Electric charge susceptibility in 2+1 flavour QCD on an anisotropic lattice

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The FASTSUM Collaboration presents its first results for the electric charge susceptibility in QCD using $2+1$ dynamical flavours of Wilson quark on anisotropic lattices. Spatial volumes of $(2.94 \text{ fm})^3$ are used at fixed cut-off with temperatures ranging from below T_c to $\sim 2T_c$.

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1. Introduction

The measurement of fluctuations of conserved charges can probe both the thermal state of the medium and its critical behaviour. The fluctuations are quantified by the susceptibilities, defined as second (and higher) derivatives of the free energy with respect to the chemical potential associated with the investigated charge. In QCD, taking into account the three light flavours, usually three charges are studied in the literature: baryon number, electric charge, strangeness. Their susceptibilities probe the actual degrees of freedom that carry such charges, *i.e.* quarks or their bound states.

QCD shows a very interesting phase structure [1]. The main characteristic, at zero baryon chemical potential (μ_B), is a crossover transition from a confined, chirally broken phase at low temperature (T) to a deconfined, chirally symmetric phase at high temperature called quark-gluon plasma (QGP) around $T_c \approx 150$MeV. Fluctuations can be used to probe quark deconfinement [2] by studying event-by-event fluctuations of charged particle ratios [3]. Susceptibilities show a rapid rise in the crossover region: at low temperature they are small since quarks are confined; at high temperature they are large and they approach the ideal gas limit.

There are many specific reasons why physicists are interested in studying these quantities; here we recall the following:

- the QCD transition is today reproduced in the heavy ion collision experiments at BNL (RHIC) and at CERN (LHC) where the fluctuations can be studied [4]: it is clearly very important for our understanding of the strong interaction to compare their measurements with lattice QCD determinations;

- susceptibilities can be seen as coefficients of the Taylor expansion of the free energy with respect to the chemical potentials; in this form they can be used to perform numerical studies at finite density QCD [5, 6];

- QCD may have a critical point, an endpoint of a line of first order phase transitions which extends from the μ_B-axis into the (μ_B,T) plane. Susceptibilities can probe its presence and, in particular, the baryon number susceptibility is expected to diverge at the critical point. Its position can be estimated studying the radius of convergence [7] of the Taylor series introduced in the previous paragraph;

- the susceptibilities of the conserved charges enter the study of the transport properties of the QGP via Kubo formulae [8], *e.g.* the electric charge susceptibility χ_Q connects the charge diffusion coefficient D with the electrical conductivity σ: $\sigma = \chi_Q D$.

Among the available theoretical tools, lattice calculations are probably the best for calculating the properties of QGP and in particular the susceptibilities from first principles: this approach is followed in this work. Nearly all lattice studies of susceptibilities have so far been carried out using staggered fermions. In this study we employ instead clover-improved Wilson fermions (for an earlier study using Wilson fermions see Ref. [9]).

2. Simulation details

The action that we have used is, for the gauge sector, Symanzik-improved with tree-level tadpole-improved coefficients and for the fermion sector, a $2+1$ flavour anisotropic clover action with stout-link smearing; for details see Ref. [10]. The configurations have been generated using the Chroma Library [11] on IBM Blue Gene/P and Blue Gene/Q supercomputers.

The volumes we have used are $24^3 \times N_t$, where the values of N_t, together with the corresponding temperature and the number of configurations generated, are given in Table 1.

N_t	40	36	32	28	24	20	16
T [MeV]	141	156	176	201	235	281	352
N_{cfg}	500	500	1000	1000	1000	1000	1000

Table 1: Some simulation parameters.

We used anisotropic lattices with a physical anisotropy $\xi \equiv a_s/a_t = 3.5$: the temporal lattice spacing, measured using M_Ω to set the scale, is $a_t = 0.03506(23)$ fm ($a_t^{-1} = 5.63(4)$ GeV) and $a_s = 0.1227(8)$ fm; for details see Ref. [12]. Moreover, $M_\pi/M_\rho = 0.446(3)$ and $M_\pi = 392(4)$ MeV, *i.e.* 2.9 times bigger than the physical value.

3. Definitions and observables

Introducing the quark chemical potentials μ_u, μ_d, μ_s and the charges $q^u = +\frac{2}{3}$, $q^d = q^s = -\frac{1}{3}$, for each flavour (we use also here the correspondence: 1 $\leftrightarrow$ up, 2 $\leftrightarrow$ down, 3 $\leftrightarrow$ strange and also in the following $l \to$ light, $s \to$ strange) we define the following quantities:

- quark number densities: $n_i = \frac{T}{V}\frac{\partial \ln Z}{\partial \mu_i}$;

- quark number susceptibilities: $\chi_{ij} = \frac{T}{V}\frac{\partial^2 \ln Z}{\partial \mu_i \partial \mu_j}$.

Introducing the electric charge chemical potential μ_Q, the electric charge Q and its susceptibility χ_Q are given by:

$$Q = \frac{T}{V}\frac{\partial \ln Z}{\partial \mu_Q} = \sum_{i=1}^{3} q^i n_i \,, \qquad \chi_Q = \frac{\partial Q}{\partial \mu_Q} = \sum_{i=1}^{3}(q^i)^2 \chi_{ii} + \sum_{i \neq j}^{3} q^i q^j \chi_{ij}. \tag{3.1}$$

We now introduce the following terms (M is the fermion matrix):

$$T_1^i = \langle \frac{T}{V}\text{Tr}\left[M^{-1}\frac{\partial M}{\partial \mu_i}\right]\rangle \,, \quad T_2^i = \langle \frac{T}{V}\text{Tr}\left[M^{-1}\frac{\partial^2 M}{\partial \mu_i^2}\right]\rangle \,,$$

$$T_3^{ij} = \langle \frac{T}{V}\text{Tr}\left[M^{-1}\frac{\partial M}{\partial \mu_i}\right]\text{Tr}\left[M^{-1}\frac{\partial M}{\partial \mu_j}\right]\rangle \,, \quad T_4^i = \langle \frac{T}{V}\text{Tr}\left[M^{-1}\frac{\partial M}{\partial \mu_i}M^{-1}\frac{\partial M}{\partial \mu_i}\right]\rangle \,, \tag{3.2}$$

which we can be used to determine the quantities:

$$n_i = T_1^i \,; \tag{3.3}$$

$$\chi_{ii} = -(T_1^i)^2 + T_2^i + T_3^{ii} - T_4^i \,; \tag{3.4}$$

$$\chi_{ij} = -T_1^i T_1^j + T_3^{ij} \quad (\text{here } i \neq j) \,. \tag{3.5}$$

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Note that $T_1^i = 0$ for zero chemical potentials, in fact $n_i = 0$ and $Q = 0$; therefore there is no need to compute this quantity numerically.

The simplest quantity we can determine is the isospin susceptibility (defining $\mu_I = \mu_d - \mu_u$):

$$\chi_I = \frac{T}{V}\frac{\partial^2 \ln Z}{\partial \mu_I^2} = \frac{1}{4}\frac{T}{V}\left[\frac{\partial^2 \ln Z}{\partial \mu_u^2} + \frac{\partial^2 \ln Z}{\partial \mu_d^2} - 2\frac{\partial^2 \ln Z}{\partial \mu_u \partial \mu_d}\right] = \frac{1}{4}\sum_{i=1}^{2}\left[T_2^i - T_4^i\right]. \tag{3.6}$$

We note that it depends only on the terms T_2 and T_4 but not T_3 which, from a numerical point of view, is the most expensive quantity to determine since it comes from a disconnected diagram.

Below we compare our results at high temperature with the expressions for free massless fermions in the continuum limit, which read:

$$\chi_I \rightarrow \frac{T^2}{2}; \tag{3.7}$$

$$\chi_Q \rightarrow T^2 \sum_{i=1}^{3} q_i^2 , \tag{3.8}$$

where $\sum_{i=1}^{3} q_i^2 = 2/3$.

Moreover, we also compare the susceptibilities with those obtained from free Wilson fermions, which can be determined analytically starting from the following expression for the baryon density, valid for N_f flavours and N_c colours:

$$n_B^{free}(\mu) = \frac{8N_f N_c}{N_s^3 N_t}\sum_{k_4,k_i}\frac{iP_4\sin(k_4+i\mu)\left[1-2P_s\sum_i\cos k_i\right]}{\left[1-2P_s\sum_i\cos k_i - 2P_4\cos(k_4+i\mu)\right]^2 + 4P_s^2\sum_i\sin^2 k_i + 4P_4^2\sin^2(k_4+i\mu)} ,$$

where $i = 1,2,3$, k_i are the discretised momenta, the coefficients P_4 and P_s are given by:

$$P_4 = \nu_t/(m + \nu_t + 3/\gamma_f) , \quad P_s = \nu_s/\left[2\ \xi_0\ (m + \nu_t + 3/\gamma_f)\right],$$

and $\nu_t = 1$, $\nu_s = \gamma_g/\gamma_f$ and $\xi_0 = \gamma_g$ (γ_g is the bare gauge anisotropy and γ_f is the bare fermion anisotropy). Note that when we compare with our data, γ_f has to be replaced with ξ, the physical value. This relation was determined following the approach discussed in Sec. 4.2.4 of Ref. [13].

4. A few technical aspects

We estimated the traces of Eq. (3.2) using N_v noise vectors η_i; for connected terms, *i.e.* T_2, T_4, we used just $N_v = 9$ noise vectors but for the disconnected term, *i.e.* T_3, we used $N_v = 200$ noise vectors for $N_t = 40$ and $N_v = 100$ for the others. As discussed in Ref. [14] the term T_3, which contain two traces, has a significantly larger variance than the other terms and therefore needs a larger number of random vectors. It is worth noting that in this case the standard error of the mean falls like the inverse of the number of noise vectors (not like the square root of it) so that increasing N_v has an evident effect in the final result.

As discussed in Ref. [15] the most efficient way to determine the square of a trace is by the following relation:

$$(\text{Tr}A)^2 = \frac{2}{N_v(N_v-1)}\sum_{i>j=1}^{N_v}\eta_i^\dagger A\eta_i\ \eta_j^\dagger A\eta_j , \tag{4.1}$$

i.e. the diagonal terms are not taken into account because they would introduce a bias in the final result given by a term whose relative significance is $O(1/N_v)$.

We tested the effect of *dilution* [16, 17] in the colour and Dirac space but we did not see any improvement in the final results. A dilution test done with $N_t = 40$ has brought the following results: we have noted a reduction of the errors in the real part of T_1 by a factor ~ 2, and in the imaginary part of T_2 by a factor ~ 3; in all other cases the effect of dilution has been counterproductive. This is not a surprise because dilution has a positive effect only if the off-diagonal elements of a matrix dominate the diagonal ones, therefore the effect depends strongly on the observable under consideration[1].

5. Results

In this Section we present our preliminary results. In Figure 1 (Left) we present the result for the isospin susceptibility, normalising it with respect to the continuum expectation at high temperature, Eq. (3.7). As can be seen for $T \gtrsim 270$MeV the value is systematically higher than the expected one, *i.e.* unity, for free massless fermions living in a continuum spacetime. This is a lattice artefact which is a consequence of combined effect of our fixed cut-off approach and the small number of *effective* sites in the temporal direction ($N_t/\xi = 4.6, 5.7, 6.8, \ldots$). This is evident looking at the dashed-red line which shows the same quantity for free massless lattice fermions, *i.e.* taking into account the effect of discretisation of the spacetime.

In Figure 1 (Right) we compare directly the result with that of massless free Wilson fermions. Here the discretisation effects are clearly taken into account and for $T \gtrsim 250$MeV the value of χ_I is above 85% of the Stefan-Boltzmann value. In the figure we plot moreover the result with two values of the fermion anisotropy: the physical one, $\gamma_f = \xi = 3.5$, and the bare one, $\gamma_f = 3.4$. The importance of using the correct value for the parameter γ_f to compare our results with the Stefan-Boltzmann limit is evident.

The contribution of the different terms to the susceptibilities are shown in Figure 2 (Left). We can see that the main contribution to the final value of the susceptibilities is given by the terms T_2 and T_4; note also the appreciable difference between the light and the strange quarks.

From Figure 2 (Left) we can see moreover the contribution of the disconnected term T_3. As discussed in Ref. [14] it is expected that this term is negative, basically as a consequence of hopping parameter expansion analysis. Hard thermal loop (HTL) perturbation theory showed a decade ago [19] that $\chi_{ij} = T_3^{ij}$ should be different from zero, showing a clear correlation between different flavours. Recent lattice calculations [18] have shown a clear dip for the off-diagonal term (in the crossover region). Our results, both for diagonal and off-diagonal contributions, show that it is compatible with zero, either at low and high temperature: this is probably a consequence of our relatively large pion mass.

The electric charge susceptibility is presented in Figure 2 (Right). Here we present this quantity normalised with respect to the high temperature behaviour expected for free massless fermions living in a continuum spacetime, Eq. (3.8). The cut-off effects are clearly present at high temperature as for Figure 1 (Left). The rapid rise of χ_Q, signalling the transition from the confined phase to the deconfined phase, is evident around $T_c \sim 150$MeV.

[1]See Eq. (20) of Ref. [16].
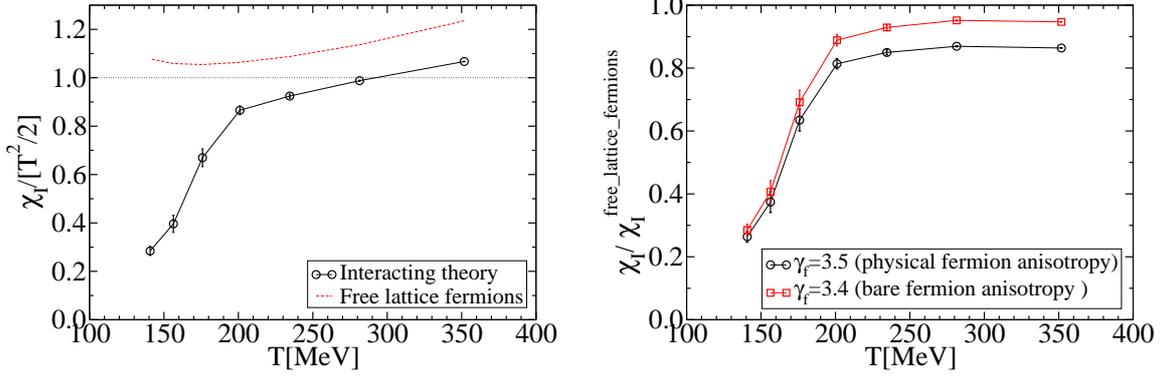
Figure 1: (Left) χ_I normalised using the high temperature expected behaviour (for free massless fermions living in a continuum spacetime). For comparison the same quantity for free massless lattice fermions is plotted. (Right) χ_I normalised with respect to the same quantity calculated for free massless lattice fermions using two values for the fermion anisotropy.

In this preliminary figure, we have included all terms of Eq. (3.2) only for a few values of the temperature (see legend). Taking into account the results of Figure 2 (Left) and the fact that the disconnected contribution has had little effect at those temperatures where the electric charge susceptibility has been calculated, we can infer it will also have little affect for the other temperatures.
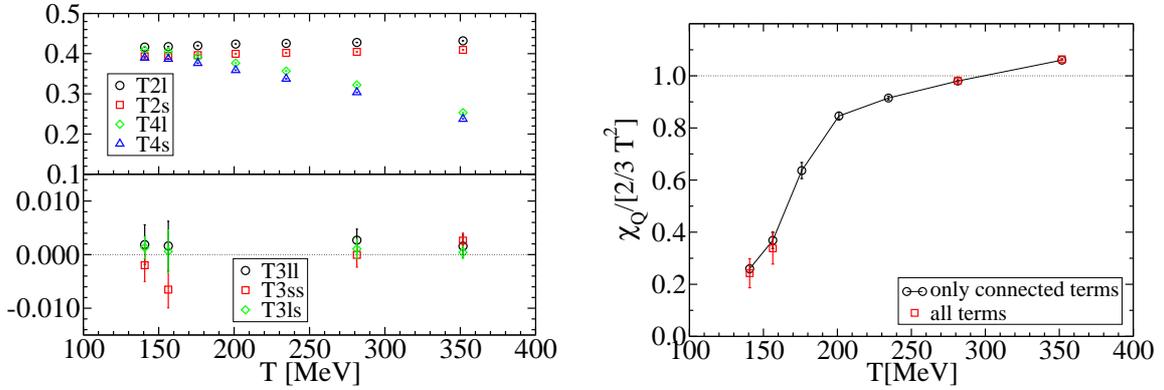
Figure 2: (Left) Terms T_2, T_4 and T_3. (Right) χ_Q normalised using the expected high temperature behaviour (for free massless fermions living in a continuum spacetime).

6. Conclusion and outlook

We have presented here our preliminary calculations of isospin and electric charge susceptibility in $2+1$ flavour QCD on anisotropic lattices using a fixed cut-off approach to explore a range of temperature which goes from below T_c to $\sim 2T_c$. We are completing the determination of the susceptibilities on the volume 24^3 on all the configurations at our disposal. When this is complete, we

plan to combine these results with the measurement of the electrical conductivity, see Refs. [20], to determine the charge diffusion coefficient D. Moreover, by an appropriate combination of the terms of Eq. (3.2), we will determine the other relevant susceptibilities, in particular the one associated with the baryon number, χ_B.

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