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Spectrum of the effective SU(3) Hamiltonian in a small volume computed by path-integral Monte Carlo integration

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Using a simple Monte Carlo integration method for quantum-mechanical problems on a "time lattice" the mass gaps of the low-lying states of Lüscher's effective Hamiltonian with and without massless fermions for a small volume are computed. While there is good agreement between this method and previous Rayleigh-Ritz-type calculations in the case of SU(2), notable differences are found in the case of SU(3) for most states. The statistical and systematic errors are competitive with those of the variational method. Having no dependence on basis set size, the Monte Carlo method is a good alternative to the Rayleigh-Ritz calculations also for SU(3). An extension of the method to intermediate volumes including fermions is definitely possible.

I. INTRODUCTION

While QCD perturbation theory allows the computation of many processes at high momentum transfer or small distances because the running coupling constant is small there, large-distance or low-momentum predictions such as the mass spectrum and the question of quark and gluon confinement are thwarted by the infrared divergence of the renormalized coupling constant. One systematic approach pioneered by Lüscher to control the infrared problem is to work in a small periodic volume, which provides a discrete momentum spectrum of the fields. As long as the box is small enough the spacing between momenta is large and the renormalized coupling constant is small enough for perturbation theory to apply; i.e., one is allowed to treat higher momentum modes as a perturbation to the lower modes. So integrating out all spatially nonconstant modes of the gauge fields in one-loop perturbation theory Lüscher obtained the first terms of an effective Hamiltonian for the spatially constant fields in a small cubic box of length L with periodic boundary conditions [1]. The corresponding Lagrangian has the form

$$L = g^{2/3}(1+g^2\kappa_2) \times (\tfrac{1}{2}\dot{c}_i^a\dot{c}_i^a + \tfrac{1}{4}f^{abe}f^{ecd}c_i^a c_j^b c_i^c c_j^d) + g^{4/3}\kappa_1 c_i^a c_i^a + g^{8/3}(\kappa_3 s^{abcd}c_i^a c_i^b c_j^c c_j^d + \kappa_4 s^{abcd}c_i^a c_i^b c_i^c c_i^d)\ , \quad (1.1)$$

where g is the renormalized coupling constant, and the c_i^a are the constant gauge fields in the temporal gauge scaled with $Lg^{-2/3}$. The dot means differentiation with respect to $\tau = t/L$, f^{abc} are the structure constants of SU(N), s^{abcd} is the totally symmetric invariant tensor, and summation over spatial index i and color index $a = \{1, \ldots, N^2-1\}$ is implied. The κ factors result from the momentum summation of the one-loop quantum corrections to the classical Hamiltonian. Higher-order terms were computed by Koller and van Baal [2], but are not used here, because they give only very small corrections that this method of obtaining the mass gap cannot show, and would only prevent a comparison of the results obtained from this method with the Rayleigh-Ritz calculations of Lüscher and Münster [3], Ziemann [4], and Weisz and Ziemann [5]. The effective Hamiltonian has N^3 degenerate "vacua" due to symmetry under the so-called "central conjugations" [1]. For small g the N^3 "potential wells" can be considered as separate, while for g of order 1 tunneling between the "vacua" sets in and breaks the degeneracy [2]. In this paper only the small-g case is considered corresponding to volumes with a box length of about one correlation length ξ of the scalar glueball, i.e., $z = mL = L/\xi \approx 1$. The so-called intermediate volume range extends to about five correlation lengths. Comparison with lattice-gauge-theory Monte Carlo computations shows that for bigger box lengths the effective Hamiltonian approximation breaks down [6].

In a theory with n_F massless fermion fields one can integrate out the fermion fields completely and obtain again an effective Hamiltonian for the constant gauge fields [7–10]. Choosing antiperiodic boundary conditions the form of the effective Hamiltonian for the potential well centered around $c_i^a = 0$ is the same as in the pure gauge theory, only the κ coefficients are changed, whereas the other potential wells are also lifted, thereby removing the vacuum degeneracy.

For pure gauge fields the spectrum was determined by variational methods for SU(2) and SU(3) in small [3–5] and intermediate volumes [2,11,12]. In the case of SU(3) in a small volume [4,5] the number of basis functions for the variational method was rather small for some states. As is well known, a too-small basis for the trial wave functions causes a systematic overestimation of the energy levels by the Rayleigh-Ritz method. It also seems that in intermediate volumes a determination of the spectrum including fermions is possible only by using the Monte Carlo (MC) method for quantum-mechanical problems, as introduced by Kripfganz and Michael for SU(2) in small [8] and intermediate (Kripfganz and Michael [9] and Michael [10]) volumes. Of course, the MC method is plagued by finite-size effects, finite-time-step errors, statistical errors, and the like, but in order to cover the in-

TABLE I. Expressions for operators for the various irreps measured. P denotes parity and C charge conjugation. The first column uses the notation of [4], while the second gives explicit expressions. The summation convention is always used.

irrep^{PC}	Notation of [4]	Explicit
E_2^{++}		$c_1^a c_1^a - c_2^a c_2^a$ and cyclic; $c_1^a c_1^a + c_2^a c_2^a - 2c_3^a c_3^a$ and cyclic
T_2^{++}	(ij)	$c_i^a c_j^a$; $i \neq j$
A_1^{++}	(ii)	$c_i^a c_i^a$
A_1^{-+}	$\mathrm{Im}[\epsilon_{ijk}(ijk)]$	$\epsilon_{ijk} f^{abc} c_i^a c_j^b c_k^c$
A_1^{+-}	$\mathrm{Im}[(ij)(kll)(ijkmm)]$	$(c_i^f c_j^f)[c_i^a c_j^b d^{abp} f^{pcg} c_k^c (d^{qrs} c_k^q c_l^r c_l^s) d^{gde} c_m^d c_m^e]$
T_2^{-+}	$\mathrm{Im}[\epsilon_{klm}(klm)(ij)]$	$(\epsilon_{klm} f^{abc} c_k^a c_l^b c_m^c) c_i^d c_j^d$
T_2^{+-}	$\mathrm{Im}[(ik)(jkll)]$	$(c_i^f c_k^f)(c_j^a c_k^b f^{abe} d^{ecd} c_m^c c_m^d)$
T_1^{++}	$\mathrm{Re}[(jl)(lkmm)\epsilon_{ijk}]$	$(c_j^f c_l^f)(c_i^a c_k^b d^{abe} d^{ecd} c_m^c c_m^d)\epsilon_{ijk}$
T_1^{-+}	$\mathrm{Im}[(jkk)(ijll)]$	$(d^{fgh} c_j^f c_k^g c_k^h)(c_i^a c_j^b f^{abe} d^{ecd} c_m^c c_m^d)$
T_1^{+-}	$\mathrm{Im}[\epsilon_{ijk}(jkll)]$	$-\epsilon_{ijk}(c_j^a c_k^b f^{abe} d^{ecd} c_l^c c_l^d)$
T_1^{--}	(ijj)	$d^{abc} c_i^a c_j^b c_j^c$
A_2^{--}	(ijk)	$d^{abc} c_i^a c_j^b c_k^c$

termediate volume range in the presence of fermions also for SU(3), it seems mandatory to extend the MC method to this group. Hopefully the accuracy achievable will be high enough to allow a useful comparison with SU(3) lattice calculations with dynamical fermions in the corresponding volume range.

As a first step toward this goal the mass gaps for the various glueball states for SU(3) in small volumes were computed with the Monte Carlo method on a large time lattice, in order to check the accuracy and feasibility of such a computation. Despite the above-mentioned difficulties of this method it was found that the mass gaps are smaller than those computed by variational methods and the statistical and estimated systematic errors are competitive with the error of the variational method caused by the finite basis set size.

II. MONTE CARLO INTEGRATION

As the rotational symmetry of the system is broken by the torus topology, the effective Lagrangian contains a term [the last in (1.1)] that breaks the O(3) symmetry. The remaining symmetry is that of the cubic group and so the states measured were chosen as irreducible representations (irreps) of this group. Additional symmetries are parity P and charge conjugation C [only for SU(3)]. Table I shows the operators measured for each state. A vectorized (odd-even) Metropolis Monte Carlo routine is used to compute the spectrum ([8,9] and references therein). After every 20th sweep [15th for SU(3)] through the time lattice the correlation functions of the various representations of the "glueball states" are measured. Vector and tensor state operators were constructed for all possible space directions. The correlation functions were checked for invariance against permutation of the coordinate axes and then averaged over all space directions. For the determination of the mass gaps from the correlation functions see [9,10].

In the case of SU(2) the data are binned [13] in 128 bins of 250 measurements. The number of thermalization updates correspond to 16 bins. The error bars are computed with the data partitioned into 128, 64, 32, and 16 bins, respectively and the largest is given. Most data points were obtained with a time step of 0.2 on a lattice of 400 sites. For the highest g values also time steps of 0.15 and 0.1 on a corresponding larger time lattice were probed to check for finite-time-step errors. For SU(3) the data were binned in 400 bins of 40 measurements. The number of

TABLE II. SU(3) pure gauge theory mass ratios $z(\mathrm{irrep}^{PC})/z_{E^{++}}$ for $g=0$ obtained by Rayleigh-Ritz [4,5], MC results for four g values, and variational results [11] for $g=0.4$.

	$g^2=0$ [5]	'$g^2=0$'	$g^2=0.01$	$g^2=0.05$	$g^2=0.16$	$g^2=0.16$ [11]
$z_{E^{++}}$	0	0	0.448(10)	0.715(9)	0.956(8)	0.993
$z(\mathrm{irrep}^{PC})/z_{E^{++}}$						
T_2^{++}	1.000	1.013(13)	1.006(27)	0.994(19)	0.990(13)	1.078
A_1^{++}	1.230	1.25(2)	1.28(5)	1.25(11)	1.23(4)	1.309
A_1^{-+}	2.30	2.35(5)	2.45(5)	2.63(4)	2.78(4)	3.22
A_1^{+-}	6.80	5.49(14)	5.56(20)	5.61(16)	5.87(20)	6.45
T_2^{-+}	3.71	3.42(5)	3.63(10)	3.77(5)	3.98(8)	4.18
E^{-+}	3.71	3.45(5)	3.61(7)	3.76(6)	3.95(6)	
T_2^{+-}	4.20	4.05(7)	4.22(7)	4.39(6)	4.72(6)	4.94
E^{+-}	4.20	4.09(5)	4.22(7)	4.38(7)	4.68(7)	
T_1^{++}	>3.3	3.99(6)	4.15(10)	4.42(9)	4.60(10)	3.28
T_1^{-+}	4.60	4.87(7)	4.99(10)	5.19(9)	5.33(16)	5.39
T_1^{+-}	2.39	2.72(5)	2.84(7)	2.93(6)	3.22(5)	3.48
T_1^{--}	1.97	1.82(3)	1.83(4)	1.86(4)	1.86(4)	1.90
A_2^{--}	1.73	1.55(2)	1.57(4)	1.57(3)	1.57(2)	1.67

initialization sweeps corresponds to 24 bins. The errors of the z values and the mass ratios were computed using the jackknife method ([14] and references therein) for 400,200, . . . , 25 bins, and if there is no plateau value the largest error is given. The results quoted in Table II for SU(3) pure gauge theory are all obtained with a time step of 0.15 and 320 time slices in the periodic time lattice. A variation of the time step to 0.2 shows no deviation beyond the statistical error, which is larger than for SU(2) because of limitations in computer time. (The production of one bin needs 150 sec on an IBM 3090.) For g much smaller than 0.1 the MC method becomes unpractical, because the mass gaps go to zero with vanishing g. As for $g \to 0$ the lowest-order terms (the classical Lagrangian) dominate, the mass gaps are proportional to $g^{2/3}$, and so the mass ratios are independent of g; one can simulate the mass ratios for $g=0$ by discarding all higher-order terms in the effective Lagrangian and performing the simulation at a conveniently chosen g. Since the mass-ratio curves are almost flat near $z=0$, the z values in the gap that cannot be measured could be obtained by interpolation.

III. RESULTS AND DISCUSSION

(a) SU(2): For this group the Monte Carlo (MC) method was first used by Kripfganz and Michael [8,9] and the reproduction of their results serves only to illustrate the accuracy of the method. Figures 1 and 2 show rather good agreement between the Monte Carlo and the variational methods, as also reported in [9]. The solid line marks the results of Lüscher and Münster [3], and the dotted line is obtained with three massless fermions using van Baal's results [7]. For SU(2) a notable time-step error is observed for large z_{E^+} as the mass ratios for A_1^- and T_2^- diminish somewhat going from time step 0.2 over 0.15 down to 0.1. (An appropriately longer time lattice is always used to keep the physical time extent constant.) This reduction of the mass ratios is caused mainly by an increase of z_{E^+} by about one percent for each decrease of the time step, while the increments of the z values for T_2^+ and A_1^- are slightly smaller, and $z_{T_2^-}$ shows no dependence on time step at all. The $z_{A_1^+}$ value changes by three to five percent on going from time step 0.2 to 0.1, but the statistical error is rather large anyway. So there seems to be no plateau value reached by decreasing the time step, and although it is possible that the remaining deviations of the MC points in Fig. 1 would disappear if one could go to smaller time steps, as the autocorrelation grows with decreasing time step, this is unfortunately unpractical. With the given statistics the difference between the curves with and without three fermion flavors could not be resolved using this method for z_{E^+} smaller than 0.5 for the A_1^- and T_2^- states and for z_{E^+} smaller than 0.75 for the A_1^+ state. Since the Hamiltonian scales with $g^{2/3}$ in lowest order, mass ratios are independent of g and therefore of z_{E^+} to this order. The term in the effective Lagrangian which causes the main deviation of the mass ratios from a constant value for all z_{E^+} is κ_1, because the κ_3 and κ_4 factors are 1 and 2 orders of magnitude smaller. As κ_1 is reduced by including fermions, it is obvious that the mass-ratio curves have to become more flat and meet the pure gauge curves in the limit $g \to 0$, i.e., $z_{E^+} \to 0$. The A_1^- state seems to lie a lit-

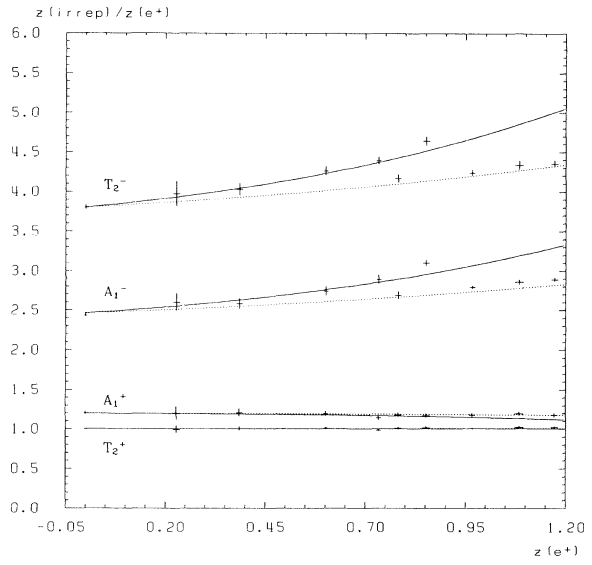

FIG. 1. SU(2) mass ratios $m(\text{irrep}^P)/m(E^+) = z(\text{irrep}^P)/z(E^+)$, plotted against Lüscher's scaling variable z_{E^+}. (P denotes parity.) In ascending order the states shown are T_2^+, A_1^+, A_1^-, T_2^-. The solid line shows the results of Lüscher and Münster [3], while the dotted line is obtained using van Baal's results [7] for $n_F=3$. All mass ratios are determined with a time step of 0.2, except the last two with the highest z_{E^+}, for which a time step of 0.1 is used. This holds for pure gauge as well as for the case with fermions.

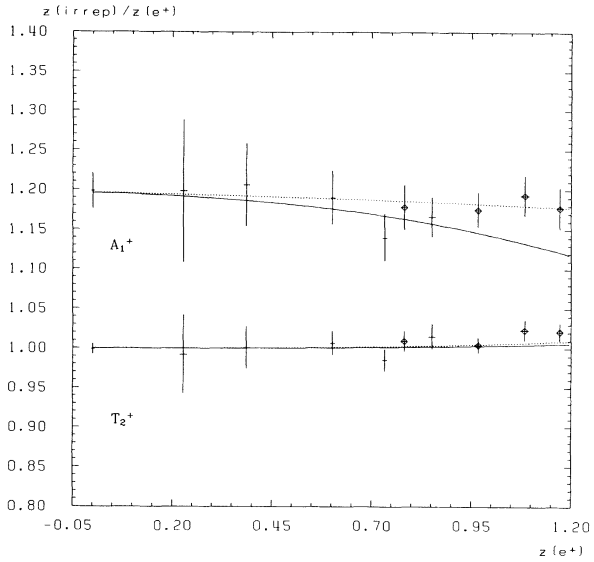

FIG. 2. Same plot as for Fig. 1 showing only $m(A_1^+)/m(E^+)$ and $m(T_2^+)/m(E^+)$. Crosses with diamonds denote the data points obtained with $n_F=3$.

tle below the variational result and to increase more strongly with increasing z_{E^+}, but the difference is small and this observation may be an overinterpretation of the data. The splitting caused by the last term in the effective Lagrangian of the E^+ and T_2^+ states, which should combine in the infinite-volume limit to the 2^+ glueballs, is of course not resolved by the MC method in the small-volume range, because the κ_4 factor is too small. For pure gauge fields tunneling sets in around $z_{E^+}=0.9$ whereas with three fermion fields tunneling occurs shortly before $z_{E^+}=1.2$. This shows up in the MC computation by a sudden increase of $z_{T_2^+}$ relative to z_{E^+}. However, since the MC routine used for this work is not stable for this g value, no z ratios are given here.

(b) SU(3): Table II displays the MC results for pure gauge fields, the results of Vohwinkel for the lowest value of g given in [11], and also the mass ratios Ziemann [4] and Weisz and Ziemann [5] obtained at $g=0$. Although in [5] mass ratios for all relevant $z_{E^{++}}$ values are given, only those for $g=0$ are quoted here, because a comparison at other g values would show qualitatively the same results. Rather good agreement is found for the E^{++}, T_2^{++}, A_1^{++}, and A_1^{-+} states. The difference between the MC and variational result of [11] for E^{++} is a 4σ deviation and may be caused by the inclusion of sixth-order terms in the effective Hamiltonian by Vohwinkel or finite basis set size effects (although estimated to be smaller than two percent) or the finite-time-step error of the MC method. As for the scalar A_1^{++} the connected correlation function has to be computed to determine the mass gap; the statistical error is rather large. So no improvement in accuracy is gained compared with the variational method. However, for the A_1^{+-}, T_2^{-+}, T_2^{+-}, E^{+-}, A_2^{--}, and T_1^{--} states the results show the mass gaps notably reduced in comparison with the variational calculations. This is certainly the effect of a too-small basis set in the Rayleigh-Ritz-type calculations, since a variation of the time step to 0.2 shows no deviation within the error. Unfortunately, the correlation functions for A_1^{--}, E^{--}, and T_2^{--} provided no mass estimate worth quoting. Regarding the results of Table II one has to note the following when comparing with the variational results.

The T_1 is an irreducible representation of the cubic group that is contained not only in the spin-1 representation but also in the spin-3 (and higher spin) representation of the rotation group. That means T_2 and A_2 combine with T_1 to a spin-3 state if the rotational invariance is unbroken. So the T_1^{--} should be degenerate with A_2^{--} or smaller in mass. However, because the term in the Lagrangian breaking the rotational symmetry is so small and the T_1^{--} operator constructed is a spin-1 operator when rotational invariance is unbroken, it projects almost completely on the T_1^{--} belonging to the 1^{--} state. So only the A_2^{--} correlation function gives the mass gap of the 3^{--} spin state.

Similarly, the T_1^{++} operator projects not on the T_1^{++} belonging to the spin 4^{++}, which Vohwinkel found to be the spin state containing T_1^{++} with the smallest mass, but on 1^{++}. Unfortunately, the value obtained by MC does not agree with the mass value given in [11] for the next highest T_1^{++} not belonging to 4^{++}. That the rotational symmetry is unbroken in small volumes is shown in addition by the degeneracy of T_2^{+-} and E^{+-}, which belong to the 2^{+-} state, as well as T_2^{-+} and E^{-+} belonging to 2^{-+}.

The slight deviation of the T_1^{-+} at $g=0$ in comparison with the variational computation could be explained by the fact that an excited state is nearby (at 4.86, if one scales the result of Vohwinkel linearly down to $g=0$). This could lead to the measurement of an effective mass value which is bigger than the real mass gap.

The effect of fermions with antiperiodic boundary conditions on the mass ratios is smaller for SU(3) than for SU(2) because the bosonic part of the κ_1 coefficient, which determines the slope of the mass-ratio curves for the various states, is proportional to N in case of SU(N), whereas the fermionic part is independent of N. Because for SU(3) most mass-ratio curves are rather flat even for $n_F=3$ only a minor effect is to be expected for small volumes. With the statistics accumulated to date no meaningful prediction or comparison with van Baal's rescaling formula [7] is possible, so the publication of these results is postponed until the accuracy is high enough.

IV. CONCLUSIONS

It was shown that one can obtain reliable results for the low-lying mass states of the effective SU(3) Lagrangian with a path-integral Monte Carlo method, which is not affected by basis set size effects like the Rayleigh-Ritz method. This is shown by comparing the lower mass gap estimates obtained by MC with the variational results [5] for states where only a small basis was constructed. With improvements regarding computational efficiency and finite-time-step error [15,16], the Monte Carlo method should also give results that are competitive with the variational method in intermediate volumes. As nobody has been able so far to include fermions in the Rayleigh-Ritz method, the use of this Monte Carlo method is presently the only way which offers the hope of providing predictions for SU(3) lattice-gauge-theory computations with dynamical fermions in intermediate volumes.

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