Archives

QCD with Dynamical Quarks at Finite Temperature: Spectral Structure in the Mesonic Channels⁺

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ABSTRACT

We study the mesonic spectrum of finite temperature QCD with dynamical Wilson quarks. We use anisotropic lattices and measure meson propagators both in the "temperature" (Euclidean time) and in the space direction. We extract from the former "pole-masses", which have been inaccessible to conventional analyses and which turn out to be different from the "screening-masses" obtained from the spatial propagators. This behaviour parallels that observed in quenched QCD calculations and indicates strong plasma effects in the region just below T_c where this calculation has been done.

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presenting our analysis (Section 3) and discussing the results (Section 4).

2. Formulation of the problem

a) Finite temperature correlation functions on anisotropic lattices

Since Monte Carlo calculations proceed from a Euclidean lattice formulation of the original quantum field theoretical model, it is natural to work in the imaginary time formalism to realize a finite temperature theory. In this formalism the Euclidean "time" axis is not simply related by a Wick "rotation" to the real time axis of the original Minkowski-space, finite temperature QFT. Therefore the basis of this and related analyses implies conceptually three steps:

i) Starting from the given QFT in Minkowski space at finite temperature we consider the Fourier transforms of its Green functions which can be defined by analytic continuation over the whole complex energy plane.

ii) Employing the "imaginary time" formalism we write down "temperature Green functions" for which the Fourier transforms are defined only on a discrete set of points (the "Matsubara frequencies") on the imaginary axis of the complex energy plane.

The relation between these two steps is given by the observation that the finite temperature, real time Green functions and the "temperature Green Functions" are related by identifying their Fourier transforms on their common support, that is, at the Matsubara frequencies [5], [6].

iii) Discretizing the Euclidean QFT of step ii) we can obtain its "temperature Green functions" from a partition function defined on a lattice with periodic boundary conditions on its fourth axis, which is taken to be of fixed physical extension $\beta = 1/T$ and therefore may be called the "temperature axis".

The quantities measured in this way are discretized "temperature Green functions", e.g., for a scalar field:

$$G_{\beta}(\tau, \mathbf{x}; \tau', \mathbf{x}') = \langle (T_{\tau} \phi(\tau, \mathbf{x}) \phi(\tau', \mathbf{x}')) \rangle \quad (2.1)$$

Here the double brackets indicate a trace with $e^{-\beta H}$ and T_{τ} means Euclidean time-ordering for the Heisenberg operators

$$\phi(\tau, \mathbf{x}) = e^{\tau H} \phi(0, \mathbf{x}) e^{-\tau H} \quad (2.2)$$

1. Introduction

The behaviour of QCD at non-zero temperature, particularly in the vicinity of the deconfining transition, is still not well understood, in spite of the intensive attention it has received [1]. One of the lessons from the recent discussion is that the so-called "screening" properties of the hadrons, which show up in connection with propagation in the spatial directions (and which have been the main subject of the previous analyses), do not seem sufficient to characterize the phenomena occurring in this region [2] [3]. This is related to the breaking of the Lorentz invariance due to the finite temperature and requires the study of the correlations along the (Euclidean) "temporal" direction [4]. Such analyses are more involved than the usual study of propagators, because in the imaginary time formalism the "time" axis is in fact a "temperature" axis, of finite physical length, and the behaviour of the correlation functions with this variable cannot be directly interpreted as time dependence. The analysis of the spectral function therefore requires a clean separation of non-vanishing contributions from the excited states. This can be achieved, for instance, by doing fits with sufficiently many parameters to permit a good description of the spectral function. To provide the information necessary for such a fit we must ensure a large number of points in the time direction (i.e., a large number of Matsubara frequencies in the Fourier transform). Hence we need a very fine discretization of the "time" axis, while we still can live with a coarser one for the space directions if the corresponding cut-off is already high enough to permit scaling. This situation can be realized with anisotropic lattices, which have different discretization lengths a_{σ} (a_{τ}) for the space (time) directions.

This program has been accomplished for quenched QCD showing both the feasibility of the approach and the significance of its results [4]. Here we develop this program for the full QCD with dynamical Wilson fermions. Since most of the general discussion can be found in [4], we shall refer to this paper for general considerations concerning both the formulation and the method (see also [5]), and restrict ourselves here to a short recollection of the problem (Section 2) before

This leads to the so-called KMS condition [5]:

$$G_\beta(\tau, \mathbf{x}; 0, 0) = G_\beta(\tau + \beta, \mathbf{x}; 0, 0) \quad (2.3)$$

Usually one does not measure G_β , but the related functions G_β^μ obtained by partial Fourier transformation:

$$G_\beta^\mu(x_\mu, \{p_\nu, \nu \neq \mu\}) = \Pi_{\nu \neq \mu} F_{x_\nu, p_\nu}^{-1} G_\beta(\tau, \mathbf{x}; 0, 0) = F_{x_\mu, p_\mu} K_\beta(\zeta, \mathbf{p}) \quad (2.4)$$

where $p_4 = \zeta$ and for $\mu = 4$ the Fourier transform is taken discrete (with $\zeta = \zeta_n = 2\pi T n$: the Matsubara frequencies). $K_\beta(\zeta, \mathbf{p})$ is the full Fourier transform of the (Euclidean) temperature Green functions Eq.(2.1). Since we still have rotational symmetry, we shall only differentiate between the "Euclidean time" ("temperature") propagators $\mu = 4$ (G_β^τ) and the "space" ones, $\mu \neq 4$ (G_β^σ). Of course, for $\beta \rightarrow \infty$ they coincide, due to the restored Euclidean symmetry.

Going now from the Hamiltonian formulation to the Euclidean path integral, the temperature Green functions Eq.(2.1) (or (2.4)) are simply obtained as correlations taken with an ensemble defined with periodic boundary conditions in τ (antiperiodic for fermionic variables), to ensure the corresponding KMS condition (see Eq.(2.3)):

$$G_\beta(\tau, \mathbf{x}) = \langle \phi(\tau, \mathbf{x}) \phi(0, 0) \rangle_\beta \equiv \frac{1}{Z} \int d[\phi] \phi(\tau, \mathbf{x}) \phi(0, 0) e^{-\int_0^\beta d\tau \int d\mathbf{x} L_E(\phi)} \quad (2.5)$$

with Z the partition function, L_E the Euclidean Lagrangian density corresponding to H , and classical variables ϕ . Eq.(2.5) is well defined on the lattice. Notice that there is no analytic continuation involved at this stage. Finally, the relation to the original, finite temperature, real time QFT of step i) implies an interpolation from the Matsubara frequencies and an analytic continuation of $K_\beta(\zeta, \mathbf{p})$ in $z = i\zeta$ to obtain the spectral functions of the corresponding Green functions at finite temperature. The interpolation and analytic continuation are well defined if the general analytic properties are under control (which in principle includes the necessity of a scaling analysis, if we work at finite cut-off - i.e., with a finite number of Matsubara frequencies).

Since what we directly measure are the statistical averages Eq.(2.5), the actual procedure is to make an ansatz for the spectral function which, by following the

steps i) to iii) leads to an ansatz for the correlation functions Eq.(2.5), to be fitted to the data. This is in principle nothing new for lattice calculations, since it is exactly what one does also at zero temperature. However, in the latter case, since the imaginary time is related to the real time by a simple Wick rotation and the Euclidean time axis is not bounded in principle, we may expect that in distant correlations only the lowest state will survive and an exponential ansatz would be realistic enough. At finite temperature, however, not only do we expect the original particle pole contributions to the spectral function to broaden (the poles move on the second sheet), but we also expect to have non-vanishing admixture of the higher excitations at all available distances. This requires a more refined fit ansatz and many data points (besides, of course, small errors). See Fig. 1 for an illustration of the problem.

b) Finite temperature calculations on anisotropic lattices

In agreement with the above discussion, finite temperature models are realized on the lattice by taking periodic (antiperiodic) boundary conditions for the bosonic (fermionic) fields in the "time" direction and by choosing a renormalization which relates the continuum and the thermodynamic limits, to wit:

$$\begin{aligned} N_\sigma &\rightarrow \infty \\ a &\rightarrow 0 \end{aligned} \quad (2.6)$$

$$N_\tau \rightarrow \infty, \quad a_\tau \rightarrow 0, \quad \text{fixed } T$$

with

$$T = \frac{1}{t_\tau} = \frac{1}{N_\tau a_\tau} = \frac{\xi}{N_\tau a}, \quad a = a_\sigma, \quad \xi = a_\sigma / a_\tau \quad (2.7)$$

Clearly enough, using a large cut-off anisotropy ξ allows us to meet both conditions of producing a high temperature and of ensuring a large number of lattice points in the "time" direction N_τ even for moderately weak coupling.

Anisotropic lattices have been already applied for some time [7], [8], [9]. An anisotropic lattice model is defined with the help of anisotropic nearest-neighbour couplings (bare couplings), while ξ itself is not a parameter of the lattice model, like also the cut-offs a_σ and a_τ , but emerges in the frame of a renormalization

procedure. The latter is performed at zero temperature and consists of tuning the bare coupling anisotropies γ_i such as to achieve isotropy for physical quantities with a single rescaling of distances by a factor ξ , to wit:

$$\bar{O}_{m\sigma}(\gamma_1, \gamma_2, \dots) = \bar{O}_{m\sigma}(\xi\gamma_1, \xi\gamma_2, \dots); \quad m = 1, 2, \dots \quad (2.8)$$

where the averages $\bar{O}_{m\sigma}$, $\bar{O}_{m\tau}$ are some correlation function over n sites in space (time) direction, respectively. This procedure is called calibration (see, e.g., Ref. 9) and may be non-trivial in a theory like QCD where we have more couplings which must be tuned simultaneously, since the physical isotropy condition amounts to implicit constraints among them. Assume, however, that we work at values of the anisotropies, γ'_i , near the "physical" ones, γ_i , (which fulfils Eqs.(2.8) with a given ξ); then we can write for the observables entering Eqs.(2.8) [10], [4]:

$$\bar{O}_m(\gamma_i) = \frac{\int O_m \exp(-S(\gamma_i))}{\int \exp(-S(\gamma_i))} = \frac{\int O_m \exp(-S(\gamma'_i) + \Delta S + C)}{\int \exp(-S(\gamma'_i) + \Delta S + C)} \quad (2.9)$$

with S : the action, and:

$$\Delta S = S' - S = S(\gamma'_i) - S(\gamma_i) = - \sum_i Q_i \Delta \gamma_i \quad (2.10)$$

Expanding the exponentials in ΔS we get for the isotropic averages

$$\bar{O}_m = \langle O_m \rangle = \langle O_m \rangle' + \sum_i \Delta \gamma_i (\langle O_m Q_i \rangle' - \langle O_m \rangle' \langle Q_i \rangle') \quad (2.11)$$

A fit to Eqs.(2.8) and (2.11) will then produce both γ_i and ξ without further tuning. In Eq.(2.9) C is of course redundant, but choosing it to be $- < \Delta S >$ we see that it is not ΔS (an extensive quantity) which controls the quality of the approximation, but its fluctuation $\Delta S - < \Delta S >$ which only grows as the square root of the volume.

3. Analysis for full QCD

a) General formulae

The action for QCD on anisotropic lattices is given by

$$S_{YM} = -\frac{1}{3}\beta \left[\frac{1}{\gamma_G} \text{ReTr}(\Box_\sigma) + \gamma_G \text{ReTr}(\Box_\tau) \right], \quad S_F = -\bar{\Psi} W \Psi \quad (3.1)$$

$$W = 1 - \kappa_\sigma \left(\sum_i (\Gamma_{+i} U_i T_i + \Gamma_{-i} T_i^* U_i^*) + \gamma_F (\Gamma_{+4} U_4 T_4 + \Gamma_{-4} T_4^* U_4^*) \right)$$

$$\Gamma_{\pm\mu} = r \pm \gamma_\mu, \quad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$$

Here U_μ are the link variables ($SU(3)$ fundamental matrices) and $\Psi, \bar{\Psi}$ the site variables representing n_F flavours of Wilson fermions. T_μ are lattice translation operators. Periodic (antiperiodic) boundary conditions are assumed for the boson (fermion) field in all directions. The hopping parameter κ_σ is related to the bare quark mass by

$$\kappa_\sigma = \frac{1}{2(M + (3 + \gamma_F)r)} \quad (3.2)$$

and γ_G, γ_F are the two coupling anisotropies

$$\gamma_G = \sqrt{\beta_\tau / \beta_\sigma}; \quad \beta = \sqrt{\beta_\sigma \beta_\tau} = \frac{1}{g^2} \quad (3.3a)$$

$$\gamma_F = \frac{\kappa_\tau}{\kappa_\sigma}; \quad \kappa = \sqrt{\kappa_\sigma \kappa_\tau} \quad (3.3b)$$

They have to be tuned such that the renormalization at zero temperature can be done in terms of one cut-off a and one cut-off anisotropy ξ , as described in the preceding section:

$$\xi = a_\sigma / a_\tau, \quad a_\sigma = a \quad (3.4)$$

In our analysis we work with lattices of $6^2 \times 8 \times N_\tau$ points and employ $n_f = 2$ flavours.

b) Calibration

The calibration is done on a lattice with $N_\tau = 24$ at $\beta = 5.3$, $\gamma_G = 2.3$, $k_\sigma = 0.0995955$ and using as starting point for the method described in Section 2b) the value

$$\gamma'_F = 3 \quad (3.5)$$

We then make a simultaneous fit to the isotropy conditions Eqs.(2.8) and (2.11) including both Wilson loops and meson propagators, with γ_F and ξ as free parameters. See Fig. 2. As a result we obtain for the physical isotropy point

$$\gamma_F = 3.04824, \quad \xi = 3.44 \quad (3.6)$$

Since the correction is small and the fit good we renounce iterating the procedure in order to save computer time.

c) Calculation

After calibration we reduce N_τ in order to increase the temperature. The calculation is done on an $6^2 \times 8 \times 14$ lattice at:

$$\beta = 5.3, \quad \gamma_G = 2.3, \quad k_\sigma = 0.0995955, \quad \gamma_F = 3.04824, \quad (\xi = 3.44) \quad (3.7)$$

We use the HMC algorithm and perform about 1500 trajectories (of 100 steps each) including 1165 trajectories for thermalization (the first 1000 without fermions). We use about 80 configurations, each taken 4 or 5 trajectories apart and measure meson propagators both in the "time" and in the space direction. The configurations seem to be thermalized and the statistics of the propagators appears satisfactory (see Figs. 3, 4).

The simulation has been done on the Fujitsu VP-400 vector machine of the University of Karlsruhe.

4. Results and discussion

As explained in Sections 1 and 2, in fitting the meson propagators we need to account for two kinds of effects:

- i) the breaking of the hypercubic symmetry of the physical Euclidean lattice (that is, for physical distances) due to the non-zero temperature, and
- ii) the complicated structure of the spectral contributions in the propagators.

Since we only measured correlations of the type Eq.(2.4) we account for point i) by using independent sets of parameters in the "time" and in the space directions. Our aim is to determine the "pole-masses" defining the dominant low-energy structure in the meson channels, and showing up in the "time" behaviour of the

τ -propagators, and compare them with the "screening-masses" obtained from the σ -propagators. Since in the τ -propagators the excited state contributions vanish nowhere we used fit ansätze with the low-energy structure parameterized by a pole and the higher excitations collectively parameterized by a pole or by a continuum. To diminish the danger of bias in the comparison with "screening-masses" we used the same type of ansatz for the spatial propagators, although here the physical distances permitted by our lattice are up to a factor two larger than in the "time" direction. Our ansätze are hence of the type:

$$G^{(\alpha)}(x_\alpha, p \neq \alpha = 0; T) =$$

$$C_\alpha(T) \frac{\cosh(M_\alpha(T)(N_\alpha/2 - x_\alpha))}{2M_\alpha(T) \sinh(M_\alpha(T)N_\alpha/2)} + E_\alpha(T; N_\alpha, x_\alpha) \quad (4.1)$$

with $\alpha = \sigma, \tau$, $x_\alpha = z, t$ and $N_\alpha = N_3, N_\tau$, respectively. E_α represents the higher excitations. In the 4-parameter fit we take for E

$$E_\alpha^P(T; N_\alpha, x_\alpha) = C'_\alpha(T) \frac{\cosh(M'_\alpha(T)(N_\alpha/2 - x_\alpha))}{2M'_\alpha(T) \sinh(M'_\alpha(T)N_\alpha/2)} \quad (4.2)$$

and in the 5-parameter fit we take

$$E_\alpha^C(T; N_\alpha, x_\alpha) = C'_\alpha(T) \int_0^\infty d\omega \frac{\cosh((\omega + M'_\alpha(T))(N_\alpha/2 - x_\alpha))}{2 \sinh((\omega + M'_\alpha(T)N_\alpha/2)(\omega + M'_\alpha(T))^{1+\eta_\alpha(T)})} \quad (4.3)$$

which corresponds to a continuum contribution:

$$\theta_{(\omega - M'_\alpha(T))\omega^{-\eta_\alpha(T)}} \quad (4.4)$$

The fits were done by the routine MRQMIN [11]. The results are given in Table 1. Since the σ -propagators provide at most 5 data points fits with more than 4 parameters are not meaningful for them. The parameters for the higher energy part E are not given in the Table since we do not try to assign physical meaning to E : it is there only in order to take the trash and allow us to separate the low-energy signal. As can be seen from Fig. 4a, the fit ansatz seems to be able to produce a clean low energy contribution.

As one can read from Table 1 the dependence on the fit ansatz of the "pole-masses" is rather weak, remaining at the level of 5%, which is the general level of uncertainty anyway - as indicated by a jack-knife treatment of the fit-data. A larger sensitivity seems however to affect the "screening-masses" (which is understandable considering the small number of points in the σ -propagator). See also Fig. 4b. Defining a distance dependent "effective mass" in the usual way, and fitting with $1/n$ and $1/n^2$ corrections we obtain asymptotic values for m_σ which are larger than those given by the two pole-fit. For m_τ , all tests are consistent with each other.

We should, however, remain aware of the fact that retrieving the low energy signal from the τ -propagators is a sensitive affair and its reliability should be improved by taking more points (larger lattices) to allow further refined fits and by using also other operators, to allow cross-analysis.

Considering now the results as they stand, we first remark that they acknowledge the same kind of behaviour as we observed in the quenched QCD calculation [4], although (mainly because of the uncertainty in m_σ) this behaviour appears less clear here. To help the comparison we notice that in this simulation - see Eq.(3.7) - the effects of the dynamical quarks seem to be strong concerning the renormalization aspects, less strong in the dynamics itself. Both the cut-off a and the cut-off anisotropy ξ are strongly affected by the presence of the quarks: the latter is shifted from the value 3.0 to the value 3.44 while the former is reduced by nearly a factor 2 (this is taken care of in our simulation by choosing $\beta = 5.3$ instead of $\beta = 5.7$ for the quenched case). On the other hand, we have rather massive quarks as can be seen from a ratio π/ρ of about 0.9 and pion correlation lengths of at most 1 (in units of a^{-1}). The high temperature (slightly below T_c) thus mainly affects the gluonic degrees of freedom, while T/m_π remains rather small (less than 1/4). Hence it is not surprising that a similar behaviour to that of the quenched simulation is observed here and the quality of the results is not good enough to judge upon significant differences. Therefore for the physical situation implied by this simulation, similar conclusions can be drawn as in [4], in particular:

i) the dispersion law of the mesons seems to be strongly modified by the temperature and not in the expected way (the latter supposes plasma effects to slow down the propagation of "particle" modes, leading to "screening-masses" higher than the "pole-masses" - the converse effect to what we observe; this picture, however, is correct only for small momenta).

ii) the temperature effects already appear before T_c , indicating a non-trivial physics in the transition region. However, since we only measured at one temperature we cannot verify here the more detailed observations from the quenched case.

A more refined analysis should try to obtain the full dispersion law, measuring propagators not only at zero "transverse" three-momenta (see Eqs.(2.4),(4.1)), and should ensure a larger number of points in both "time" and "space" directions to allow for better fit ansätze. Such a calculation should also allow us to obtain more information on the structure of the hadrons at finite temperature by making the relation to the corresponding wave functions. We are presently starting such a project.

We want to stress here, as a general conclusion, that all these observations (and also the broad discussion going on presently) indicate the necessity and usefulness of calculations involving more refined correlation functions, especially involving Euclidean "time" distances. Calculations involving only spatial distances are undoubtedly significant for the phenomena at finite temperature, but one is misled in interpreting "screening" correlation functions in terms of particle masses or wave functions for compound systems (for a discussion of these and related matters we also refer to the foregoing paper [4] as well as to further literature [12]). In fact, in view of the Euclidean formulation, "screening" properties are directly relevant for the particle propagation in a zero-temperature QFT with squeezed spatial volume (in one of the space directions), while their interpretation in terms of the finite temperature, infinite volume QFT problem with which we started is more involved. The Lorentz symmetry breaking due to the finite temperature forces a physical anisotropy of the phenomena and requires correspondingly more complex analyses from us. Global or fixed momentum observables, like susceptibilities, can give information on threshold behaviour but they cannot identify effective structures. For the physical processes going on at temperatures around T_c the latter are the relevant quantities, however, since they describe the coupling of the hadrons to effective modes in the plasma. To obtain information about the effect of temperature on the structure of hadrons we need therefore to describe the propagation in the "time" variable and study hadronic correlation functions with detailed dependency on both energy and three-momentum. The main conclusion from this and the foregoing paper [4] should be the evidence for the interest and feasibility of this program.

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TABLE 1

channel	two-pole fit	pole & cont.	asympt. eff. mass
$m_{\rho^+ a_\sigma}^{\rho^+ a_\sigma}$	1.43	1.37	1.38
$m_{\rho^0 a_\sigma}^{\rho^0 a_\sigma}$	1.1		1.3
$m_{\rho^- a_\sigma}^{\rho^- a_\sigma}$	1.53	1.47	
$m_{\phi a_\sigma}^{\phi a_\sigma}$	1.36		

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Table Captions

Table 1: Lower masses from two-pole (4-parameter) and pole and continuum (5-parameter) fits in the pseudoscalar and vector channels at $\beta = 5.3$, $\gamma_G = 2.3$, $\kappa_\sigma = 0.0995955$, $\gamma_F = 3.04824$, $\xi = 3.44$ with $N_\tau = 14$ implying a temperature $T = 0.2457a^{-1}$. Also given are asymptotic values obtained from distance dependent "effective masses" fitted with $1/n$ and $1/n^2$ corrections, as an indication for the uncertainties of the results. Since for the (larger) masses in the vector channel all the effects are rather small, we did not make further tests for them.

Figure Captions

- 1 Energy plane with Matsubara frequencies for a boson field (a) and an illustration of the expected spectral function (b) and its approximations in the frame of the two-pole (c) and a pole-and-continuum (d) fit ansatz. The cross on the real axis in Fig 1a) indicates the peak of the discontinuity across the cut induced by a presumed particle pole pushed on the second sheet at non-zero temperature.
- 2 χ^2 for the simultaneous fit of Wilson loops and meson propagators measured on the $6^2 \times 8 \times 24$ lattice at the approximative isotropy point $\gamma'_F = 3$, Eq.(3.5). The curves correspond to fixed values of ξ , the abscissa represents γ_F (ξ and γ_F are the two fit parameters).
- 3 Iteration history of the plaquettes after coupling to the quarks.
- 4a Pion τ -propagator at the isotropy point Eq.(3.7) on the $6^2 \times 8 \times 14$ lattice ($T = 0.2457a^{-1}$). Full line is the pole-and-continuum fit, dotted line the contribution of the (low energy) pole (rescaled to the bottom of the propagator), dashed line that of the (high energy) continuum (rescaled to the top of the propagator).
- 4b Pion σ -propagator at the isotropy point Eq.(3.7) on the $6^2 \times 8 \times 14$ lattice ($T = 0.2457a^{-1}$). Full line is the two-poles fit, dotted line the contribution of the lower pole (rescaled to the bottom of the propagator), dashed line that of the higher one (rescaled to the top of the propagator).

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Fig2

Fig3a

plaquette value

Fig3b

Fig4a

Fig4b