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A systematic effect in hadron mass calculations

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In our attempt to reproduce recent work by Hamber and Parisi we have discovered some important aspects of Monte Carlo calculations of the mass spectrum of lattice QCD. In particular, we find that, for typical values of the input parameters, the hadron propagators reach their asymptotic form only at a lattice distance which is larger than that available in previous calculations. This will have some numerically important effects on the results. We also suggest the use in certain cases of nonperiodic boundary conditions which can increase the maximum available distance on a given lattice.

Recently, Hamber and Parisi have presented a lattice Monte Carlo computation of hadron masses in an SU(3) lattice gauge theory.[1,2] Because of the significance of their results, we have attempted to repeat the calculation. In so doing, we have discovered some important features of the problem which, we feel, should be pointed out at this time.

The basic idea of these calculations is as follows. One generates, with standard Monte Carlo methods, a series of SU(3) lattice gauge-field configurations which are in "equilibrium" according to the pure gauge action. Quark propagators (usually Wilson,[3] $r=1$, fermions) in each background gauge configuration are computed by some numerical matrix-inversion technique and are then combined through appropriate spin and color sums to form hadron propagators which, in turn, are averaged over configurations. This is the so-called "quenched approximation"[4–6,1,2] because the back effect of the quarks on the gauge fields through the fermion determinant (i.e., the sum of closed quark loops) is not taken into account.

Hadron masses can then be extracted from the behavior of the hadron propagators at long distances in one lattice direction (the "time" direction). For convenience, the propagators are typically first averaged over the perpendicular ("spatial") directions.[5,6,2] For an infinite lattice, the time behavior is then simply a sum of decaying exponentials with the decay constants given by the masses of the possible intermediate states that can be created by the given hadron field. We thus have

$$G(t)\equiv\sum_{\vec{x}}\langle 0|\chi(\vec{x},t)\bar{\chi}(\vec{0},0)|0\rangle = \sum_i c_i e^{-m_i t}\,, \qquad (1)$$

where χ is some hadron field (made out of two or more quark fields), m_i are the masses of intermediate states with the right quantum numbers (the hadron of interest and its radial excitations), and the c_i are the corresponding squares of the wave functions at the origin. In order to extract masses reliably from $G(t)$, one should compute it out to values of t large enough so that only the lowest-mass state contributes. One thereby determines that mass. One may then attempt to find the mass of the first excited state by subtracting out the ground-state behavior. The process may even be repeated, but the errors, of course, increase at each stage. If large enough values of t for the above procedure are not available, one may try a multiparameter fit at intermediate t values. This is inherently very risky, however, since there are typically only a small number of points to fit and one does not know, *a priori,* how many parameters to fit them with.

In Refs. 1 and 2, the lattice size used was predominantly $5^3\times 8$, with $6^3\times 10$ and $6^3\times 12$ also used in a few cases. (The largest dimension of each lattice is the time direction.) Since periodic boundary conditions were imposed in the time direction, the greatest value of t that could be employed to extract meson masses was half the lattice size, namely 4 (or sometimes 5 or 6). This is because the periodic boundary conditions force the meson propagators to rise after t passes the lattice midpoint. The mesons can propagate just as easily in either direction in time. Thus the propagators are fit to $A\cosh m(L/2-t)$ at the midpoint ($t=L/2$) rather than a pure exponential $A\exp(-mt)$. Of course, such a fit assumes that all higher mass states have already died out by $t=L/2$, an assumption that does not appear to be quite justified for the range of parameters used in Refs. 1 and 2. When we attempt to repeat their calculation at $1/g_0{}^2=1.0$ ($\beta=6.0$) and Wilson[3] $K=0.145$ on an effectively much longer lattice (see below), we find that the pseudoscalar and vector-meson propagators are not saturated by the lowest-mass intermediate state before a distance of 7 or 8 lattice spacings; we determine masses about 20—30 % lower than those quoted in Refs. 1 and 2. Similar discrepancies are also found at higher K values (lower quark masses).[7] When Hamber and Parisi try a two-mass fit to the meson masses at the lattice midpoint, they find only a 5% reduction. We believe this shows the inherent difficulty of such fits, especially, in the case of periodic boundary conditions, for mesons near the lattice midpoint. The propagator there is a sum of approximately flat hyperbolic cosines which cannot easily be distinguished from each other.

For baryons, the situation is slightly better since the lowest-mass states, created at zero total momentum by the upper components of a combination of quark operators, propagate only forward in time. (Backward-moving states can be created with significant amplitude by upper components only with large relative momentum and hence with higher mass.) Thus, one might expect the baryon propagators at the lattice midpoint to be a sum only of falling exponentials. A two-mass fit, which Hamber and Parisi again perform at the midpoint, might be expected to work better here than for mesons. Indeed, although we again find that one must go out to a distance of 7 or 8 lattice spacings (at $1/g_0{}^2=1.0$, $K=0.145$) for the lowest-mass state to dominate, the mass we find is only about 10—15 % lower than those determined in Refs. 1 and 2 from fits at a distance of about 4 (or slightly greater).

From the above discussion, it is clear that one wants to examine the hadron propagators at large distances. To accomplish this without resorting to lattice sizes much bigger than those used by Hamber and Parisi (which would be impractical), we imposed nonperiodic boundary conditions on the quarks in the time direction.[8] (Periodic boundary conditions were kept on the quarks in space and on the gauge fields in all directions.) In general, the nonperiodic choice was "free" boundary conditions. The quark field at sites just beyond and just inside the edge of the lattice in the time direction are defined to have the same value. This effectively doubles the lattice size in the time direction, since all hadron propagators now behave as a sum of falling exponentials across the entire lattice. Of course, one must check that the boundary conditions do not do violence to the quantities calculated. We did this by holding gauge field configurations fixed and then calculating the hadron propagators ($K=0.145$, $1/g_0{}^2=1.0$) for a variety of boundary conditions on the quarks: "free," "fixed" (the quark field set equal to zero at the sites beyond the edge of the lattice in the time direction), periodic, and "free on a sublattice" (i.e., a new boundary imposed well inside the original lattice boundary). In all cases, large variations in the masses (up to 20%) were found right on the boundaries, but already at one site in from the boundary effects were typically only 2—3 % (the maximum even seen was 6%), and in the interior the effects were almost always much less than 1%. The boundary effects on noninteracting quarks were also calculated and were found to be very small everywhere in the interior. Of course, as the midpoint of the lattice is approached, there are always large differences between periodic boundary conditions and all the other choices, but this is due to the nature of the periodic boundary conditions, as explained above. In our analysis, we always throw out the points on the boundary. We keep the points one in from the edge, but one should be aware that there is a slight (2—3 %) systematic downward pull on those points in the data presented here. One should also be aware that as the hadron masses decrease (increasing K toward K_c) the boundary conditions will have larger effects. In the range of K in which we are working (which is essentially the same as that used in Refs. 1 and 2) this does not appear to be a problem. The region very close to K_c, where the boundary conditions might be expected to cause more severe problems, is inaccessible to the present matrix inversion techniques.

Our data at $1/g_0{}^2=1.0$ was taken on lattices of size $6^3\times 10$ and $6^3\times 13$, with two different starting configurations on the $6^3\times 10$ lattice. At least 700 Monte Carlo passes with 15 metropolis hits per site were performed before taking data; approximately half the data comes from lattices that had more than 3000 passes (beyond 500 passes no systematic trend was apparent). There were, in general, 100 passes between configurations on which propagators were calculated, but we twice waited more than 1000 passes to ensure more complete statistical independence among groups of runs. A straightforward Gauss-Seidel[9,4—6,1—2] iterative matrix-inversion technique was used. We stopped iterating when the quark propagators changed by less than 1% over the previous 4 iterations (about 50—100 iterations total at the values of K investigated); hadron masses were changing by less than 0.01%.

Figures 1—4 show our results for four different hadrons at $1/g_0{}^2=1.0$, $K=0.145$. We graph the dimensionless quantity $m(t)$ versus lattice distance t, where $m(t)$ is defined by

$$m(t)=\ln\left[\frac{G(t-1)}{G(t)}\right], \tag{2}$$

with $G(t)$ given by (1). In the limit of large t, $m(t)$

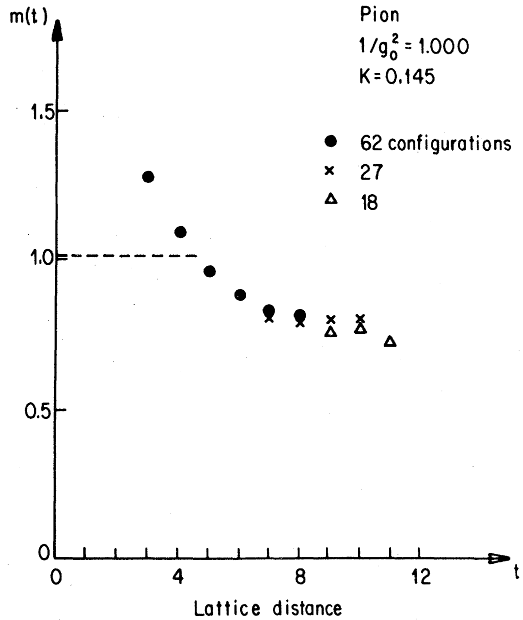

FIG. 1. The behavior of the effective lattice mass $m(t)$ as a function of lattice time distance t for the pseudoscalar ("pion") at $1/g_0{}^2=1.000$ and $K=0.145$. ● label values averaged over 62 gauge-field configurations. × and △ label values averaged over considerably fewer configurations for which a lattice longer in the time direction (13 versus 10 sites) was used. The horizontal dashed line indicates the mass extracted by Hamber and Parisi at the same parameters.

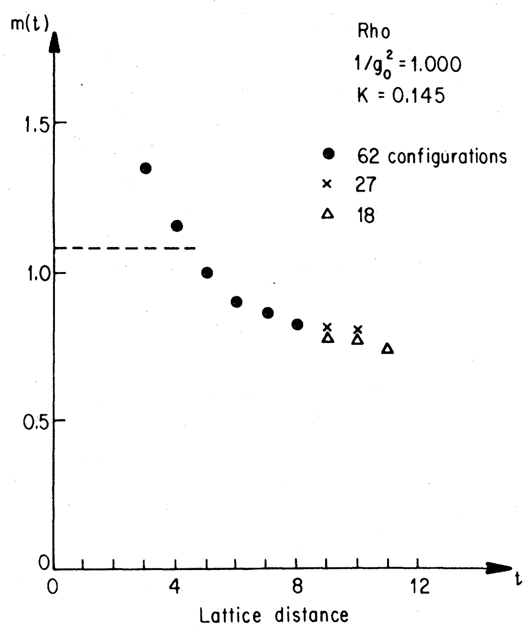

FIG. 2. Same as in Fig. 1 but for the ρ.

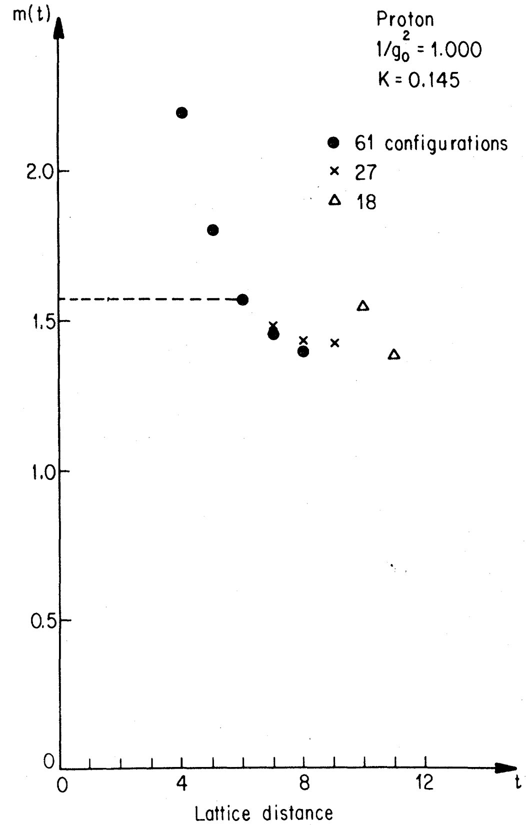

FIG. 3. Same as in Fig. 1 but for the proton.

approaches the lattice mass of the hadron of interest. A total of 62 configurations on the two different lattice sizes ($6^3\times10$, $6^3\times13$) were averaged to find the propagators for $t\leq8$; for $t>8$, just the results from the $6^3\times13$ lattice were used. (Since there were only 27 configurations for $t=9$ and 10, and 18 configurations for $t=11$, these points should not be taken quite as seriously as the points for $t<8$.) To give some sense of the statistical errors involved, we also plot separately the results of the $6^3\times13$ configurations wherever this subaverage can be distinguished from the average over all the available configurations. In general statistical errors tend to increase with t since the numerical fluctuations in the propagators decrease more slowly than the propagators themselves. A horizontal line on each graph indicates that value of the mass for the hadron of interest as quoted in Ref. 2.

For the pion and the ρ (Figs. 1 and 2), a rather clear leveling off of $m(t)$ occurs at $t=7$ or 8. As mentioned above, the value of $m(t)$ when it levels off is about 20—30% below the mass given by Hamber and Parisi. However, our data is consistent with theirs in the following sense. In each case, $m(t)$ evaluated at the maximum value of t available

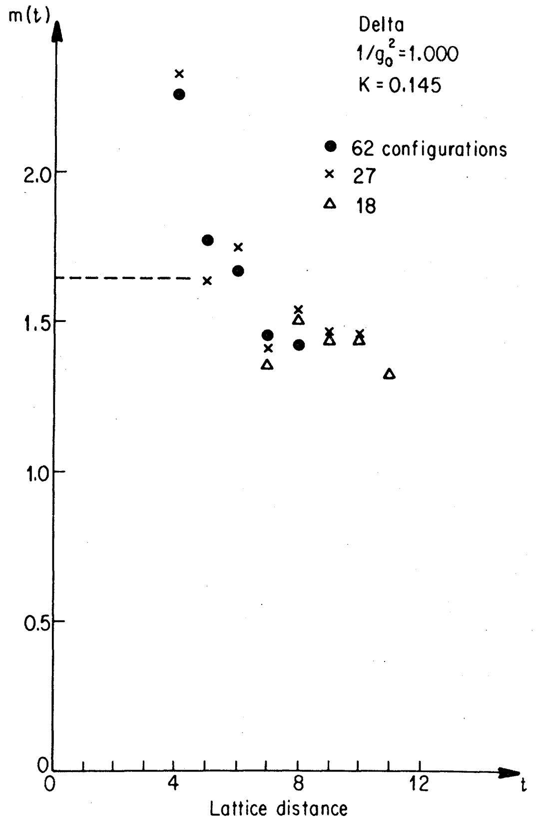

FIG. 4. Same as in Fig. 1 but for the Δ.

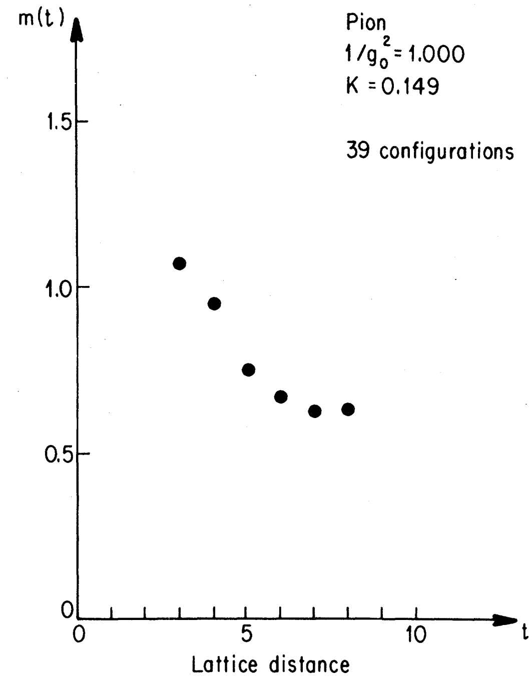

FIG. 5. Similar to Fig. 1 except that the $K=0.149$. (●) label values averaged over 39 gauge-field configurations. The lattice had 10 sites in the time direction.

in Refs. 1 and 2 ($t \simeq 4$ to 5), is roughly equal to the number quoted there.

The situation is similar for the baryons (proton and Δ, Figs. 3 and 4). However the errors tend to be somewhat larger—not surprising since they involve the cube, rather than the square, of quark propagators. Here the masses, at their apparent leveling-off point, are only about 10—15% below the values in Ref. 2. Furthermore, those values correspond to distances of 5 or 6 on our plots. This seems to indicate that the two-mass fit employed in Ref. 2 "stretches" somewhat the lattice size, enabling them effectively to calculate the mass at a point beyond where the fit is performed.

We have also taken some data (with the $6^3 \times 10$ lattice only) at other K values for this same value of $1/g_0^2$ (1.0). Figures 5 and 6 present the results for the pion and the proton at $K=0.149$. The effects are similar to those seen at $K=0.145$. Hamber and Parisi do not present results at this particular K value, but our pion again seems about 20—30% below the value we get by interpolating their data. For the proton, there is no real evidence yet for the leveling off of $m(t)$; it is clear that data on a larger lattice is needed.

Finally, some attempt was also made to investigate the problem also at $1/g_0^2=0.90$. We worked there on a $5^3 \times 10$ lattice. The effects seen there were qualitatively similar to those at $1/g_0^2=1.0$, with the masses appearing to level off at smaller distances in lattice units since the lattice spacing is larger at stronger coupling. However, the fluctuations were quite large,[10] especially for the baryons, even after averaging over 40 configurations. This is perhaps due to the fact that $1/g_0^2=0.90$ is in the middle of the transition region from weak to strong coupling. We therefore do not feel ready to present graphs like Figs. 1—4 for this coupling. The statistical errors are under study—it may be possible to get better data by throwing out a few wildly fluctuating runs.

It may be surprising to some readers (it was to us) that one has to go out such a large number of lattice spacings (7—8 at $1/g_0^2=1.0$, $K=0.145$) in order to see the hadron masses level off. To get some feeling for the numbers involved, we examined a very crude model in which two quarks are nonrelativistically bound into mesons by a linear potential. Using[11] $a^{-1}=1250$ MeV at $1/g_0^2=1.0$ and the level value of $ma \simeq 0.8$ from Fig. 2 gives a ρ mass of about 1000 MeV at $K=0.145$. If we imagine this ρ to be made of two quarks of constituent mass $\simeq 500$ MeV, we can calculate the excited-state masses with

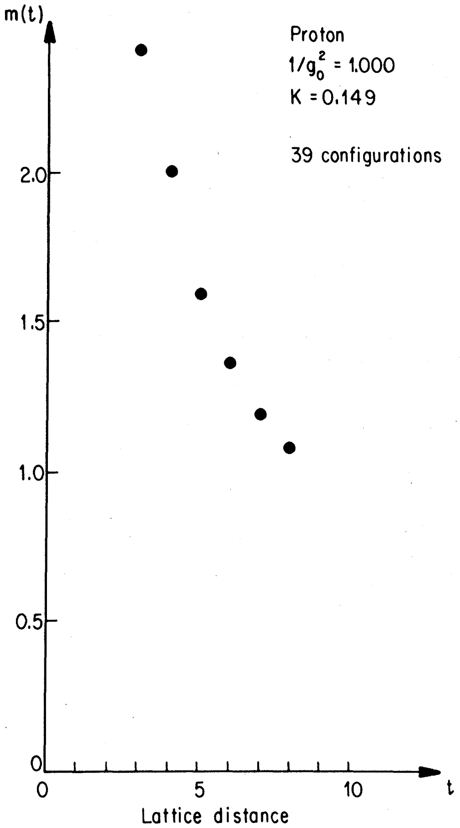

FIG. 6. Same as in Fig. 5 but for the proton.

our crude model and ask, for example, at what lattice distance $m(t)$ would be within 20% of its asymptotic value. We get $t \simeq 3$–4, which is not wildly different from what is seen in Fig. 2.

We wish to emphasize an important point here. While Figs. 1–4 show fairly clearly that the lattices used were large enough in the time direction to allow the hadron propagators to reach their asymptotic behavior, we can draw no conclusions from them about the adequacy of the spatial size of the lattice. Such graphs enable one to read off the mass of the lowest state in a periodic box of the given spatial size; they have nothing to say about the stability of the mass to changes in this size. Indeed the spatial dimension here is rather small (~ 1fm) and there may be large finite-size effects. To investigate these effects one must change (preferably increase) the spatial length; work on this is in progress.

Another point that bears reemphasis is that the results presented here refer only to hadron masses at specific values of K and not yet to physical hadron masses. The physical masses come only from an extrapolation from lower K values toward $K = K_c$, the value of K for which the pion is physical (approximately massless).[12] Lacking data at enough different K values to perform this extrapolation, we cannot yet quote results for physical hadron masses. We do note, however, that the values of K presented here (0.145, 0.149) are in the middle to upper range of the values used in Refs. 1 and 2, so the 20–30% effects found here are expected to produce some significant changes in their results. Our own values for hadron masses will be presented in a future publication.

Finally, one must keep in mind that all this work is in the context of the "quenched" approximation.[4–6,1,2] Only after the masses are extracted in a reliable way and the finite-size effects are under control, will one be able to test accurately this approximation.

In summary, we feel that the two most important conclusions of our work up to this point are the following.

(1) For typical values of the parameters $1/g_0^2$ and K (values which are used in Refs. 1 and 2 and which are more or less demanded by practical considerations such as manageable lattice sizes, reasonably fast convergence of matrix-inversion techniques, and a desire to be as much as possible in the weak-coupling regime) large lattice distances are necessary in order to see the asymptotic behavior of hadron propagators.

(2) In order to extend as far as possible the maximum available lattice, it is useful to impose nonperiodic boundary conditions on the quarks. Even if one throws out a few sites next to the boundary, there is a considerable advantage over periodic boundary conditions on any reasonably large-sized lattice.

Note added. While this work was being written up we received a report by Don Weingarten, Indiana University Report No. IUHET-82 (unpublished). He also finds some evidence, albeit at stronger coupling ($1/g_0^2 = 0.67, 0.93, 0.95$) and with considerably fewer configurations (8) than were used here, that the lattices used in Refs. 1 and 2 were not long enough in time direction. He gives his own version of the extrapolation to physical masses.

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[3]K. Wilson, in *New Phenomena in Subnuclear Physics,* Proceedings of the 14th Course of the International School of Subnuclear Physics, Erice, 1975, edited by A. Zichichi (Plenum, New York, 1977).

[4]E. Marinari, G. Parisi, and C. Rebbi, Nucl. Phys. B190 [FS3], 734 (1981).

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[6]E. Marinari, G. Parisi, and C. Rebbi, Phys. Rev. Lett. 47, 1795 (1981); H. Hamber, E. Marinari, G. Parisi, and C. Rebbi, Phys. Lett. B108, 314 (1982).

[7]An extrapolation to near zero quark mass must be performed in all such calculations. We do not yet have enough data at a sufficient number of K values to perform this extrapolation reliably, so we are not able to say how much the physical masses are changed by this effect.

[8]We thank Jonathan Sapirstein for first suggesting to us that some kind of nonperiodic boundary conditions would be useful for this problem.

[9]S. D. Conte and Carl de Boor, *Elementary Numerical Analysis: An Algorithmic Approach* (McGraw-Hill, New York, 1972).

[10]The fluctuations were sometimes large enough to cause the baryon propagators to change sign at large distances.

[11]E. Pietarinen, Nucl. Phys. B190 [FS3], 349 (1981); M. Creutz, Phys. Rev. Lett. 45, 313 (1980).

[12]The best way to extrapolate in K is to use the same set of gauge fields for each K value (our configurations at $K=0.149$ are a subset of these at $K=0.145$, and we will use this subset in doing the final extrapolation). This reduces the effects of fluctuations on the extrapolation processes and also reduces Gauss-Seidel convergence time since the propagators at one value of K may be used as input for the next K value.