Taylor expansions on Lefschetz thimbles

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(Received 7 August 2020; accepted 15 February 2021; published 26 February 2021)

Thimble regularization is a possible solution to the sign problem, which is evaded by formulating quantum field theories on manifolds where the imaginary part of the action stays constant (Lefschetz thimbles). A major obstacle is due to the fact that one in general needs to collect contributions coming from more than one thimble. Here we explore the idea of performing Taylor expansions on Lefschetz thimbles. We show that in some cases we can compute expansions in regions where only the dominant thimble contributes to the result in such a way that these (different, disjoint) regions can be bridged. This can most effectively be done via Padé approximants. In this way multi-thimble simulations can be circumvented. The approach can be trusted provided we can show that the analytic continuation we are performing is a legitimate one, which thing we can indeed show. We briefly discuss two prototypal computations, for which we obtained a very good control on the analytical structure (and singularities) of the results. All in all, the main strategy that we adopt is supposed to be valuable not only in the thimble approach, which thing we finally discuss.

DOI: 10.1103/PhysRevD.103.034513

I. INTRODUCTION: THIMBLE REGULARIZATION AND SINGLE THIMBLE DOMINANCE

Lattice regularization provides an effective framework for a nonperturbative definition of quantum field theories. It also enables numerical computations: in the Euclidean formulation, a lattice-regularized QFT resembles a statistical physics problem, the functional integral defines a decent probability measure and Monte Carlo simulations are viable. However, this is not always the case. When a complex action is in place, we have no probability measure to start with and there is no obvious way to set up a Monte Carlo scheme. This is one consequence of what is known as the sign problem. Among other theories, QCD at nonzero chemical potential is plagued by a sign problem and at the moment we have no effective way to tackle the investigation of its (supposedly rich) phase diagram by lattice methods (for a clean explanation of the sign problem in the framework of QCD see [1]; for an up-to-date account of the status of the efforts to constrain the QCD phase diagram see [2]).

Thimble regularization is an elegant (attempt at a) solution to the sign problem. Following seminal papers by Witten [3,4], it has been introduced with the idea that the sign problem can be beaten at a fundamental level. Thimble regularization is conceptually simple: one changes the domain of integration by complexifying the degrees of freedom and defines the theory on manifolds where the imaginary part of the action stays constant. These manifolds are the so-called Lefschetz thimbles [5,6]. In practice, the method has many subtleties. A major one has to do with a fundamental feature, i.e., the so-called thimble decomposition. While there are cases in which a single contribution (attached to the so-called dominant thimble) accounts for the solution of the problem at hand, in general a given quantity is computed summing contributions attached to many thimbles. This feature in turn has to do with the occurrence of Stokes phenomena. The latter take place at given points in the space of the parameters which define the theory: for certain values of the parameters there is no meaningful thimble decomposition. While *at those points* there is no thimble decomposition, *across those points* there is a discontinuity in thimble decompositions, which nevertheless does not generally imply a discontinuity in physical results. This basic feature will play a major role in the following.

In the original formulation [5] a single thimble dominance conjecture was put forward. The underlying idea is very simple: one defines the theory as the functional integral restricted to the dominant thimble, i.e., the one associated to the absolute minimum of the real action. From

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very general (semiclassical) arguments, this contribution is expected to be more and more enhanced in the thermodynamic limit. At a more fundamental level, the regularization of a field theory on the dominant thimble defines a local quantum field theory with exactly the same symmetries, the same number of degrees of freedom (belonging to the same representations of the symmetry groups) and the same local interactions as the original theory. Moreover, the perturbative expansion on the dominant thimble is exactly the same computed in standard perturbation theory in the original formulation. Quite interestingly, in the case of the relativistic Bose gas this approximation proved to work very well [7]. The Bose gas was of course only one success. Needless to say, if the dominant thimble dominance hypothesis held true for a wide range of theories, that would be a major success: numerical simulations for thimble regularization would be in the end not that difficult. The Thirring model was shown to be a (first) counterexample: in this case the dominant thimble does not capture the (complete) correct result [8,9]. This was a major motivation for the exploration of alternative formulations somehow inspired by thimbles. The idea of deforming the original domain of integration is indeed a very general one (from this point of view the complexification of the degrees of freedom is quite an obvious thing to do). Alternatives to thimble regularization were put forward, e.g., the holomorphic flow [9] or various definitions of sign-optimized manifolds, possibly selected by deep-learning techniques [10–12]; for a recent, nice review of most of these ideas see [13].

In this work we want to explore the idea of performing Taylor expansions on Lefschetz thimbles. All in all, the main idea is to compute Taylor expansions in different regions of the parameter space of a given theory, namely around points where only the dominant thimble contributes to the result one is interested in. This could seem somehow a lucky scenario, but we argue that this can quite often be the case. Through multiple expansions these (different, disjoint) regions can be bridged and in this way multi-thimbles simulations can be circumvented. This bridging can most effectively be obtained via Padé approximants. The question then should be: "Can we trust this bridging?" The answer is yes if we can prove that we are going through a legitimate analytic continuation. Needless to say, working with Taylor expansions we are aiming at a control on analytic contributions to the result and we will be blind to any nonperturbative effect in the expansion parameter.[1] Most noticeably, in the simple examples we preliminarily discuss in this work, we show that we can have a very good control on the analytic structure (and singularities) of the results. We stress that this good control is coming from multiple Taylor expansions at different points (in the end, different values for the chemical potential) and Padé approximants. While all this is discussed in the framework of (and motivated by) thimble regularization, it is important to recognize in what we do an overall strategy that does not apply only to this regularization. This is in a sense a strategy which can go well beyond thimbles.

The paper is organized in a such a way that a minimal prior knowledge of the subject is assumed. In Sec. II we collect the basics of thimble regularization; in particular, we define what a thimble decomposition is and we mention a couple of approaches to multiple thimbles simulations we have been testing in the last few years; the main content of the section is the focus on Stokes phenomena. Section III contains the basic description of the computational method we propose together with a discussion of preliminary results for a couple of theories, which (while admittedly simple) are supposed to be valuable prototypes. Conclusions IV are meant to recognize to which extent the strategy we discuss can go beyond the application to thimble regularization.

II. THIMBLE DECOMPOSITION AND STOKES PHENOMENA: A STORY OF CONTINUITY AND DISCONTINUITIES

A. Basics of thimble decomposition and basic multiple thimbles computations

Let us summarize the general problem by writing

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

$$= \frac{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)}\int_{\mathcal{J}_\sigma} dz e^{-S_R(z)}O(z)e^{i\omega(z)}}{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)}\int_{\mathcal{J}_\sigma} dz e^{-S_R(z)}e^{i\omega(z)}} \tag{1b}$$

$$= \frac{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)}Z_\sigma\langle O e^{i\omega}\rangle_\sigma}{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)}Z_\sigma\langle e^{i\omega}\rangle_\sigma} \tag{1c}$$

It is assumed that $S(x) = S_R(x) + iS_I(x)$. x stands collectively for the *real* degrees of freedom of our original problem and z for the degrees of freedom that are the *complexification* of the latter. (1) is the original formulation of the problem, while (1b) is the thimble decomposition as expected from Lefschetz/Picard theory. p_σ are critical points where $\partial_z S = 0$. The thimbles $\mathcal{J}_\sigma$ attached to each critical point are the union of all the steepest ascent paths (SA) which are the solutions of

$$\frac{d}{dt}z_i = \frac{\partial\bar{S}}{\partial\bar{z}_i}$$

stemming from a given critical point (initial condition). Both numerator and denominator (i.e., the partition function) of (1a) are rewritten as a linear combination of

[1] We stress that the nonperturbative effects we are talking about are not the ones in the coupling constant, i.e., the ones we are most often concerned with.

integrals computed on the thimbles attached to critical points; the sum is formally extended to all of them, but the coefficients n_σ can be zero for possibly many critical points. Actually $n_\sigma = 0$ for a critical point when the associated *unstable* thimble (the union of the steepest descent paths stemming from the critical point) does not intersect the original integration manifold. While the (constant) phase $e^{-iS_I(p_\sigma)}$ is factored in front of each integral, yet another phase enters the integrands. This is the so-called *residual phase* [14] ($e^{i\omega}$) which accounts for the orientation of the thimbles with respect to the embedding manifold.[2] In (1c) $\langle O\rangle$ is rewritten by defining

$$\langle X\rangle_\sigma \equiv \frac{\int_{\mathcal{J}_\sigma} dz e^{-S_R} X}{\int_{\mathcal{J}_\sigma} dz e^{-S_R}} \equiv \frac{\int_{\mathcal{J}_\sigma} dz e^{-S_R} X}{Z_\sigma}.$$

Stated in this way, the thimble decomposition is a linear combination of expectation values computed on single thimbles, with coefficients proportional to the Z_σ. As a result, multiple thimbles simulations amount to a given prescription for obtaining, in one way or another, (a) the contribution attached to each given thimble $\langle O\rangle_\sigma$ contributing to the result and (b) the relative weights in (1c). Actually, (b) turns out to be a harder task than (a). Despite the difficulties, there are cases in which we could attempt and succeed in multiple thimbles simulations. While these are admittedly preliminary steps in an interesting direction, they are worth mentioning, if only to appreciate the peculiar circumstances under which they worked out.

There are cases in which not only it turns out that non-null contributions come from a limited number of thimbles, but also a few of the latter are related to each other due to symmetries. One possible strategy in such cases is the one which was successful for QCD in $0+1$ dimensions [15]. In that case (due to a symmetry which is in place) the correct result was obtained by taking into account only two contributions according to

$$\langle O\rangle = \frac{\langle Oe^{i\omega}\rangle_{\sigma_1} + \alpha\langle Oe^{i\omega}\rangle_{\sigma_2}}{\langle e^{i\omega}\rangle_{\sigma_1} + \alpha\langle e^{i\omega}\rangle_{\sigma_2}}. \quad (2)$$

(2) is yet another rewriting of the thimble decomposition. All in all, all our ignorance of relative weights is in such a case coded in one single parameter, i.e., α. The value of the latter can be fixed assuming one known measurement as a normalization point. We can then predict the value of other observables. It is obvious that in such a way we give up the hope of a first principles derivation of relative weights. This is very much in the spirit of general frameworks for (nonperturbative) renormalization. Quite interestingly, this appears to be possible also in the framework of the Thirring model [16].

It should be stressed that relative weights are quite easy to obtain in a semiclassical approximation, which is also referred to as the *Gaussian approximation*. This suggests another strategy: one starts with the relative weights as computed in such an approximation and then compute corrections as the simulations proceeds. Once again, this is not expected to work efficiently in every case. A case of success was a minimal version of the so-called heavy dense approximation for QCD [17]. Yet another proposal for “reweighting Lefschetz Thimbles” was put forward in [18].

B. Deeper into the problem: Stokes phenomena

Multiple thimbles simulations are a hard problem and solutions so far have been admittedly a partial success. Our goal here is to find an alternative to them which goes beyond the naive single thimble prescription. In order to proceed, let us have a look at Stokes phenomena: these control the basic mechanism of the thimble decomposition. The main lesson to take home is that a thimble decomposition is never given once and forever. In the following we provide a simplified, informal discussion. The interested reader is strongly referred to [19] for a nice discussion of the subject in the context of the Thirring model.

Loosely speaking, we have a thimble decomposition when the union of a given number of thimbles is a convenient deformation of the original domain of integration, just like in standard applications of the Cauchy theorem. It is clear that the deformation provided by thimbles is not the only possible one (this is, e.g., the spirit of [9–12]). Strictly speaking, thimbles provide a basis of the relative homology group which the integration cycle we are interested in belongs to. It is a very convenient basis because the imaginary part of the action stays constant on thimbles. It is also a very convenient basis because the coefficients in the linear combination reconstructing a given path (the n_σ) are integers. Moreover (as already said) we have a criterion to establish which thimbles do not enter a decomposition: $n_\sigma = 0$ whenever the unstable thimble associated to a given critical point does not intersect the original domain of integration.[3] This has an important consequence, which is quite clear pictorially. As they are different solutions of the same (first order) differential equation subject to different initial conditions, *different thimbles can not cross each other*. Put in a simple-minded (but maybe effective) way, they act as *barriers to each other*: when the union of a given number of thimbles provide a *correct* decomposition of the original integration contour, other thimbles are simply kept out.

In order to gain some insight, in Fig. 1 we plot what the problem looks like in a simple toy model, i.e., the 0-dim ϕ^4

[2] Thimbles are manifolds of the same (real) dimension of the original manifold the theory was formulated on, but they are embedded in a manifold of twice that dimension.

[3] It can be shown that the n_σ have the meaning of intersection numbers.

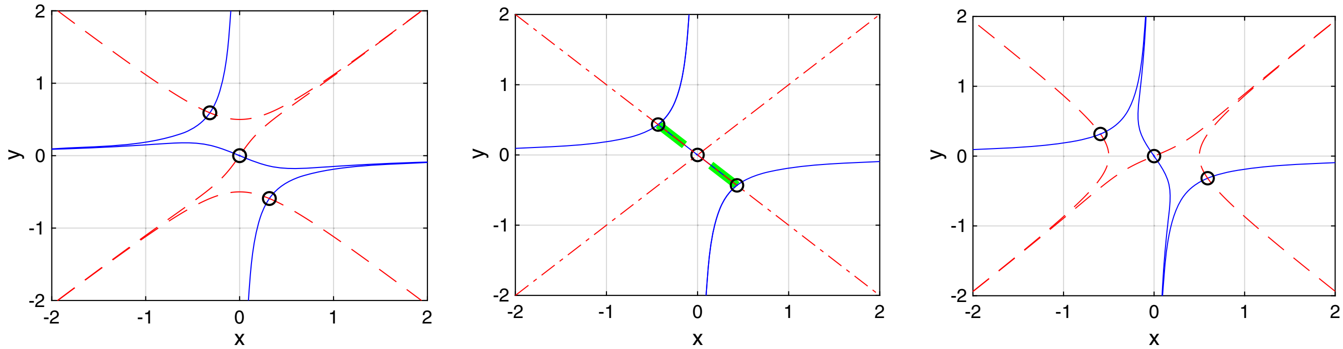

FIG. 1. Thimbles structure for a 0-dim ϕ^4 toy model: continuous (blue) lines are stable thimbles; dashed (red) lines are unstable thimbles. The three panels refer to different points in the parameter space of the theory. In the middle, an example of a Stokes phenomenon. For further details, see [20].

theory. The problem amounts to computing simple one-dimensional integrals (see [20]) defined via a "partition function"

$$Z = \int_{\mathbb{R}} \mathrm{d}\phi e^{-S(\phi)} \qquad S(\phi) = \frac{1}{2}\sigma\phi^2 + \frac{1}{4}\lambda\phi^4$$

where we take $\lambda \in \mathbb{R}^+$ and $\sigma \in \mathbb{C}$, which makes the "action" S complex. In the following we will keep fixed $\sigma_I > 0$,[4] so that the thimble decomposition is decided by the value of σ_R. We have three critical points, for which we adhere to the same notation of [20], labeling them as $\phi_0 = 0$ and $\phi_\pm = \pm\sqrt{-\frac{\sigma}{\lambda}}$. In the following discussion of Fig. 1 we encourage the reader to look at it having in mind the general picture and that is why we will keep the references to the actual model to a minimum.

In the left panel, we can see the correct thimble decomposition at a given point of the parameter space of the theory (namely $\sigma_R > 0$); stable thimbles are depicted as continuous (blue) lines: as it is manifest, one single thimble is enough to get a correct deformation of the original domain of integration (the latter being the real axis).[5] Probing different points in the parameter space, one finds that critical points and associated thimbles do move around in the manifold embedding the original one (i.e., the complexified manifold). As they smoothly move around, they are always subject to the constraint of not crossing each other. Thus the thimbles that contribute to the decomposition of the original domain of integration keep on keeping the others out.

There is only one way thimbles can cross each other: we need two thimbles to sit on top of each other. This means that two different critical points are connected by a SA/SD path, i.e., the stable thimble of one sits on top of the unstable thimble of the other. When this occurs we are in presence of a Stokes phenomenon: see the central panel (here $\sigma_R = 0$). As it is clear from the figure, *at a Stokes phenomenon the thimble decomposition fails*.

After a Stokes phenomenon has occurred, the *relative* arrangement of thimbles can change and a different thimble decomposition is in place (see right panel, where $\sigma_R < 0$).

The toy model we referred to is a trivial example: one can recognize the occurrence of a Stokes phenomenon by direct inspection. One could then think that tracking Stokes phenomena could be an almost impossible task in a typical case. This is not the case, since we have a clear signal that a Stokes phenomenon *can* occur: when two critical points are connected as described above, the imaginary part of the action takes the same value. To look for Stokes phenomena, we change the values of the parameters describing the theory; let us denote collectively these parameters by ξ. As the ξ vary, a critical point p_σ moves around and the value of the imaginary part of the action associated to it (and to the stable and unstable thimbles attached to it) describes a curve $S_I^{(\sigma)}(\xi)$. In order that a Stokes phenomenon occurs, two curves need to intersect, i.e., $S_I^{(\sigma)}(\xi_0) = S_I^{(\sigma')}(\xi_0)$. For a beautiful description of the procedure which we just sketched, we refer the interested reader to [19].

We end this sketchy discussion with a trivial, but in practice relevant observation. Reconstructing the correct thimble decomposition is not necessarily the end of story. It can well be that one (or more) thimble(s) entering the correct thimble decomposition is (are) so damped with respect to other contributions that its (their) contribution is *de facto* negligible. There are cases in which this is evident from the semi-classical approximation: this has to do with the $e^{-S_R(p_\sigma)}$ that can be factored in front of the integral associated to a critical point p_σ and which was one of the main rationales for the single thimble dominance hypothesis.

C. Discontinuities vs continuity

Stokes phenomena mark *discontinuities in the thimble decomposition* and one is left with the problem of fixing the

[4]This is the same choice of [20].

[5]Note how only one unstable thimble intersects the original domain of integration; unstable thimbles are depicted as dashed (red) lines.

values of the n_σ. With this respect, points where Stokes phenomena occur act as borders. In our simple example (Fig. 1): on one side of the border (left panel, $\sigma_R > 0$) one single thimble is relevant and we have a single non-trivial n_σ, i.e., $n_0 = 1$ and $n_\pm = 0$; on the other side (right panel, $\sigma_R < 0$) three thimbles are relevant and we need to fix the correct values of n_0 and $n_\pm$. A key point is that *discontinuity in the thimble decomposition does not imply a discontinuity in a physical observable* we can be interested in. This is quite clear in the 0-dim ϕ^4 toy model: Z is given in terms of a modified Bessel function $Z = \sqrt{\frac{\sigma}{2\lambda}} e^{\frac{\sigma^2}{8\lambda}} K_{-\frac{1}{4}}(\frac{\sigma^2}{8\lambda})$, which has no singularity whatsoever across the Stokes point. In other words, our original path integral (on the original domain of integration) is not aware of any thimble decomposition. It is the shape and relative orientation of the thimble attached to the critical point $\phi_0 = 0$ (the only relevant one for $\sigma_R > 0$) which abruptly changes across the Stokes point ($\sigma_R = 0$). As a consequence, as the thimble attached to $\phi_0 = 0$ changes, its contribution also abruptly changes: not surprisingly, it is actually discontinuous as we cross $\sigma_R = 0$. It is right the sum of the three contributions coming from all the thimbles which in turn ensures the continuity of the observable. Therefore, one way of fixing the n_σ values is to ensure continuity of an observable (or possibly more than one), which is exactly what was done in [20] to obtain $n_0 = -1$ and $n_\pm = +1$ in the region $\sigma_R < 0$. We will come back to the 0-dim ϕ^4 toy model in Appendix: it will have more to tell us with respect to the mechanism we are discussing. In the following we take a step forward in a more general framework.

The determination of the n_σ is not the only point we want to make, nor the most important one. The main message we want to deliver is that

(i) across points where Stokes phenomena occur, we generally have discontinuity of thimble decompositions and continuity of physical observables and *this continuity can build a bridge over different regions*;

(ii) the natural candidates to build the bridge are *Taylor expansions*.

Of course we cannot blindly assume that thimble discontinuity about a point will never be accompanied by a discontinuity in any physical observable for any model. Still, it is quite a general argument that the path integral itself is not aware of any thimble decomposition. Most of the observables we are concerned with enter the partition function in a smooth way (the typical example is QCD, where we have a negative exponential of the chemical potential μ coupled with the number density term). The most likely scenario of having a discontinuity in physical observables is at phase transitions, which in general do not have to do with Stokes phenomena.

III. TAYLOR EXPANSIONS ON THIMBLES

To circumvent multiple thimbles simulations by computing Taylor expansions we want to

(1) find at least two points where one single thimble contributes to the result, either strictly speaking or *de facto*, and compute Taylor expansions at those points;

(2) bridge the gap in between the regions where the previous computations are performed: in principle one could show that the Taylor expansions join smoothly; in practice, at a given order of the expansions, Padé approximants can do (much) better;

(3) show that the Padé approximants provide a fairly good control on the singularity structure in the complex plane; first of all, this can confirm the correctness of the procedure (remember the big question: do the radii of convergence enable the analytic continuation we have been trying?); also, this can possibly provide *in se* extra insight into the theory at hand.

The approach is based on Taylor expansions (which we eventually trade for Padé approximants) and those are expansions in $\frac{\mu}{X}$, where X is a dimensionful parameter, i.e., a mass m or the temperature T. It is therefore clear that we will be blind to any nonperturbative effect in $\frac{\mu}{X}$. We stress that the latter are not the nonperturbative effects we are most often concerned with (i.e., those in the coupling constant).

Strictly speaking we have no rigorous proof the method will work. In particular, in the case in which a Stokes point is accompanied by a discontinuity in the physical variable we are interested in, Taylor expansions would fail to bridge the regions to the left and right of the point in question.[6] Still, as we have already made the point, we expect that this is not the general case and to show that our program can indeed be accomplished we present two examples. Although simple, we will argue that they display general enough features to support the hope that the method has a potential for further applications.

1-dim Thirring model We can now fill the gap that was originally pointed out in [8,9]. The action of the 1-dim Thirring model is

$$
\begin{aligned}
S &= \beta \sum_n (1 - \cos(x_n)) - \log(\det D) \det D \\
&= \frac{1}{2^{L-1}} \left(\cosh\left(L\hat{\mu} + i \sum_n x_n \right) + \cosh(L \sinh^{-1}(\hat{m})) \right)
\end{aligned}
$$

The chemical potential $\hat{\mu}$ and the mass $\hat{m}$ are given in lattice units. We work at fixed value of mass m (and of β) and there is a single parameter controlling the sign problem, namely

[6] Notice that in such a case one would *a posteriori* recognize the inconsistency; in other words, inconsistency would be manifest from the Taylor expansions themselves. One would rather scan the parameter space and look for other regions to start the procedure and if that can be accomplished one would eventually get a confirmation of the discontinuity from the singularity structure of the result (see later).

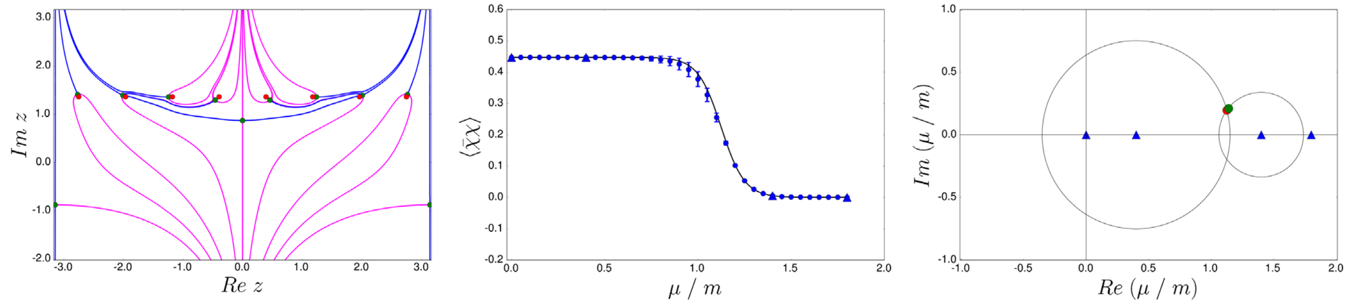

FIG. 2. (Left panel) The flow lines highlighting the thimbles structure of the 1-dim Thirring model at $\frac{\mu}{m} = 1.4$: stable thimbles are depicted in blue, unstable thimbles in magenta. The dominant thimble is associated to the critical point sitting at $\Re(z) = 0$. The critical point σ_1 is the closest to the latter to the right (there is a mirror image to the left as well): notice that the unstable thimble associated to it does not intersect the original domain of integration (which is on the real axis). (Center panel) The chiral condensate as obtained from the analytic solution (continuous black line) and from our Padé approximant (we plot points instead of a continuum line so that the size of errors are easier to spot.). The points providing input to the evaluation of Padé are marked as triangles. (Right panel) Singularity of the solution in the complex plane: red point computed from the analytic solution, green point is the only pole of our Padé approximant. We plot the radii of convergence which are relevant for the expansions at hand: our analytic continuation indeed stands on firm ground.

μ. We can obtain a dimensionless quantity by taking the ratio $\frac{\mu}{m} = \frac{\hat{\mu}}{\hat{m}}$. Since the analytic result is known, the single thimble approximation was shown not to account for the correct result on the entire $\frac{\mu}{m}$ axis. In our new approach the problem is solved and in Fig. 2 we display the essential features of our results: as an example, we show results for the chiral condensate $\langle\bar{\chi}\chi\rangle$ (parameters are $L = 8$, $\beta = 1$, $m = 2$). We can argue that all the requirements of the program that we sketched above can be met. There is a preliminary point we have to make. For real β a Stokes phenomenon is potentially present up to a given value of $\frac{\mu}{m}$: this involves the dominant thimble p_{σ_0} and another critical point. We denote the latter $p_{\sigma_{\bar{0}}}$, following the notation of [19]. The problem can be easily solved by adding a small imaginary part to β: in this way a Stokes phenomenon does not take place, a thimble decomposition is in place and while $p_{\sigma_{\bar{0}}}$ could in principle give a contribution to the result, this is *de facto* negligible due to the huge difference $S_R(p_{\sigma_{\bar{0}}}) \gg S_R(p_{\sigma_0})$. This solves the problem and any further reference to this point will be omitted in the following.

(1) A first value of $\frac{\mu}{m}$ for which only the dominant thimble p_{σ_0} accounts for the correct result can be found in a very fundamental, yet simple way. The range of values S_I can take on the real axis depends on the values of $\hat{\mu}$ and $\hat{m}$ and, below a given value of $\frac{\mu}{m}$, this range is limited. By explicit computation of the $S_I^{(\sigma)}(\frac{\mu}{m})$ we can show that no unstable thimble associated to a critical point p_σ other that the dominant one can intersect the original domain of integration below a given value $\frac{\mu_0}{m}$.[7] Thus for $\frac{\mu}{m} < \frac{\mu_0}{m}$ we can easily select a first point at which the dominant thimble provides the only contribution to the result. We picked $\frac{\mu}{m} = 0.4$ and computed the Taylor expansion up to the second derivative.

We now need to find a second value of $\frac{\mu}{m}$ at which the dominant thimble accounts for the complete result and compute the Taylor expansion on it. In principle we could study the crossing mechanism between the different curves $S_I^{(\sigma)}(\frac{\mu}{m})$ (see subsection II B). In practice there is a much simpler way to proceed. First of all, we point out that the asymptotic value of $\langle\bar{\chi}\chi\rangle$ is known: for large enough values of μ the chiral condensate is zero. We notice that for $\frac{\mu}{m} = 1.4$ the value of $\langle\bar{\chi}\chi\rangle$ computed on the dominant thimble is very close to zero. By inspecting the values of $S_R(p_\sigma)$ for thimbles other than the fundamental one, we find that, for $\frac{\mu}{m} = 1.4$, $S_R(p_\sigma) \gg S_R(p_{\sigma_0})$ for all the critical points but three, that we denote σ_1, $\sigma_{\bar{1}}$, $\sigma_{\bar{2}}$.[8] Two of them ($\sigma_{\bar{1}}$ and $\sigma_{\bar{2}}$) have values of the real action which are lower than $S_{\min}$, which is the minimum value S_R takes on the original domain of integration: because of this, the unstable thimbles associated to them can't intersect the original domain of integration. As for σ_1, in this simple model it does not take that much to show that the unstable thimble attached to it does not intersect the original domain of integration (see the left panel of Fig. 2). We conclude that the dominant thimble σ_0 can account for the complete result at this value of $\frac{\mu}{m}$. We have thus selected the second point we were looking for; at this point the series has been computed up to the fifth derivative. One might object that we made use of the explicit query for intersections between the original domain of integration and a given unstable thimble, which thing is

[7]The value of $\hat{m}$ is held fixed.

[8]We once again adhere to the notation of [19].

quite hard to do in a less simple theory. In the second example we will proceed in a different way: in principle one could follow the same approach also in this case.[9]

(2) In order to bridge the gap in between the two values of $\frac{\mu}{m}$ at which Taylor expansions on the dominant thimble have been computed, one could try to show that the two Taylor expansions do smoothly join. This would actually ask for computing quite a large number of derivatives at the lower value of the chemical potential (as one can see, the curve is quite flat nearby). As we have already pointed out, a Padé approximant can do better. In the middle panel of Fig. 2 we plot the interpolation we got from a Padé approximant on top of the analytic result. In order to appreciate how this solves the problem of the inconsistency of single thimble computations we refer the reader to the figures in [8].

(3) From the middle panel of Fig. 2 one can see that actually four points were taken into account in our Padé procedure (see the four triangles in the plot). On top of the two points we discussed previously, two other points enter and act as extra constraints: the values of the condensate at $\frac{\mu}{m} = 0$ and for $\frac{\mu}{m}$ high enough are known and thus they can be taken into account.[10] The right panel in the figure provides us with a confirmation that the overall procedure is under good control. Since the analytic solution is known, we know that the latter displays a singularity in the complex plane. As one can see, our Padé approximant study captures it quite well: see the green and red points practically on top of each other. The detection of the (expected) singularity is indeed very stable with respect to variations in the number of orders that we take into account. One can thus inspect the convergence radii of our Taylor expansions and it is indeed confirmed that what we got is a legitimate analytic continuation. This is not the only relevant point. The knowledge of the analytic structure of the solution provides *in se* extra insight into the theory at hand. Needless to say, this is quite often one of the main piece of information we will be interested in.

The present computation is essentially only a proof of concept; the extraction of the continuum limit on a line of constant physics has been obtained as well and will be reported elsewhere [21].

(The simplest version of) heavy dense QCD In subsection II A we mentioned the multiple thimbles simulation of heavy dense QCD. We now go back to that theory via the application of the Taylor expansion method we suggest in this paper; the interested reader can compare results with what we discussed in [17]. We are dealing with the effective formulation that can be obtained from QCD by a combined strong-coupling and hopping parameter expansion. One ends up with a 3d effective theory, whose only degrees of freedom are Polyakov loops [22–24]. We tackle the simplest version of the theory, described by the action[11]

$$
\begin{aligned}
S &= S_G + S_F \\
&= -\lambda \sum_{\langle x,y\rangle} (\mathrm{Tr} W_x \mathrm{Tr} W_y^\dagger + \mathrm{Tr} W_x^\dagger \mathrm{Tr} W_y) \\
&\quad - 2\sum_x \ln\left(1 + h_1 \mathrm{Tr} W_x + h_1^2 \mathrm{Tr} W_x^\dagger + h_1^3\right).
\end{aligned}
$$

Here $\lambda = u^{N_t} e^{N_t \cdot (4u^4 + 12u^5 - 14u^6 - 36u^7 + \ldots)}$, $h_1 = (2ke^{\hat{\mu}})^{N_t}$, $u \approx \frac{\beta}{18}$, k is the hopping parameter and $W_x = \prod_{t=1}^{N_t} U_0(x,t)$ is the Polyakov loop. The theory can be refined by adding to the fermionic part a sum extended over nearest neighbors, which couples degrees of freedom sitting at different lattice points. The truncation at hand amounts to neglecting $O(k^2)$ terms in the hopping parameter expansion. Moreover we are concerned with the cold regime, where $N_t \gg 1$, $\lambda \approx 0$; in these conditions the gauge term of the action is negligible (and is indeed neglected). With no interaction among different degrees of freedom W_x, one can write the sum over the degrees of freedom in the action simply as $\sum_{x=1}^{L} \ln(1 + \ldots)$; we studied the model with $L = 8$.[12] Despite its simplicity, the theory displays a sign problem. Also, it displays features that are interesting in our approach: we will have the chance to do something different from what we did in the context of the Thirring model. We stress that also in this case there is a single parameter controlling the sign problem. We work at fixed values of T and m, so that only μ varies and it enters the game through the combination which defines $h_1 = (2ke^{\hat{\mu}})^{N_t} = e^{-\frac{(m-\mu)}{T}}$. Notice that (being m and T fixed) this parameter can be $h_1 < 1$ or $h_1 > 1$ depending on μ being $\mu < m$ or $\mu > m$. Figure 3 displays our results for the quark number density (normalized to 1). We plot results versus the ratio $\frac{\mu}{m}$, the value of m being fixed by

[9] We will see that we need to have a known value (which one can trust as correct) and reconstruct the latter by our Taylor expansion. In this case the asymptotic value at large enough values of $\frac{\mu}{m}$ is the natural candidate (possibly to be reached in a two/three steps procedure).

[10] Notice that at $\frac{\mu}{m} = 0$ there is no sign problem and thus one could even quite easily compute a high order Taylor expansion.

[11] Also in this case, we use the hat notation for lattice (dimensionless) quantities.

[12] Notice that in the limit in which we work, with interaction among degrees of freedom missing, dimensionality is a somehow odd concept: $L = 8$ can be interpreted as a tiny 2^3 3d system (this is the canonical HDQCD, coming from actual QCD), but this is not the only possible interpretation. One could think of a $L = 8$ 1d system (in which case one would have started from $1 + 1$ QCD).

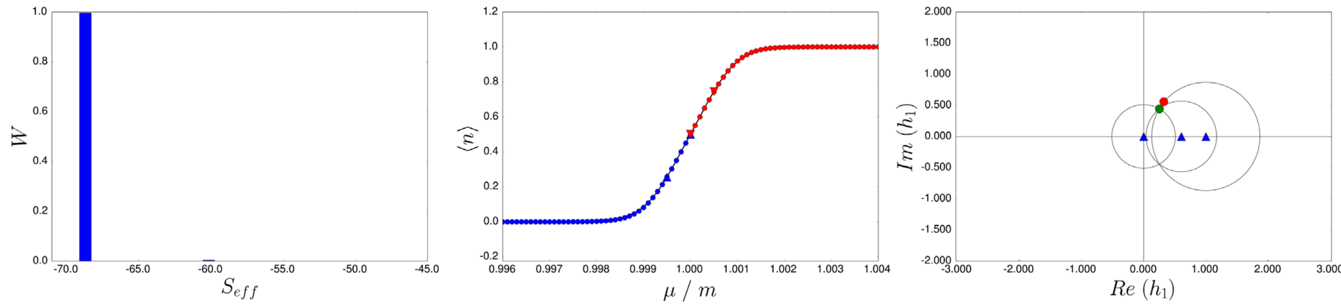

FIG. 3. Left panel: semiclassical evaluation of the relative weight of different thimbles at $\frac{\mu}{m} = 0.9995$: weights are plotted vs the value of the (real) action. The dominant thimble has *de facto* weight 1 (it is very hard to detect the weight of the thimble with action near the value −60). Center panel: the known analytic value for the quark number density is correctly reproduced over the entire relevant range of $\frac{\mu}{m}$ via the Padé approximant; the points entering the computation are marked as triangles (see main text for details). Right panel: the known singularity of the solution as analytically known (red point) and as reconstructed by the Padé approximant (green point).

$k = 0.0000887$. The value of T is fixed by $N_t = 116$. Also in this case, we can argue that all the requirements we formulated for the application of our new program can be met.

(1) To find two points at which a Taylor expansion can be computed on the dominant thimble, we revert this time to a different strategy. We notice that at $\frac{\mu}{m} = 1$ (the point that sits in the middle of the relevant region) there is no sign problem at all; thus computing a Taylor expansion poses no problem. We pick two points, to the right ($\mu > m$) and to the left ($\mu < m$) at which we will compute Taylor expansions on the dominant thimble. We argue that computations on the dominant thimble at those points provide us with the complete result by checking that the results obtained by Taylor expansions smoothly (we would say perfectly actually) join the result we get at $\frac{\mu}{m} = 1$ (of whose correctness we are certain). Remember once again that we are concerned with analytic contributions and we will be blind to any nonperturbative effect in the expansion parameter. As an extra confirmation, in the left panel of Fig. 3 we plot the relative weights of different thimbles as computed from the semiclassical (*Gaussian*) approximation at those values of $\frac{\mu}{m}$ (the dominant thimble virtually saturates the normalization; the weight of the least depressed thimble—other than the dominant one—is hardly visible in the figure). In the center panel of Fig. 3 one can inspect the location of the two points we selected (once again, they are marked as triangles).

(2) While we plot results as a function of $\frac{\mu}{m}$, our expansions are not computed in powers of the latter variable. The natural parameter for the expansion is $h_1 = e^{-\frac{(\mu-m)}{T}}$: we actually expand in h_1 (for $\mu < m$) and in h_1^{-1} (for $\mu > m$). More precisely, we expand up to the second derivative with respect to h_1 at $\frac{\mu}{m} = 0.9995$ and we supplement as extra constraints the values of the observable and its first derivative at $\frac{\mu}{m} = 0$ and $\frac{\mu}{m} = 1$; we expand up to the second derivative with respect to h_1^{-1} at $\frac{\mu}{m} = 1.0005$ and we supplement as extra constraints the values of the observable and its first derivative at $\frac{\mu}{m} = 1$ and at a value of $\frac{\mu}{m}$ large enough (which is fixed by saturation). Also in this case, we plot in Fig. 3 (center panel) the result obtained out of a Padé approximant.

(3) Knowing the analytic solution, also in this case we know of a singularity in the complex plane. In the right panel of Fig. 3 we display how this is fairly well reconstructed. The conclusion is once again that the procedure we followed is *a posteriori* proved correct: the convergence radii of the expansions on which we build our construction indeed show that the latter is a legitimate analytic continuation.

In both the cases we presented we have looked for points where the dominant thimble accounts for the complete result and computed the Taylor expansion on the dominant thimble itself. We notice that this is not the only possible case. In Appendix we come back to the 0-dim ϕ^4 toy model and show how at the expansion points computations do not need to be performed on the same thimble nor the latter necessarily needs to be the dominant one. Having said this, we also notice that computations on the dominant thimble most often prove to be easier than on other ones.[13]

IV. CONCLUSIONS AND OUTLOOK

We discussed a new strategy to circumvent multiple thimbles simulations in the Lefschetz thimble regularization of a lattice field theory. The idea is to explore the space of the parameters describing the theory and find (at least) two points at which the dominant thimble accounts for the full result: as we saw, there could be different strategies to attain this. We do expect that in between these two points

[13] In [21] we will show that, while we are able to compute on a thimble which is not the dominant one, this is usually (much) harder than computing on the dominant thimble.

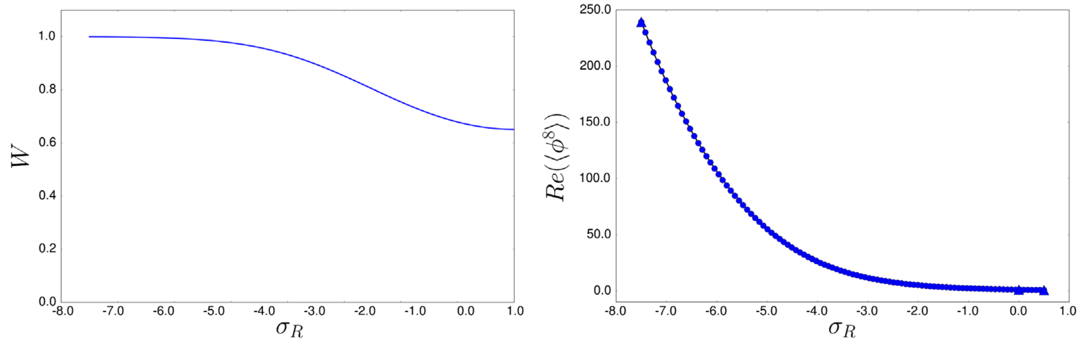

FIG. 4. Left panel: we plot for the 0-dim ϕ^4 toy model the semiclassical evaluation of the relative weight of thimbles attached to $\phi_\pm$ critical points. Weight is plotted vs σ_R. The weight of ϕ_0 is $1 - W$. Right to the left of the Stokes point ($\sigma_R = 0$) the three thimbles provide comparable contributions, while as σ_R gets more and more negative the weight of $\phi_\pm$ is more and more enhanced. Right panel: the value of the moment $\langle \phi^8 \rangle$ is correctly reproduced over the entire negative semiaxis $\sigma_R < 0$ via the Padé approximant; the points entering the computation are marked as triangles, where at the point to the left the expansion is computed on the thimble attached to ϕ_+ (or ϕ_-; see main text for details).

Stokes phenomena can occur, so that a non trivial thimble decomposition can be in place. While Stokes phenomena introduce discontinuities in the thimble decomposition of the integrals we are interested in, they do not determine in general discontinuities in physical results. Taylor expansions can thus bridge the different (disjoint) regions where we can compute on the dominant thimble only. We are thus aiming at computing the analytic dependence of our result on the parameter expansion, being blind to any possible nonperturbative contribution.[14] Not surprisingly, Padé approximants turn out to be the most effective tool to implement our program. In particular, they give us the chance to inspect the analytic structure of our results in the complex plane and thus the convergence radius of our expansions, so that our construction can be *a posteriori* proved to be a legitimate analytic continuation. In a quite natural way, computing multiple Taylor expansions in the complex plane in order to get information out of Padé approximants can be a legitimate approach beyond thimbles, no matter what is the strategy used to obtain the different expansions. In the end, singularities in the complex plane are quite often one of the most valuable pieces of information we look for.

ACKNOWLEDGMENTS

This work has received funding from the European Unions Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 813942 (EuroPLEx). We also acknowledge support from I. N. F. N. under the research project *i.s. QCDLAT*. This research benefits from the HPC (High Performance Computing) facility of the University of Parma, Italy.

[14]We stress once again that these are not the *standard* nonperturbative effects in the coupling.

APPENDIX: AGAIN ON THE 0-DIM ϕ^4 TOY MODEL

As already pointed out, in our computations of the 0-dim ϕ^4 toy model we take the coefficient of the quartic contribution $\lambda > 0$, which thing ensures convergence of the integral. We also keep fixed the imaginary part of the coefficient of the quadratic contribution at a value $\sigma_I > 0$. Because of this, the thimble decomposition depends on the value of σ_R only and the latter is the parameter in which we have to expand in order to implement our program.

By simple inspection of Fig. 1 it is pretty obvious that in the region $\sigma_R < 0$ we cannot find a point where the dominant thimble accounts for the entire result. On the other side, in Fig. 4 we show that there is a region in which the result is essentially coming from the two thimbles attached to $\phi_\pm$ only (ϕ_+ and ϕ_- are related by a symmetry, so that one single computation is needed).

In the left panel of Fig. 4 we show the semiclassical computation of the relative weight of the thimbles attached to $\phi_\pm$. All in all, the overall picture is the following: as we cross the Stokes point $\sigma_R = 0$ coming from the right (i.e., from the region $\sigma_R > 0$, where the dominant thimble is enough to compute the correct result) we go through a region where all the three thimble are needed (the correct combination being computed according to the continuity argument discussed in Sec. II B), but then the more we proceed to the left (i.e., the more negative σ_R) the more the weight is concentrated in the contribution attached to $\phi_\pm$. This suggests to implement our procedure computing the Taylor expansions at points like those depicted in the right panel of Fig. 4, where at the point to the left the expansion is computed on the thimble attached to ϕ_+ (or to ϕ_-; because of symmetry this is equivalent). Once again the Padè approximant successfully reproduces the correct result. This is an example in which our procedure is implemented by computing Taylor expansions on different thimbles in different regions. While this is conceptually important, we notice that quite often computing on a thimble different from the dominant one is numerically more challenging (we will provide evidences of this in [21]). With this respect, the fact that the results presented in Sec. III could be obtained computing on the dominant thimble only can be regarded as a nice feature (even if this is not the only possible scenario in which we can think of an application of our method).

[1] P. de Forcrand, Simulating QCD at finite density, Proc. Sci. LAT2009 (**2009**) 010.

[2] O. Philipsen, Constraining the QCD phase diagram at finite temperature and density, Proc. Sci. LATTICE2019 (**2019**) 273.

[3] E. Witten, Analytic continuation of Chern-Simons theory, AMS/IP Stud. Adv. Math. **50**, 347 (2011).

[4] E. Witten, A new look at the path integral of quantum mechanics, arXiv:1009.6032.

[5] M. Cristoforetti, F. Di Renzo, and L. Scorzato (AuroraScience Collaboration), New approach to the sign problem in quantum field theories: High density QCD on a Lefschetz thimble, Phys. Rev. D **86**, 074506 (2012).

[6] 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, J. High Energy Phys. 10 (2013) 147.

[7] M. Cristoforetti, F. Di Renzo, A. Mukherjee, and L. Scorzato, Monte Carlo simulations on the Lefschetz thimble: Taming the sign problem, Phys. Rev. D **88**, 051501 (2013).

[8] H. Fujii, S. Kamata, and Y. Kikukawa, Monte Carlo study of Lefschetz thimble structure in one-dimensional Thirring model at finite density, J. High Energy Phys. 12 (2015) 125; 09 (2016) 172(E).

[9] A. Alexandru, G. Basar, P. F. Bedaque, G. W. Ridgway, and N. C. Warrington, Sign problem and Monte Carlo calculations beyond Lefschetz thimbles, J. High Energy Phys. 05 (2016) 053.

[10] A. Alexandru, P. F. Bedaque, H. Lamm, and S. Lawrence, Deep learning beyond Lefschetz thimbles, Phys. Rev. D **96**, 094505 (2017).

[11] A. Alexandru, P. F. Bedaque, H. Lamm, and S. Lawrence, Finite-density Monte Carlo calculations on sign-optimized manifolds, Phys. Rev. D **97**, 094510 (2018).

[12] Y. Mori, K. Kashiwa, and A. Ohnishi, Toward solving the sign problem with path optimization method, Phys. Rev. D **96**, 111501 (2017).

[13] A. Alexandru, G. Basar, P. F. Bedaque, and N. C. Warrington, Complex paths around the sign problem, arXiv:2007.05436.

[14] M. Cristoforetti, F. Di Renzo, G. Eruzzi, A. Mukherjee, C. Schmidt, L. Scorzato, and C. Torrero, An efficient method to compute the residual phase on a Lefschetz thimble, Phys. Rev. D **89**, 114505 (2014).

[15] F. Di Renzo and G. Eruzzi, One-dimensional QCD in thimble regularization, Phys. Rev. D **97**, 014503 (2018).

[16] K. Zambello and F. Di Renzo, On the Lefschetz thimbles structure of the Thirring model, Proc. Sci. LATTICE2019 (**2019**) 211.

[17] K. Zambello and F. Di Renzo, Towards Lefschetz thimbles regularization of heavy-dense QCD, Proc. Sci. LATTICE2018 (**2018**) 148.

[18] 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**, 044 (2018).

[19] H. Fujii, S. Kamata, and Y. Kikukawa, Lefschetz thimble structure in one-dimensional lattice Thirring model at finite density, J. High Energy Phys. 11 (2015) 078; Erratum, J. High Energy Phys. 02 (2016) 036.

[20] F. Di Renzo and G. Eruzzi, Thimble regularization at work: From toy models to chiral random matrix theories, Phys. Rev. D **92**, 085030 (2015).

[21] F. Di Renzo and K. Zambello, Settling an old story: Solution of the Thirring model in thimble regularization (to be published).

[22] M. Fromm, J. Langelage, S. Lottini, and O. Philipsen, The QCD deconfinement transition for heavy quarks and all baryon chemical potentials, J. High Energy Phys. 01 (2012) 042.

[23] 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**, 122001 (2013).

[24] J. Langelage, M. Neuman, and O. Philipsen, Heavy dense QCD and nuclear matter from an effective lattice theory, J. High Energy Phys. 09 (2014) 131.