TESTING IMAGINARY VS. REAL CHEMICAL POTENTIAL IN FINITE-TEMPERATURE QCD

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One suggestion for determining the properties of QCD at finite temperatures and densities is to carry out lattice simulations with an imaginary chemical potential whereby no sign problem arises, and to convert the results to real physical observables only afterwards. We test the practical feasibility of such an approach for a particular class of physical observables, spatial correlation lengths in the quark-gluon plasma phase. Simulations with imaginary chemical potential followed by analytic continuation are compared with simulations with real chemical potential, which are possible by using a dimensionally reduced effective action for hot QCD. We find that for imaginary chemical potential the system undergoes a phase transition at $|\mu/T| \approx \pi/3$, and thus observables are analytic only in a limited range. However, utilising this range, relevant information can be obtained for the real chemical potential case.

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1. Introduction

Given the applications to cosmology and heavy ion collision experiments, it is important to determine the properties of QCD at finite temperatures and baryon densities. For instance, one would like to know the locations of any phase transitions, and the properties of the quark-gluon plasma phase such as its free energy density, or pressure, as well as the spatial and temporal correlation lengths felt by various types of excitations in the system.

Because the theory is strongly coupled, the only practical first principles method available for addressing these questions is lattice simulations. While there has been steady improvement in the accuracy of results at vanishing baryon density [1], the case of a non-vanishing density is still largely open, despite much work [1]–[10]. Indeed, introducing a non-vanishing density, or chemical potential, is difficult because it leads to a measure which is not positive definite (this is the so called sign problem), whereby standard Monte Carlo techniques fail.

In this paper we focus on one of the suggestions for how a finite density system could eventually be addressed with practical lattice simulations. The idea is to first inspect an imaginary chemical potential, whereby the sign problem temporarily disappears, and then relate this to the case of a real chemical potential. Let us denote by μ the chemical potential for quark number Q, and by μ_B the chemical potential for baryon number $B = Q/3$: then $\mu = \mu_B/3$. By $\mu_R, \mu_I \in \mathbb{R}$ we denote the real and imaginary parts of μ:

$$\mu = \mu_R + i\mu_I. \tag{1.1}$$

It is easy to see, by going to momentum space, that physical observables are periodic in μ_I with the period $2\pi T$.

There are then two types of suggestions for how an imaginary $\mu = i\mu_I$ could be utilised to obtain information on a system with a real chemical potential, $\mu = \mu_R$. The first idea is related directly to the equation of state, and employs the canonical partition function at fixed quark number ([2, 3] and references therein):

$$Z(T, Q) = \frac{1}{2\pi T} \int_{-\pi T}^{+\pi T} d\mu_I \, Z(T, \mu = i\mu_I) \, e^{-i\mu_I Q/T}, \tag{1.2}$$

where the grand canonical partition function,

$$Z(T, \mu) = \mathrm{Tr}\, e^{-(\hat{H} - \mu\hat{Q})/T}, \tag{1.3}$$

has been evaluated with an imaginary chemical potential. Here $\hat{H}$ and $\hat{Q}$ denote the Hamiltonian and quark number operators, respectively, while Q is a number. With an

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imaginary chemical potential, $Z(T, \mu = i\mu_I)$ or rather the ratio $Z(T, \mu = i\mu_I)/Z(T, 0)$, can be determined using standard lattice techniques [6]. What remains is to perform the integral in Eq. (1.2). Of course, this gets more and more difficult in the thermodynamic limit $Q \to \infty$, because oscillations reappear in the Fourier transform. In addition, a Legendre transform would be needed to go from $Z(T, Q)$ to a system in an ensemble with a real chemical potential, $Z(T, \mu = \mu_R)$.

The second idea ([9] and references therein) is that, away from possible phase transition lines, the partition function and expectation values for various observables should be analytic in their arguments, in particular in μ/T. Thus, we may attempt a general power series ansatz for the functional behaviour in μ/T, determine a finite number of coefficients with an imaginary chemical potential, and finally analytically continue to real values.

In this letter we study the latter suggestion within the framework of a dimensionally reduced effective theory. As we shall review in the next section, at temperatures sufficiently above the phase transition, the thermodynamics of QCD can be represented, with good practical accuracy, by a simple three-dimensional (3d) purely bosonic theory. This can also be done with a chemical potential, both real and imaginary [11]. We then use this theory to measure the longest static correlation lengths in the system for both cases. We find that, for small $|\mu/T|$, the observables are well described by a truncated power series with coefficients determined by fits. We then inspect how well the analytically continued series describes the real data. In principle the free energy density could be addressed with similar effective theory methods [12], but this requires a number of high-order perturbative computations which are not available at the moment for $\mu \neq 0$.

2. Effective theory

2.1. Action

The effective theory emerging from hot QCD by dimensional reduction [13]–[19],[11], is the SU(3)+adjoint Higgs model with the action

$$S = \int d^3x \left\{ \frac{1}{2} \mathrm{Tr}\, F_{ij}^2 + \mathrm{Tr}\, [D_i, A_0]^2 + m_3^2 \mathrm{Tr}\, A_0^2 + i\gamma_3 \mathrm{Tr}\, A_0^3 + \lambda_3 (\mathrm{Tr}\, A_0^2)^2 \right\}, \qquad (2.1)$$

where $F_{ij} = \partial_i A_j - \partial_j A_i + ig_3[A_i, A_j]$, $D_i = \partial_i + ig_3 A_i$, F_{ij}, A_i, and A_0 are all traceless 3×3 Hermitian matrices ($A_0 = A_0^a T_a$, etc), and g_3^2 and λ_3 are the gauge and scalar coupling constants with mass dimension one, respectively. The physical properties of

the effective theory are determined by the three dimensionless ratios

$$x = \frac{\lambda_3}{g_3^2}, \quad y = \frac{m_3^2(\bar{\mu}_3 = g_3^2)}{g_3^4}, \quad z = \frac{\gamma_3}{g_3^3}, \tag{2.2}$$

where $\bar{\mu}_3$ is the $\overline{\text{MS}}$ dimensional regularization scale in 3d. These ratios are via dimensional reduction functions of the temperature $T/\Lambda_{\overline{\text{MS}}}$ and the chemical potential $\mu/\Lambda_{\overline{\text{MS}}}$, as well as of the number N_f of massless quark flavours. (The inclusion of quark masses is also possible in principle.) For the case $\mu = 0$, we refer to [19].

Compared with the case $\mu = 0$, the dominant changes in the action due to a small chemical potential are [11]

$$z: 0 \to \frac{\mu}{T} \frac{N_f}{3\pi^2}; \quad y: y \to y\left(1 + \left(\frac{\mu}{\pi T}\right)^2 \frac{3N_f}{2N_c + N_f}\right), \tag{2.3}$$

where $N_c = 3$. Thus, one new operator is generated in the effective action, and one of the parameters which already existed, gets modified.

For real chemical potential, $\mu = \mu_R$, the effective action is thus complex, whereas for imaginary chemical potential, $\mu = i\mu_I$, it is real.

2.2. Ranges of validity

There are several requirements for the effective description in Eq. (2.1) to be reliable. They are all related to a sufficiently "weak coupling", or effective expansion parameter, for a given $T/\Lambda_{\overline{\text{MS}}}, \mu/\Lambda_{\overline{\text{MS}}}, N_f$. Let us briefly reiterate them here.

First, the perturbative expansions for the effective parameters in Eq. (2.2) have to be well convergent. Inspecting the actual series up to next-to-leading order, it appears that this requirement is surprisingly well met even at temperatures not much above the critical one [19].

Second, the higher dimensional operators arising in the reduction step which are not included in the effective action in Eq. (2.1), should only give small corrections. This condition is met if the dynamical mass scales described by the effective theory are smaller than the ones $\sim 2\pi T$ that have been integrated out. In pure Yang-Mills theory, there is evidence that this can be sufficiently satisfied at temperatures as low as $T \sim 2\Lambda_{\overline{\text{MS}}}$ [14],[19]–[23],[11]. However, when fermions are included and a *real* chemical potential is switched on, some of the mass scales increase (see below), and the effective description will become less accurate.

Third, the effective 3d theory represents the 4d theory reliably only when it lies in its symmetric phase [19, 24]. Indeed, for $N_f = 0$ QCD has a so called Z(N)-symmetry [25, 26], and this symmetry is not fully reproduced by the effective theory.

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The 4d Z(N) symmetry is however spontaneously broken for $N_f = 0$ in the deconfined phase, and even explicitly broken for $N_f > 0$. Consequently the requirement to be in the symmetric phase is easier to control for $N_f > 0$. Furthermore, the situation gets even better for real $\mu \neq 0$. In the effective theory this can be seen, for instance, from the fact that the mass parameter y in Eq. (2.3) grows, which makes it more difficult to depart from $A_0 \sim 0$. Another stabilising factor is that the unphysical minima correspond to non-zero expectation values for $\mathrm{Tr}\, A_0^3$ [24], and the imaginary term $\sim i\mathrm{Tr}\, A_0^3$ in the action in Eq. (2.1) disfavours such minima according to the standard argument [27].

On the other hand, an *imaginary* chemical potential $\mu = i\mu_I$, favours Z(N) symmetry breaking. Utilising the perturbative effective potential [28], we find that the lowest broken minimum becomes degenerate with the symmetric one already at $\mu_I/T = \pi/3$, and increasing μ_I further it eventually becomes lower than our minimum. Thus there is a (first order) "phase transition". In the effective theory, this phase transition is triggered by the decrease of the mass parameter y in Eq. (2.3). Moreover, in this case the term $\sim \mathrm{Tr}\, A_0^3$ in the action in Eq. (2.1) favours the effective theory remnant of one of the broken Z(N) minima.

This phase transition limits the applicability of the effective theory with imaginary chemical potential, since only the symmetric phase is a faithful representation of the 4d theory [19, 24]. (For one suggestion on how perhaps to circumvent this problem at least for $N_f = 0$, which we shall however not dwell on here, see [29].) In a way, this problem is related to the fact that as one approaches $\mu_I/T = \pi$, fermions start to obey Bose-Einstein statistics and become "light" infrared sensitive degrees of freedom (see also [28]), whereby it is no longer legitimate to integrate them out.

In summary, the effective theory roughly loses its accuracy with a real chemical potential once even the longest correlation length is shorter than $\sim 1/(2\pi T)$, and with an imaginary chemical potential once $|\mu/T|$ exceeds unity. Fortunately, this range of validity contains the parameters that are phenomenologically most relevant. Indeed, heavy ion collision experiments at and above AGS and SPS energies can be estimated to correspond to $\mu_B/T \lesssim 4.0$ [30], or a quark chemical potential $\mu/T \lesssim 1.3$.

2.3. Observables and their parametric behaviour

As we have mentioned, the physical observables which we shall study are spatial correlation lengths: we consider operators living in the (x_1, x_2)-plane, and measure the correlation lengths in the x_3-direction.

In the presence of $\mu \neq 0$, there are only two different quantum number channels to be considered, distinguished by the two-dimensional parity P in the transverse plane.

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The lowest dimensional gauge invariant operators in the scalar ($J = 0$) channels are:

$$J^P = 0^+ : \quad \text{Tr}\, A_0^2, \text{Tr}\, F_{12}^2, \text{Tr}\, A_0^3, \text{Tr}\, A_0 F_{12}^2, ...$$
$$J^P = 0^- : \quad \text{Tr}\, F_{12}^3, \text{Tr}\, A_0^2 F_{12}, \text{Tr}\, A_0 F_{12}, ... \quad (2.4)$$

The corresponding 4d operators can be found in [31]. We shall measure whole cross correlation matrices between all (smeared) operators in these channels, but mostly focus on their lowest eigenstates, corresponding to the longest correlation lengths in the 4d finite temperature system. We denote the "energies" of these eigenstates, viz. inverses of correlation lengths, by m. We also examine the overlap of operators of different field contents onto the eigenstates.

Since a change $\mu \to -\mu$ can be compensated for by a field redefinition $A_0 \to -A_0$ in Eq. (2.1), all physical observables must be even under this operation. In the original 4d theory the same statement follows from compensating $\mu \to -\mu$ by a C (or CP) operation. Moreover, since there are no massless modes at $\mu = 0$, we expect the masses to be analytic in μ away from phase transitions. For small values of μ/T, the inverse correlation lengths may thus be written as

$$\frac{m}{T} = c_0 + c_1 \left(\frac{\mu}{\pi T}\right)^2 + c_2 \left(\frac{\mu}{\pi T}\right)^4 + \mathcal{O}\left(\left(\frac{\mu}{\pi T}\right)^6\right) . \quad (2.5)$$

We have chosen to include πT in the denominators, because the chemical potential appears with this structure in the effective parameters, cf. Eq. (2.3). Of course, the radii of convergence of such expansions are not known a priori.

Here we first check to what extent a truncated series of the type in Eq. (2.5) can accurately describe the data. In the range where this is possible, we determine the $\{c_i\}$ with $\mu = i\mu_I$, and check if the analytically continued result reproduces the independent measurements carried out with $\mu = \mu_R$.

3. Simulations

3.1. Simulation methods

We simulate the theory at several μ/T. The values chosen, together with the corresponding continuum parameters, are listed in Table 1. Discretization and lattice–continuum relations [32] are implemented as in [11]. As discussed there, finite volume and lattice spacing effects are expected to be smaller or at most of the same order as the statistical errors for the parameter values we employ. Compared with [11], we have

$\frac{|\mu|}{T}$	$\frac{|\mu|^2}{(\pi T)^2}$	real μ		imaginary μ	
		y	z	y	z
0.50	0.0253	0.49218	0.0338	0.47382	$0.0338i$
0.75	0.0570	—	—	0.46235	$0.0507i$
1.00	0.1013	0.51970	0.0675	0.44630	$0.0675i$
1.25	0.1583	0.54035	0.0844	0.42565	$0.0844i$
1.50	0.2280	0.56558	0.1013	0.40042	$0.1013i$
1.75	0.3103	0.59540	0.1182	—	—
2.00	0.4053	0.62981	0.1351	—	—
3.00	0.9119	0.81333	0.2026	—	—
3.75	1.4248	0.99914	0.2533	—	—
4.00	1.6211	1.07026	0.2702	—	—

Table 1: *The parameters used for $\mu \neq 0$ (cf. Eq. (2.2)). All correspond to $T = 2\Lambda_{\overline{\rm MS}}$, $N_f = 2$. In addition, $x = 0.0919$, $g_3^2 = 2.92T$, $\beta = 21$, volume $= 30^3$, where β determines the lattice spacing (for the detailed relations employed here, see [11]).*

increased the statistics and included many new values of μ/T, in order to carry out more precise fits.

For real $\mu = \mu_R$, the action in Eq. (2.1) with parameters as in Eq. (2.3) is complex, which precludes direct Monte Carlo simulations. We must thus carry out simulations using a reweighting technique, which has been explained in detail in [11]. There it was found that physically realistic lattice volumes may be simulated for chemical potentials up to $\mu_R/T \lesssim 4$. For imaginary $\mu = i\mu_I$, the action in Eq. (2.1) with parameters as in Eq. (2.3) is real, and correspondingly we simulate the full action using a Metropolis update.

3.2. Results

As a first result, let us note that, as has been the case in several related theories [33, 21, 11], we again observe a dynamical decoupling of operators, such that operators involving scalars (Tr A_0^2, Tr $A_0 F_{12}^2$ etc.) and purely gluonic operators (Tr F_{12}^2 etc.) have a mutual overlap consistent with zero. The correlation matrix thus assumes an approximately block diagonal form. We find that the gluonic states remain extremely insensitive to μ/T, and agree well with the masses found in $d = 3$ pure gauge theory [34]. This situation is illustrated in Fig. 1.
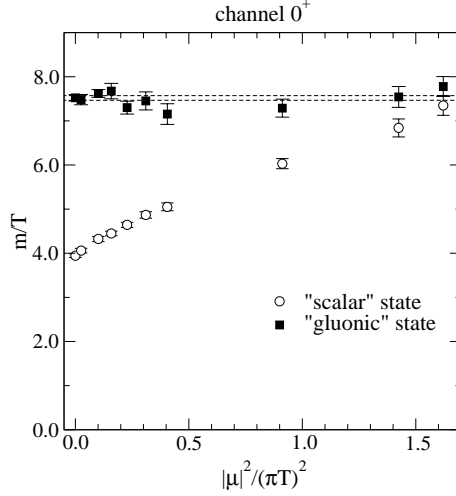
Figure 1: *Inverse correlation lengths in the channel 0^+, for real μ/T. "Scalar" states ($\mathrm{Tr}\, A_0^2$ etc) do depend on μ/T, while "gluonic" states ($\mathrm{Tr}\, F_{12}^2$ etc) are practically independent of it. For comparison, the horizontal band indicates the 3d pure glue result for $\mathrm{Tr}\, F_{12}^2$ [34], converted to our units via $g_3^2 = 2.92T$.*
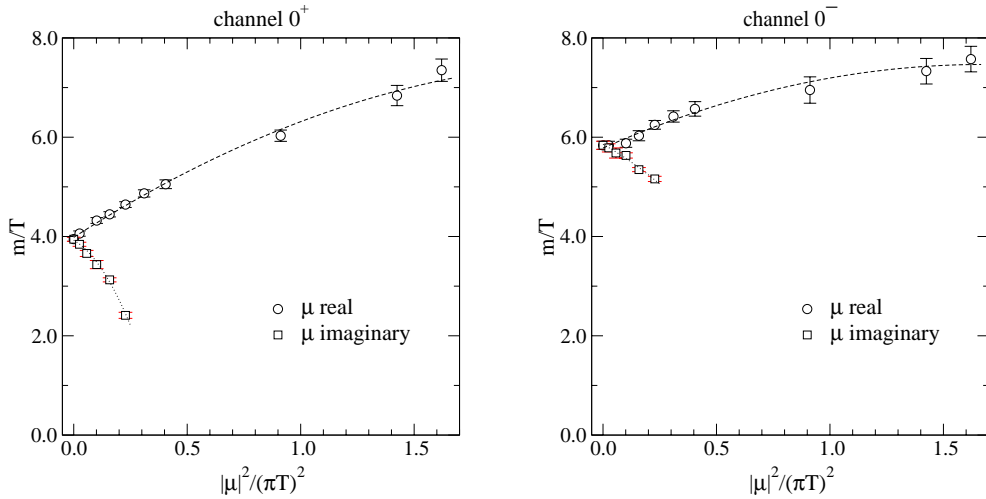

Figure 2: *Left: Inverses of longest correlation lengths in the channel 0^+, for real and imaginary μ. Right: the same for 0^-. The lines are fits according to Eq. (2.5).*

The scalar states, on the other hand, show a marked dependence on μ/T, with their masses increasing for real μ and decreasing for imaginary values. For both small real and small imaginary μ/T, the ground state in each channel is scalar in nature, and we plot these states in Fig. 2.

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N_R	$\mu_R^{\max}/T$	c_0^R	c_1^R	c_2^R	χ^2/dof	Q
5	1.50	3.952 (37)	3.89 (99)	-3.92 (449)	0.175	0.840
7	2.00	3.956 (35)	3.54 (52)	-2.06 (144)	0.145	0.965
8	3.00	3.965 (32)	3.22 (27)	-1.06 (33)	0.216	0.956
10	4.00	3.983 (30)	2.94 (20)	-0.61 (16)	0.607	0.751
N_I	$\mu_I^{\max}/T$	c_0^I	c_1^I	c_2^I	χ^2/dof	Q
5	1.25	3.952 (38)	4.73 (157)	-3.07 (933)	0.090	0.914
6	1.50	3.925 (35)	2.64 (96)	-16.89 (443)	1.004	0.390

Table 2: *Fitting the N_R lowest real μ and the N_I lowest imaginary μ masses in the channel 0^+. The numbers in parentheses indicate the error of the last digit shown, the coefficients refer to Eq. (2.5), the sub and superscripts R,I denote real or imaginary μ, and Q is the quality of the fit.*

N_R	$\mu_R^{\max}/T$	c_0^R	c_1^R	c_2^R	χ^2/dof	Q
5	1.50	5.839 (69)	-0.54 (167)	10.33 (722)	0.029	0.971
7	2.00	5.804 (63)	1.22 (91)	2.06 (246)	0.429	0.788
8	3.00	5.770 (57)	2.18 (47)	-0.90 (65)	0.655	0.658
10	4.00	5.782 (54)	2.01 (35)	-0.60 (23)	0.546	0.800
N_I	$\mu_I^{\max}/T$	c_0^I	c_1^I	c_2^I	χ^2/dof	Q
5	1.25	5.818 (71)	0.36 (195)	-16.36 (1087)	0.298	0.742
6	1.50	5.857 (65)	2.57 (116)	-2.53 (465)	0.858	0.462

Table 3: *Fitting the N_R lowest real μ and the N_I lowest imaginary μ masses in the channel 0^-. The notation is the same as in Table 2.*

Because of the different qualitative behaviours of 3d gluonic and scalar states, we may expect to observe a change in the nature of the ground state excitation at some μ_R. Indeed, Fig. 1 suggests a level crossing at $\mu/T \sim 4.0$. This would mean that the longest correlation length in the thermal system does not get arbitrarily short with increasing density, but rather stays at a constant level. Note that the value of m/T at this crossing is already so large that the effective theory may be inaccurate quantitatively, and in fact in the full 4d theory the flattening off could take place much earlier. However, the qualitative effect should be the same.

Next, let us discuss the applicability of the power series ansatz in Eq. (2.5). To this end we perform fits over a range $|\mu| = 0...\mu^{\max}$ to the inverses of the longest correlation lengths, both for real and imaginary μ. For imaginary μ, we can follow the "analytically continued" metastable branch as long as tunnelling into an unphysical minimum does not become a problem, which in practice means $\mu_I/T \lesssim 1.5$.

The results are shown for the 0^+ channel in Table 2, and for the 0^- channel in Table 3. Examining these fits we see that in all cases we have good fits, as demonstrated by the low $\chi^2/$dof and good Q values. In the case of real μ we find stable and well constrained values for the coefficients as we increase the size of the fitting range. For imaginary μ, due to the breakdown of the effective theory at large values of μ_I/T, we have fewer significant data points, and consequently the coefficient of the quartic term is much less constrained.

As our main result, we can now state that we observe good evidence for analytic continuation in the first non–trivial term, with c_1^R consistent with c_1^I in the 0^+ channel and similarly for the 0^- states. Unfortunately, the data is not accurate enough to make a similar statement for c_2^R, c_2^I. Extremely precise measurements would be needed, because the range in $|\mu/T|$ available to imaginary chemical potential simulations is very limited. On the other hand, from the phenomenological point of view the first non-trivial coefficient is sufficient, since the series expansion turns out to be in powers of $\mu^2/(\pi T)^2$, which is small in the most important practical applications. Thus, for phenomenological purposes, it does not seem necessary to invest an extra amount of effort on a more precise determination of the masses in the imaginary μ case.

4.   Conclusions

In this letter, we have studied the question as to what extent imaginary chemical potential simulations could be useful for determining the properties of the quark gluon plasma phase at high temperatures and finite densities. The physical observables we have measured are static bosonic correlation lengths, but the pattern should be very similar for the free energy density, as long as $T > T_c$.

The method we have used is based on a dimensionally reduced effective field theory. This way we can address both a system with a real and an imaginary chemical potential, as long as their absolute values are relatively small compared with the temperature. For larger absolute values of $\mu/T = i\mu_I/T$, there is a (first order) phase transition, and the effective description breaks down.

Despite the fact that we are only working in the quark-gluon plasma phase, we find an interesting structure in the longest correlation length, which decreases first but

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becomes constant beyond some value of μ/T, which we estimate to be $\lesssim 4.0$.

Furthermore, in the region where the effective theory is applicable, we find that direct analytic continuation does seem to provide a working tool for determining correlation lengths. For phenomenological applications, only the first two coefficients in the power series are needed, since we find the expansion parameter to be $\lesssim \mu^2/(\pi T)^2$, which is small in heavy ion collision experiments. This is good, since determining more coefficients with imaginary chemical potential would require very precise simulations.

We are thus encouraged to believe that in 4d simulations analytic continuation of imaginary chemical potential results would give physically relevant results if a good ansatz for the μ-dependence is available, and would allow to go closer to T_c determining, e.g., the free energy density and the spatial correlation lengths there.

Acknowledgements

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