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Flavour Breaking Effects of Wilson twisted mass fermions

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Abstract

We study the flavour breaking effects appearing in the Wilson twisted mass formulation of lattice QCD. In this quenched study, we focus on the mass splitting between the neutral and the charged pion, determining the neutral pion mass with a stochastic noise method to evaluate the disconnected contributions. We find that these disconnected contributions are significant. Using the Osterwalder-Seiler interpretation of the *connected* piece of the neutral pion correlator, we compute the corresponding neutral pion mass to study with more precision the scaling behaviour of the mass splitting.

1 Introduction

Wilson twisted mass fermions [1, 2] have by now been employed extensively in numerical simulations of lattice QCD, both quenched [3, 4, 5, 6, 7, 8] and unquenched [9, 10, 11, 12] with very promising results: In the quenched case, the anticipated $O(a)$-improvement for physical observables at full twist [2] has been demonstrated and, employing a definition of the critical mass derived from the vanishing of the PCAC quark mass [13, 14, 15], it has also been demonstrated numerically [5, 6, 8] and analytically [15] that $O(a^2)$ effects are small for physical quantities even at low values of the pion mass of about 270 MeV. These results are very encouraging, in particular if one thinks of eventual dynamical simulations at full twist which we have just started.

One important property of the twisted mass approach is that at a non-vanishing value of the lattice spacing a, flavour symmetry is explicitly broken. This manifests itself, e.g. in the mass splitting, as a non-vanishing difference of the charged m_{π^+} and the neutral m_{π^0} pion masses. Of course, this phenomenon is a pure cut-off effect which is expected to vanish, at full twist, quadratically with the lattice spacing when the continuum limit is approached. We will concentrate in this work on the difference $m_{\pi^0} - m_{\pi^+}$ to study the flavour breaking effects and their lattice spacing dependence. We will compute the neutral pion mass from the connected and disconnected pieces of the corresponding correlation function using the stochastic noise source method of refs. [16, 17] for the disconnected diagrams. In quenched studies, the disconnected contributions to flavour singlet correlators are known to be pathological - having a double pole structure. Note, however, that for the twisted mass situation even in the quenched approximation in the continuum limit the full neutral pion correlation function (connected plus disconnected parts) is a well-defined correlator since at $a = 0$ the flavour symmtry is restored and the twisting is just a formal rotation that leaves the theory invariant. Therefore the continuum limit of the neutral pion correlator evaluated at a non-vanishing value of the lattice spacing can be taken. Additionally, we consider another definition of the neutral pion mass from the connected piece of the twisted mass neutral pion correlator alone, using the Osterwalder-Seiler interpretation [18, 19] of this correlator. This last procedure is only valid in the quenched approximation and will mainly provide a more accurate estimate of the scaling properties of the flavour breaking cut-off effects, checking the strength of the $O(a^2)$ cut-off effects.

We will work with two definitions for the critical quark mass. The first is the point where the pion mass vanishes, the second, where the PCAC quark mass vanishes. In the following we will refer to the first situation as the "pion definition" and to the second situation as the "PCAC definition" of the critical point. Both definitions lead to an $O(a)$-improvement, but they can lead to very different $O(a^2)$ effects [15], in particular at small pion masses. In the language of twisted mass lattice QCD, tuning to the critical quark mass corresponds to working at full twist. In refs. [5, 6] we presented results from both definitions of the critical bare quark mass and demonstrated that the PCAC definition shows indeed small scaling violations even when the pion mass is taken to be as low as 270 MeV. Here we are interested to see, whether also for the pion mass difference a similar situation occurs.

While it is the primary goal of this paper to study the strength of flavour breaking effects in Wilson twisted mass QCD, another interesting question is the evaluation of the disconnected diagrams themselves within this approach. Such disconnected diagrams are needed in many physical problems such as the computation of the pseudoscalar and scalar flavour singlet masses, the decay of the ρ-meson, the phenomenon of string breaking and contributions to the vacuum polarisation tensor. In addition, if one thinks of simulations with mixed actions, it becomes again important to know, how reliably the disconnected diagrams can be computed. It is hence of an essential interest to know whether the disconnected pieces can be computed with a reasonable number, say $O(100-500)$, of independent gauge field configurations and $O(10-50)$ stochastic noise vectors.

2 Wilson twisted mass fermions

The Wilson twisted mass action in the so-called twisted basis can be written [2] as

$$S[U,\chi,\bar{\chi}] = a^4 \sum_x \bar{\chi}(x)(D_W + m_0 + i\mu\gamma_5\tau_3)\chi(x) \equiv \bar{\chi} D_{\mathrm{tm}} \chi \ , \tag{1}$$

where the Wilson-Dirac operator D_{W} is given by

$$D_{\mathrm{W}} = \sum_{\mu=0}^{3} \frac{1}{2}[\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\nabla_\mu^*\nabla_\mu] \tag{2}$$

and ∇_μ and ∇_μ^* denote the usual forward and backward derivatives and the Wilson parameter r was set to 1.

The situation of full twist and hence automatic $O(a)$ improvement arises when m_0 in eq. (1) is tuned towards a critical bare quark mass m_{c}. We use for our simulations the hopping representation of the Wilson-Dirac operator with $\kappa = (2am_0+8)^{-1}$ and hence this critical quark mass corresponds to a critical hopping parameter $\kappa_{\mathrm{c}} = (2am_{\mathrm{c}}+8)^{-1}$. As remarked in the introduction, in this paper we will use the pion and the PCAC definitions of κ_{c} to realize full twist.

We consider the local bilinears $P^\pm = \bar{\chi}\gamma_5\frac{\tau^\pm}{2}\chi$ and $P^0 = \bar{\chi}\chi$ (corresponding to the scalar operator in the twisted basis), where χ denotes a mass-degenerate doublet of up and down quarks. From these operators we extract the charged m_{π^+} and neutral m_{π^0} pseudoscalar masses from the correlation functions:

$$\begin{aligned} C_{\pi^+}(x_0) &= a^3 \sum_{\mathbf{x}} \langle \left[P^+(x)P^-(0)\right]_{\mathrm{con}} \rangle \ , \\ C_{\pi^0}(x_0) &= a^3 \sum_{\mathbf{x}} \langle \left[P^0(x)P^0(0)\right]_{\mathrm{con}} + \left[P^0(x)P^0(0)\right]_{\mathrm{disc}} \rangle \end{aligned} \tag{3}$$

where

$$\left[P^0(x)P^0(0)\right]_{\rm disc} = \left[{\rm tr}D_{\rm tm}^{-1}\right](x)\left[{\rm tr}D_{\rm tm}^{-1}\right](0) \tag{4}$$

with the vacuum contribution to ${\rm tr}D_{\rm tm}^{-1}$ being subtracted and the trace taken over colour and Dirac indices. We indicate in eqs. (3) the connected (con) and the disconnected (disc) pieces of the correlation function and denote by [ ] the fermionic contractions only.

We also checked the operator $A_0^3 = \bar{\chi}\gamma_0\gamma_5\frac{\tau^3}{2}\chi$ to compute the neutral pion correlation function which has the advantage to not develop a vacuum contribution. However, we found that this operator is very noisy for the disconnected contribution and could not be used to extract a signal. We see two possible explanations for this behaviour. The first is that the operator itself is proportional to the pion mass. Hence, the signal becomes small at low values of the pion mass while the error remains roughly constant. The other reason can be that in the free theory the correlation function is identically zero since from the fermionic contractions there remains only a ${\rm tr}\gamma_0$. Consequently, the correlation function starts with a $a^2g_0^2$ behaviour, leading again to a possible small signal. We cannot disentangle what is the major effect for the observed large fluctuations in the A_0^3 correlation function, or, whether it is a mixture of both. Anyway, we conclude that the A_0^3 operator is, from a practical point of view, not a suitable operator to study the neutral pion correlation function.

3 Results

In this section we present our simulation results. We use a stochastic source method, for which we only employ the PCAC definition for the critical point. We will also use the connected part of the neutral pion correlation function which we interprete with the help of the Osterwalder-Seiler action. For this part, we use both, pion and PCAC definitions of the critical point.

3.1 Stochastic source method

The correlation function for the neutral pion in eq. (3) has a connected piece as well as a disconnected piece. While the connected piece can be computed by standard methods using local or smeared sources, we evaluate the disconnected piece by stochastic source methods. We follow here the techniques used in refs. [20, 21], in particular we used a stochastic source method with variance reduction as described in the appendix of ref. [20]. Given a number of gauge field configurations, see table 1 for our statistics, we performed the evaluation of the disconnected piece of the correlation function for a number N_Φ stochastic noise vectors Φ. We found that for $N_\Phi = 24$ the contribution of the stochastic sources to the total error is less or comparable to the error from the gauge field average. Hence, for the stochastic estimate of the disconnected pieces of the correlation function $C_{\pi^0}(x_0)$ in eq. (3) we

$\mathrm{N_{meas}}$	β	κ_{c}	μa	$m_{\pi^0}a(\mathrm{tot})$	$m_{\pi^0}a - m_{\pi^+}a$
400	6.0	0.157409	0.0038	0.19(2)	0.07(2)
400	6.0	0.157409	0.0076	0.19(2)	0.02(2)
400	6.0	0.157409	0.0109	0.23(2)	0.02(2)
100	5.85	0.162379	0.0050	0.28(5)	0.12(5)
100	5.85	0.162379	0.0100	0.25(5)	0.02(5)
100	5.85	0.162379	0.0144	0.28(6)	0.00(6)

Table 1: *The number of gauge field configurations N_{meas} as well the values of β, κ_{c} and μ we have used for the stochastic source method. We give the values of the neutral pion mass m_{π^0} evaluated from fits to the full correlation function $C_{\pi^0}(x_0)$ in eq. (3) and the mass splitting $m_{\pi^0} - m_{\pi^+}$. Data for the charged pion mass m_{π^+} and the neutral pion mass computed from the connected piece of the correlation function can be found in tables 4 and 5. The computations used $N_\Phi = 24$ stochastic noise sources to determine the disconnected pieces of the correlation functions.*

always used $N_\Phi = 24$. We measure the disconnected contributions for both local and fuzzed (non-local) [22] operators which gave consistent results. Let us mention that we used as a check the stochastic source method also for the connected piece of the correlation functions in eq. (3) and found full agreement with the computation by standard methods. In table 1 we give the parameter values for β, μ and κ_{c} that we have used for the analysis using the stochastic source method. Note that here we only employ the PCAC definition of κ_{c} to realize full twist. Table 1 contains our results for the neutral pion mass m_{π^0} and the mass splitting $m_{\pi^0} - m_{\pi^+}$.

In fig. 1 we show, as an example, the ratio of the correlation functions of the neutral and the charged pion at $\beta = 6.0$ and $\mu a = 0.0038$. We show the ratio of the correlation functions for the connected part only and for the full correlation function including the disconnected piece. Clearly, the ratio of these correlation functions is not constant and does not assume a value of one as would be the case for a situation where no flavour violation appears. In fact, the deviations from one of the correlation function ratio appears to be rather large indicating strong flavour breaking effects. Note, however, that these effects are substantially larger when only the connected pieces are considered and the addition of the disconnected piece reduces the flavour symmetry violation significantly. We also remark that the ratio of pion correlators is closer to 1.0 at $\beta = 6.0$ compared to $\beta = 5.85$. This indicates that the flavour breaking effects become small when the continuum limit is approached as can also be seen from the comparison of $\Delta m = m_{\pi^0} - m_{\pi^+}$ in table 1. We will come back to this point in the next section. The time dependence of the ratio in the graph reflects the fact that the mass splitting Δm is non-vanishing and positive. The solid lines in fig. 1 are the ratio of the fit functions obtained by separate fits to the neutral and charged pion correlation functions.

We also considered the flavour splitting between the charged and neutral states of the scalar meson with $I = 1$, the a_0. Consider the correlation function of the bilinear operator $a_0^0 = \bar{\chi}\gamma_5\chi$ and the mass splitting with the corresponding charged state a_0^+ where the correlation function for a_0^0 again has a disconnected piece. As for the π, we find that the disconnected contribution to a_0^0 is such as to reduce the flavour violation from that observed with the connected piece alone. However, both correlation functions (for a_0^0 and a_0^+) become negative as t increases, demonstrating the failure of the quenched approximation. We finally remark that also for the a_0^+, a_0^0 system the flavour breaking effects are reduced when moving from $\beta = 5.85$ to $\beta = 6.0$ indicating that this effect will disappear in the continuum limit.

3.2 Osterwalder-Seiler interpretation

The calculation of the disconnected piece for the neutral pion correlation function leads to a rather large error for the neutral pion mass. One may wonder, whether the neutral pion mass could not be extracted from the connected piece of this correlation function alone. However, in principle neglecting the disconnected diagram may lead to a correlator that does not have an interpretation in terms of a local operator and so does not have an interpretation in terms of the transfer matrix. One way out of this problem is to use the Osterwalder-Seiler (OS) action to interprete the connected piece of the twisted mass neutral pion correlation function. As we will see, the connected piece can provide, at least in the here used quenched approximation, a sensible definition of the neutral pion mass. This will allow us to test the scaling behaviour of the mass splitting in Wilson twisted mass QCD.

In the Osterwalder-Seiler (OS) action [18, 19] the τ_3 matrix of eq. (1) is replaced by a unit matrix in flavour space. With such an action there is no flavour breaking and the difference between neutral and charged pion masses vanishes, $m_{\pi^+} = m_{\pi^0}$. For the OS action,

$$C^{\mathrm{OS}}_{\pi^+}(x_0) = C^{\mathrm{OS}}_{\pi^0}(x_0) \tag{5}$$

where no disconnected piece appears. In contrast, for the twisted mass action we have

$$C^{\mathrm{tm}}_{\pi^0}(x_0) = (C^{\mathrm{tm}}_{\pi^0}(x_0))_{\mathrm{con}} + (C^{\mathrm{tm}}_{\pi^0}(x_0))_{\mathrm{disc}} \ . \tag{6}$$

Now, the crucial observation is that

$$C^{\mathrm{OS}}_{\pi^0}(x_0) = (C^{\mathrm{tm}}_{\pi^0}(x_0))_{\mathrm{con}} \ . \tag{7}$$

Thus $(C^{\mathrm{tm}}_{\pi^0}(x_0))_{\mathrm{con}}$ can be interpreted as the correlation function of a local operator and has therefore a standard transfer matrix decomposition. In particular, the exponential decay of $(C^{\mathrm{tm}}_{\pi^0}(x_0))_{\mathrm{con}}$ will allow us to extract the neutral pion mass and, since we can neglect the disconnected piece, the correlation function can be evaluated with good precision. Let us, nevertheless, emphasise that it is the main goal of this investigation to check whether the mass splitting shows the expected $O(a^2)$ lattice artifacts and to estimate the size of the flavour breaking effects.

β	5.85	6.00	6.20
a (fm)	0.123	0.093	0.068
r_0/a	4.067	5.368	7.360
L/a	16	16	24
T/a	32	32	48
	pion definition of κ_c		
N_{meas}	378	387	260
$\mu_1 a$	0.0050	0.0038	0.0028
$\mu_2 a$	0.0100	0.0076	0.0055
$\mu_3 a$	0.0200	0.0151	0.0111
$\mu_4 a$	0.0400	0.0302	0.0221
$\mu_5 a$	0.0600	0.0454	0.0332
$\mu_6 a$	0.0800	0.0605	0.0442
$\mu_7 a$	0.1000	0.0756	0.0553
	PCAC definition of κ_c		
N_{meas}	500	400	300
$\mu_1 a$	0.0050	0.0038	0.0028
$\mu_2 a$	0.0100	0.0076	0.0055
$\mu_3 a$	0.0200	0.0151	0.0111
$\mu_4 a$	0.0400	0.0302	0.0221
$\mu_5 a$	0.0600	0.0454	0.0332
$\mu_6 a$	0.0800	0.0605	0.0442
$\mu_7 a$	0.1000	0.0756	0.0553

Table 2: *Simulation parameters*

In table 2 we give the simulation parameters and the statistics of our quenched runs. We give in table 3 the values for the critical hopping parameter obtained from the pion and the PCAC definitions of the critical mass. Finally, we show in table 4 our results for the charged pion mass and in table 5 for the neutral pion mass. Note that the data in tables 3 and 4 are the same as in ref. [6] and are only given here for completeness.

In fig. 2 we show the relative difference $(m_{\pi^0} - m_{\pi^+})/m_{\pi^+}$ as a function of $(a/r_0)^2$, where $r_0 = 0.5$ fm is the Sommer parameter [23]. For the plot we use data from the pion definition (open circles) and the PCAC definition (filled circles) fixing the pion mass to be 297 MeV and 382 MeV.

Fig. 2 demonstrates that the scaling of the mass splitting is consistent with an a^2 behaviour as expected. On the other hand, as we already discussed in the previous section, the flavour breaking effects turn out to be rather large. For the case of the conventional twisted theory, with disconnected contributions to the π^0 included, the errors are sufficiently large that a precise estimate of the scaling behaviour of the

β	pion κ_c	PCAC κ_c
5.85	0.161662(17)	0.162379(93)
6.0	0.156911(35)	0.157409(72)
6.2	0.153199(16)	0.153447(32)

Table 3: *Critical values of the hopping parameters obtained from the vanishing of the pseudoscalar meson mass (pion κ_c) and from the vanishing of the PCAC mass (PCAC κ_c).*

β	5.85	6.00	6.20
	$m_{\pi^+}a$ (pion κ_c)		
$\mu_1 a$	0.1682(26)	0.1385(66)	0.1004(27)
$\mu_2 a$	0.2256(22)	0.1764(42)	0.1298(23)
$\mu_3 a$	0.3122(19)	0.2373(32)	0.1768(17)
$\mu_4 a$	0.4452(14)	0.3335(22)	0.2463(15)
$\mu_5 a$	0.5535(12)	0.4134(17)	0.3037(13)
$\mu_6 a$	0.6488(13)	0.4839(16)	0.3546(12)
$\mu_7 a$	0.7358(12)	0.5491(14)	0.4021(11)
	$m_{\pi^+}a$ (PCAC κ_c)		
$\mu_1 a$	0.1640(23)	0.1217(66)	0.0934(24)
$\mu_2 a$	0.2289(17)	0.1708(50)	0.1276(21)
$\mu_3 a$	0.3232(13)	0.2396(33)	0.1779(18)
$\mu_4 a$	0.4606(11)	0.3403(22)	0.2492(13)
$\mu_5 a$	0.5701(10)	0.4214(17)	0.3071(12)
$\mu_6 a$	0.6658(9)	0.4925(14)	0.3588(10)
$\mu_7 a$	0.7530(9)	0.5579(14)	0.4062(9)

Table 4: *Pseudoscalar meson masses $m_{\pi^+}a$ for all simulation points.*

mass difference cannot be obtained. However, we have shown that the size of the flavour breaking effects is reduced when the disconnected piece of the correlation function is included.

Another somewhat surprising observation is that the flavour breaking effect is larger for the PCAC definition of κ_c than for the pion definition of κ_c. We interpret this phenomenon in the following way: for Wilson twisted mass fermions at non-vanishing twist angle it is not possible to conserve *simultaneously* parity and flavour symmetry. Using the PCAC definition of κ_c, parity is restored as well as possible, leading to a large violation of flavour symmetry. When using the pion definition of κ_c one looses somewhat on the parity violation but gains on the flavour symmetry. This interpretation follows from an analytical study in the framework of Wilson chiral perturbation theory [24, 13]. With ω the twist angle, it is shown in these

β	5.85	6.00	6.20
	$m_{\pi^0}a$ (pion κ_c)		
$\mu_1 a$	0.245(12)	0.1858(84)	0.1150(47)
$\mu_2 a$	0.2989(63)	0.2202(43)	0.1419(27)
$\mu_3 a$	0.3759(58)	0.2751(28)	0.1887(16)
$\mu_4 a$	0.4974(31)	0.3621(20)	0.2563(12)
$\mu_5 a$	0.5983(25)	0.4371(17)	0.3119(12)
$\mu_6 a$	0.6887(23)	0.5047(14)	0.3615(11)
$\mu_7 a$	0.7726(23)	0.5670(14)	0.4082(10)
	$m_{\pi^0}a$ (PCAC κ_c)		
$\mu_1 a$	0.319(14)	0.2183(92)	0.123(10)
$\mu_2 a$	0.3510(79)	0.2458(51)	0.1537(50)
$\mu_3 a$	0.4137(44)	0.2929(29)	0.1970(22)
$\mu_4 a$	0.5276(24)	0.3746(20)	0.2615(14)
$\mu_5 a$	0.6255(22)	0.4478(15)	0.3163(12)
$\mu_6 a$	0.7143(19)	0.5150(14)	0.3655(12)
$\mu_7 a$	0.7969(18)	0.5782(13)	0.4120(11)

Table 5: *Neutral pion masses $m_{\pi^0}a$ coming from the connected correlators for all simulation points.*

references that the mass splitting is proportional to $\sin(\omega)$ indicating a maximal flavour symmetry violation at maximal twist angle.

4 Conclusion

In this paper we have studied the flavour breaking effects of Wilson twisted mass lattice QCD in the quenched approximation. We focussed on the example of the mass splitting of the neutral to charged pion. While the charged pion mass has been computed with standard methods, we evaluated the neutral pion correlator by means of a stochastic source method. The absolute errors from the stochastic evaluation of disconnected contributions do not decrease with increasing t, unlike for the connected case. Since the pions we use are relatively light and the disconnected contribution to the π^0 propagators is relatively large, we are in a very favourable situation to evaluate disconnected contributions. We found that about 24 stochastic sources are sufficient to keep the fluctuations from the stochastic noise under control and at a comparable level to the error from the gauge field average. This allows an evaluation of the disconnected contribution out to large t. The disconnected contribution to the π^0 is indeed large and reduces the apparent flavour violation substantially. We remark that the mass splitting $\Delta m = m_{\pi^0} - m_{\pi^+}$ comes out to be positive which is consistent with an Aoki phase scenario in the quenched approximation of lattice QCD. In addition, using the Osterwalder-Seiler interpretation of the twisted mass neutral pion correlation function, we computed the neutral pion mass using solely the connected piece of the neutral pion correlator which gives a more accurate result, albeit for a less familiar theory.

Our results reveal that, for the situation of full twist as has been realized in this work, the mass splitting and hence the flavour breaking effects vanish with a rate that is quadratic in the lattice spacing as expected and at a level characterised by $r_0^2(m_{\pi^0}^2 - m_{\pi^+}^2) = c(a/r_0)^2$ with $c \approx 10$. Note that without adding the disconnected piece, this value of c can easily be twice bigger. On the other hand, for a fixed value of the lattice spacing of, say, $a = 0.1$ fm, the flavour breaking effects are substantial and are not negligible. Indeed, comparing to a quenched simulation for naive staggered fermions with Wilson gauge action [25], one finds a similar size of the flavour splitting effects encountered for the pion mass at a similar lattice spacing with a value of $c \approx 40$. It will be very interesting to see, whether for dynamical fermions the value of c would change. The only source of information is presently provided by dynamical improved staggered fermions [26] which give a value of c similar in magnitude to the value we found above. One should keep in mind, however, the caveats of the improved staggered simulations using the fourth root trick [27, 28].

The inclusion of the disconnected piece in the analysis turned out to be crucial to reduce the flavour breaking effects. An interesting observation is that with the PCAC definition of the critical point that reduces parity violations as much as possible, the connected contributions to the flavour breaking effects are larger than with a definition of the critical point that leaves some parity violations. We interpret this phenomenon as arising since it is not possible to simultaneously keep both effects small and that there is a trade-off between both.

The work presented here has been performed in the quenched approximation and it is the aim of the paper to obtain a first insight into the flavour breaking effects in Wilson twisted mass QCD. It is clear that the quenched approximation, in particular in the flavour singlet aspects, has conceptual short comings. This we see clearly for example in the correlator of a_0 which turns negative. Nevertheless, we think that the quenched approximation has provided useful insight into the flavour breaking effects of Wilson twisted mass fermions. Of course, it will be very interesting, to investigate flavour singlet quantities also for full QCD in this setup.

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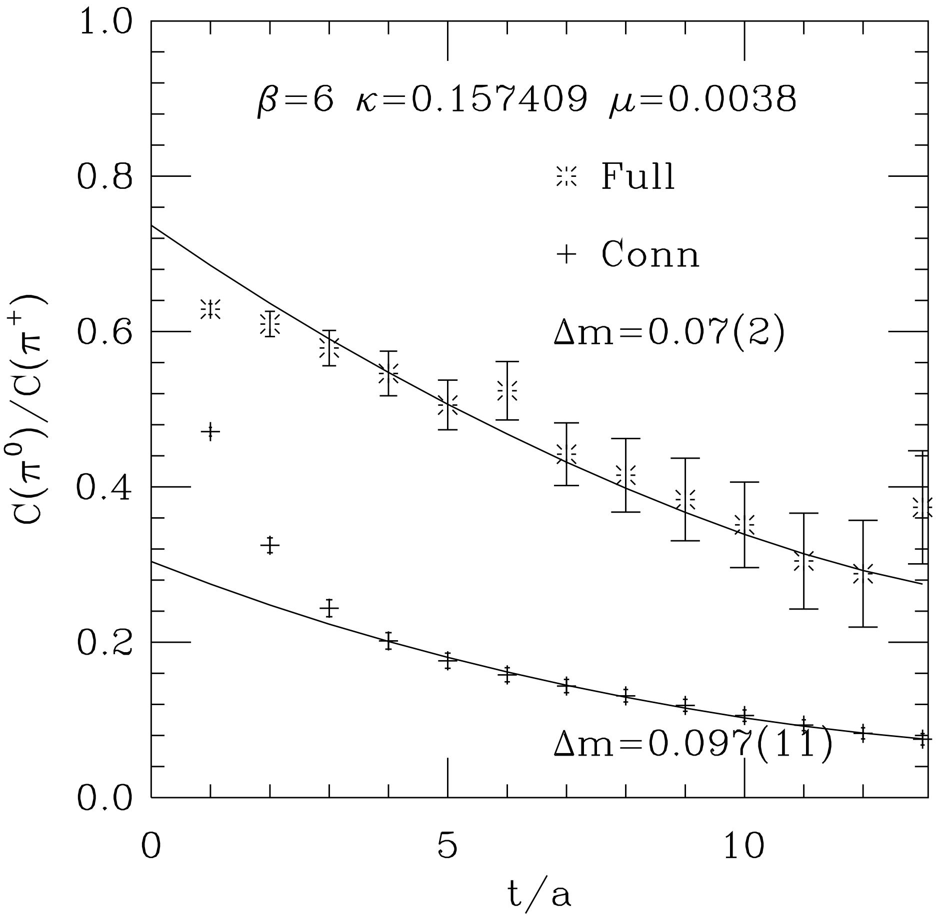

Figure 1: Correlation function ratios (for local operators only) of the neutral to the charged pion correlation functions for both the full correlation functions in eq. (3) and taking only the connected part of the neutral pion correlation function. The solid lines are the corresponding ratios from the fits to these correlation functions. We also indicate the values of mass splitting $\Delta m = m_{\pi^0} - m_{\pi^+} > 0$, see also table 1.

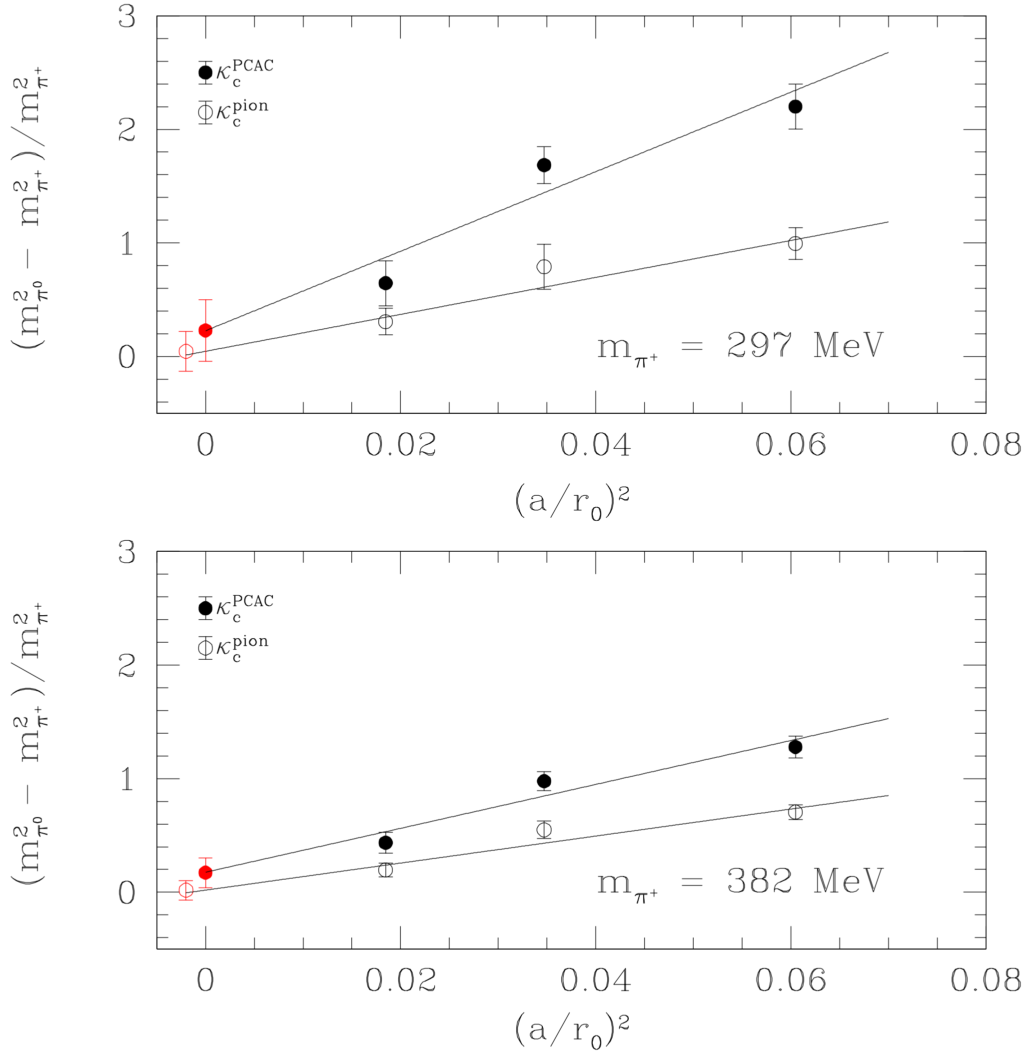

Figure 2: Relative pion mass difference as function of $(a/r_0)^2$ at two fixed values of the charged pion mass employing the pion and the PCAC definitions of the critical point.