THE SMALL-VOLUME EXPANSION OF GAUGE THEORIES COUPLED TO MASSLESS FERMIONS

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Received 16 March 1988

The small-volume expansion of the low-lying glueball states for SU(2) and SU(3) gauge theory, coupled to massless fermions with periodic and antiperiodic boundary conditions, is determined. For SU(3) with periodic boundary conditions the vacuum is eightfold degenerate and breaks part of the cubic group spontaneously. In all cases the scalar-to-tensor mass ratio $m_{4^{++}}/m_{E^{++}}$ is 1.1 to 1.3 as in the pure-gauge case. We also discuss chiral symmetry.

1. Introduction

In this paper we wish to apply the approach of the zero-temperature small-volume expansion [1] to SU(N) (for N = 2, 3) gauge theories coupled to massless fermions with spatially periodic and antiperiodic boundary conditions. The number of flavours n_f will be arbitrary (but small enough in order not to destroy asymptotic freedom). Some explicit predictions for three flavours will be given as an example. This work is aimed at understanding the mechanism of confinement and chiral-symmetry breaking, starting from the fundamental QCD lagrangian. Asymptotic freedom will guarantee calculability at small volumes. For large volumes one has the important results of Lüscher [2] and of Gasser and Leutwyler [3], especially for controlling the finite-volume errors in lattice gauge theory. However, these large-volume expansions leave undetermined a number of, in principle, calculable constants.

It was claimed in ref. [4] that chiral symmetry is broken even when going to small volumes, due to condensation of zero-energy fermion modes. We will show that actually expanding around the true quantum vacuum, no such zero-energy fermion modes occur, so chiral symmetry is unbroken in small volumes [3].

Another motivation for our study is the comparison of analytic results with Monte Carlo data [5]. Limitations in computational power will allow a better approach to the continuum in small volumes [6]. In this context we compute the contribution of massless fermions to the effective hamiltonian of the zero-momentum gauge fields, yielding a generalization of Lüscher's effective hamiltonian [1]. The fermions contribute through vacuum polarization effects, which are computed to one-loop order. The spectrum of the effective hamiltonian will give the low-lying glueball masses in a small volume and, as in the pure-gauge case, these are of the order $g^{2/3}/L$. On the other hand, since there are no zero-energy fermion modes, the pion has a mass of order 1/L and hence glueballs cannot decay into pions in a small volume (the "femto universe" [7]; this reference also contains a very clear overview of the many aspects of nonperturbative QCD.) Therefore, we need not address the issue of coupling to flavour-singlet mesons. Nevertheless this is an important issue, since this coupling determines the decay modes for the glueballs. In principle, however, the glueball wave function (not to be confused with the wave function for the effective hamiltonian) allows one to determine the mixing with the flavour-singlet states, but this issue will not be pursued any further in this paper.

A surprising result for SU(3) with periodic boundary conditions is that the vacuum is eightfold degenerate and the set of vacua form an orbit under the group of coordinate reflections. As a consequence the mass gap will go to zero for small volumes. Tunneling effects will have to be included in order to go to intermediate volumes, as in the pure-gauge case [8], but a detailed study of the appropriate nonperturbative dynamics will be left for the future.

2. Boundary conditions and chiral symmetry

Let us begin by specifying the boundary conditions for the gauge and fermion fields on a cube of sides $L \times L \times L$ ($n \in \mathbb{Z}^3$)

$$A_{i}(\mathbf{x} + \mathbf{n}L) = A_{i}(\mathbf{x}),$$

$$\Psi_{+}(\mathbf{x} + \mathbf{n}L) = (\pm 1)^{n_{1} + n_{2} + n_{3}}\Psi_{+}(\mathbf{x}).$$
(1)

Hence, the vector fields and Ψ_{\pm} are periodic, whereas Ψ_{\pm} is antiperiodic. Naively, one would expand around $A_i = 0$, $\Psi_{\pm} = 0$, but the following argument will show that this is not obviously correct. The periodic boundary conditions for the gauge fields remain unchanged under the twisted gauge transformations of 't Hooft [9]

$$g_{k}(\boldsymbol{x} + \boldsymbol{n}L) = \exp(2\pi \boldsymbol{i}\boldsymbol{n} \cdot \boldsymbol{k}/N) g_{k}(\boldsymbol{x}), \qquad (2)$$

but the boundary conditions for the fermion fields in the fundamental representation of SU(N) change to

$$\hat{\Psi}_{\pm}(\mathbf{x} + \mathbf{n}L) = (\pm 1)^{n_1 + n_2 + n_3} \exp(2\pi i \mathbf{k} \cdot \mathbf{n}/N) \hat{\Psi}_{\pm}(\mathbf{x}), \qquad (3)$$

where $\hat{\Psi}_{\pm}(x) = g_k(x)\Psi_{\pm}(x)$. However, operators like the hamiltonian remain invariant under the gauge transformations g_k and therefore one could just as well

claim that perturbation theory is defined by expanding around $\Psi_{\pm} = 0$, $A_i(\mathbf{x}) = -ig_k^{-1}(\mathbf{x}) \partial_i g_k(\mathbf{x})$, (which is equivalent to expanding around $\hat{\Psi}_{\pm} = 0$, $\hat{A}_i = 0$.) Due to the presence of the fermions this will, in general, be a state with a different energy.

The various candidate vacua, thus obtained, can be distinguished by the Polyakov line

$$P_{j} = \frac{1}{N} \operatorname{Tr} \left[P \exp \left(i \int_{0}^{L} A_{j} \left(\mathbf{x} + t \mathbf{e}_{j} \right) dt \right) \right], \tag{4}$$

evaluated at the vacuum. These Polyakov lines have to take values in the centre of the gauge group when evaluated at the quantum vacua (otherwise gauge invariance would be spontaneously broken) and they transform under eq. (2) by multiplying with an element of the centre.

For SU(2) $P_j = \pm 1$ and we expect the vacuum to have maximal symmetry. Indeed we will show that for periodic boundary conditions $P_j = -1$ for all *j* (hence $\Psi_+ = 0$, $A_i = 0$ is a *false* vacuum), whereas for antiperiodic boundary conditions, $P_j = 1$ for all *j* (here $\Psi_- = 0$, $A_i = 0$ is the *true* vacuum). By taking $\mathbf{k} = (1, 1, 1)$ in eq. (3) we see that both cases are related by a gauge transformation. This observation is well known in lattice gauge theory [10] but the implication for the vacuum ambiguity was never realized.

For SU(3) and antiperiodic boundary conditions we likewise find $P_j = 1$ for all j, but with periodic boundary conditions $P_j = 1$ will correspond to a false vacuum. The lowest energy in this case is achieved for $P_j(l) = \exp(2\pi i l_j/3)$ with $l_j = \pm 1$. Reflection in the *i*th coordinate will change the sign of l_i and we therefore have an eightfold-degenerate vacuum which forms an orbit under the coordinate reflections Z_2^3 .

The proof that the above vacua are not false vacua will be given after we have discussed the implication for chiral-symmetry breaking. Chiral-symmetry breaking is believed to be associated with condensation of zero-energy fermion modes, and indeed for the two-dimensional Gross-Neveu model [11] (exactly solvable in the large N-limit) this causes chiral symmetry to be broken even in small volumes [12]. Expanding around $\Psi = 0$, $A_i = 0$, one would then expect a similar behaviour for gauge theories coupled to massless fermions [4]. However, one can easily convince oneself that zero-energy modes for the fermions in perturbation theory will only occur when

$$\Psi(\mathbf{x} + \mathbf{n}L) = \left(\prod_{j=1}^{3} P_j^{n_j}\right) \Psi(\mathbf{x}), \qquad (5)$$

where P_j is the value of the Polyakov line in the true vacuum. This criterion is clearly not satisfied for the vacua we identified and, in lowest order, chiral symmetry will be unbroken.

Actually, we claim that even if eq. (5) were fulfilled, no chiral-symmetry breaking would occur. To see this we compute, for periodic fermion fields in a fixed

zero-momentum gauge-field background A_i , the lowest order contribution to $\langle \overline{\Psi}\Psi \rangle$. This yields

$$\left\langle \overline{\Psi}\Psi\right\rangle = \frac{mNn_{\rm f}}{L^3\sqrt{m^2 + 2\operatorname{Tr}(A^2)}} + O(m/L^2).$$
(6)

For $A_i = 0$, $m \to 0$ we indeed get the result [4] $\langle \overline{\Psi}\Psi \rangle = Nn_f/L^3$. However, one is *not* allowed to take the limit $m \to 0$ before averaging over the gauge-field fluctuations and this is easily seen to wipe out the non-zero value of $\langle \overline{\Psi}\Psi \rangle$ for $m \to 0$. (Note, that for the Gross-Neveu model the fermions are *not* coupled to a gauge field and our argument does *not* apply to that model.) Thus, chiral symmetry will not be broken perturbatively through the presence of zero-energy fermion modes, and to all orders in perturbation theory, $\langle \overline{\Psi}\Psi \rangle = 0$ for massless fermions. It should be noted, however, that $\langle \overline{\Psi}\Psi \rangle$ is not a good order parameter for spontaneous chiral-symmetry breaking in a finite volume (for the same reason that the magnetization in the Ising model will only be non-zero in the thermodynamic limit).

Finally, we wish to remark that breaking of chiral $SU(n_f) \times SU(n_f)$ down to the diagonal flavour symmetry group $SU(n_f)$ should not be confused with breaking of chiral $U_A(1)$ through instantons [13]. However, using the consistency conditions imposed by the axial anomaly, 't Hooft showed that spontaneous chiral-symmetry breaking seems unavoidable in QCD [14], which suggests that this breaking of chiral symmetry is dynamically realized through the breakdown of the chiral $U_A(1)$ symmetry.

3. The effective potential

We will compute, in this section, the contribution of the fermions to the effective potential, which depends on the parameters of the classical vacua. These parameters are the same as for the pure-gauge theories (the fermion fields are zero), and are given by the set of spatially constant, abelian, gauge fields [1] (parametrizing the vacuum valley)

$$A_i(\mathbf{x}) = \frac{C_i^a}{L} T_a \equiv \frac{C_i \cdot T}{L}, \qquad (7)$$

modulo periodic (homotopically trivial) gauge transformations, leaving the abelian and constant properties invariant. In eq. (7), T_a are the (N-1) generators for the Cartan subalgebra, explicitly

SU(2):
$$T_1 = \frac{1}{2}\sigma_3 = \frac{1}{2}\text{diag}(1, -1);$$

SU(3): $T_1 = \frac{1}{2}\lambda_3 = \frac{1}{2}\text{diag}(1, -1, 0),$
 $T_2 = \frac{1}{2}\lambda_8 = \frac{1}{(2\sqrt{3})}\text{diag}(1, 1, -2).$ (8)

To be more precise, this describes one connected component, related to the others by the homotopically non-trivial periodic gauge transformations. Concentrating on one such component is equivalent to ignoring instanton effects [15].

If $\mu^{(i)}$, i = 1, 2, ..., N are the (N - 1)-dimensional weight vectors of the fundamental representation (i.e. $T_a = \text{diag}(\mu_a^{(1)}, ..., \mu_a^{(N)})$), one easily generalizes Lüscher's result for the effective potential [1] to include the fermions

$$V_{\rm eff}^{\pm}(C_i^a) = \frac{1}{2} \sum_{i \neq j=1}^N \hat{V}_1(C \cdot (\mu^{(i)} - \mu^{(j)})) - n_f \sum_{i=1}^N \hat{V}_1(C \cdot \mu^{(i)} + C_{\pm}), \qquad (9)$$

(up to a possible overall constant), where

$$\hat{V}_{1}(\mathbf{x}) = \frac{4}{\pi^{2}L} \sum_{\mathbf{n}\neq\mathbf{0}} \frac{\sin^{2}(\frac{1}{2}\mathbf{n}\cdot\mathbf{x})}{(\mathbf{n}^{2})^{2}},$$
(10)

 $C_{+}=0$ (periodic boundary conditions for the fermions) and $C_{-}=(\pi, \pi, \pi)$ (antiperiodic boundary conditions for the fermions). Note, that $\{\mu^{(i)} - \mu^{(j)}\}$ are the weights of the adjoint representation, i.e. the roots $\{\alpha\}$ (ref. [15], appendix D). Eq. (9) follows straightforwardly from (ref. [16])

$$\int_{0}^{T} \mathrm{d}t \, V_{\mathrm{eff}}(C_{i}^{a}) = \ln \left[\frac{\mathrm{det}' (-D_{\mu}^{2}(B)) \mathrm{det}(\not D(B))^{n_{t}}}{\mathrm{det}' (W_{\mu\nu}(B))^{1/2}} \right], \tag{11}$$

with $\not D(B)$ the Dirac operator at $B_i = C_i \cdot T/L$.

The correct quantum vacuum is now given by the minimum of V_{eff} . Since $\hat{V}_1(x)$ has its minimum at $x = \mathbf{0} \pmod{2\pi}$ and its maximum at $x = C_{-} \pmod{2\pi}$ [15], the true vacuum for antiperiodic boundary conditions is given by $\mu^{(i)} \cdot \mathbf{C} = \mathbf{0} \pmod{2\pi}$. Note that $\mu^{(i)} \cdot \mathbf{C}$ are not independent, since $\sum_i \mu^{(i)} \cdot \mathbf{C} = \operatorname{Tr}(T \cdot \mathbf{C}) = \mathbf{0}$ and that the Polyakov lines evaluated at $\mathbf{A} = \mathbf{C} \cdot T/L$ are given by

$$P_{j}(C_{i}^{a}) = \frac{1}{N} \operatorname{Tr}\left(\exp(iC_{j} \cdot T)\right)$$
$$= \frac{1}{N} \sum_{k=1}^{N} \exp(i\mu^{(k)} \cdot C_{j}).$$
(12)

Hence, for antiperiodic boundary conditions we confirm the quantum vacuum to be unique with $P_j = 1$. For periodic boundary conditions the situation is more complicated, however. As mentioned before, $\exp(iC_j \cdot T)$ should be in the centre of SU(N) for C_j^a corresponding to the proper vacuum and hence at the vacuum for all $i \neq j, \ \mu^{(i)} \cdot C = \mu^{(j)} \cdot C \pmod{2\pi}$, or for all i

$$\mu^{(i)} \cdot C = \frac{2\pi}{N} l \pmod{2\pi}, \qquad l_j = 0, 1, \dots, (N-1).$$
(13)

At this value, $V_{\text{eff}}^+(C) = -Nn_f \hat{V}_1(2\pi l/N)$, which is minimal for SU(2) and SU(3) if all $l_j = \pm 1$. Hence, for SU(2) we have $P_j = -1$ and the vacuum is unique. Note that for SU(2) the periodic and the antiperiodic cases are related by the gauge transformation $g_{(1,1,1)}$, which transforms P_j to $-P_j$.

For SU(3) the vacuum is eightfold degenerate with $P_j = \exp(l_j 2\pi i/3)$, $l_j = \pm 1$. In perturbation theory we will only expand around one of the quantum vacua. Since these vacua are related by coordinate reflections, a symmetry of the full effective hamiltonian, each choice is equivalent. The vacua of eq. (13) are related to $C_i^a = 0$ by the gauge transformation $g_i(x)$. Hence, expanding around $\Psi_+(x) = 0$, $\mu^{(i)} \cdot A(x) = 2\pi l/NL$ is equivalent to expanding around $\hat{\Psi}_+(x) = 0$, $\hat{A}_i(x) = 0$ provided operators are properly transformed before computing the expectation value. We will, therefore, express the effective hamiltonian in terms of

$$c_{i}^{a} = \frac{1}{L^{2}} \int d_{3}x \, 2 \operatorname{Tr}(\hat{A}_{i}(x)T_{a}),$$
$$\hat{A}_{i}(x) = g_{I}(x)A_{i}(x)g_{I}^{-1}(x) - ig_{I}(x)\partial_{i}g_{I}^{-1}(x), \qquad (14)$$

where a now runs from 1 to $N^2 - 1$, with T_a a hermitian basis of the Lie algebra and $\text{Tr}(T_a T_b) = \frac{1}{2} \delta_{ab}$. The effective hamiltonian was computed with the "dynamical background field" calculation exactly as in the pure-gauge case [15, 16]. The background field is $\hat{A}_i^a = c_i^a/L$, the pure-gauge Feynman rules are those of ref. [17] $(\mathbf{m} = \mathbf{0})$ and the rules which include the fermions are given in fig. 1 with (γ_{μ} are the



Fig. 1. Feynman rules which contain fermion lines. For the remaining, purely bosonic Feynman rules, see ref. [17].

Dirac matrices)

$$\mathscr{V}_{7} = \left(\frac{i\delta_{ab}}{k_{\mu}\gamma^{\mu} + i\epsilon}\right)_{\alpha\beta}, \qquad \mathbf{k} = \frac{2\pi}{L}(\mathbf{n} + \mathbf{n}_{0}),$$
$$\mathscr{V}_{8} = -i(\gamma_{\mu})_{\alpha\beta}(T_{c})_{ab}\delta_{p_{\mu},q_{\mu}+r_{\mu}}.$$
(15)

For antiperiodic boundary conditions $n_0 = \frac{1}{2}(1,1,1)$ and for periodic boundary conditions $n_0 = l/N$, i.e. for SU(2) $n_0 = \frac{1}{2}(1,1,1)$ and for SU(3) we choose $n_0 = \frac{1}{3}(1,1,1)$ (the other seven possibilities can be obtained by coordinate reflections.)

The results up to one loop will be expressed in terms of the background field c_i^a and the renormalized coupling constant at the scale $\mu = 1/L$ in the minimal subtraction scheme [18]

$$g^{-2}(L) = -2b_0 \ln(L\Lambda_{\rm MS}) + \frac{b_1}{2b_0^2} \ln\left[-2\ln(L\Lambda_{\rm MS})\right],$$

$$b_0 = \frac{1}{(4\pi)^2} \left(\frac{11}{3}N - \frac{2}{3}n_{\rm f}\right),$$

$$b_1 = \frac{1}{(4\pi)^4} \left(-\frac{34}{3}N^2 + \frac{10}{3}Nn_{\rm f} + (N^2 - 1)n_{\rm f}/N\right).$$
 (16)

4. The effective hamiltonian for SU(2)

For SU(2) we find the following result for the effective hamiltonian in the zero-momentum gauge fields

$$H_{\rm eff} = -\frac{1}{2L} \left(\frac{1}{g^2} + \tilde{\alpha}_1 \right)^{-1} \frac{\partial^2}{\partial c_i^{a2}} + V_{\rm T}(c) + V_1(c) + \cdots,$$

$$L \cdot V_{\rm T}(c) = \frac{1}{4} \left(\frac{1}{g^2} + \tilde{\alpha}_2 \right) F_{ij}^a F_{ij}^a + \tilde{\alpha}_3 F_{ij}^a F_{ij}^a c_k^b c_k^b + \tilde{\alpha}_4 F_{ij}^a F_{ij}^a c_b^b c_j^b + \tilde{\alpha}_5 (\det c)^2 + \cdots,$$

$$V_1(c) = \hat{V}_1(\mathbf{r}) - 2n_i \hat{V}_1(\frac{1}{2}\mathbf{r} + \mathbf{C}_-) - 2|\mathbf{r}|/L,$$

$$= \frac{1}{L} \left(\tilde{\kappa}_1 c_i^a c_i^a + 3(\tilde{\kappa}_3 - \tilde{\kappa}_4) c_i^a c_i^a c_j^b c_j^b + 5\tilde{\kappa}_4 c_i^a c_i^a c_i^b c_i^b + \tilde{\kappa}_7 \prod_{i=1}^3 (c_i^a c_i^a) + \cdots \right), \quad (17)$$

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where

$$r_{i} = \sqrt{c_{i}^{a}c_{i}^{a}}, \qquad F_{ij}^{a} = -\varepsilon_{abc}c_{i}^{a}c_{j}^{b},$$
$$\tilde{\alpha}_{i} = \alpha_{i} - 2n_{f}\alpha_{i}', \qquad \tilde{\kappa}_{i} = \kappa_{i} - 2n_{f}\kappa_{i}'. \qquad (18)$$

The constants $\alpha_i, \alpha'_i, \kappa_i, \kappa'_i$ are given in table 1. The primed coefficients are as momentum sums similar to those for the pure-gauge case [16], but with the momenta shifted over $2\pi n_0/L$.

$$\frac{1}{g^{2}} + \tilde{\alpha}_{1} = \frac{1}{g_{0}^{2}} - \frac{7d+1}{4d} \sum_{(0)} \frac{L^{d}}{|\mathbf{k}|^{3}} + \frac{2n_{f}(d-1)}{8d} \sum_{(\frac{1}{2})} \frac{L^{d}}{|\mathbf{k}|^{3}},$$

$$\frac{1}{g^{2}} + \tilde{\alpha}_{2} = 8(\tilde{\kappa}_{4} - \tilde{\kappa}_{3}) + \frac{1}{g_{0}^{2}} - 2\left(1 + \frac{(d-1)(d-6)}{24d}\right) \sum_{(0)} \frac{L^{d}}{|\mathbf{k}|^{3}}$$

$$+ \frac{2n_{f}(2d-3)}{12d} \sum_{(\frac{1}{2})} \frac{L^{d}}{|\mathbf{k}|^{3}},$$

$$\alpha_{1}' = \frac{1}{144\pi^{2}} - 3\kappa_{2}',$$

$$\alpha_{2}' = \frac{1}{72\pi^{2}} - 3\kappa_{2}' + 8(\kappa_{4}' - \kappa_{3}'),$$

$$\alpha_{3}' = \frac{1}{64} L^{5} \sum_{(\frac{1}{2})} \left(\frac{1}{3|\mathbf{k}|^{5}} - \frac{35k_{1}^{2}k_{2}^{2}}{4|\mathbf{k}|^{9}} + \frac{189k_{1}^{2}k_{2}^{2}k_{3}^{2}}{4|\mathbf{k}|^{11}}\right),$$

$$\alpha_{4}' = \frac{1}{64} L^{5} \sum_{(\frac{1}{2})} \left(\frac{36k_{1}^{2}k_{2}^{4}}{2|\mathbf{k}|^{11}} - \frac{189k_{1}^{2}k_{2}^{2}k_{3}^{2}}{2|\mathbf{k}|^{11}}\right),$$

$$\alpha_{5}' = \frac{1}{64} L^{5} \sum_{(\frac{1}{2})} \left(\frac{1}{|\mathbf{k}|^{5}} - \frac{63k_{1}^{2}k_{2}^{2}k_{3}^{2}}{|\mathbf{k}|^{11}}\right),$$
(19)

where d is the dimension of space, g_0 is the bare coupling constant and

$$\sum_{(0)} = \sum_{k=2\pi n/L \neq 0}, \qquad \sum_{(n_0)} = \sum_{k=2\pi (n+n_0(1,1,1))/L}.$$
 (20)

For the remaining coefficients see ref. [16] or below.

 TABLE 1

 Coefficients for the SU(2) effective hamiltonian. The primed coefficients give the fermionic contribution per Weyl component

$\kappa_{1} = -0.30104661$ $\kappa_{2} = -6.3319840 \times 10^{-3}$ $\kappa_{3} = 5.6289546 \times 10^{-4}$ $\kappa_{4} = -1.5687855 \times 10^{-3}$ $\kappa_{5} = 4.9676959 \times 10^{-5}$ $\kappa_{6} = -5.5172502 \times 10^{-5}$ $\kappa_{7} = -1.2423581 \times 10^{-3}$	$\begin{aligned} \alpha_1 &= 2.1810429 \times 10^{-2} \\ \alpha_2 &= 7.5714590 \times 10^{-3} \\ \alpha_3 &= -1.1130266 \times 10^{-4} \\ \alpha_4 &= -2.1475176 \times 10^{-4} \\ \alpha_5 &= -1.2775652 \times 10^{-3} \end{aligned}$
$\kappa'_{1} = -2.1272012 \times 10^{-2}$ $\kappa'_{2} = 2.2421241 \times 10^{-4}$ $\kappa'_{3} = 3.5180967 \times 10^{-5}$ $\kappa'_{4} = 1.5850480 \times 10^{-4}$ $\kappa'_{5} = -2.8659656 \times 10^{-6}$ $\kappa'_{6} = 1.1578663 \times 10^{-5}$ $\kappa'_{7} = -7.9447492 \times 10^{-5}$	$\begin{aligned} \alpha_1' &= 3.098211 \times 10^{-5} \\ \alpha_2' &= 1.7211922 \times 10^{-3} \\ \alpha_3' &= 3.0178786 \times 10^{-5} \\ \alpha_4' &= 3.2156523 \times 10^{-5} \\ \alpha_5' &= -3.2271736 \times 10^{-5} \end{aligned}$

To obtain the perturbative expansion we add $2n_f \hat{V}_1(\pi, \pi, \pi)$ to eq. (17) and rescale the fields as

$$c_i^a \to g^{2/3} \left(1 - \frac{1}{6} (\tilde{\alpha}_1 + \tilde{\alpha}_2) g^2 \right) c_i^a,$$
 (21)

which yields Lüscher's effective hamiltonian [1] with n_f dependent coefficients

$$L \cdot H_{\rm eff} = g^{2/3} H_0 + g^{4/3} \tilde{\kappa}_1 c_i^a c_i^a + g^{8/3} (\tilde{\kappa}_2 + \frac{8}{3} (\tilde{\kappa}_4 - \tilde{\kappa}_3)) H_0 + 3g^{8/3} (\tilde{\kappa}_3 - \tilde{\kappa}_4) c_i^a c_i^a c_j^b c_j^b + 5g^{8/3} \tilde{\kappa}_4 c_i^a c_i^b c_i^b + \dots, \qquad (22)$$

with

$$H_0 = -\frac{1}{2} \frac{\partial^2}{\partial c_i^{a2}} + \frac{1}{4} F_{ij}^a F_{ij}^a.$$
(23)

This deviates slightly from Lüscher's [1] expression, but is equivalent to it by the use of the virial theorem, which implies $(\phi_0, F_{ij}^{a2}\phi_0) = \frac{4}{3}(\phi_0, H_0\phi_0)$ (here ϕ_0 is the eigenfunction of H_0). Energies, labelled by the representations of the cubic group are again given by a power series in $g^{2/3}$, but now with coefficients $\tilde{\epsilon}_i$ which depend on the number of flavours

$$L \cdot E = g^{2/3} \tilde{\epsilon}_1 + g^{4/3} \tilde{\epsilon}_2 + g^2 \tilde{\epsilon}_3 + g^{8/3} \tilde{\epsilon}_4 + O(g^{10/3}),$$

$$\tilde{\epsilon}_1 = \epsilon_1, \quad \tilde{\epsilon}_2 = \rho \epsilon_2, \quad \tilde{\epsilon}_3 = \rho^2 \epsilon_3, \quad \rho = \tilde{\kappa}_1 / \kappa_1,$$

$$\tilde{\epsilon}_4 = \rho^3 \epsilon_4 + \left[\tilde{\kappa}_2 + \frac{8}{3} (\tilde{\kappa}_4 - \tilde{\kappa}_3) - \rho^3 (\kappa_2 + \frac{8}{3} (\kappa_4 - \kappa_3)) \right] \epsilon_1$$

$$+ 3 \left[\tilde{\kappa}_3 - \tilde{\kappa}_4 - \rho^3 (\kappa_3 - \kappa_4) \right] \eta_1 + 5 \left[\tilde{\kappa}_4 - \rho^3 \kappa_4 \right] \eta_2, \quad (24)$$

	A_1^+	A_1^+	A_1^-	E^+	T_2^+
η_1	18.348	55.96	27.1518	41.55	41.55
η_2	8.8134	30.18	11.6048	25.10	19.47
$\tilde{\tilde{\epsilon}}_1(3)$	4.116720	6.386359	8.786713	6.0145	6.0145
$\tilde{\epsilon}_{2}(3)$	-0.676567	-1.135974	-0.855423	-1.039	-1.039
$\tilde{\epsilon}_3(3)$	-0.039464	-0.145	-0.024888	- 0.090	-0.090
$\tilde{\epsilon}_{4}(3)$	-0.02188	-0.0382	-0.0485197	-0.0732	-0.0023

 TABLE 2

 Coefficients for the perturbative expansion of the energy for a few low-lying states in SU(2)

where ε_i were calculated by Lüscher and Münster [1] and η_i are the expectation values

$$\eta_1 = \left(\phi_0, c_i^a c_i^a c_j^b c_j^b \phi_0\right), \qquad \eta_2 = \left(\phi_0, c_i^a c_i^a c_i^b c_i^b \phi_0\right). \tag{25}$$

They are given in table 2 for a few states, together with $\tilde{\epsilon}_i$ as an example for three flavours. One can easily generate the results for other flavours by using eq. (24).

We note that for the first three orders in perturbation theory there is a simple scaling of the energies

$$L \cdot E(n_{\rm f}, g) = \rho^{-1} L \cdot E(0, \rho^{3/2} g).$$
⁽²⁶⁾

Masses, which are obtained as the energy differences with the ground state, scale similarly, whereas mass ratios $r_{\rm R} = m_{\rm R}/m_{A_1^+}$ scale with $z_{A_1^+} \equiv m_{A_1^+} \cdot L$ to this order as:

$$r_{\rm R}(n_{\rm f}, z_{A^+}) = r_{\rm R}(0, \rho z_{A^+}).$$
⁽²⁷⁾

Since $\rho = (1 - 0.14132n_f)$ is smaller than 1, the mass ratios in the presence of dynamical fermions have a weaker z-dependence than in the pure-gauge case, which suggests that the perturbative expansion remains valid for larger values of z. Indeed, this is what a crude nonperturbative analysis shows. Such an analysis is based on the fact that V_{eff} has local minima, which are false vacua, separated from the true vacuum by a potential barrier, and perturbation theory is typically expected to break down for the energy level in question, once this energy reaches the saddle point (the minimal potential one has to overcome to go to the false vacuum). We find the following heights $\delta V(n_f)$ for the saddle point above the vacuum:

$$L \cdot \delta V(0) = 3.210, \qquad L \cdot \delta V(1) = 3.576,$$

 $L \cdot \delta V(2) = 3.984, \qquad L \cdot \delta V(3) = 4.432.$ (28)

As an example we take again three flavours and equate E for the first excited A_1^+ state to δV . From this we find that the perturbative expansion should hold up to $g \sim 0.76$, which corresponds to $z_{A_1^+} \sim 1.5$ and $m_{A_1^+}/m_{E^+} \sim 1.18$. This is to be compared with the pure-gauge case, where perturbation theory for the same state breaks down at $g \sim 0.54$, for which $z_{A_1^+} \sim 1.0$. For SU(2) we therefore predict the low-lying glueball states to be arranged as in the pure-gauge case, independent of the boundary conditions for the fermions. Moreover, the spatial Polyakov line will have a single-phase structure, which clusters around (+1) - 1 with (anti-)periodic boundary conditions for the fermions.

5. The effective hamiltonian for SU(3)

The techniques to calculate the effective hamiltonian for SU(3) are essentially the same as for SU(2). We will restrict ourselves to one-loop and fourth order in the background field. In the following

$$F_{ij}^a = -f_{abc}c_i^b c_j^c, \qquad (29)$$

with f_{abc} the SU(3) structure constants. The coefficients of $-\frac{1}{2}\partial^2/\partial c_i^{a^2}$ and $F_{ij}^{a^2}$ were determined by a one-loop calculation; the remaining coefficients are determined by expanding the effective vacuum-valley potential. For this the following identities will be helpful ($\mu^{(i)}$ are the weights introduced earlier)

$$\delta_{ab} = 2 \sum_{k=1}^{3} \mu_{a}^{(k)} \mu_{b}^{(k)} ,$$

$$d_{abc} = \frac{4}{3} \sum_{k=1}^{3} \mu_{a}^{(k)} \mu_{b}^{(k)} \mu_{c}^{(k)} ,$$

$$s_{abcd} = 18 \sum_{k=1}^{3} \mu_{a}^{(k)} \mu_{b}^{(k)} \mu_{c}^{(k)} \mu_{d}^{(k)} .$$
(30)

In this equation a, b, c and d run only over the generators of the Cartan subalgebra (i.e. in our conventions over 1 and 2), $d_{abc} = 2 \operatorname{Tr}(\{T_a, T_b\}T_c)$ and s_{abcd} is the symmetric tensor introduced by Lüscher [1]. We note that, for SU(3), [19]

$$s_{abcd} = \frac{3}{4} \left(\delta_{ab} \delta_{cd} + \delta_{ac} \delta_{bd} + \delta_{ad} \delta_{bc} \right), \tag{31}$$

(for SU(N), N > 3, no similar reduction of s_{abcd} to delta functions exists.)

Using the fact that δ and d are irreducible SU(3) invariant tensors, the extension to fourth order in the fields, from the vacuum valley to all background fields, is unique up to $F_{ij}^{a^2}$. The result will, therefore, be expressed in terms of the Taylor

coefficients of \hat{V}_1

$$n_{0} \neq 0, \qquad M_{i_{1} \dots i_{n}}^{(n_{0})} = \frac{\partial^{n} \hat{V}_{1}(C)}{\partial C_{i_{1}} \dots \partial C_{i_{n}}} \bigg|_{C = 2\pi n_{0}(1,1,1)},$$

$$n_{0} = 0, \qquad M_{i_{1} \dots i_{n}}^{(0)} = \frac{\partial^{n} (\hat{V}_{1}(C) - 2|C|)}{\partial C_{i_{1}} \dots \partial C_{i_{n}}} \bigg|_{C = 0}.$$
(32)

Note that the $M_{i_1\cdots i_n}^{(n_0)}$ are fully symmetric with respect to its indices and further are related by S_3 (e.g. $M_{11} = M_{22} = M_{33}$, $M_{12} = M_{13} = M_{23}$ etc.) Furthermore, $M_{i_j}^{(1/3)}$ is negative definite (with two of its eigenvalues equal $M_{11}^{(1/3)} - M_{12}^{(1/3)}$ and the other eigenvalue equal $M_{11}^{(1/3)} + 2M_{12}^{(1/3)}$), which guarantees that $\mu^{(i)} \cdot C = 2\pi/3(1,1,1)$ is a minimum of $V_{\text{eff}}^+(C_i^a)$.

We find the following expression for the SU(3) effective hamiltonian

$$L \cdot H_{eff} = -\frac{1}{2} K_{ij} \frac{\partial^2}{\partial c_i^a \partial c_j^a} + V(c_i^a),$$

$$(K^{-1})_{ij} = \frac{1}{g^2} + \alpha_1^{(n_0)} \quad \text{for} \quad i = j,$$

$$= -n_i \beta^{(n_0)} \quad \text{for} \quad i \neq j,$$

$$V(c_i^a) = \frac{1}{4} \left(\frac{1}{g^2} + \alpha_2^{(n_0)}\right) F_{ij}^a F_{ij}^a + \frac{1}{2} n_f \beta^{(n_0)} \sum_{i \neq j} F_{ik}^a F_{jk}^a + \frac{1}{4} \left(3M_{ij}^{(0)} - n_f M_{ij}^{(n_0)}\right) c_i^a c_j^a$$

$$- \frac{1}{8} n_f M_{ijk}^{(n_0)} d_{abe} c_i^a c_j^b c_k^e + \frac{1}{432} \left(9M_{ijkm}^{(0)} - n_f M_{ijkm}^{(n_0)}\right) s_{abde} c_i^a c_j^b c_k^d c_m^e, \quad (33)$$

where $\alpha_1^{(n_0)}$, $\alpha_2^{(n_0)}$ and $\beta^{(n_0)}$ are determined by

$$\frac{1}{g^2} + \alpha_1^{(n_0)} = \frac{1}{g_0^2} - 3\frac{(7d+1)}{8d}\sum_{(0)}\frac{L^d}{|\boldsymbol{k}|^3} + \frac{2n_f(d-1)}{8d}\sum_{(n_0)}\frac{L^d}{|\boldsymbol{k}|^3},$$

$$\frac{1}{g^2} + \alpha_2^{(n_0)} = \frac{1}{g_0^2} - 3\left(1 + \frac{(d-1)(d-6)}{24d}\right)\sum_{(0)}\frac{L^d}{|\boldsymbol{k}|^3} + \frac{2n_f(2d-3)}{12d}\sum_{(n_0)}\frac{L^d}{|\boldsymbol{k}|^3},$$

$$\beta^{(n_0)} = \sum_{(n_0)}\frac{L^d k_1 k_2}{4|\boldsymbol{k}|^5} = \frac{1}{24}\left(2M_{1112}^{(n_0)} + M_{1123}^{(n_0)}\right).$$
(34)

In table 3 we give the values of $M^{(n_0)}$ for $n_0 = 0$, $n_0 = \frac{1}{2}$ and $n_0 = \frac{1}{3}$. The following relations of $M^{(n_0)}$ with κ_i and κ'_i hold

$$M_{11}^{(0)} = 2\kappa_1, \ M_{1111}^{(0)} = 24(3\kappa_3 + 2\kappa_4), \qquad M_{1122}^{(0)} = 24(\kappa_3 - \kappa_4),$$

$$M_{11}^{(1/2)} = 8\kappa_1', M_{1111}^{(1/2)} = 384(3\kappa_3' + 2\kappa_4'), \qquad M_{1122}^{(1/2)} = 384(\kappa_3' - \kappa_4'); \qquad (35)$$

furthermore, we have

$$\alpha_{1}^{(n_{0})} = 1.5 \left(\frac{1}{36\pi^{2}} - 3\kappa_{2} \right) - 2n_{f} \left(\frac{1}{144\pi^{2}} - 3\kappa_{2}^{(n_{0})} \right),$$

$$\alpha_{2}^{(n_{0})} = 1.5 \left(\frac{1}{18\pi^{2}} - 3\kappa_{2} \right) - 2n_{f} \left(\frac{1}{72\pi^{2}} - 3\kappa_{2}^{(n_{0})} \right),$$

$$\kappa_{2}^{(1/2)} = \kappa_{2}', \qquad \kappa_{2}^{(1/3)} = 4.856880 \times 10^{-4}.$$
(36)

The case of $n_0 = \frac{1}{2}$ gives the results for antiperiodic boundary conditions. For periodic boundary conditions of the fermion fields one has to choose $n_0 = \frac{1}{3}$.

To obtain the perturbative expansion we rescale the fields as in eq. (21)

$$c_i^a \to g^{(2/3)} \left(1 - \frac{1}{6} \left(\alpha_1^{(n_0)} + \alpha_2^{(n_0)} \right) g^2 \right) c_i^a,$$
(37)

and find (using eq. (29), H_0 is still given by eq. (23))

$$L \cdot H_{eff} = g^{2/3} H_0 + \frac{1}{4} g^{4/3} \left(3M_{ij}^{(0)} - n_f M_{ij}^{(n_0)} \right) c_i^a c_j^a - \frac{1}{8} g^2 n_f M_{ijk}^{(n_0)} d_{abe} c_i^a c_j^b c_k^e + g^{8/3} \left(1.5 \kappa_2 - 2n_f \kappa_2^{(n_0)} \right) H_0 + \frac{1}{432} g^{8/3} \left(9M_{ijkm}^{(0)} - n_f M_{ijkm}^{(n_0)} \right) s_{abde} c_i^a c_j^b c_k^d c_m^e + \frac{1}{2} g^{8/3} n_f \beta^{(n_0)} \sum_{i \neq j} \left(-\frac{\partial^2}{\partial c_i^a \partial c_i^a} + F_{ik}^a F_{jk}^a \right) + \cdots$$
(38)

For the case of antiperiodic boundary conditions in the fermions, H_{eff} is exactly of the same form as in ref. [1] but with coefficients depending on the number of flavours. (To be specific one makes the following replacements in Lüscher's expression for the SU(3) pure gauge effective hamiltonian: $a_1 \rightarrow a_1 - 2n_f \kappa'_1$, $a_3 \rightarrow a_3 - \frac{8}{3}n_f(\kappa'_3 - \kappa'_4) a_4 \rightarrow a_4 - \frac{40}{3}n_f \kappa'_4$.) The quantum vacuum is unique with a single phase structure for the Polyakov loops P_j , clustering around 1. The effective hamiltonian has the symmetries of the full cubic group and charge conjugation C

$$C: \qquad c_i \cdot T \to -(c_i \cdot T)^* = -(c_i \cdot T)^t. \tag{39}$$

	$n_0 = 0$	$n_0 = \frac{1}{2}$	$n_0 = \frac{1}{3}$
M _{ii}	$-6.0209322 \times 10^{-1}$	$-1.70176098 \times 10^{-1}$	$-1.25941522 \times 10^{-1}$
M _{ii}	0.0	0.0	$-6.03866725 \times 10^{-2}$
M _{iii}	0.0	0.0	$-1.88451162 imes 10^{-1}$
 М _{ін і}	0.0	0.0	$4.40270126 \times 10^{-2}$
Min	0.0	0.0	$4.07658227 \times 10^{-1}$
М.,,,	$-3.4773231 \times 10^{-2}$	$1.62260164 imes 10^{-1}$	$1.38599356 imes 10^{-1}$
M	5.1160343×10^{-2}	$-4.73563539 \times 10^{-2}$	$-3.55259501 \times 10^{-2}$
Miiri	0.0	0.0	$4.25447526 \times 10^{-2}$
Maria	0.0	0.0	$-3.61684403 \times 10^{-2}$

TABLE 3 Taylor coefficients of \hat{V}_1 . No summations over repeated indices is implied, $i \neq j \neq k$ run from 1 to 3 and M is symmetric in its indices

For the first three non-trivial orders we have, again, exactly the same scaling behaviour of eqs. (26) and (27), but with

$$\rho = (3\kappa_1 - 4n_f\kappa_1')/(3\kappa_1) = (1 - 0.09421 n_f).$$
⁽⁴⁰⁾

To this order the results can, therefore, be read off from those of ref. [20], using eqs. (26) and (27). We will not determine the dependence of the fourth order term on the number of flavours, expecting this dependence to be relatively weak, like for SU(2).

For $n_f = 3$, $\rho^{-1} \sim 1.394$ and the saddle point, similar to what was discussed for SU(2), has a height of $L \cdot \delta V \sim 7.834$ above the vacuum. Therefore, perturbation theory is expected to break down at $g \sim 0.64$ for the first excited A_1^{++} state, which corresponds to $z_{A_1^{++}} \sim 1.8$. (In this case we have to compare δV with the energy difference of the SU(2) groundstate energy [21].)

Finally, we will discuss the consequences of our results for the energy levels of SU(3) with periodic boundary conditions for the fermions. As observed before, the coordinate-reflection symmetry is broken, since the values of P_j are not invariant under these symmetries. Moreover, since P_j is complex, charge conjugation is also spontaneously broken. However, since charge conjugation C has the same effect as overall parity P on the value of this Polyakov loop, evaluated in the quantum vacua, the simultaneous parity and charge conjugation transformation is still a symmetry. That is, CP is conversed but C and P are separately broken spontaneously. Indeed, only terms in the expansion of the effective hamiltonian, which are odd in the tensor d_{abc} , break either parity or charge conjugation, but are invariant under their combined action. The other symmetries of the perturbative vacuum are the coordinate permutations S₃ (up to a possible conjugation with coordinate reflections). Irreducible representations of S₃ × CP are denoted by A_1^k , E^k and A_2^k , with $k = \pm 1$ the eigenvalue of CP. The representations A_1 and A_2 are singlets and E is a

doublet. Each perturbative state is eightfold degenerate and tunneling between the vacua will lift the degeneracies and restore the full symmetries (of the cubic group and charge conjugation.) The perturbative ground state is an A_1^+ state, which will split into the following representations of $O(3, Z) \times C$: $A_1^+ \rightarrow A_1^{++}, T_2^{--}, T_2^{++}, A_1^{--}$. Alternatively, these states can be classified by the eigenvalues p_j of the coordinate reflections. The A_1^{++} corresponds to all $p_j = 1$; T_2^{--} , to one out of the three $p_j = -1$; T_2^{++} , to two out of the three $p_j = -1$; and A_1^{--} corresponds to all $p_j = 1$; T_2^{--} , to use study the eigenvalues P_j by the eigenvalue SU(2) gauge theory [8, 16].) We therefore have the surprising result that at small volumes the mass gap is exponentially small. Furthermore, each spatial Polyakov loop P_j has a two-phase structure, at sufficiently weak coupling, clustering around $\exp(2\pi i/3)$ and $\exp(-2\pi i/3)$. No clustering around 1 should occur.

Concerning perturbation theory we can obtain the low-order results from those of Weisz and Ziemann [20], depending on the representation in question. Since reflection symmetry is already broken at second order in perturbation theory $(M_{ij}^{(1/3)}$ is not diagonal), there are two possibilities: (i) states A_1^{PC} , E^{PC} and A_2^{PC} which do not split since they are already representations of $S_3 \times CP$. Their energies are given by

$$L \cdot E = \epsilon_1 g^{2/3} + \epsilon_2 \left(1 - \frac{M_{11}^{(1/3)} n_f}{6\kappa_1} \right) g^{4/3} + \mathcal{O}(g^2), \qquad (41)$$

where the $O(g^2)$ term requires more information than can be extracted from [20]; (ii) states T_1^{PC} and T_2^{PC} which are not invariant under coordinate reflections and will hence split into irreducible representations of $S_3 \times CP$ (into (E^k, A_2^k) and (E^k, A_1^k) , respectively, where k is the eigenvalue of CP). This splitting occurs to order $g^{4/3}$ since $M_{ij}^{(1/3)}c_i^a c_j^a$ is not invariant under coordinate reflections. In this case we can only extract the lowest order energy, which does not depend on the number of flavours, from ref. [20].

A safe estimate for $z_{A_1^{++}}$, below which the mass gap is exponentially small, is the value of 1.6 estimated for the pure-gauge case, as the value below which electric flux is suppressed [21]. A more detailed analysis of nonperturbative effects is beyond the scope of this paper. However, we can expect that the ratio $m_{A_1^{++}}/m_{E^{++}}$ (the scalar-to-tensor glueball mass ratio) remains relatively constant with a value of 1.2–1.3 and that the perturbative results (eq. (42) together with the results of ref. [20]) remain valid up to at least $z_{A_1^{++}} \sim 1.5$.

This is consistent with the Monte Carlo results of ref. [5] where the following ratios were measured: $m_{A_1^{++}}/m_{E^{++}} = 1.31 \pm 0.17$ at $z_{A_1^{++}} = 3.08 \pm 0.24$, $m_{A_1^{++}}/m_{E^{++}} = 1.62 \pm 0.30$ at $z_{A_1^{++}} = 3.24 \pm 0.30$ and $m_{A_1^{++}}/m_{E^{++}} = 1.69 \pm 0.40$ at $z_{A_1^{++}} = 3.52 \pm 0.60$. However, the fermion mass used in ref. [5] is relatively high and a direct comparison has to wait until the mass dependence is included in the analytic calculations. This dependence is, however, expected to be small because the mass ratios only weakly depend on the fermionic contributions. To lowest order, glueball masses are independent of this fermion mass since to order $g^{2/3}$ there is no n_f dependence.

6. Conclusions

We have started to investigate the effect of dynamical massless fermions, in the continuum for gauge theories in a finite cubic volume, on the low-lying spectrum for the glueball states. Already, at the order which allows one to identify the proper quantum vacuum, we found unexpected results. In particular, for periodic boundary conditions in the spatial directions imposed on the fermions, no zero-energy modes for the fermions arose and for SU(3) we found an unexpected rich vacuum structure, whose more direct consequences should be easily verifiable in Monte Carlo studies. We hope that some of the present work can serve as a testing ground for the fermionic algorithms developed [22]. A comparison with existing Monte Carlo results [5] for SU(3) was possible, but one needs to include nonperturbative corrections in the spirit of the pure-gauge case [8, 16] and a fermion-mass term in order to make a direct comparison.

Except for the case of SU(3) with periodic boundary conditions imposed on the fermions, the small-volume expansion is remarkably similar to the pure-gauge case [1,20], as expressed in terms of the scaling in eqs. (26) and (27), valid up to and including third order in $g^{2/3}$. We should stress, however, that there is no reason to expect this scaling to hold even approximately in larger volumes.

As for the pure-gauge case no claim is made that the results will give predictions for infinite-volume mass ratios and the interest is mainly theoretical. It would, however, be desirable for some SU(2) Monte Carlo glueball-spectrum calculations with dynamical fermions to become available, since intermediate-volume analytic calculations for SU(2) seem feasible, whereas those for SU(3) at present appear impractical. Certainly, in the pure-gauge case these intermediate-volume calculations give good results, at least for the lowest-lying states, and seem to bring us to the point where confining effects set in [6, 8, 16]. This conclusion is supported by the recent finite-temperature analysis [23]. In the presence of massless fermions one would likewise expect the intermediate-volume calculation (based on using the effective hamiltonian presented here, supplemented with boundary conditions in configuration space, which are dictated by symmetries and Gribov horizons [16]) to bring us to the point where spontaneous breaking of chiral symmetry starts to manifest itself.

Andreas Gocksch was the first to urge me to look at fermions in a small volume, for which I thank him. I am greatly indebted to Jack Smith, whose valuable time was spent on ensuring that I could use my Stony Brook computer programmes at CERN. Many of those programmes were to a large extent developed by Jeff Koller and I thank him for the fruitful collaboration of the previous two years. I also wish to thank Jürg Gasser, Frithjof Karsch, Apoorva Patel and Akira Ukawa for fruitful discussions and Ulrich Baur for his help to run TEX.

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