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Thermal momentum distribution from path integrals with shifted boundary conditions

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For a thermal field theory formulated in the grand canonical ensemble, the distribution of the total momentum is an observable characterizing the thermal state. We show that its cumulants are related to thermodynamic potentials. In a relativistic system for instance, the thermal variance of the total momentum is a direct measure of the enthalpy. We relate the generating function of the cumulants to the ratio of (a) a partition function expressed as a Matsubara path integral with shifted boundary conditions in the compact direction, and (b) the ordinary partition function. In this form the generating function is well suited for Monte-Carlo evaluation, and the cumulants can be extracted straightforwardly. We test the method in the SU(3) Yang–Mills theory and obtain the entropy density at three different temperatures.

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I. INTRODUCTION

Thermal field theory is a theoretical tool of central importance in condensed matter physics, plasma physics, nuclear physics and cosmology [1, 2]. Obtaining first-principles predictions from a thermal field theory is often challenging, since it describes an infinite number of degrees of freedom subject to both quantum and thermal fluctuations. New theoretical concepts and more efficient computational techniques are still needed in many contexts, particularly when weak-coupling methods are inapplicable.

In this work we exploit the global symmetries of a thermal theory to define the contributions to the partition function of states with given quantum numbers, and show that they are well suited for *ab initio* Monte-Carlo computations. Our main results, which are based on spatial translation invariance, concern the relative contribution to the partition function of states with total momentum $\boldsymbol{p}$. These contributions form the probability distribution of $\boldsymbol{p}$, whose cumulants can be related in a simple manner to the equation of state by using Lorentzian or Galilean invariance. For instance, in Quantum Chromodynamics (QCD) at zero baryon chemical potential μ, the variance of the total momentum measures the entropy of the system. As we will see shortly, the generating function K of the cumulants of the momentum distribution can be expressed as a ratio of two partition functions. The latter are represented by Euclidean path integrals with different boundary conditions for the fields in the time direction, and their ratio can therefore be computed by standard Monte Carlo techniques.

While the following theoretical discussion extends to a wide class of theories, we illustrate our ideas numerically in the $SU(3)$ Yang–Mills theory, where we determine the entropy density of the system at three different temperatures. Crucially, the method can be applied to QCD, since the hermiticity properties of finite-difference operators are not affected by our 'shifted' boundary conditions, and hence the actions to be used in the simulations are always real at $\mu = 0$. As an example of an application to a non-relativistic system, it can also be employed in the study of neutron matter in the Euclidean approach of [3].

There are already several established methods to compute the thermodynamic properties of gauge theories [4–7]. They require either a vacuum subtraction or a renormalization constant to be determined, facts which make it difficult to apply them at arbitrarily high and low temperatures. Our method avoids these problems, and has the further advantage that a Symanzik improvement of the action (i.e. a suppression of the discretization errors [8, 9]) automatically leads to a corresponding improvement in the thermodynamic quantities. Computationally, the method is rather expensive, since it consists in calculating a ratio of partition functions. However our experience shows that, even with a simple algorithm, physics results can be obtained with commonly available computing resources.

II. MOMENTUM DISTRIBUTION

Recent progress in lattice field theory has made it possible to define and compute by Monte Carlo simulations the relative contribution to the partition function due to states carrying a given set of quantum numbers associated with exact symmetries of a theory [10, 11]. Here we apply these techniques to a finite temperature and density system in the grand canonical ensemble (or the canonical ensemble if there is no conserved particle number). The relative contribution to the partition function of the states with momentum $\boldsymbol{p}$ is given by

$$\frac{R(\beta,\mu,\boldsymbol{p})}{L^3} = \langle \hat{\mathrm{P}}^{(\boldsymbol{p})}\rangle = \frac{\mathrm{Tr}\{e^{-\beta(\hat{H}-\mu\hat{N})}\hat{\mathrm{P}}^{(\boldsymbol{p})}\}}{\mathrm{Tr}\{e^{-\beta(\hat{H}-\mu\hat{N})}\}} \qquad (1)$$

where the trace is over all the states of the Hilbert space, $\hat{\mathrm{P}}^{(\boldsymbol{p})}$ is the projector onto those states with total momentum $\boldsymbol{p}$, $\beta = 1/T$ is the inverse temperature, $\hat{H}$ the Hamiltonian, $\hat{N}$ the particle number and L the linear size of the system. The generating function K associated with the momentum distribution is defined as

$$e^{-K(\beta,\mu,\boldsymbol{z})} = \frac{1}{L^3} \sum_{\boldsymbol{p}} e^{i\boldsymbol{p}\cdot\boldsymbol{z}} \, R(\beta,\mu,\boldsymbol{p}) \; . \tag{2}$$

The connected cumulants are obtained from it as follows,

$$\frac{K_{\{2n_1,2n_2,2n_3\}}}{(-1)^{n_1+n_2+n_3+1}} = \frac{\partial^{2n_1}}{\partial \boldsymbol{z}_1^{2n_1}} \frac{\partial^{2n_2}}{\partial \boldsymbol{z}_2^{2n_2}} \frac{\partial^{2n_3}}{\partial \boldsymbol{z}_3^{2n_3}} \frac{K(\boldsymbol{z})}{L^3}\Big|_{\boldsymbol{z}=0} \, , \tag{3}$$

where they have been normalized so as to have a finite limit when $L \to \infty$ and the (β, μ) dependence has been suppressed. Finally, we can write

$$R(\beta, \boldsymbol{p}) = \int d^3\boldsymbol{z} \, e^{-i\boldsymbol{p}\cdot\boldsymbol{z}} \, \frac{Z(\beta,\mu,\boldsymbol{z})}{Z(\beta,\mu)}, \tag{4}$$

where $Z(\beta,\mu,\boldsymbol{z}) = \mathrm{Tr}\,\{e^{-\beta(\hat{H}-\mu\hat{N})+i\hat{\boldsymbol{p}}\boldsymbol{z}}\}$ is a partition function in which states of momentum $\boldsymbol{p}$ are weighted by a phase $e^{i\boldsymbol{p}\cdot\boldsymbol{z}}$. The shifted partition function $Z(\beta,\mu,\boldsymbol{z})$ can be expressed as a path integral in Euclidean time by adopting the 'shifted' boundary conditions

$$\phi(\beta, \boldsymbol{x}) = \pm\phi(0, \boldsymbol{x} + \boldsymbol{z}) \tag{5}$$

with the $+(-)$ sign for bosonic (fermionic) fields respectively. From Eqs. (2) and (4), the generating function can be written as the ratio of two partition functions,

$$e^{-K(\beta,\mu,\boldsymbol{z})} = \frac{Z(\beta,\mu,\boldsymbol{z})}{Z(\beta,\mu)} \; , \tag{6}$$

i.e. two path integrals with the same action but different boundary conditions. In a renormalizeable theory it therefore has a finite and universal continuum limit.

We remark that in the large volume regime, the momentum distribution can be expressed at each value of $\boldsymbol{p}$ as a saddle point expansion. Its leading term in $1/L^3$, for a system with a finite correlation length, is a Gaussian with a width equal to the second cumulant. Near a second-order phase transition on the other hand, the relative size of the fourth and second cumulants can serve to characterize a universality class.

III. CONNECTION TO THERMODYNAMICS

In thermal field theories, there is a connection between the cumulants of the momentum distribution and thermodynamic functions. In relativistic theories, the reason is that the momentum density $\pi_i \equiv T_{0i}$ can be chosen to coincide with the energy flux. In non-relativistic theories, the particles are the only carriers of momentum, and therefore the momentum density (divided by the mass m of the particles) coincides with the particle number flux [12]. The relation

$$\int d^3\boldsymbol{x} \langle \hat{\pi}_i(x)\, \hat{\pi}_i(0)\rangle_c \overset{L\to\infty}{=} \begin{cases} \langle \hat{H}\, \hat{T}_{ii}\rangle_c & \text{(rel.)} \\ m\langle \hat{N}\, \hat{T}_{ii}\rangle_c & \text{(non-rel.)} \end{cases} \tag{7}$$

then follows from the Ward identities associated with (a) the conservation of momentum and (b) the conservation of energy (particle number) respectively in the relativistic (non-relativistic) case. In a fluid at rest the pressure $p(T)$ is given by the thermal average of the stress tensor $\langle \hat{T}_{ij}\rangle = \delta_{ij} p(T)$, and the relations $\frac{\partial p}{\partial \mu}(T,\mu) = n$, $\frac{\partial p}{\partial T}(T,\mu) = s$, $Ts + \mu n = e + p$ hold in the thermodynamic limit. We thus obtain

$$K_{2,0,0}(\beta,\mu) = \begin{cases} T(e+p) & \text{(rel.)} \\ Tmn & \text{(non-rel.).} \end{cases} \tag{8}$$

Alternatively, Eq. (8) can be derived using the linear response formulae and adopting hydrodynamics as a low-momentum description [13–15].

Relativistic theories at $\mu = 0$ constitute an important special case that we investigate in more detail, since it is relevant both to heavy-ion collisions [16] and to the physics of the early universe [17, 18]. First, the relation $e + p = Ts$ implies that the thermal variance of the momentum is a direct measure of the entropy of the system. Secondly, by establishing a recursion relation among the cumulants based on the Ward identities, it is possible to show that the fourth order cumulants are related to the specific heat of the system [19],

$$c_v = \frac{K_{4,0,0}}{3T^4} - \frac{3\,K_{2,0,0}}{T^2} = \frac{K_{2,2,0}}{T^4} - \frac{3\,K_{2,0,0}}{T^2}. \tag{9}$$

Combining second and fourth cumulants, one can thus obtain the speed of sound $c_s^2 = \frac{s}{c_v}$. One may prove [19] that in conformal field theories, the generating function is completely determined by its first non-zero cumulant,

$$\frac{K_{\rm CFT}(\beta,\boldsymbol{z})}{L^3} = \frac{s_{\rm CFT}(T)}{4}\left(1 - \frac{1}{(1+T^2\boldsymbol{z}^2)^2}\right). \tag{10}$$

Thirdly, it can be shown [19] that finite volume effects in $K_{2,0,0}$ are exponentially small in $m(T)\cdot L$, where $m(T)$ is the lightest screening mass in the theory, and the prefactor is explicitly known [20]. In summary, the cumulants can be used to calculate thermodynamic properties.

IV. NUMERICAL IMPLEMENTATION AND RESULTS

There are many potential applications of formulae (8,9). As an illustration we consider the $SU(3)$ lattice Yang–Mills theory defined in a cubic box of volume L^3 with periodic boundary conditions, at temperature $\beta = 1/T$ and lattice spacing a. Our goal is to show that the entropy density can be computed in the thermodynamic and continuum limit.

Lat	$6/g_0^2$	β/a	L/a	r_0/a	$K(\beta,\boldsymbol{z},a)$	$\frac{2K(\beta,\boldsymbol{z},a)}{\lvert\boldsymbol{z}\rvert^2T^5L^3}$
A_1	5.9	4	12	4.48(5)	17.20(11)	5.10(3)
A_{1a}	5.9	4	16	4.48(5)	40.71(15)	5.089(19)
A_2	6.024	5	16	5.58(6)	13.05(10)	4.98(4)
A_3	6.137	6	18	6.69(7)	7.32(8)	4.88(6)
A_4	6.337	8	24	8.96(9)	4.32(16)	5.12(19)
A_5	6.507	10	30	11.29(11)	2.62(17)	4.9(3)
B_1	6.572	4	12	12.28(12)	22.22(11)	6.58(3)
B_{1a}	6.572	4	16	12.28(12)	53.47(16)	6.684(20)
B_2	6.747	5	16	15.34(15)	17.11(15)	6.53(6)
B_3	6.883	6	18	18.14(18)	9.61(9)	6.40(6)
B_4	7.135	8	24	24.5(3)	5.42(17)	6.42(20)
B_5	7.325	10	30	30.7(4)	3.32(18)	6.1(3)
C_1	7.234	4	16	27.6(3)	57.44(25)	7.18(3)
C_2	7.426	5	20	34.5(4)	36.5(4)	7.13(8)
C_3	7.584	6	24	41.4(5)	24.7(4)	6.94(12)

TABLE I. Lattice parameters and numerical results with $\boldsymbol{z} = (2, 0, 0)$. The quantity in the last column is the estimator for the entropy density, see Eq. (15).

Even though the lattice breaks continuous translation invariance, discrete translations remain as exact symmetries of the lattice action. They suffice to define K at finite lattice spacing precisely as in section (II). The function $K(\beta,\boldsymbol{z},a)$ defined on the lattice differs by $O(a^2)$ effects from its continuum counterpart.

The canonical partition function is given as usual by

$$Z(\beta) = \mathrm{Tr}\{e^{-\beta\hat{H}}\} = \int D[U]\, e^{-S(U)}\ , \qquad (11)$$

where we suppress the dependence of Z on a and $D[U]$ is the Haar measure over the gauge links $U_\mu(x_0,\boldsymbol{x})$, for $\mu = 0, 1, 2, 3$ and for each lattice point $(x_0,\boldsymbol{x})$. For definiteness we choose the action $S(U)$ to be the standard Wilson plaquette action [21], whose bare coupling we denote by g_0^2 (for unexplained notation see Ref. [10]).

The most straightforward way to compute $Z(\beta,\boldsymbol{z})/Z(\beta)$ as given in Eq. (6) is to define a set of $(n+1)$ systems with partition functions $\mathcal{Z}(\beta, r_0)\ \ldots\ \mathcal{Z}(\beta, r_n)$, where r is a real parameter, with actions $\overline{S}(U, r)$ designed in such a way that the relevant phase spaces of successive integrals overlap and that $\mathcal{Z}(\beta, r_0) = Z(\beta,\boldsymbol{z})$ and $\mathcal{Z}(\beta, r_n) = Z(\beta)$. We can then write the identity

$$\frac{Z(\beta,\boldsymbol{z})}{Z(\beta)} = \prod_{i=0}^{n-1} \frac{\mathcal{Z}(\beta, r_i)}{\mathcal{Z}(\beta, r_{i+1})}\ , \qquad (12)$$

where $r_i = i\cdot\varepsilon$ and $\varepsilon = 1/n$. If one defines the 'reweighting' observable as

$$O(U, r_{i+1}) = e^{\overline{S}(U,r_{i+1})-\overline{S}(U,r_i)}\ , \qquad (13)$$

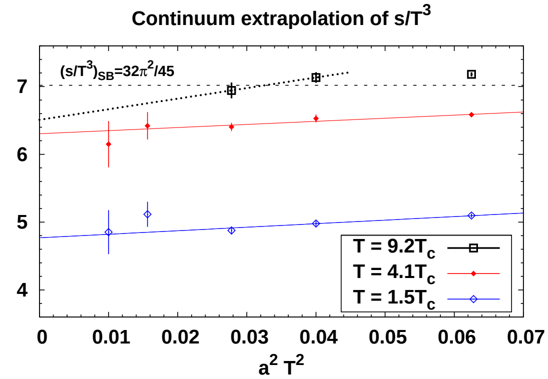

FIG. 1. Scaling behavior of s/T^3, see Eq. (15). The Stefan-Boltzmann value reached in the high-T limit is also displayed.

then the ratio $\mathcal{Z}(\beta, r_i)/\mathcal{Z}(\beta, r_{i+1})$ in Eq. (12) can be computed as its expectation value on the ensemble of gauge configurations generated with the action $\overline{S}(U, r_{i+1})$ [10]. The generating functional can thus be written as

$$K(\beta,\boldsymbol{z},a) = -\sum_{i=0}^{n-1} \ln\left\{\frac{\mathcal{Z}(\beta, r_i)}{\mathcal{Z}(\beta, r_{i+1})}\right\}. \qquad (14)$$

The continuum limit value of the second cumulant is obtained from a discrete lattice by a limiting procedure,

$$\frac{s(T)}{T^3} = \frac{K_{2,0,0}(\beta)}{T^5} = \lim_{a\to 0} \frac{2K(\beta,\boldsymbol{z},a)}{\lvert\boldsymbol{z}\rvert^2 T^5 L^3}\ , \qquad (15)$$

where $\boldsymbol{z} = (n_z a, 0, 0)$, the integer n_z being kept fixed when $a \to 0$. The continuum value of the entropy is thus approached with $O(a^2)$ corrections.

If the set of interpolating systems is chosen so that the error of each contribution in the sum is comparable and $n = (L/a)^3$, then the cost of the simulations for a given relative precision on $K(\beta,\boldsymbol{z},a)$, at fixed value of $\boldsymbol{z}$, scales approximatively as a^{-7}, while it remains roughly constant as a function of L. Each derivative of K at the origin requires an extra factor $\propto a^{-2}$ in statistics and therefore in the overall cost. Such a cost figure does not take into account autocorrelation times, and it depends heavily on the particular algorithm that we have implemented. More refined algorithms may lead to a significant speedup.

We have calculated the entropy at three temperatures, 1.5, 4.1 and $9.2T_c$, see Table I for the numerical results. The update algorithm used is the standard combination of heatbath and overrelaxation sweeps [22–24]. The only changes over the standard algorithm reside (a) in the computation of the 'staples' that determine the contribution to the action of a given link variable $U_\mu(x)$ and (b) in the more frequent updating of the two time-slices on which the observable has its support.

The bare coupling g_0^2 was tuned using the data of [25] in order to match lattices of different β/a to the same temperature. Motivated by a study of the free case, we chose $n_z = 2$. The scaling behavior of the entropy density is displayed in Fig. 1. We observe that the cutoff effects are quite mild. Our continuum results at the two lower temperatures are compatible with published results [26, 27], and the results at $9.2T_c$ are new.

V. FINAL REMARKS

In this Letter we have introduced the generating function of cumulants of the total-momentum distribution and a new way of computing it. As an application, we have shown that the second cumulant is a measure of the enthalpy (or particle density in the non-relativistic case, see Eq. (8)), and calculated the enthalpy density of gluons at three different temperatures. The ideas presented in this paper have further interesting applications.

One application is the determination of the partial pressures of different symmetry sectors (labeled by continuous as well as discrete quantum numbers) in the confined phase of QCD, since this will allow for a far more stringent test of the hadron resonance gas model than has been possible so far. The latter model postulates that the QCD pressure is due to the sum of the partial pressures of all zero-temperature resonances of width $\Gamma \lesssim T$, and is an important ingredient in the phenomenology of heavy-ion collisions (see for instance [28]). Beyond the pressure, any observable can be calculated in the restricted ensemble where certain quantum numbers assume prescribed values.

Our method has a 'kinematic' character, and the lattice action is the only ingredient in the calculation. It is conceivable that the boundary conditions adopted in this paper can be used to formulate Symanzik improvement conditions [8, 9], or to compute the constants needed to define an energy-momentum tensor which satisfies the Ward identities in the continuum limit [29].

We stress that the generating function $K(\beta, \mu, \boldsymbol{z})$ is of intrinsic interest, beyond giving access to basic thermodynamic quantities. It can be used to assess how nearly scale-invariant the system is at a given temperature, see Eq. (10). In QCD at finite baryon density and in the low-temperature limit, the generating function K is an order parameter for the spontaneous breaking of translation invariance. Finally, it may be of interest in analytic treatments, where it is more convenient to absorb the shift $\boldsymbol{z}$ into the action [30]. The propagators are then modified, the parameter $i\boldsymbol{z}/\beta$ playing the role of an external velocity parameter.

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