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Pion in a Box

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Abstract

The residual mass of the pion in a finite spatial box at vanishing quark masses, the mass gap, is computed with two flavors of dynamical clover fermions. The result is compared with predictions of chiral perturbation theory in the δ regime.

Understanding finite size effects has always been an important issue in lattice studies of QCD. For an accurate determination of hadron observables it is of foremost importance to account for finite volume corrections. In addition, finite size effects can provide valuable information on the low-energy physics of the system. As lattice calculations are reaching the physical pion mass, the impact of finite volume will become pronounced. The main effect is caused by modified pion dynamics arising from the boundary conditions being imposed on the system.

In a finite spatial box chiral symmetry does not break down spontaneously. This results in a mass gap, even if the quark masses vanish. The physics behind that is described by a simple quantum mechanical rotator [1], whose energy levels can be computed from an expansion of the chiral effective theory in the δ regime $m_\pi L \ll 1, T \gg L$, where L (T) is the spatial (temporal) extent of the box. We are now in the position to probe the pion mass near the chiral limit and account for this effect. What makes this problem attractive, beyond the computational task of solving QCD in a finite volume, is that it is a universal feature of quantum mechanics, which is only constrained by the symmetry of the system. For a previous attempt of extracting the mass gap see [2].

In a series of papers Leutwyler [1], Hasenfratz and Niedermayer [3] and Hasenfratz [4] have computed the energy levels for two flavors of dynamical quarks to leading (L), next-to-leading (NL) and next-to-next-to-leading (NNL) order. The mass gap, *i.e.* the residual mass of the pion in the chiral limit, up to NNL order turns out to be

$$m_\pi^{\rm res} = \frac{3}{2F_\pi^2 L^3(1+\Delta)} \tag{1}$$

with

$$\begin{aligned}\Delta = & \frac{2}{F_\pi^2 L^2}\, 0.2257849591 \\ & + \frac{1}{F_\pi^4 L^4}\left[0.088431628 - \frac{0.8375369106}{3\pi^2}\left(\frac{1}{4}\ln(\Lambda_1 L)^2 + \ln(\Lambda_2 L)^2\right)\right],\end{aligned} \tag{2}$$

where F_π is the pion decay constant, and Λ_i are the intrinsic scale parameters of the low-energy constants [5],

$$\bar{l}_i = \ln\left(\frac{\Lambda_i}{m_\pi^{\rm phys}}\right)^2 . \tag{3}$$

Our simulations are performed with the Wilson gauge action and two flavors of mass-degenerate $O(a)$ improved Wilson fermions on a range of lattice volumes with periodic (antiperiodic) boundary conditions in the spatial (temporal) direction. Two values of the gauge coupling, $\beta = 5.29$ and 5.40, have been selected here. The hopping parameters and the lattice volumes of the individual runs are listed in Table 1. It is convenient to express the scale in terms of the force parameter r_0. In the chiral limit we find $r_0/a = 6.201(25)$ and 6.946(44), respectively. We set the scale by the nucleon mass, which gives $r_0 = 0.467$ fm [6]. This translates into lattice spacings $a = 0.075$ and 0.067 fm.

The quark masses are computed from the ratio (see *e.g.* [7], and references therein)

$$am_q = \frac{\langle a\partial\mathcal{A}_4(t)P(0)\rangle}{\langle P(t)P(0)\rangle} \tag{4}$$

at $t \gg a$, where $\mathcal{A}_\mu$ is the improved axial vector current [8],

$$\mathcal{A}_\mu = A_\mu + c_A\, a\partial_\mu P\,, \tag{5}$$

β	$\kappa_{\rm sea}$	$V\,[a^4]$
5.29	0.13400	$16^3 \times 32$
5.29	0.13500	$16^3 \times 32$
5.29	0.13550	$16^3 \times 32$
5.29	0.13550	$24^3 \times 48$
5.29	0.13590	$16^3 \times 32$
5.29	0.13590	$24^3 \times 48$
5.29	0.13620	$24^3 \times 48$
5.29	0.13632	$24^3 \times 48$
5.29	0.13632	$32^3 \times 64$
5.29	0.13632	$40^3 \times 64$
5.29	0.13640	$40^3 \times 64$
5.40	0.13500	$24^3 \times 48$
5.40	0.13560	$24^3 \times 48$
5.40	0.13610	$24^3 \times 48$
5.40	0.13625	$24^3 \times 48$
5.40	0.13640	$24^3 \times 48$
5.40	0.13640	$32^3 \times 64$
5.40	0.13660	$32^3 \times 64$

Table 1: Parameters of the lattice data sets used in this analysis.

and A_μ and P are the standard axial vector current and pseudoscalar density, respectively. The quark masses show practically no finite size effects beyond the statistical errors. In Table 2 we give the results from the largest lattices. Unlike the quark masses, the pion masses show significant finite size effects. The results obtained on the various volumes are shown in Table 2 as well. The pion masses from the lattices in Table 1 are printed in roman. They reach as low as 170 MeV.

Some of the pion masses at the larger quark masses are only known on 16^3 and 24^3 lattices. Furthermore, we miss one pion mass at the smallest quark mass on the 24^3 lattice at $\beta = 5.40$. In these cases the pion masses have been extrapolated to the 'missing' volumes by means of the $O(p^4)$ finite size shift formula [9]

$$\frac{m_\pi(L) - m_\pi}{m_\pi} = -\sum_{\vec{n}\neq 0} \frac{x}{2\lambda}\left[I^{(2)}_{m_{PS}}(\lambda) + xI^{(4)}_{m_{PS}}(\lambda)\right], \tag{6}$$

valid in the p regime $m_\pi L \gg 1$, with

$$x = \frac{m_\pi^2}{16\pi^2 F_\pi^2}, \quad \lambda = m_\pi |\vec{n}|\, L, \tag{7}$$

β	$\kappa_{\rm sea}$	am_π				am_q
		$L/a = 16$	$L/a = 24$	$L/a = 32$	$L/a = 40$	
5.29	0.13400	0.5767(11)				0.08781(18)
5.29	0.13500	0.4206(9)	*0.4195(9)*			0.05113(10)
5.29	0.13550	0.3325(13)	0.3270(6)	*0.3268(6)*	*0.3268(6)*	0.03293(8)
5.29	0.13590	0.2518(15)	0.2395(5)	*0.2388(5)*	*0.2388(5)*	0.01873(4)
5.29	0.13620		0.1552(6)	*0.1534(6)*	*0.1532(6)*	0.00792(4)
5.29	0.13632		0.1106(12)	0.1075(9)	0.1034(8)	0.00369(3)
5.29	0.13640				0.066(1)	0.00137(2)
5.40	0.13500		0.4030(4)	*0.4030(4)*		0.05641(5)
5.40	0.13560		0.3123(7)	*0.3121(7)*		0.03612(5)
5.40	0.13610		0.2208(7)	*0.2200(7)*		0.01930(4)
5.40	0.13625		0.1902(6)	*0.1889(6)*		0.01431(3)
5.40	0.13640		0.1538(10)	0.1504(4)		0.00932(3)
5.40	0.13660		*0.0947(11)*	0.0867(11)		0.00274(4)

Table 2: The pion and bare quark masses on the various lattices. The roman numbers are from our simulations on the quoted volumes, while the italic numbers have been obtained by extrapolation as described in the text.

where

$$\begin{aligned} I^{(2)}_{m_{PS}}(\lambda) &= -B^0(\lambda)\,, \\ I^{(4)}_{m_{PS}}(\lambda) &= \left(-\frac{55}{18} + 4\bar{l}_1 + \frac{8}{3}\bar{l}_2 - \frac{5}{2}\bar{l}_3 - 2\bar{l}_4\right) B^0(\lambda) \\ &\quad + \left(\frac{112}{9} - \frac{8}{3}\bar{l}_1 - \frac{32}{3}\bar{l}_2\right) B^2(\lambda) + S^{(4)}_{m_{PS}}(\lambda)\,, \\ S^{(4)}_{m_{PS}}(\lambda) &= \frac{13}{3} g_0 B^0(\lambda) - \frac{1}{3}\left(40 g_0 + 32 g_1 + 26 g_2\right) B^2(\lambda) \end{aligned} \tag{8}$$

with

$$B^0(\lambda) = 2K_1(\lambda)\,, \quad B^2(\lambda) = 2K_2(\lambda)/\lambda\,. \tag{9}$$

We take $F_\pi = 92.4\,\mathrm{MeV}$ throughout this paper. The Taylor coefficients g_i are

$$g_0 = 2 - \frac{\pi}{2}\,, \quad g_1 = \frac{\pi}{2} - \frac{1}{2}\,, \quad g_2 = \frac{1}{2} - \frac{\pi}{8}\,. \tag{10}$$

The first (second) expression in the square brackets of eq. (6) corresponds to $O(p^2)$ ($O(p^4)$) corrections in the Lagrangian. The low-energy parameters $\bar{l}_1$, $\bar{l}_2$ and $\bar{l}_4$ are taken from [5]:

$$\bar{l}_1 \simeq -0.4\,, \quad \bar{l}_2 \simeq 4.3\,, \quad \bar{l}_4 \simeq 4.4\,, \tag{11}$$

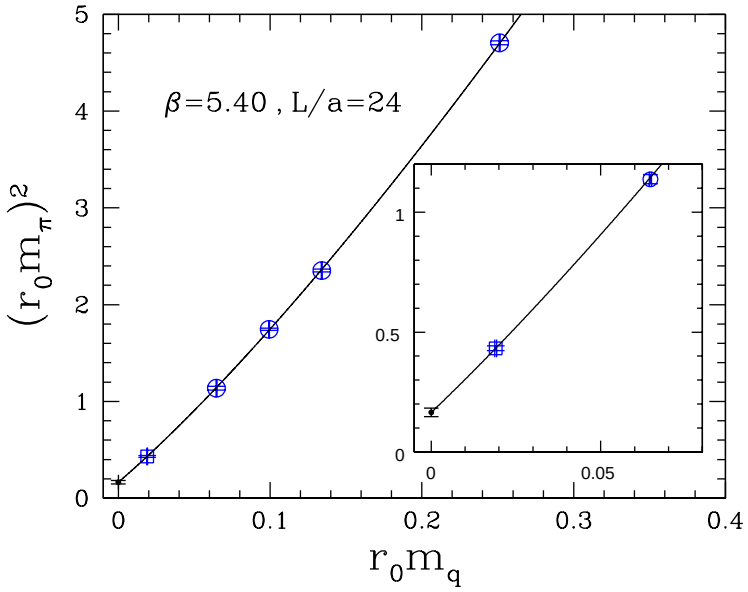

Figure 1: The pion mass squared against the quark mass on the 24^3 lattice at $\beta = 5.40$, together with the chiral fit (12). The circles refer to the roman numbers in Table 2, obtained directly on the quoted lattice, while the square is the extrapolated value and refers to the italic number in Table 2.

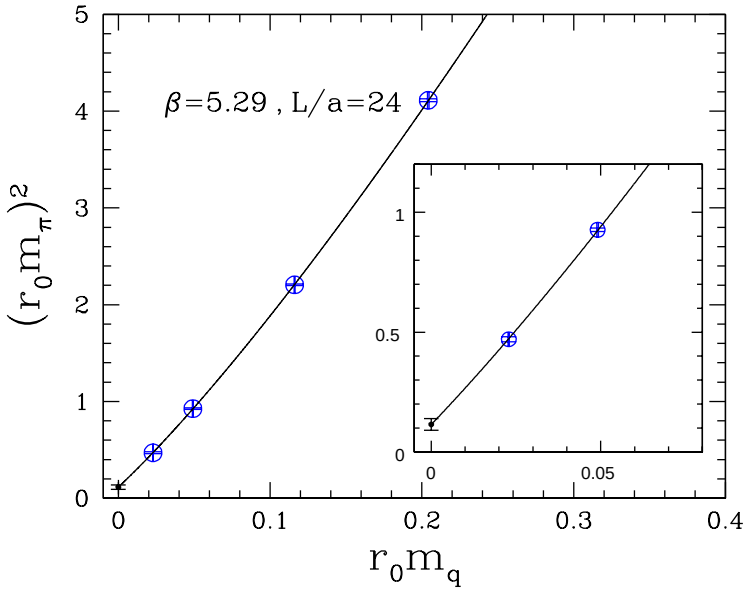

Figure 2: The pion mass squared against the quark mass on the 24^3 lattice at $\beta = 5.29$, together with the chiral fit (12). The circles refer to the roman numbers in Table 2, obtained directly on the quoted lattice. The extrapolated value referring to the italic number in Table 2 is not shown here.

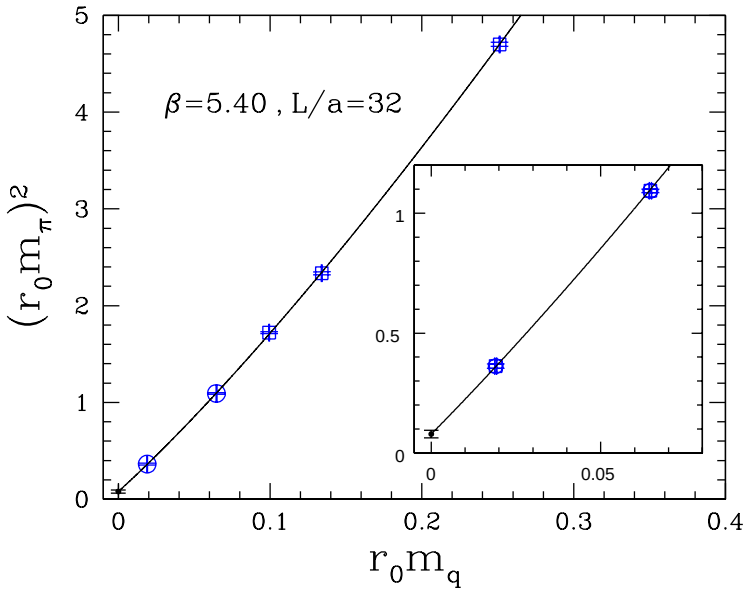

Figure 3: The pion mass squared against the quark mass on the 32^3 lattice at $\beta = 5.40$, together with the chiral fit (12). The circles refer to the roman numbers in Table 2, obtained directly on the quoted lattice, while the squares are the extrapolated values and refer to the italic numbers in Table 2.

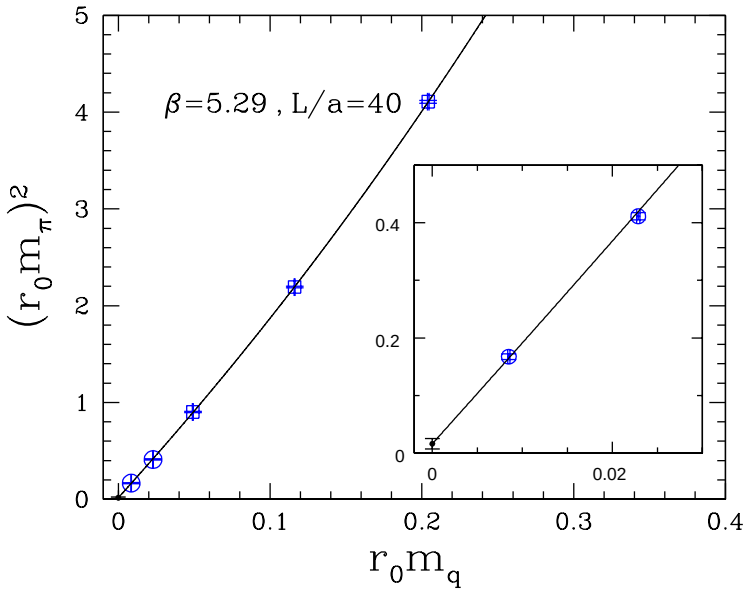

Figure 4: The pion mass squared against the quark mass on the 40^3 lattice at $\beta = 5.29$, together with the chiral fit (12). The circles refer to the roman numbers in Table 2, obtained directly on the quoted lattice, while the squares are the extrapolated values and refer to the italic numbers in Table 2.

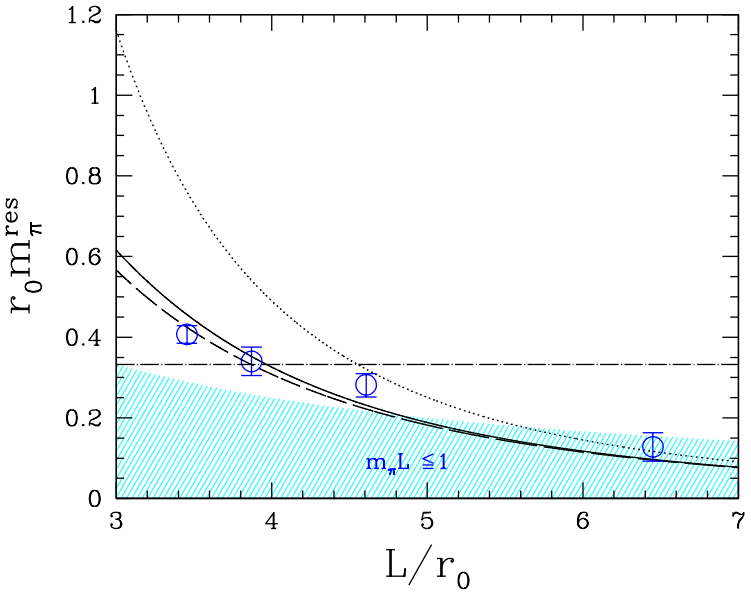

Figure 5: The mass gap as a function of lattice size for $(\beta, L/a)$=(5.40, 24), (5.29, 24) (5.40, 32) (5.29, 40), from left to right. The solid (dashed) [dotted] curve is the prediction of the chiral effective theory to NNL (NL) [L] order. The shaded area corresponds to $m_\pi L \leq 1$, indicating the δ regime. The dashed-dotted horizontal line marks the position of the physical pion mass. We have set $F_\pi = 92.4\,\mathrm{MeV}$, and the scale parameters Λ_1, Λ_2 have been taken from [5], as stated in eq. (11).

while $\bar{l}_3 = 4.2$ is taken from our fit of the pion masses in Figs. 1 – 4 (see Table 3). The extrapolated numbers are printed in italics in Table 2. As the extrapolation concerns mainly the larger quark masses, any small error inherent in the extrapolation should not affect our final result significantly. All masses in question are in the p regime.

In Figs. 1 – 4 we plot the pion mass squared against the quark mass on the 24^3 lattices at $\beta = 5.40$ and $\beta = 5.29$, on the 32^3 lattice at $\beta = 5.40$, and on the 40^3 lattice at $\beta = 5.29$. We fit the data by the formula

$$(r_0 m_\pi)^2 = A + B\, r_0 m_q \left[1 + C\, r_0 m_q \, \ln(D\, r_0 m_q)\right] , \tag{12}$$

which allows for a residual pion mass, $A = (r_0 m_\pi^{\mathrm{res}})^2$, in the chiral limit, and at larger quark masses turns over to the $O(p^4)$ chiral expansion valid in the p regime [5]. This is to say, eq. (12) interpolates between the energy levels in the δ and the p regime.

As we are working at fixed L, we are actually fitting the mass dependence of $m_\pi(L)|_L$ rather than m_π, and one might expect corrections to the fit formula, which cannot be accounted for by our ansatz (12). However, this is not the case. In Fig. 6 in the Appendix we compare the leading finite size correction in the p regime with the leading contribution to the mass gap in the δ regime. At our smallest quark mass the correction to m_π (in fact to the difference $m_\pi - m_\pi^{\mathrm{res}}$) turns out to be a

β	L/a	L [fm]	$(r_0 m_\pi^{\rm res})^2$	$m_\pi^{\rm res}$ [MeV]	$\bar{l}_3$
5.40	24	1.61	0.166(18)	172(9)	4.05(17)
5.29	24	1.81	0.116(24)	144(15)	4.22(32)
5.40	32	2.15	0.080(16)	119(12)	4.18(13)
5.29	40	3.01	0.016(9)	54(14)	4.26(31)

Table 3: The residual pion mass $m_\pi^{\rm res}$ and the low-energy constant $\bar{l}_3$.

fraction of the statistical error only for $L/a = 40$ and 32, and about the size of the statistical error for $L/a = 24$. Moreover, the corrections in the p regime are about a factor of 12 smaller than the mass gap.

The individual fits are shown in Figs. 1 – 4. On each of our lattices we obtain a residual mass, which is distinctly above zero. The results are summarized in Table 3. Barring any finite size effects, the low-energy constant $\bar{l}_3$ is given by

$$\bar{l}_3 = \ln\left(\frac{\Lambda_3}{m_\pi^{\rm phys}}\right)^2, \quad \ln(r_0\Lambda_3)^2 = 32\,\pi^2\,(r_0 F_\pi)^2\,\frac{C}{B}\ln\left(\frac{B}{D}\right). \tag{13}$$

The numbers of the individual fits are listed in Table 3. The average value turns out to be $\bar{l}_3 = 4.2(2)$, which lies at the upper end of the results reported in the literature [10].

In Fig. 5 we finally compare the residual pion masses of Table 3 with the prediction (1) of the chiral effective theory. We notice that the chiral series seems to have converged for $L/r_0 \gtrsim 5$, and below that the NL and NNL order results differ only by a few percent. We find good agreement with the NNL order formula [4] for all our lattice volumes, ranging from $L/r_0 \approx 3.5$ to ≈ 6.5. This is a bit surprising, as our results are barely touching the δ regime. The horizontal line in Fig. 5 shows the position of the physical pion mass. To capture the physics of light pions, and the spontaneous breakdown of chiral symmetry, the spatial extent of the lattice should be $L \gtrsim 3\,$fm, such that $m_\pi^{\rm res} \ll m_\pi^{\rm phys}$.

With precise data at (say) $L/r_0 \approx 6$, and quark masses at – or close to – the physical point, it should be possible to determine F_π accurately. The advantage of such a calculation is that it does not demand renormalization of the axial vector current. A fit of (1) to $m_\pi^{\rm res}$ on our largest lattice, $L/a = 40$ at $\beta = 5.29$ (the rightmost data point in Fig. 5), gives the pion decay constant in the chiral limit

$$F \equiv F_\pi|_{m_\pi=0} = 78^{+14}_{-10}\,\text{MeV} \tag{14}$$

(still using $r_0 = 0.467\,$fm), which is in the right ball-park [11], but not accurate enough to be useful yet. Due to the relatively small correction of the NNL order contribution it will, however, not be possible to determine the low-energy constants $\bar{l}_1$ and $\bar{l}_2$ reliably.

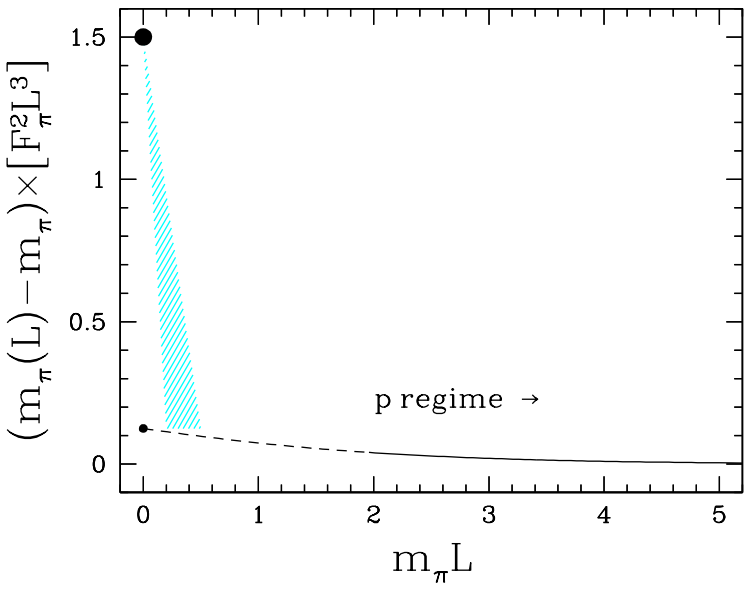

Figure 6: The leading contribution to the finite size mass shift of the pion, in units of $(F_\pi^2 L^3)^{-1}$, as a function of $m_\pi L$ (solid and dashed curve), compared with the leading order contribution to the mass gap (solid circle). Within the shaded area $m_\pi(L) \times F_\pi^2 L^3$ drops from $3/2$ at $m_\pi L = 0$ to $1/8$ at $1/F_\pi^2 L^2 \ll m_\pi L \ll 1$.

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Appendix

In Fig. 6 we show the leading $O(p^2)$ finite size correction to the mass of the pion,

$$m_\pi(L) - m_\pi = \frac{m_\pi^3}{16\pi^2 F_\pi^2} \sum_{\vec{n}\neq 0} \frac{K_1(m_\pi|\vec{n}|L)}{m_\pi|\vec{n}|L}\,, \tag{15}$$

together with the mass gap (or energy gap) to leading order,

$$m_\pi^{\rm res} = \frac{3}{2F_\pi^2 L^3}\,. \tag{16}$$

According to eq. (25) of [1], the finite volume shift drops by a factor of 12 from $3/2F_\pi^2L^3$ to $1/8F_\pi^2L^3$ in the shaded region. Incidentally (?), the p regime finite size correction formula (15) extrapolates to exactly the same value, $1/8F_\pi^2L^3$, in the chiral limit. For small $m_\pi L$ we can express the sum over $\vec{n}$ in eq. (15) by an integral:

$$m_\pi(L) = m_\pi + \frac{m_\pi^3}{16\pi^2F_\pi^2}\int_0^\infty d\nu\, 4\pi\nu^2\,\frac{K_1(m_\pi\nu L)}{m_\pi\nu L}\,. \tag{17}$$

Changing the variable ν to $\mu = m_\pi\nu L$, we obtain

$$m_\pi(L) = m_\pi + \frac{1}{4\pi F_\pi^2L^3}\int_0^\infty d\mu\,\mu\,K_1(\mu)\,. \tag{18}$$

The integral is known analytically,

$$\int_0^\infty d\mu\,\mu\,K_1(\mu) = \frac{\pi}{2}\,, \tag{19}$$

giving

$$m_\pi(L) = m_\pi + \frac{1}{8F_\pi^2L^3} \tag{20}$$

as the small $m_\pi L$ limit of (15). The $O(p^4)$ contribution to the mass shift would be suppressed by another factor of L^{-2}.

An analytical curve, that smoothly connects the mass gap of the δ regime with the $O(p^4)$ correction formula of the p regime, would be very valuable.

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