PROCEEDINGS OF SCIENCE

Taylor expansions and Padé approximations for Lefschetz thimbles and beyond

Kevin Zambello,* **Francesco Di Renzo and Simran Singh**

Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma and INFN, Gruppo Collegato di Parma, I-43124 Parma, Italy

E-mail: kevin.zambello@pr.infn.it, francesco.direnzo@pr.infn.it, simran.singh@unipr.it

Deforming the domain of integration after complexification of the field variables is an intriguing idea to tackle the sign problem. In thimble regularization the domain of integration is deformed into an union of manifolds called Lefschetz thimbles. On each thimble the imaginary part of the action stays constant and the sign problem disappears. A long standing issue of this approach is how to determine the relative weight to assign to each thimble contribution in the (multi)-thimble decomposition. Yet this is an issue one has to face, as previous work has shown that different theories exist for which the contributions coming from thimbles other than the dominant one cannot be neglected. Historically, one of the first examples of such theories is the one-dimensional Thirring model. Here we discuss how Taylor expansions can be used to by-pass the need for multi-thimble simulations. If multiple, disjoint regions can be found in the parameters space of the theory where only one thimble gives a relevant contribution, multiple Taylor expansions can be carried out in those regions to reach other regions by single thimble simulations. Better yet, these Taylor expansions can be bridged by Padé interpolants. Not only does this improve the convergence properties of the series, but it also gives access to information about the analytical structure of the observables. The true singularities of the observables can be recovered. We show that this program can be applied to the one-dimensional Thirring model and to a (simple) version of HDQCD. But the general idea behind our strategy can be helpful beyond thimble regularization itself, i.e. it could be valuable in studying the singularities of QCD in the complex μ_B plane. Indeed this is a program that is currently being carried out by the Bielefeld-Parma collaboration.

The 38th International Symposium on Lattice Field Theory, LATTICE2021 26th-30th July, 2021 Zoom/Gather@Massachusetts Institute of Technology

*Speaker

PoS(LATTICE2021)336

1. Thimble regularization

The sign problem is the main obstacle to study quantum field theories (such as QCD) at finite density by lattice simulations. On the lattice the physical observables have the form

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

where Z is the partition function and $S(x)$ is the action of the system. Assuming $S(x)$ is real, the Boltzmannian factor $e^{-S(x)}$ is a well-defined probability distribution for importance sampling and the integrals can be calculated by Monte Carlo. Unfortunately at finite density the action is in general complex-valued.

An intriguing solution to sidestep the sign problem is to complexify the degrees of freedom of the theory and deform the contour of integration of the integrals in such a way that the sign problem disappears (or is mitigated). Thimble regularization provides a way to find a suitable deformation [1, 2]. After complexifying the degrees of freedom, $x \mapsto z$, one looks for the stationary points of the action $S(z)$, i.e. the points z_σ such that $\partial_z S|_{z_\sigma} = 0$. For each critical point z_σ one can define a manifold, the (*stable*) Lefschetz thimble $\mathcal{J}_\sigma$, as the set of the solutions of the steepest ascent (SA) equations originating from the critical points, i.e. the set of all paths $z(t)$ such that $\frac{dz_i}{dt} = \frac{\partial \overline{S}}{\partial \overline{z}_i}$ and $z_i(-\infty) = z_{i,\sigma}$. Due to the properties of the SA equations the imaginary part of the action stays constant on each thimble and the real part of the action is always increasing.

According to the Picard-Lefschetz theory, the original integrals can be decomposed to a sum of integrals over the thimbles,

$$\langle O\rangle = \frac{\int dx\, O(x) e^{-S(x)}}{\int dx\, e^{-S(x)}} = \frac{\sum_\sigma n_\sigma e^{-iS_I^\sigma} \int_{\mathcal{J}_\sigma} dz\, O(z)\, e^{i\omega} e^{-S_R(z)}}{\sum_\sigma n_\sigma e^{-iS_I^\sigma} \int_{\mathcal{J}_\sigma} dz\, e^{i\omega} e^{-S_R(z)}}$$

In place the original integrals we have linear combinations of integrals over the thimbles and the latter are not affected by the sign problem. The reason is that the contribution from the imaginary part of the action is constant and can be factorized out. A complex *residual* phase, $e^{i\omega}$, still appears in the integrals. This phase comes from the orientation of the thimble in the embedding manifold. This results in a *residual* sign problem, but in practice this is usually found to be a mild one and can be taken care of by reweighting. The integer coefficients n_σ, known as intersection numbers, can be zero, therefore not all the thimbles do necessarily contribute. Geometrically the intersection numbers count the number of intersections between the original domain of integration and the *unstable* thimbles. These are defined as the solutions of the steepest descent (SD) equations originating from the critical points. The imaginary part of the action is constant on the *unstable* thimbles and the real part of the action is always decreasing. Now if we define the thimble contribution

$$\langle \bullet \rangle_\sigma = \frac{\int_{\mathcal{J}_\sigma} dz\, \bullet\, e^{-S_R}}{\int_{\mathcal{J}_\sigma} dz\, e^{-S_R}} = \frac{\int_{\mathcal{J}_\sigma} dz\, \bullet\, e^{-S_R}}{Z_\sigma}$$

we can rewrite the thimble decomposition formula as

$$\frac{\int dx\, O(x) e^{-S(x)}}{\int dx\, e^{-S(x)}} = \frac{\sum_\sigma n_\sigma e^{-iS_I^\sigma} Z_\sigma \langle O e^{i\omega}\rangle_\sigma}{\sum_\sigma n_\sigma e^{-iS_I^\sigma} Z_\sigma \langle e^{i\omega}\rangle_\sigma}$$

The original integrals are now decomposed to a sum of thimble contributions $\langle \bullet \rangle_\sigma$ that can be calculated numerically by Monte Carlo simulations. These contributions are weighted by the partition function Z_σ. Calculating these weights is hard and this could be regarded as one of the main obstacles to multi-thimble calculations. Yet this is an issue one has to face, as previous work has shown that different theories exist for which the contributions coming from thimbles other than the dominant one cannot be neglected [3–7]. Some proposals to address the issue have been made in the literature [5, 6, 8, 9]. Here we discuss what we think is a more promising approach where the need to calculate the weights is actually bypassed.

2. Taylor expansions and Padé approximants

The idea we propose is to take advantage of the changes the thimble structure is subject to as we move within the parameter space of the theory [10]. The union of the stable thimbles appearing in the thimble decomposition is a deformation of the original contour of integration. The thimble structure changes as we modify the parameters of the theory. Being solutions of the same differential equations starting from different initial conditions, the stable thimbles cannot cross each other. Therefore the stable thimbles appearing in the decomposition act as barriers, preventing the other stable thimbles from entering the decomposition. When a Stokes phenomenon takes place, however, the stable thimble attached to a critical point overlaps the unstable thimble attached to another critical point. After a Stokes phenomenon, a new (old) stable thimble can enter (leave) the decomposition and its intersection number suddenly changes. There is a discontinuity in the thimble decomposition. However this does not imply that the observables themselves are discontinuous. Hence if only one *relevant*[1] thimble is left in the decomposition after a Stokes phenomenon takes place at μ_c, we can think of reaching the region $\mu < \mu_c$ before the Stokes by a Taylor expansion calculated around a point $\mu_0 > \mu_c$ after the Stokes,

$$\langle O \rangle(\mu) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n \langle O \rangle}{\partial \mu^n} |_{\mu_0} (\mu - \mu_0)^n$$

The Taylor coefficients can be calculated from one-thimble simulations, bypassing de facto the necessity of calculating the weights of the thimbles.

If multiple suitable expansion points $\mu_0^{(k)}$ are available, the Taylor coefficients can also be used to build a multi-point Padé approximant. That is we look for a rational function $R_{n,m}(\mu) = p_n(\mu)/q_m(\mu)$ that matches the Taylor coefficients, i.e. $(\partial^j_{\mu^j} R_{n,m})(\mu_0^{(k)}) = (\partial^j_{\mu^j} \langle O \rangle)(\mu_0^{(k)})$. These Padé approximants improve the convergence properties of the series and allow to extract information on the singularities structure. The location of the true singularities of the observable in the complex μ plane can be inferred from the location of the uncancelled roots of the denominator.

3. Applications

As a first application we have applied our strategy to the one-dimensional Thirring model [3, 4, 11] with parameters $L = 8$, $\beta = 1$, $m = 2$. We have calculated Taylor expansions in term of

[1] Here we must consider two possible cases: (1) only the *dominant* thimble $\mathcal{J}_{\sigma_0}$ has a non-zero intersection number and (2) also other thimbles have a non-zero intersection number but their contribution is exponentially suppressed because $S_R(\sigma_i) \gg S_R(\sigma_0)$.

the dimensionless parameter $\frac{\mu}{m}$. As expansion points we have selected four points where only one thimble gives a relevant contribution, i.e. $\frac{\mu}{m} = 0.0, 0.4, 1.4$ and 1.8. Up to some value $\frac{\mu_0}{m} > 0.4$ only two unstable thimbles have an imaginary part of the action in the range taken by S_I on the original domain of integration. These are the thimbles attached to two critical points that we denote by σ_0 and $\sigma_{\bar{0}}$. The contribution from the second critical point is depressed, as $S_R(\sigma_{\bar{0}}) \gg S_R(\sigma_0)$. Therefore only σ_0 gives a relevant contribution at $\mu = 0.0, 0.4$. On the other hand at $\frac{\mu}{m} = 1.4, 1.8$ all critical points but three have a real part of the action much greater than $S_R(\sigma_0)$ and their contributions are depressed. Two out of the three critical points have a real part of the action lower than the minimum taken on the original domain of integration, hence they cannot enter the decomposition as their unstable thimbles cannot intersect the original domain of integration. It can explicitly be checked that the unstable thimble attached to the remaining critical point, which we denote by σ_1, does not intersect the original domain of integration, while the unstable thimble attached to σ_0 does [10]. Therefore σ_0 gives the only relevant contribution also at $\frac{\mu}{m} = 1.4, 1.8$.

The left picture of fig. 1 shows the results obtained for the scalar condensate from the Padé interpolation of the Taylor coefficients calculated at $\frac{\mu}{m} = 0.0, 0.4, 1.4$ and 1.8 respectively up to order $0, 2, 5$ and 0. The numerical results (error bars) are in good agreement with the analytical result (solid line). The right picture shows how the stable, uncancelled root of the denominator of the Padé approximant (blue point) matches very well the singularity of the analytical solution (red point) on the complex $\frac{\mu}{m}$ plane. In ref. [12] we have also repeated this analysis towards the continuum limit.

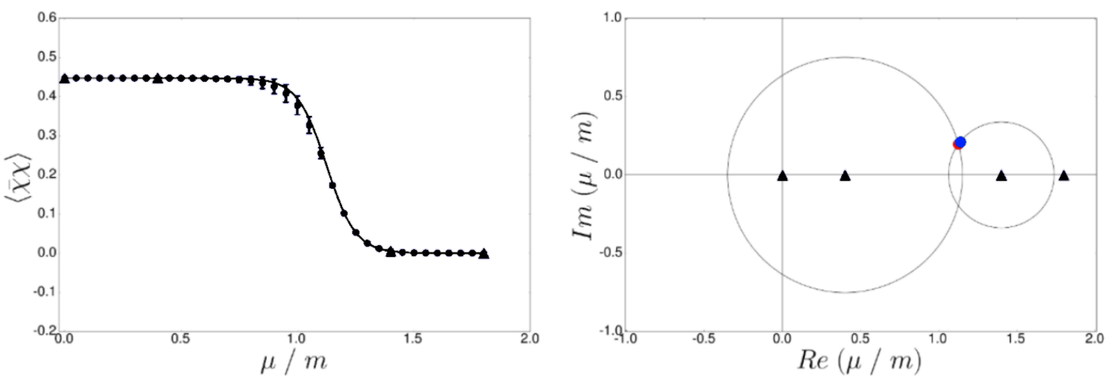

Figure 1: Results for the one-dimensional Thirring model

As a second application we have considered the simple version of heavy-dense QCD [13, 14] that we had initially investigated in ref. [6]. We have used the parameters $N_s^3 = 2^3, N_t = 116$ and $k = 0.0000887$. We have calculate Taylor expansions in term of the dimensionless parameter $h_1 = (2ke^{\hat{\mu}})^{N_t} = e^{-\frac{\mu - m}{T}}$ (actually we expanded in term of h_1 for $\mu < m$ and in term of h_1^{-1} for $\mu > m$). This is the natural expansion term, as the chemical potential μ enters the lattice action only through h_1. As expansion points we chose $\frac{\mu}{m} = 0.9995, 1.0000, 1.0005$. From a semiclassical calculations we have concluded that at these chemical potentials the contributions from all but the fundamental thimble are depressed [10].

The results for the number density from Padé are shown in the left picture of fig. 2, using different colors for the $\mu < m$ and $\mu > m$ branches. The Padé interpolation for the left branch has been calculated using as inputs the Taylor coefficients up to order 2 and 1 respectively at $\frac{\mu}{m} = 0.9995$ and 1.0000. We also added an extra constraint for the observable and its first derivative at $\frac{\mu}{m} = 0$. Similarly for the right branch we used the Taylor coefficients up to order 1 and 2 at $\frac{\mu}{m} = 1.0000$ and 1.0005, adding as extra constraint the asymptotic values of the observable and its first derivative at large chemical potentials. Also in this second application the numerical results (error bars) are in agreement with the analytical solution (solid line). The right picture shows that also in this case the uncancelled root of the denominator of the approximant (blue point) matches fairly well the singularity of the observable (red point) in the complex h_1 plane.

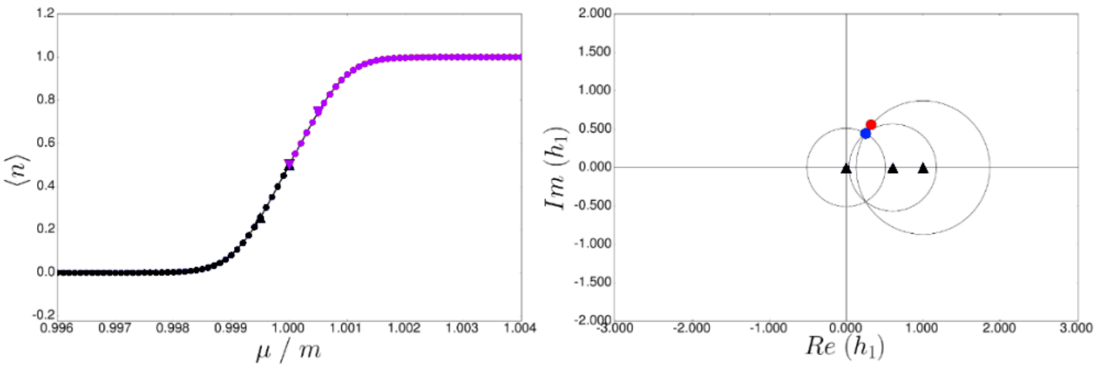

Figure 2: Result for heavy-dense QCD

4. Applications beyond thimble regularization

As we've seen in the examples we've examined in the previous section, merging different Taylor series by Padé not only improves the convergence properties of the series, but it also returns information on the singularities structure of the observables. This is something that can be valuable in lattice QCD calculations. One might be able to extract hints on the location of critical points in the QCD phase diagram. We stress that the strategy we have put in place is applicable with any calculation method that gives access to Taylor expansions around multiple points. A natural question is whether the strategy can be fruitful when applied to lattice calculation at imaginary chemical potentials (where there is no sign problem).

We have been exploring this line of research in collaboration with the Bielefeld group [15, 16]. Indeed we were able to locate a few singularities in the complex μ_B plan. For instance the left picture of fig. 3 shows the approximant we have built for the imaginary part of the baryon number density. The approximant was built from the lattice data obtained at $O(10)$ imaginary baryon chemical potentials for the number density and its $1st$ and $2nd$ order derivatives. The right picture of fig. 3 shows how two roots of the denominator (red squares) survive the cancellation with roots of the numerator (blue points). The location of these roots is stable with respect to variations of the inputs we use for Padé and it signals the presence of a genuine singularity.

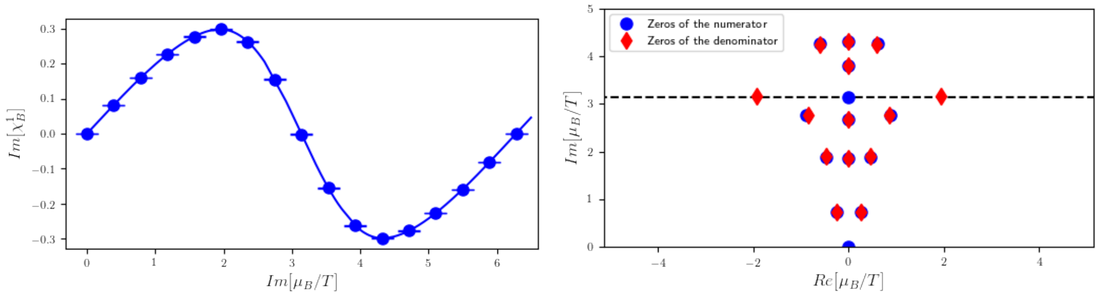

Figure 3: Results from lattice QCD calculations at imaginary μ_B

5. Conclusions

One of the main issues that prevents the application of thimble regularization to realistic theories is the calculation of the relative weights of the thimble contributions.

We argue that one can exploit the thimble structure of a theory to bypass the need for such calculations. If one can find multiple *good* points in the parameter space of the theory where only one thimble contribution matters, one can calculate different Taylor expansions around these points. The Taylor coefficients can be calculated by one-thimble simulations. The Taylor series can then be bridged by Padé approximants in order to reach *bad* regions where more than one relevant thimble enter the thimble decomposition. Moreover by studying the poles of the Padé approximants one is able to extract information about the singularities structure of the theory.

We also argue that this strategy has potential applications beyond thimble regularization itself. Indeed, any calculation method that is good enough to give access to multiple expansion points can be used to build multi-point Padé approximants. Specifically, the strategy can be useful to hunt for singularities in the phase diagram of QCD by merging Taylor series calculated at imaginary chemical potentials.

6. Acknowledgments

This work was supported by the European Union Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 813942 (EuroPLEx) and by the I.N.F.N. under the research project i.s. QCDLAT. This research used computing resources made available (i) by CINECA on Marconi and Marconi 100 under both the I.N.F.N-CINECA agreement and the ISCRA C program, (ii) by the University of Parma on its HPC (High Performance Computing) facility, (iii) by the Gauss Centre for Supercomputing on the Juwels GPU nodes at the Jülich Supercomputing Centre and (iv) by the Bielefeld University on the Bielefeld GPU-Cluster.

References

[1] M. Cristoforetti *et al.* [AuroraScience], *New approach to the sign problem in quantum field theories: High density QCD on a Lefschetz thimble*, Phys. Rev. D **86** (2012), 074506 doi:10.1103/PhysRevD.86.074506 [arXiv:1205.3996 [hep-lat]].

[2] H. Fujii, D. Honda, M. Kato, Y. Kikukawa, S. Komatsu and T. Sano, *Hybrid Monte Carlo on Lefschetz thimbles - A study of the residual sign problem*, JHEP **10** (2013), 147 doi:10.1007/JHEP10(2013)147 [arXiv:1309.4371 [hep-lat]].

[3] H. Fujii, S. Kamata and Y. Kikukawa, *Monte Carlo study of Lefschetz thimble structure in one-dimensional Thirring model at finite density*, JHEP **1512** (2015) 125 Erratum: [JHEP **1609** (2016) 172] doi:10.1007/JHEP12(2015)125, 10.1007/JHEP09(2016)172 [arXiv:1509.09141 [hep-lat]].

[4] H. Fujii, S. Kamata and Y. Kikukawa, *Lefschetz thimble structure in one-dimensional lattice Thirring model at finite density*, JHEP **1511** (2015) 078 Erratum: [JHEP **1602** (2016) 036] doi:10.1007/JHEP02(2016)036, 10.1007/JHEP11(2015)078 [arXiv:1509.08176 [hep-lat]].

[5] F. Di Renzo and G. Eruzzi, *One-dimensional QCD in thimble regularization*, Phys. Rev. D **97**, no. 1, 014503 (2018) doi:10.1103/PhysRevD.97.014503 [arXiv:1709.10468 [hep-lat]].

[6] K. Zambello and F. Di Renzo, *Towards Lefschetz thimbles regularization of heavy-dense QCD*, PoS LATTICE **2018** (2018) 148 doi:10.22323/1.334.0148 [arXiv:1811.03605 [hep-lat]].

[7] M. Ulybyshev, C. Winterowd and S. Zafeiropoulos, *Lefschetz thimbles decomposition for the Hubbard model on the hexagonal lattice*, Phys. Rev. D **101** (2020) no.1, 014508 doi:10.1103/PhysRevD.101.014508 [arXiv:1906.07678 [cond-mat.str-el]].

[8] S. Bluecher, J. M. Pawlowski, M. Scherzer, M. Schlosser, I. O. Stamatescu, S. Syrkowski and F. P. G. Ziegler, *Reweighting Lefschetz Thimbles*, SciPost Phys. **5**, no. 5, 044 (2018) doi:10.21468/SciPostPhys.5.5.044 [arXiv:1803.08418 [hep-lat]].

[9] J. M. Pawlowski, M. Scherzer, C. Schmidt, F. P. G. Ziegler and F. Ziesché, *Simulating Yang-Mills theories with a complex coupling*, Phys. Rev. D **103** (2021) no.9, 094505 doi:10.1103/PhysRevD.103.094505 [arXiv:2101.03938 [hep-lat]].

[10] F. Di Renzo, S. Singh and K. Zambello, *Taylor expansions on Lefschetz thimbles*, Phys. Rev. D **103** (2021) no.3, 034513 doi:10.1103/PhysRevD.103.034513 [arXiv:2008.01622 [hep-lat]].

[11] A. Alexandru, G. Basar and P. Bedaque, *Monte Carlo algorithm for simulating fermions on Lefschetz thimbles*, Phys. Rev. D **93** (2016) no.1, 014504 doi:10.1103/PhysRevD.93.014504 [arXiv:1510.03258 [hep-lat]].

[12] F. Di Renzo and K. Zambello, *Settling an old story: solution of the Thirring model in thimble regularization*, submitted [arXiv:2109.02511 [hep-lat]].

[13] M. Fromm, J. Langelage, S. Lottini, M. Neuman and O. Philipsen, *Onset Transition to Cold Nuclear Matter from Lattice QCD with Heavy Quarks*, Phys. Rev. Lett. **110** (2013) no.12, 122001 doi:10.1103/PhysRevLett.110.122001 [arXiv:1207.3005 [hep-lat]].

[14] M. Fromm, J. Langelage, S. Lottini and O. Philipsen, *The QCD deconfinement transition for heavy quarks and all baryon chemical potentials*, JHEP **01** (2012), 042 doi:10.1007/JHEP01(2012)042 [arXiv:1111.4953 [hep-lat]].

[15] C. Schmidt, J. Goswami, G. Nicotra, F. Ziesché, P. Dimopoulos, F. Di Renzo, S. Singh and K. Zambello, *Net-baryon number fluctuations*, Acta Phys. Pol. B Proc. Suppl. 14, 241 (2021) [arXiv:2101.02254 [hep-lat]].

[16] P. Dimopoulos, L. Dini, F. Di Renzo, J. Goswami, G.Nicotra, C. Schmidt, S. Singh, K. Zambello and F. Ziesché, *A contribution to understanding the phase structure of strong interaction matter: Lee-Yang edge singularities from lattice QCD*, submitted [arXiv:2110.15933 [hep-lat]].