Susceptibilities, the Specific Heat and a Cumulant in Two-Flavour QCD

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Abstract

We study the quark mass dependence of various response functions, which contribute to chiral susceptibilities and the specific heat in the staggered fermion formulation of two-flavour QCD. This yields information about the critical exponents \( \alpha \), \( \beta \) and \( \delta \). In the case of the chiral susceptibility, obtained as derivative of the chiral order parameter with respect to the quark mass, we calculate all contributions. This allows to construct a cumulant of the order parameter, which is a scaling function and yields a direct determination of the critical exponent \( \delta \). All our results are consistent with a second order phase transition.
1) Introduction

In contrast to QCD with three or more light flavour degrees of freedom, where numerical simulations seem to indicate that the finite temperature chiral symmetry restoring phase transition is first order, there is increasing evidence that the two-flavour theory has a second order phase transition in the limit of vanishing quark masses. At least in the parameter range studied so far in the staggered formulation of lattice QCD, no signs of a first order transition have been observed [1]. In fact, in a recent analysis [2] of the existing Monte Carlo data for pseudo-critical couplings, $g_c(m_q)$, at non-vanishing quark mass, one of us has shown that the functional dependence on $m_q$ is consistent with the scaling behaviour expected for a chiral phase transition with critical exponents in the universality class of a 3-d $O(4)$ symmetric $\sigma$-model [3,4]. Still, even in the class of $O(4)$ symmetric models the occurrence of first order phase transitions can not be ruled out easily [3,5]. A careful analysis of the nature of the chiral transition is thus asked for.

In most of the existing studies of the chiral phase transition in the staggered fermion formulation of two-flavour QCD [6,7] the critical parameters have been determined through a subjective inspection of the dependence of the chiral order parameter or the Polyakov loop expectation value on the gauge coupling. In Ref. [8] the volume and quark mass dependence of the critical couplings have been examined by locating the maximum of the variance of these quantities. They are, however, not directly related to bulk thermodynamic quantities and predictions for their scaling behaviour can, therefore, not directly be obtained from properties of the two-flavour partition function, ie. the singular part of the corresponding free energy. A priori it thus is not clear in how far these quantities can give information on the critical exponents of two-flavour QCD. We will discuss this question here in detail.

In this paper we will study susceptibilities and the specific heat obtained from second derivatives of the partition function,

$$C_V = \frac{1}{VT^2} \frac{\partial^2}{\partial (1/T)^2} \ln Z ,$$

$$\chi_m = \frac{T}{V} \frac{\partial^2}{\partial m_q^2} \ln Z ,$$

$$\chi_t = -\frac{T}{V} \frac{\partial^2}{\partial m_q \partial (1/T)} \ln Z .$$

The determination of the maxima of these quantities will allow us to give a precise quantitative definition of the pseudo-critical couplings at non-vanishing values of the quark mass. We will discuss the scaling behaviour of these couplings as well as that of the peak heights in the response functions.
From $\chi_m$ and the chiral order parameter

$$\langle \bar{\psi} \psi \rangle = \frac{N_F T}{4 V} \frac{\partial}{\partial m_q} \ln Z$$

(2)

we will construct the cumulant

$$\Delta = \frac{m_q \chi_m}{\langle \bar{\psi} \psi \rangle} ,$$

(3)

which allows a direct investigation of the zero-mass critical coupling as well as the critical exponent $\delta$ [9]. In such an analysis it is particularly important to determine the complete chiral susceptibility, $\chi_m$, i.e. taking into account also the contribution from the connected part in the product of the quark bilinears.

This paper is organized as follows. In the next section we will summarize basic relations for the critical behaviour of thermodynamic quantities in the vicinity of a second order phase transition, which is controlled by the temperature as well as an external symmetry breaking field, i.e. the quark mass. In section 3 we discuss the observables from which critical exponents for QCD with dynamical quarks on the lattice are calculated. In section 4 our Monte Carlo data for various response functions is presented for three values of the quark mass on lattices of size $8^3 \times 4$. The determination of the critical exponents $\alpha$, $\beta$ and $\delta$ is discussed. Finally we give our Conclusions in section 5.

2) Scaling Relations

If the chiral phase transition in two-flavour QCD is second order, the critical behaviour of thermodynamic quantities will be controlled by two external parameters, the reduced temperature $t = (T - T_c)/T_c$ and the symmetry breaking field $h \equiv m_q/T$. In the staggered formulation of lattice regularized QCD these two dimensionless couplings are given by

$$t = \frac{6}{g^2} - \frac{6}{g_c^2(0)} ,$$

$$h = m_q N_\tau .$$

(4)

Here $g_c^2(0)$ denotes the critical coupling on a lattice of temporal extent $N_\tau$ in the limit of vanishing bare quark mass. For non-vanishing values of the quark mass, a pseudo-critical coupling, $g_c^2(m_q)$, can, for instance, be defined as the location of a peak in one of the susceptibilities or the specific heat defined in eq. (1).

In the vicinity of the critical point the behaviour of bulk thermodynamic quantities is governed by thermal ($y_t$) and magnetic ($y_h$) critical exponents, which characterize the scaling behaviour of the singular part of the free energy density,

$$f(t, h) \equiv -\frac{T}{V} \ln Z = b^{-1} f(b^{y_t} t, b^{y_h} h) .$$

(5)
Here \( b \) is an arbitrary scale factor. It is expected that the chiral phase transition in QCD can be described by an effective, three dimensional theory for the chiral order parameter, which in the case of two-flavour QCD would amount to an \( O(4) \) symmetric spin model \([3,4]\). Still the generic structure of this effective theory leaves open the possibility of a first order transition \([3,5]\). A quantitative analysis of the scaling behaviour of thermodynamic quantities is needed to further support the existence of a second order phase transition in the zero quark mass limit. In the staggered lattice discretization of QCD the situation gets even more involved due to the fact that flavour symmetry is partially broken by \( O(a) \) terms, where \( a \) is the lattice spacing. Correspondingly, at least at large lattice spacings, the relevant symmetry group is \( O(2) \) \([9]\), which would lead to somewhat different critical exponents and even might influence the order of the phase transition \([9]\). It remains to be seen if and when the full flavour symmetry is effectively restored on lattices with small but finite spacings.

The scaling behaviour of the specific heat and susceptibilities is controlled by the critical exponents \( \alpha = (2y_t - 1)/y_t, \beta = (1 - y_h)/y_t \) and \( \delta = y_h/(1 - y_h) \). Their numerical values for \( O(2) \) and \( O(4) \) symmetric spin models in three dimensions are given in Table I.

|     | \( \alpha \)     | \( \beta \)   | \( \delta \) | \( z_\alpha \) | \( z_m \) | \( z_t \) |
|-----|------------------|---------------|---------------|---------------|-----------|-----------|
| \( O(2) \) | -0.007(6) | 0.3455(20) | 4.808(7) | -0.004(3) | 0.792(1) | 0.394(2) |
| \( O(4) \) | -0.19(6)  | 0.38(1)    | 4.82(5)    | -0.10(3)   | 0.793(3) | 0.34(1)  |

Table I: Critical exponents of 3-d \( O(N) \) symmetric spin models \([4,10,11]\).

The exponents \( z_m \) and \( z_t \) characterize the scaling behaviour of susceptibilities as defined in eq. (6). The exponent \( z_\alpha \) is defined in eq. (10) and describes the leading mass-dependence of the specific heat peak.

Eq. (5) can be used to extract scaling laws for various quantities, valid in the vicinity of the critical point. For the location and height of the maximum in the susceptibilities one finds

\[
    t_{\text{max}} = c \, m_q^{1/\beta \delta},
\]

\[
    \chi_{m,\text{max}} = c_m \, m_q^{-z_m} = c_m \, m_q^{1/\delta - 1},
\]

\[
    \chi_{t,\text{max}} = c_t \, m_q^{-z_t} = c_t \, m_q^{(\beta - 1)/\beta \delta}.
\]

For finite values of the quark mass the pseudo-critical couplings defined through peaks in \( \chi_m \) or \( \chi_t \) can, of course, differ. The exponents \( z_t \) and \( z_m \), which control the scaling behaviour of the thermal and chiral susceptibilities are also given in Table I.
Similarly we obtain for the scaling behaviour of the chiral order parameter on the zero-mass critical point \((t = 0)\) as well as on the line of pseudo-critical couplings \((t = t_{\text{max}})\),

\[
\langle \bar{\psi}\psi \rangle = c_{\psi}m_q^{1/\delta} \ .
\] (7)

In the case of spin models the analysis of cumulant ratios, which themselves are scaling functions, has proven to be useful. The simplest ratio one can consider in the case of QCD is the ratio of the second and first derivative of the free energy with respect to the quark mass, ie. the ratio

\[
\Delta(t, h) = \frac{1}{N_f \langle \bar{\psi}\psi \rangle} \frac{h \chi_m}{\langle \bar{\psi}\psi \rangle} .
\] (8)

As can be seen again from eq. (5) this ratio is a scaling function, which only depends on the combination \(y = th^{-1/\beta\delta}\). A consequence of this is that \(\Delta(t = 0, h)\) is unique for all values of \(h\) (of course, modulo corrections from the regular part of the free energy). Outside the critical region the order parameter \(\langle \bar{\psi}\psi \rangle\) is expected to depend linearly on the quark mass, \(\langle \bar{\psi}\psi \rangle = c_0 + c_1m_q\) with \(c_0\) being non-zero for \(t < 0\) and zero otherwise. From this one obtains

\[
\Delta(t, h) \equiv Q\left( th^{-1/\beta\delta} \right) = \begin{cases} 
1 & \text{if } t < 0, h \to 0 \\
1/\delta & t = 0 \\
0 & t > 0, h \to 0 
\end{cases} .
\] (9)

Similarly one can analyze the scaling behaviour of the specific heat peak. Like in the case of the susceptibilities, the quark mass dependence of its location is given by \(t_{\text{max}}\) defined in eq. (6). However, unlike for the susceptibilities discussed above, the analytic calculations for the exponent \(\alpha\) suggest that the specific heat does not diverge in the zero quark mass limit \((\alpha < 0)\) but scales as

\[
C_{V,\text{max}} = c_0 + c_1 m_q^{-z\alpha} \ ; \quad z\alpha = \alpha/\beta\delta \ .
\] (10)

The mass dependence thus is a subleading term.

3) Determination of Critical Exponents on the Lattice

In the following we will discuss the observables from which information on the critical exponents \(\alpha, \beta\) and \(\delta\) is extracted. These are various response functions which contribute to the specific heat and certain susceptibilities defined for two-flavour QCD. In particular, we will study the behaviour of three susceptibilities - the chiral \((\chi_m)\) and thermal \((\chi_t)\) susceptibilities, defined in eq. (1), as well as the Polyakov loop response function \(\chi_L\),

\[
\chi_L = N^3_f \{ \langle L^2 \rangle - \langle L \rangle^2 \} \ .
\] (11)
where \( L = \frac{1}{3} N^{-3}_\sigma \sum \vec{x} \text{Tr} \prod_{i=1}^{N_\tau} U^{\vec{x},i}_{(\vec{x},i)} \) denotes the average Polyakov loop on a lattice of size \( N_\sigma^3 \times N_\tau \). While the critical behaviour of the first two can be extracted from the structure of the free energy density, the latter is not directly related to it nor does it serve as an order parameter for a symmetry of the Lagrangian at finite quark mass. In fact, it is expected that \( \langle L \rangle \) does not show any critical behaviour (divergence) in the limit of vanishing quark mass. Nonetheless, the existing Monte Carlo investigations show the presence of a pronounced peak in the Polyakov loop response function, which reflects the sudden onset of deconfinement in the chirally symmetric phase.

On the lattice the chiral susceptibility \( \chi_m \) for \( N_F \) flavours is obtained from matrix elements of the staggered fermion matrix, \( D = m_q 1 + \sum_{\mu} D_{\mu} \), as

\[
\chi_m = \chi_0 + \chi_{\text{conn}} ,
\]

with

\[
\chi_0 = \frac{N_F}{16 N_\sigma^3 N_\tau} \left\{ \langle (\text{Tr}D^{-1})^2 \rangle - \langle \text{Tr}D^{-1} \rangle^2 \right\} ,
\]

\[
\chi_{\text{conn}} = -\frac{N_F}{4} \sum_x \langle D^{-1}(x,0)D^{-1}(0,x) \rangle .
\]

The first term, \( \chi_0 \), gives the fluctuations of the order parameter

\[
\langle \bar{\psi}\psi \rangle = \frac{N_F}{4N_\sigma^3 N_\tau} \langle \text{Tr}D^{-1} \rangle .
\]

The second term, \( \chi_{\text{conn}} \), results from the connected part appearing in the second derivative of the fermion determinant. It is the integral over the connected part of a scalar propagator.

The thermal susceptibility, \( \chi_t \), requires to calculate the derivative of the chiral condensate with respect to the temperature, which in terms of the temporal lattice spacing, \( a_\tau \), and the number of lattice points in that direction, \( N_\tau \), is given by \( T = (N_\tau a_\tau)^{-1} \). Following the standard procedure for taking derivatives with respect to the temperature on the lattice [12] we obtain

\[
\chi_t = \frac{1}{N_\tau} \frac{\partial}{\partial a_\tau} \langle \bar{\psi}\psi \rangle = \frac{1}{N_\tau} \frac{\partial}{\partial a_\tau} \left\{ \langle \bar{\psi}\psi \rangle \cdot \epsilon \right\} - \langle \bar{\psi}\psi \rangle \langle \epsilon \rangle ,
\]

where \( \epsilon \) denotes the energy density operator [12]

\[
\epsilon = 3 \left[ -\frac{6}{g^2} + 6 \frac{\partial g_s^{-2}}{\partial \xi} \right] P_\sigma + 3 \left[ \frac{6}{g^2} + 6 \frac{\partial g_t^{-2}}{\partial \xi} \right] P_\tau \\
+ \bar{\psi} D_0 \psi + \frac{\partial m_q}{\partial \xi} \bar{\psi} \psi .
\]
Here $P_{\sigma(\tau)} = \frac{1}{3} N_\sigma^{-3} N_\tau^{-1} \sum_P \text{Re Tr} \prod_{i \in P} U_i$ denotes the usual plaquette operator for space-like (timelike) plaquettes; $\bar{\psi} D_0 \psi = \frac{1}{4} N_F N_\sigma^{-3} N_\tau^{-1} \text{Tr} D_0 D^{-1}$ while $\xi = a_\sigma / a_\tau$ is the ratio of spatial and temporal lattice spacing and the derivatives in eq. (16) should be evaluated for $\xi = 1$. For further details we refer to Ref. [12].

The calculation of $\chi_t$ gets complicated due to the fact that the derivatives of the couplings with respect to the temporal lattice spacing are only known perturbatively. These perturbative relations, however, are poor approximations to the exact derivatives in the coupling regime we are presently investigating. Moreover, for a complete determination of $\chi_t$ one should also take into account the zero temperature part of the energy density, which still has to be subtracted in eq. (16). Fortunately, all this is not essential for the discussion of the scaling behaviour of $\chi_t$, i.e. its divergence in the limit of vanishing quark mass. The zero temperature terms will not show any singular behaviour at the finite temperature phase transition point and the derivatives appearing in eq. (16) can be treated as constant factors. They will not influence the singular behaviour. We thus can study separately the scaling behaviour of the different terms contributing to $\chi_t$,

$$\chi_{t,\sigma} = \langle \bar{\psi} \psi \cdot P_\sigma \rangle - \langle \bar{\psi} \psi \rangle \langle P_\sigma \rangle$$

$$\chi_{t,\tau} = \langle \bar{\psi} \psi \cdot P_\tau \rangle - \langle \bar{\psi} \psi \rangle \langle P_\tau \rangle$$

$$\chi_{t,f} = \langle \bar{\psi} \psi \cdot \bar{\psi} D_0 \psi \rangle - \langle \bar{\psi} \psi \rangle \langle \bar{\psi} D_0 \psi \rangle$$

Like in the case of the chiral susceptibility, the last response function, $\chi_{t,f}$, requires the calculation of contributions from connected diagrams. These have been omitted in the following analysis. Our results for $\chi_m$ seem to justify this. Recall that, in contrast to $\chi_m$, we are here only interested in the divergent part of $\chi_t$. For the same reason we also omit the contribution coming from the correlation of $\bar{\psi} \psi$ with the mass term in eq. (16). Due to the additional mass factor this part will not contribute to the singular behaviour of $\chi_t$. Each of the other partial contributions to the thermal susceptibilities may diverge in the zero quark mass limit. In general, they even may diverge with different critical exponents,

$$\chi_{t,x} \sim m_q^{-z_{t,x}}$$

The critical exponent, $z_t = (1 - \beta)/\beta \delta$, which controls the divergence of $\chi_t$ in the zero quark mass limit, is then given by the maximum of these three exponents

$$z_t = \max\{z_{t,\sigma}, z_{t,\tau}, z_{t,f}\}.$$
investigate the scaling behaviour of the various response functions contributing to \( C_V \);

\[
C_{V,\mu\nu} = \langle P_\mu \cdot P_\nu \rangle - \langle P_\mu \rangle \langle P_\nu \rangle
\]

\[
C_{V,D\mu} = \langle \bar{\psi} D_0 \psi \cdot P_\mu \rangle - \langle \bar{\psi} D_0 \psi \rangle \langle P_\mu \rangle
\]

\[
C_{V,DD} = \langle \bar{\psi} D_0 \psi \cdot \bar{\psi} D_0 \psi \rangle - \langle \bar{\psi} D_0 \psi \rangle \langle \bar{\psi} D_0 \psi \rangle
\]

Here \( \mu, \nu \) denote \( \sigma \) or \( \tau \). We also left out the correlations of \( P_\mu \) and \( \bar{\psi} D_0 \psi \) with the chiral condensate \( \bar{\psi} \psi \). These are given already in eq. (17) and, due to additional mass factors (see eq. (16)), certainly will not lead to a singular behaviour in the specific heat. From eq. (5) one expects that the quark mass dependence of the specific heat peak is controlled by the exponent \( z_\alpha = \alpha / \beta \delta \). In the case of the \( O(N) \) models in three dimensions the situation becomes, however, a bit more complicated due to the fact that the exponent \( \alpha \) is expected to be negative [4]. In this case the specific heat is not expected to diverge, but rather should develop a cusp at \( T_c \). Accordingly none of the response functions defined in eq. (20) is actually expected to diverge. They rather should approach a constant in the limit of vanishing quark mass, with the quark mass dependence described by eq. (10).

4) Numerical Results

We have performed calculations on an \( 8^3 \times 4 \) lattice, which may be considered to be quite a small lattice, yet, Ref. [5] shows that varying the spatial lattice extent from \( N_\sigma = 6 \) to 12 at \( N_\tau = 4 \) surprisingly does not change the pseudo-critical temperature [8]. Likewise, increasing \( N_\tau \) from 4 to 8 while keeping \( N_\sigma / N_\tau \) between 2 and 4 also does not lead to apparent differences in the scaling behaviour of the pseudo-critical points. Nonetheless, it is important to get control over finite size effects. The present analysis should thus be considered as a first step towards a quantitative determination of critical exponents in QCD with light fermions.

For the quark masses, we have chosen the values \( m_q = 0.075, 0.0375 \) and 0.02 in units of the lattice spacing \( a \). These quark masses have been selected such that they can provide additional information on the quark mass dependence of pseudo-critical couplings beyond the existing data [2]. At each value of the quark mass we have performed simulations at several values of the gauge coupling, \( 6 / g^2 \), in the pseudo-critical region. The simulations have been carried out by means of the so-called hybrid R algorithm [13]. Guided by analyses of the hybrid Monte Carlo algorithm, we have scaled the step size according to the quark mass, \( d\tau = 0.05, 0.04 \) and 0.03 (in the normalization of [13]) for \( m_q = 0.075, 0.0375 \) and 0.02 respectively. The trajectory length was fixed to \( \tau = 1 \). For the conjugate gradient inversion we have settled at a required precision of \( (\Phi - DX)^2 / \Phi^2 \leq 0.5 \times 10^{-13} \). The
autocorrelation times have been determined to $\tau_{\text{exp}} \leq 100$ trajectories right on the pseudo-critical couplings, the longest correlations being in the Polyakov loop, while away from the cross-over $\tau_{\text{exp}}$ is considerably smaller. At each value of the coupling we collected between 5000 and 10000 trajectories which then have been analyzed using a reweighting with the density of states at intermediate values of the gauge coupling [14]. Errors were computed by the jack-knife procedure.

4.1) Susceptibilities and the Specific Heat

In Fig. 1 we show the Polyakov loop response function, $\chi_L$, for three values of the quark mass. Pronounced peaks are clearly visible. Although the location of the peaks clearly depends on $m_q$, their heights do not have any significant quark mass dependence. This is consistent with the analysis presented in Ref. [8], which also suggests that the volume dependence of the peak height is small and distinctively different from the situation in the pure gauge theory.

The behaviour of $\chi_L$ is also drastically different from that of the chiral susceptibility, $\chi_m$, which is shown in Fig. 2. The rise in the peak height with decreasing quark mass as well as the shift in the critical coupling is clearly seen. In Fig. 2 the two contributions, $\chi_0$ and $\chi_{\text{conn}}$ are shown separately. The contribution from the connected part to the susceptibility is a slowly varying function in the critical region. The ratio $\chi_{\text{conn}}/\chi_0$ decreases with decreasing quark mass. However, even for $m_q = 0.02$ we find that $\chi_{\text{conn}}$ contributes about 30% to the value of $\chi_{m,\text{max}}$ and in the region of the zero quark mass critical temperature it gives the dominant contribution. This will be particularly important for our discussion of the chiral cumulant in section 4.3.

| $z_m$  | $z_{t,\sigma}$ | $z_{t,\tau}$ | $z_{t,f}$ | $z_L$  |
|-------|----------------|--------------|----------|-------|
| 0.79(4) | 0.63(7)  | 0.63(7)  | 0.65(7)  | 0.05(6)  |

Table II: Critical exponents controlling the divergence of the chiral ($m$), Polyakov loop ($L$) and various parts of the thermal susceptibilities in the limit of vanishing quark mass. Results are obtained from straight line fits to the data shown in Fig. 4.

In Fig. 3 we show the partial contributions to the thermal susceptibility, defined in eq.(17). It is apparent that all three have a similar quark mass dependence. Note also that the peak position in all three cases coincides with the pseudo-critical couplings in $\chi_L$ or $\chi_m$. 
The peak heights of all susceptibilities are shown in Fig. 4 as a function of quark mass. A fit with a powerlike singular behaviour as indicated in eq. (18) yields the critical exponents given in Table II. While the exponent \( z_L \) is compatible with being zero, we find that \( z_m \) is in remarkably good agreement with the \( O(N) \) prediction. The agreement is not that good for the exponent of the thermal susceptibility, which comes out to be about 50% larger than expected for an \( O(N) \) symmetric model. This, however, is not that unexpected as the exponent \( z_m \) is only sensitive to the magnetic exponent \( y_h \), while \( z_t \) is also related to \( y_t \). The latter gives directly the correlation length exponent \( y_t = 1/3 \nu \) and thus is expected to be more sensitive to the spatial size of the system. We can rephrase our numerical results for \( z_m \) and \( z_t \) in terms of the exponents \( y_h \) and \( y_t \). This yields

\[
y_h = 0.83 \pm 0.03 , \\
y_t = 0.69 \pm 0.07 ,
\]

which should be compared with the \( O(4) \) values \( y_h = 0.828 \) and \( y_t = 0.452 \).

As has been discussed above the various response functions contributing to the specific heat are not expected to diverge in the zero quark mass limit. Results for three of the six different response functions defined in eq.(20) are shown in Fig. 5 for the three different quark mass values studied here. A comparison with the susceptibilities displayed in Figs. 3 and 4 clearly shows that the increase in the peak height is considerably slower. However, we do not have any direct evidence for a finite limit of the peak height in the limit of vanishing quark mass. Results for the calculated peak values, \( C_{V}^{\text{max}} \), and the corresponding pseudo-critical couplings are given in Table III. We have analyzed the scaling behaviour of these peaks in two ways, which clearly show the present uncertainties in the determination of \( z_\alpha \):

(i) Assuming that the specific heat diverges in the zero quark mass limit,

one can analyze the quark mass dependence of the specific heat response functions in the same way as the various components of the susceptibilities, i.e. we fit the peak heights to eq. (10) with \( c_0 \equiv 0 \). By construction this leads to \( z_\alpha > 0 \). We find, depending on the particular response function, values for \( z_\alpha \) between 0.28 and 0.34. The best fit result yields \( z_\alpha = 0.28(6) \).

(ii) Assuming that the specific heat stays finite in the zero quark mass limit,

one can fit the peak heights to eq. (21) with \( c_0 > 0 \). By construction this leads to \( z_\alpha < 0 \). As can be seen in Fig. 5 the strongest quark mass dependence is found in the purely gluonic response functions. They lead to \( z_\alpha = -0.05(2) \).

We note that even by assuming a finite specific heat in the limit of vanishing quark mass our fits suggest a large value of the response functions in that limit. For instance we
find $C_{V,\tau}^{\text{max}}(m_q = 0) \simeq 6$. This indicates that these response function will still show quite a strong quark mass dependence also for quite small values of $m_q$, which is related to the nearly vanishing magnitude of $\alpha$ ($\alpha = 0$ corresponds to a logarithmic singularity). The upper limit for $\alpha$ obtained in this analysis, $\alpha \leq 0.34$, corresponds to an upper limit of 0.6 for the thermal exponent $y_t$. As can be seen from eq. (21) this is slightly lower than the result obtained from the analysis of the thermal susceptibility.

Further calculations at smaller quark masses are thus particularly interesting for these response functions and are needed in order to extract the thermal exponent $y_t$ and to further clarify the nature of the scaling behaviour of the specific heat in the zero quark mass limit.

| $m$   | $D\sigma$   | $D\tau$   | $\sigma\tau$ | $\sigma\sigma$ | $\tau\tau$ |
|-------|-------------|------------|---------------|-----------------|-------------|
| 0.075 | 0.0535(53)  | 0.0691(60) | 0.761(65)     | 0.807(58)       | 0.957(71)   |
|       | 5.350(4)    | 5.350(4)   | 5.348(4)      | 5.348(4)        | 5.348(4)    |
| 0.0375| 0.0722(83)  | 0.0921(97) | 0.974(45)     | 0.999(40)       | 1.193(51)   |
|       | 5.306(4)    | 5.306(4)   | 5.306(2)      | 5.306(2)        | 5.306(2)    |
| 0.02  | 0.0844(61)  | 0.1040(66) | 1.165(62)     | 1.170(53)       | 1.409(70)   |
|       | 5.282(2)    | 5.282(2)   | 5.282(2)      | 5.282(2)        | 5.282(2)    |

Table III: The peak values of various response functions contributing to the specific heat and the corresponding values of the pseudo-critical couplings.

4.2) Pseudo-Critical Couplings

The locations of the peaks in the various susceptibilities or the specific heat, which have been discussed in the previous section, can be used to define pseudo-critical couplings. Although these pseudo-critical couplings may differ for different observables at non-vanishing values of the quark mass, we found that they agreed within our numerical accuracy. We thus may quote a common pseudo-critical coupling for all the response functions analyzed by us. These are collected in Table IV.

It is quite reassuring that the pseudo-critical couplings extracted from the location of the peak in $\chi_m$, the various components of $\chi_t$ and $C_V$ agree this well. In particular this shows that the pseudo-critical couplings, extracted so far from the variation of the slope of $\langle \bar{\psi}\psi \rangle$ as a function of $6/g^2$ (this corresponds to the location of the peak in $\chi_{t,\sigma(\tau)}$) can
indeed be used to discuss the scaling behaviour of these couplings as a function of the quark mass.

| $m_q$   | $6/g_c^2$  |
|---------|------------|
| 0.075   | 5.350(4)   |
| 0.0375  | 5.306(2)   |
| 0.02    | 5.282(2)   |

Table IV: Pseudo-critical couplings determined from the location of the peak in various response functions. Errors are obtained from a jack-knife analysis of the interpolation curves resulting from a reweighting with the density of states method.

In Fig. 6 we show the quark mass dependence of the pseudo-critical couplings. Here we also include data from earlier simulations [6,7], which have been summarized in Ref. [2]. The pseudo-critical couplings have been fitted with the ansatz

$$\frac{6}{g_c^2(m_q)} = c_0 + c_1 m_q^{z_c},$$

where $c_0$ gives the critical coupling in the zero quark mass limit and $z_c \equiv 1/\beta\delta$. We find

$$\frac{6}{g_c^2(0)} = 5.243 \pm 0.010$$

$$\frac{1}{\beta\delta} = 0.77 \pm 0.14$$.

Compared to the corresponding $O(4)$ value $1/\beta\delta = 0.55(2)$ and the $O(2)$ value $1/\beta\delta = 0.60(1)$ the three parameter fit yields a larger value for this combination of exponents. However, also a two parameter fit with $1/\beta\delta$ fixed to its $O(4)$ value still yields a good $\chi^2$. We show this fit also in Fig. 6. The resulting zero quark mass critical coupling is found to be $6/g_c^2(0) = 5.222 \pm 0.003$. We also note that the result obtained for $1/\beta\delta$ is consistent with the determination of the thermal and magnetic exponents in the previous section and also suggests that in our present analysis we overestimate the value for $y_t$.

4.3) The Chiral Cumulant

The most direct procedure to determine the critical exponent $\delta$, which is independent of any ansatz for a fitting function, is given through an analysis of the chiral cumulant, defined in eq. (8). In the vicinity of the critical point this is a simple scaling function and
curves for different quark masses cross in a unique point - the zero mass critical coupling, if subleading corrections from the non-singular part of thermodynamic quantities can be ignored. In Fig. 7 we show $\Delta(6/g^2, m_q)$ for our three different quark masses. For the largest mass the pseudo-critical region was quite far away from the zero quark mass critical region and we did not attempt to extend the calculations for that mass into this regime. The simulations for the two smaller quark masses, however, have been extended into this region and we see from Fig. 7 that they indeed cross at a coupling, which is consistent with the result obtained from our fit to the pseudo-critical couplings (Fig. 6). Moreover, we find that the value of $\Delta$ at the crossing point gives an astonishingly accurate estimate of $1/\delta$. In fact, due to the rather weak dependence of $\Delta$ on the coupling $6/g^2$ in this region, we find that the exponent $1/\delta$ is much better determined than the zero quark mass critical coupling. Taking for the latter the interval of values obtained from the two fits shown in Fig. 6, i.e. $5.22 < 6/g^2(0) < 5.25$, we get for the exponent $\delta$,

$$0.21 < 1/\delta = 0.23 < 0.26.$$  \hspace{1cm} (24)

5) Conclusions

We have studied various response functions which contribute to susceptibilities and the specific heat in two-flavour QCD, simulated with staggered fermions on a lattice of size $8^3 \times 4$. We find that these observables are very well suited to localize the pseudo-critical couplings at non-vanishing values of the quark mass. At least at the moderate values of the quark mass analyzed here the height of the peaks in the susceptibilities is very well determined and can be used to investigate the scaling behaviour of these quantities. The analysis of the peak heights in the response functions as well as the quark mass dependence of the peak location yields independent observables, which can be used to determine the critical exponents $\alpha$, $\beta$ and $\delta$. Additional information on $\delta$ and the location of the zero quark mass critical point is obtained from the structure of the chiral cumulant. These exponents can be related to the two basic exponents $y_t$ and $y_h$, which characterize the scaling behaviour of the singular part of the free energy density.

Our present analysis yields a magnetic exponent $y_m$, which is consistent with the value expected for a second order phase transition controlled by $O(4)$ exponents (eq. (21)). Our result for the thermal exponent, however, turns out to be about 50% larger than the corresponding $O(4)$ value.

Clearly the errors are still quite large. However, the present results are consistent with our expectations based on the existence of a second order phase transition in the limit of
vanishing quark mass. We find it particularly reassuring, that we obtain the weakest quark mass dependence in response functions which contribute to the specific heat. We also confirm a weaker quark mass dependence of the peak of the thermal susceptibility relative to that of the chiral susceptibility. Moreover, we find that the Polyakov loop response function is insensitive to changes in the quark mass. This suggests that, indeed, the chiral symmetry restoration is the driving mechanism for the finite temperature phase transition in two flavour QCD.

We expect that in particular the thermal exponent $y_t$ is sensitive to finite lattice effects. The behaviour of the susceptibilities thus has to be studied for smaller quark masses and on larger lattices.

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References

1) For a recent review see: F. Karsch, Nucl. Phys. B (Proc. Suppl.) 34 (1994) 63.
2) F. Karsch, Phys. Rev. D49 (1994) 3791.
3) R.D. Pisarski and F. Wilczek, Phys. Rev. D29 (1984) 338.
4) F. Wilczek, Intern. J. Mod. Phys. A7 (1992) 3911; K. Rajagopal and F. Wilczek, Nucl. Phys. B399 (1993) 395.
5) J.I. Kapusta and A.M. Srivastava, The Proximal Chiral Phase Transition, NSF-ITP-94-28.
6) S. Gottlieb, Phys. Rev. D47 (1993) 3619 and references therein.
7) F.R. Brown et al., Phys. Rev. Lett. 65 (1990) 2491.
8) M. Fukugita, H. Mino, M. Okawa and A. Ukawa, Phys. Rev. D42 (1990) 2936.
9) G. Boyd, J. Fingberg, F. Karsch, L. Kärkkäinen and B. Petersson, Nucl. Phys. B376 (1992) 199.
10) G. Baker, D. Meiron and B. Nickel, Phys. Rev. B17 (1978) 1365.
11) J.C. Le Guillou and J. Zinn-Justin, Phys. Rev. B21 (1980) 3976 and J. Phys. Lett. (Paris) 46 (1985) L-137.
12) for a discussion of QCD thermodynamics on the lattice see for instance: F.Karsch, Simulating the Quark-Gluon Plasma on the Lattice, Advanced Series on Directions in High Energy Physics - Vol.6 (1990) 61, "Quark Gluon Plasma" (Ed. R.C. Hwa), Singapore 1990, World Scientific.
13) S. Gottlieb, W. Liu, D. Toussaint, R.L. Renken and R.L. Sugar, Phys. Rev. D35 (1987) 3972.
14) for a discussion of our implementation of the density of state method and references see: J. Fingberg, U. Heller and F. Karsch, Nucl. Phys. B392 (1993) 493.
Figure Captions

Figure 1: The Polyakov loop response function versus $6/g^2$ for three values of the quark mass. Shown are results from a reweighting analysis with bins of length $\Delta(6/g^2) = 0.002$ close to the pseudo-critical coupling and 0.005 elsewhere. The couplings at which simulations have actually been performed are marked by filled symbols.

Figure 2: The chiral susceptibility versus $6/g^2$ for three values of the quark mass. Results from a reweighting analysis for the disconnected part $\chi_0$ and the connected part $\chi_{\text{conn}}$ defined in eq. (13) are shown separately.

Figure 3: The three response functions which contribute to the thermal susceptibility defined in eqs. (15)-(17).

Figure 4: Peak values of the Polyakov loop response function ($\chi_L$), the chiral ($\chi_m$) and the thermal ($\chi_t$) susceptibility versus the quark mass.

Figure 5: Three response functions which contribute to the specific heat as defined in eq. (20).

Figure 6: Pseudo-critical couplings, $6/g_c^2(m_q)$, versus $h = N\tau m_q$ for $N\tau = 4$. The three new values analyzed here are shown as full diamonds. The other data points are taken from the collection given in Ref. [2]. The dashed curve is a three parameter fit with eq. (22). The solid curve is a two-parameter with this function and $z_c$ fixed to the $O(4)$ value $z_c = 0.55$.

Figure 7: The chiral cumulant, $\Delta$, versus $6/g^2$ for three values of the quark mass.
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\( \chi_m \)

\[ m_q = 0.02 \]

\[ m_q = 0.0375 \]

\[ m_q = 0.075 \]

\( 6/g^2 \)
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\( \chi_{t,0} \) for various values of \( m_q \):
- \( m_q = 0.02 \)
- \( m_q = 0.0375 \)
- \( m_q = 0.075 \)

\( \chi_{t,T} \)

\( \chi_{t,f} \)
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