}\ , \text{ with i.c. } z_i(-\infty) = z_{\sigma,i}$$



4. Along the flow the real part of the action is increasing and the imaginary part of the action is constant. Still there is a complex factor: the residual phase (orientation of the thimble in the embedding manifold).

4. thimbles decomposition:

$$\int_{\mathcal{R}} dz^n\, O(z)\, e^{-S(z)} = \sum_{\sigma} n_\sigma e^{-iS^I_\sigma} \int_{\mathcal{J}_\sigma} dz^n\, O(z)\;\; e^{-S^R}\; e^{i\omega_\sigma}$$

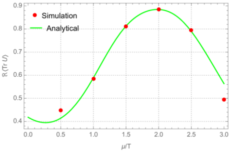
- S_R is always increasing and this ensures the convergence of the integral; S_I is constant and e^{-iS_I} can be factored out
- the sum is in principle over all the critical points, but ...
- the intersection numbers n_σ are integers numbers that count the intersections between the original contour and the unstable thimble $\mathcal{K}_\sigma \to n_\sigma$ can be zero
  - unstable thimble $\mathcal{K}_\sigma$ defined in a similar fashion to the stable thimble $\mathcal{J}_\sigma$ as the set of solutions of the SD equations, on which S_I is constant and S_R is decreasing

- thimbles decomposition formula:

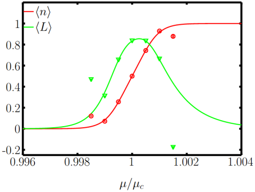
$$\langle O \rangle = \frac{\sum_\sigma n_\sigma Z_\sigma \langle O e^{i\omega} \rangle_\sigma}{\sum_\sigma n_\sigma Z_\sigma \langle e^{i\omega} \rangle_\sigma} \overset{?}{\approx} \frac{\langle O e^{i\omega} \rangle_{\sigma_0}}{\langle e^{i\omega} \rangle_{\sigma_0}}$$

how good can be the one-thimble approximation?

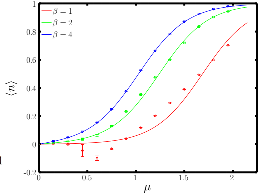
- counter-examples:



(0+1)-dimensional QCD
F. Di Renzo, G. Eruzzi
Phys. Rev. D 97, 014503 (2018)



heavy-dense QCD
F. Di Renzo, K. Zambello
PoS LATTICE2018 (2018) 148



Thirring model
F. Di Renzo, K. Zambello
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- Taylor expansions around points where only σ_0 matters

$$\langle O\rangle(\mu) = \langle O\rangle(\mu_0) + \left.\frac{\partial O}{\partial \mu}\right|_{\mu_0}(\mu-\mu_0) + \frac{1}{2}\left.\frac{\partial^2 O}{\partial \mu^2}\right|_{\mu_0}(\mu-\mu_0)^2 + \dots$$

We can use multiple Taylor expansions at different points, this itself is an improvement w.r.t. a single Taylor expansion around $\mu = 0$.

- The big improvement: interpolate all the Taylor coefficients at once using rational functions (Padé approximants).

We look for a function of the form

$$R_{n,m}(\mu) = \frac{p_n(\mu)}{q_m(\mu)} = \frac{a_0 + a_1\mu + a_2\mu^2 + \dots + a_n\mu^n}{1 + b_1\mu + b_2\mu^2 + \dots + b_m\mu^m}$$

that matches all the Taylor coefficients we calculated.

- Multi-point Padé: we determine a_i, b_i by imposing

$$\partial^j_{\mu^j} R_{n,m}(\mu^{(k)}) = \partial^j_{\mu^j} \langle O \rangle (\mu^{(k)})$$

Nonlinear system of eqs, but the problem can be linearized

$$\begin{cases} p_n(\mu^{(k)}) = \langle O \rangle(\mu^{(k)}) q_m(\mu^{(k)}) \\ p'_n(\mu^{(k)}) = \langle O \rangle'(\mu^{(k)}) q_m(\mu^{(k)}) + \langle O \rangle(\mu^{(k)}) q'_m(\mu^{(k)}) \\ p''_n(\mu^{(k)}) = \langle O \rangle''(\mu^{(k)}) q_m(\mu^{(k)}) + 2\langle O \rangle'(\mu^{(k)}) q'_m(\mu^{(k)}) + \langle O \rangle(\mu^{(k)}) q''_m(\mu^{(k)}) \\ \dots \end{cases}$$

We fix the number of expansion points $\mu^{(k)}$, then we increase the order of the derivatives until convergence.

$\Rightarrow$ improved convergence properties of the series + interesting information on singularities structure **(see also Simran's talk, today at 6:30 ET)**

(0+1)-dimensional Thirring model

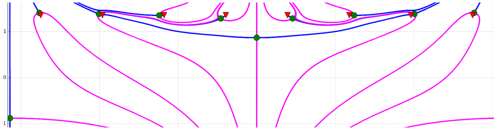
For this theory the one-thimble approximation fails.

(JHEP 12 (2015) 125, JHEP 05 (2016) 053, PoS LATTICE2019 (2020) 211)

Can we find at least a few suitable expansion points in regions where the one-thimble approximation holds?

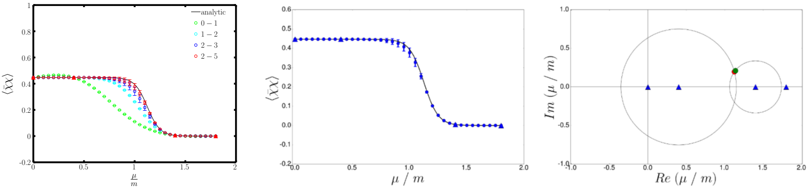
Parameters $L = 8, \beta = 1, m = 2$:

- $\frac{\mu}{m} = 0 \rightarrow$ no sign problem at all
- $\frac{\mu}{m} = 0.4 \rightarrow$ from S_I we know one thimble contributes
- $\frac{\mu}{m} = 1.4, 1.8 \rightarrow$ from S_R we know only two might contribute and ...



- Numerical results for $L = 8$:

F. Di Renzo, S. Singh, K. Zambello, Phys. Rev. D 103, 034513 (2021)



From Padé we are able to extract some information about the analytical structure of the observable.

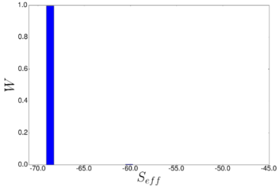
The analysis has also been repeated towards the continuum limit up to $L = 64$.

Taylor expansions on Lefschetz thimbles

Applications

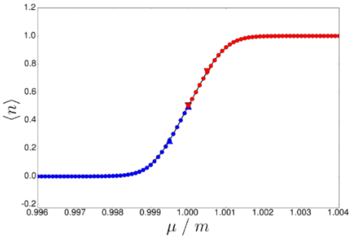
Heavy-dense QCD

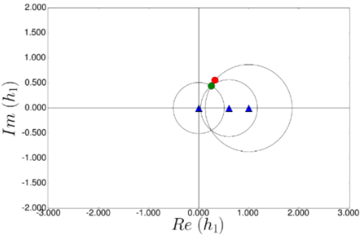
- $\frac{\mu}{m} = 1.0 \rightarrow$ no sign problem
- $\frac{\mu}{m} = 0.9995, 1.0005 \rightarrow$ thimbles other than the fundamental one are depressed



- Numerical results:

F. Di Renzo, S. Singh, K. Zambello, Phys. Rev. D 103, 034513 (2021)

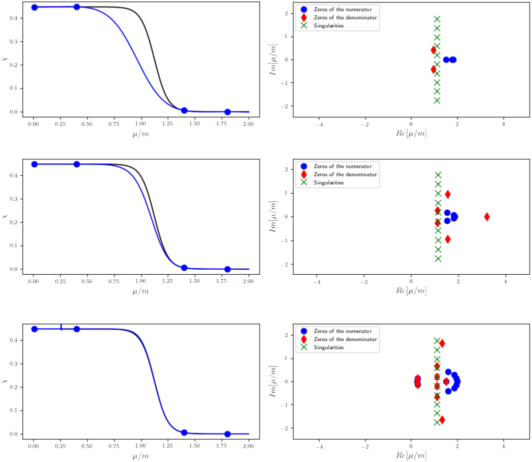




A few comments

Possible applications beyond thimbles

- A numerical experiment (add more derivatives, no errors)

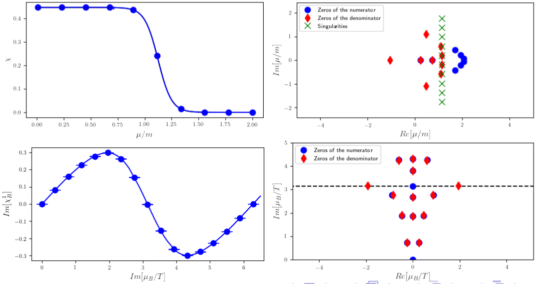


$\Rightarrow$ This method apparently returns a lot of information on singularities structure. This is right what we look for in QCD!

- This procedure works for any calculation method that gives access to multiple expansion points
- Application beyond thimbles: hunt for singularities in the QCD phase diagram by Padé interpolation of multiple Taylor expansions around points at imaginary μ.

  (see Simran's and Guido's talks, today at 6:30 and 6:45 ET)

For practical reasons in this case we have to increase the number of points instead of the order of the derivatives.



- so far thimble regularization has been applied to various models; it is now clear that the dominant thimble alone is not enough to capture the full content of a theory
- multi-thimble simulations are hard, but we have proposed a new and more powerful approach in which the need for multi-thimble simulations can be by-passed by computing and bridging different Taylor expansions; we have successfully applied this method to heavy-dense QCD and to the Thirring model
- we have found that the method is more powerful than we had anticipated, as bridging by Padé not only allowed to by-pass the need for multi-thimble simulations but it also allowed to locate the true singularities of the observables
- this idea has applications to QCD at imaginary μ

  . . . more about this in the following talks by Simran and Guido

  . . . stay tuned!