ANNALS OF PHYSICS 174, 299-371 (1987)

QCD on a Torus, and Electric Flux Energies from Tunneling

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Received May 8, 1986

The energy of 't Hooft-type electric flux in pure QCD on the hypertorus is a non-perturbative effect, caused by tunneling through a quantum-induced potential barrier. We calculate the electric flux energy using the semiclassical approximation. The problem of infrared divergences is attacked directly, and we show how to treat them consistently, using Lüscher's effective Hamiltonian approach. A toy model is first solved to demonstrate the consistency of our approach. Lüscher's effective Hamiltonian for the spatially constant modes in QCD is rederived using a Lagrangian approach with a non-local gauge-fixing term, and we show how this rigorously defines an effective action to all loop orders. The removal of the gauge degrees of freedom from the effective Hamiltonian while avoiding Gribov ambiguities is discussed in detail, as are the numerical methods required to treat this non-integrable system. Some consequences of our final result are noted.

1. INTRODUCTION

Unbroken gauge theories are plagued by infrared divergences in perturbation theory. However, the infrared region is believed to be crucial for confinement, which is a long distance feature of the theory. Our difficulties are caused by the strong increase of the effective coupling constant at large distances, the counterpart of asymptotic freedom. To be able to do perturbation theory it is therefore useful to use an infrared cutoff, and the most elegant procedure is to consider the theory in a three-dimensional box and impose periodic boundary conditions. These boundary conditions must not break the gauge invariance, so we require only gauge invariant quantities to be periodic; the gauge potential is only periodic up to a gauge transformation. In this way, 't Hooft [1] introduced gauge theories on the hypertorus. If there are no matter fields in the fundamental representation of the gauge group, electric and magnetic flux are defined by a topological property called twist. If we take the hypertorus to be a cube with sides of length L, and assume that when L gets large electric flux tubes form, then the energy of electric flux will be of the form $\sigma \cdot L$, and we recognize σ as the string tension.

However, the energy of electric flux can only be calculated analytically for small L. Lüscher [2] showed how to do perturbation theory on the hypertorus in the zero magnetic flux case. He found that to all orders in perturbation theory there is a

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degeneracy in electric flux, i.e., electric flux has no energy in perturbation theory. In a previous paper by one of us [3] it was explaned how this degeneracy is lifted by tunneling through a quantum-induced potential, and we called the associated "classical solution" a "pinchon," because it is analogous to an instanton. We expressed the dimensionless ratio of the energy of electric flux ($\Delta E(L)$) and the glueball mas $M_L(0^+)$ in terms of Lüscher's universal expansion parameter $z = M_L(0^+) \cdot L$ [4], which yields a universal (i.e., renormalization group independent) function. The large L (i.e., large z) behaviour is also known if we assume string formation and a finite glueball mass: $\Delta E(L)/M_L(0^+) \sim (\sigma/M(0^+)^2)\, z$.

We expect the formation of flux tubes to be due to non-perturbative effects. One could thus hope that in a situation where the perturbative contributions are completely absent (unlike in the case of nonzero magnetic flux), there is a smooth behaviour when going from small to large values of z, except of course at the point where the non-perturbative effect sets in.

In a paper [5] where we presented the final result for the short distance expansion of $\mathscr{E}(L) = \Delta E(L)/M_L(0^+)$ for $SU(2)$, this behaviour was indeed observed. Although Monte Carlo calculations [6] have not yet confirmed the onset of tunneling (which we predicted to occur at $z \simeq 1.2$), data is available in the range $z \cong 1.5$ to $z \simeq 8$. Despite the fact that these Monte Carlo calculations were performed on periodic lattices, we were able to identify the energy obtained from time-time correlation functions for spatial Polyakov loops in the *fundamental* representation [6] as the energy of electric flux, which was first defined by 't Hooft by using twisted boundary conditions [1]. Originally these correlation functions were used as an alternative way to calculate the string tension, so one was interested in their large z behaviour; our interpretation provides a well-defined meaning of this quantity for all z values. It becomes an important tool in probing the physics of the QCD vacuum [5].

To understand how one can relate two apparently separate fields, 't Hooft's QCD on a torus with *twisted* boundary conditions, and conventional lattice QCD with *periodic* boundary conditions, we observe that in the Hamiltonian formalism with zero magnetic flux (no twist in the spatial deirection) one also works with periodic boundary conditions. Electric flux, alternatively defined by 't Hooft as a twist in the time direction, is introduced in this case by classifying the physical states as representations of the homotopy group of allowed gauge transformations, as explained in Section 2. Similarly, on the lattice one can define 't Hooft-type electric flux using the transfer matrix approach, as explained in [32]. On the other hand, a spatial Polyakov loop in the fundamental representation creates one unit of electric flux [1]. (Details on this can be found in [8].) Time–time correlation functions of such loops thus select the energy difference between the ground state with one unit of electric flux and the ground state with zero electric flux, which is the way the energy of electric flux was defined by 't Hooft.

This paper is technical in nature. It provides a thorough discussion of the tunneling calculation and gives results contained in [11], hitherto unpublished. It furthermore gives results left out in [3, 5]. The paper is organized as follows: In Section 2

we discuss the classical vacuum. Section 3 presents a toy model closely related to the problem at hand; here we also review the effective Hamiltonian calculation based on Bloch perturbation theory. Section 4 discusses this effective Hamiltonian for $SU(2)$ Yang–Mills on T^3, but also gives a Lagrangian derivation. We work out in great detail the non-local gauge fixing introduced in [3] and show what the consequences are for the ghost interactions. It is important to note that our approach yields a *consistent* split into the spatially constant and spatially varying modes, which allows a proper and gauge-invariant treatment of infrared modes, *without* giving those modes a "mass" term (as would happen for non-zero magnetic flux or for Yang–Mills on a sphere).

Section 5 is devoted to eliminating the gauge degrees of freedom in the effective Hamiltonian. We show that a conventional approach based on gauge fixing leads to Gribov ambiguities. We also show how to decompose this Hamiltonian, which has six degrees of freedom, into a piece along the three-dimensional vacuum valley and a piece orthogonal to it.

Section 6 explains how the tunneling calculation (to the order in which we are interested) reduces to a calculation for a three-dimensional cubic lattice with a well-defined bounded potential. In Section 7 we calculate the appropriate energies using this reduction and summarize our analytic results.

These analytic results involve the perturbative energies and wavefunctions, and a contribution from transverse fluctuations along the pinchon (the instanton path). It has been shown that the effective Hamiltonian (Yang–Mills for spatially constant vectors potentials) is non-integrable [12], so to obtain these quantities, one has to resort to numerical calculations, which are described in detail in Section 8.

The results of these calculations have been presented earlier [5]. Here we describe the methods, closely connected to the route followed by Lüscher and Münster [13] for $SU(2)$.

Finally, there are four appendices, discussing respectively the properties of the one-loop effective potential, the polar decomposition, the multiloop infrared behaviour, and a discussion on generalizing our results to arbitrary gauge group.

2. The Classical Vacuum

In this section we will work in the Hamiltonian formalism of Lüscher [2]. Our base space is then the flat torus T^3, or its equivalent $\mathbf{R}^3/\Lambda$, where Λ is the lattice spanned by $\mathbf{a}^{(i)}$, $i=1, 2, 3$. We will choose the torus symmetric, of length L in each direction ($\mathbf{a}^{(i)} = L\mathbf{e}^{(i)}$), but this is only for convenience, and the calculation could be done on tori of other shapes. If the magnetic flux is zero, as will be assumed throughout, one can always choose a gauge such that the potentials themselves are periodic:

$$\mathbf{A}(\mathbf{x}+\mathbf{a}^{(i)}) = \mathbf{A}(\mathbf{x}). \tag{2.1}$$

Gauss's law then imposes the constraint that physical state vectors are invariant under any periodic, homotopically trivial gauge transformation. However, the full set of all "allowed gauge transformations" (i.e., all those that do not alter the periodicity of any periodic gauge potential), is a larger class also containing gauge transformations only periodic up to an element of the center of the gauge group. For $SU(2)$ this is just $\mathbf{Z}_2 = \{\pm 1\}$:

$$\Omega(\mathbf{x} + \mathbf{a}^{(i)}) = (-1)^{k_i} \Omega(\mathbf{x}). \tag{2.2}$$

The homotopy type is thus specified by the three integers $k_i \bmod 2$, and the winding number

$$P = \frac{1}{24\pi^3} \int_{T^3} d^3x \, \varepsilon_{ijk} \operatorname{Tr}((\Omega \partial_i \Omega^{-1})(\Omega \partial_j \Omega^{-1})(\Omega \partial_k \Omega^{-1})), \tag{2.3}$$

which (for zero magnetic flux) is an integer.

The physical state vectors are now labeled by the quantum numbers $\theta \pmod{2\pi}$ and $\mathbf{e} \pmod 2$, which are conjugate to P and $\mathbf{k}$, in the sense that if we denote the action of a gauge transformation on state vectors by $[\Omega]$, then

$$[\Omega] \, |\mathbf{e}, \theta\rangle = e^{\pi i \mathbf{k} \cdot \mathbf{e} + i\theta P} \, |\mathbf{e}, \theta\rangle. \tag{2.4}$$

The quantum number $\mathbf{e}$ is the electric flux of the state, as defined by 't Hooft [1]. In future we thus distinguish between "periodic gauge transformations," under which physical state vectors are invariant, and the "allowed gauge transformations."

Our first step is to identify the classical vacuum, which will suggest appropriate coordinates for specifying the wavefunctions. The classical potential is the positive definite expression

$$V(\mathbf{A}) = \frac{1}{2g_0^2} \int_{T^3} d^3x \operatorname{Tr}(F_{ij}^2), \tag{2.5}$$

$$F_{ij} = \partial_i A_j - \partial_j A_i + i[A_i, A_j], \tag{2.6}$$

so the classical vacuum is the set of the curvature-free ($F_{ij} = 0$) vector potentials. Because T^3 is multiconnected, these are not all gauge equivalent. To see this, consider the Wilson loop

$$W(\mathscr{C}) = \operatorname{Tr} \mathrm{P} \exp\left(i \oint_{\mathscr{C}} \mathbf{A} \cdot d\mathbf{x} \right), \tag{2.7}$$

which is invariant under infinitesimal deformations of the loop $\mathscr{C}$ if and only if the colour magnetic field is zero. (Recall that F_{ij} is given by the area derivative [9].) Thus for a vacuum configuration $W(\mathscr{C})$ is completely determined by the homotopy type of the curve $\mathscr{C}$. In a simply connected space $\mathscr{C}$ is always contractible and $W(\mathscr{C}) = 2$. However, for T^3 the homotopy type of $\mathscr{C}$ is specified by three integers n_i,

which give the winding numbers around each of the three generating circles of T^3. Hence

$$W(\mathscr{C}) = \mathrm{Tr}(U_1^{n_1} U_2^{n_2} U_3^{n_3}), \tag{2.8}$$

where

$$U_i = \mathrm{P} \exp\left(i \int_0^L A_i(s\mathbf{e}^{(i)})\, ds \right). \tag{2.9}$$

Furthermore, $W(\mathscr{C})$ does not depend on the order of U_i's, so these must commute. Let their eigenvalues be $\exp(\pm i\varphi_i)$: then, because $\mathrm{Tr}(U_i) = 2\cos\varphi_i$ is invariant under periodic gauge transformations, vacua with different values of $\cos\varphi_i$ must be inequivalent. Indeed, the vacua can be classified by $\cos\varphi_i$, since we can explicitly construct a curvature free configuration giving any desired value of $\cos\varphi_i$, viz., the constant field

$$A_i = \frac{\varphi_i}{L}\sigma_3 \equiv \frac{C_i}{L}\frac{\sigma_3}{2}, \tag{2.10}$$

with σ_i the Pauli matrices. Any other curvature-free configuration can be reduced to this form by a periodic gauge transformation. Also, one can identify

$$\begin{aligned} \varphi_i &\cong \varphi_i + 2\pi, \\ \varphi &\cong -\varphi. \end{aligned} \tag{2.11}$$

This corresponds to Lüscher's gauge-invariant labeling of the torons (i.e., classical vacua). Finally, note that an allowed gauge transformation of the type in Eq. (2.2) transforms $W(\mathscr{C})$ into $(-1)^{\mathbf{k}\cdot\mathbf{n}} W(\mathscr{C})$. Since these transformations are genuine invariances of the Hamiltonian, we make a note of how they transform the vacua:

$$\varphi_i \to \varphi_i + \pi n_i, \qquad C_i \to C_i + 2\pi n_i. \tag{2.12}$$

These transformations are generated by

$$\Omega^{(i)}(\mathbf{x}) = \exp(-\pi i x_i \sigma_3 / L). \tag{2.13}$$

In summary: the classical "vacuum valley" is parameterized by a vector $\mathbf{C}$, mod 4π, and a symmetry relates vacua $\mathbf{C}$, $-\mathbf{C}$, and $\mathbf{C} + 2\pi\mathbf{n}$ ($\mathbf{n} \in \mathbf{Z}_2^3$).

The next step is to expand the potential around the classical vacuum, so we follow Lüscher and write

$$A_k(\mathbf{x}) = \Omega(\mathbf{x}) \left(\frac{C_k \sigma^3}{2L} + g_0 q_k(\mathbf{x}) \right) \Omega^{-1}(\mathbf{x}) - i\Omega(\mathbf{x})\, \partial_i \Omega^{-1}(\mathbf{x}), \tag{2.14}$$

with the gauge condition

$$\int_{T^3} d^3x\, q_k^3(\mathbf{x}) = 0, \qquad D_i q_i(\mathbf{x}) = 0. \tag{2.15}$$

D_i is the covariant derivative in the background vacuum configuration

$$D_k = \hat{c}_k + i\,\mathrm{ad}\left(\frac{C_k \sigma_3}{2L}\right). \tag{2.16}$$

With this parameterization one finds

$$V(\mathbf{A}) = \int_{T^3} \mathrm{Tr}\{(D_i q_k(\mathbf{x}))^2 + 2ig_0(D_i q_j(\mathbf{x}))[q_i(\mathbf{x}), q_j(\mathbf{x})] - \tfrac{1}{2} g_0^2 [q_i(\mathbf{x}), q_j(\mathbf{x})]^2\}. \tag{2.17}$$

The quadratic part of V can be diagonalized by putting

$$\begin{aligned} q_i(\mathbf{x}) &= q_i^3(\mathbf{k})\, e^{2\pi i \mathbf{k}\cdot\mathbf{x}/L}\sigma_3, & \lambda^3(\mathbf{k}) &= \left(\frac{2\pi\mathbf{k}}{L}\right)^2 \qquad \mathbf{k}\neq\mathbf{0} \\ q_i(\mathbf{x}) &= q_i^+(\mathbf{k})\, e^{2\pi i \mathbf{k}\cdot\mathbf{x}/L}\frac{(\sigma_1 + i\sigma_2)}{2}, & \lambda_{\mathbf{C}}^+(\mathbf{k}) &= \left(\frac{2\pi\mathbf{k}+\mathbf{C}}{L}\right)^2 \end{aligned} \tag{2.18}$$

where $q_i^3(\mathbf{k})$ $(\mathbf{k}\neq\mathbf{0})$ and $q_i^+(\mathbf{k})$ satisfy the conditions

$$\mathbf{k}\cdot\mathbf{q}^3(\mathbf{k}) = (2\pi\mathbf{k}+\mathbf{C})\cdot\mathbf{q}^+(\mathbf{k}) = 0. \tag{2.19}$$

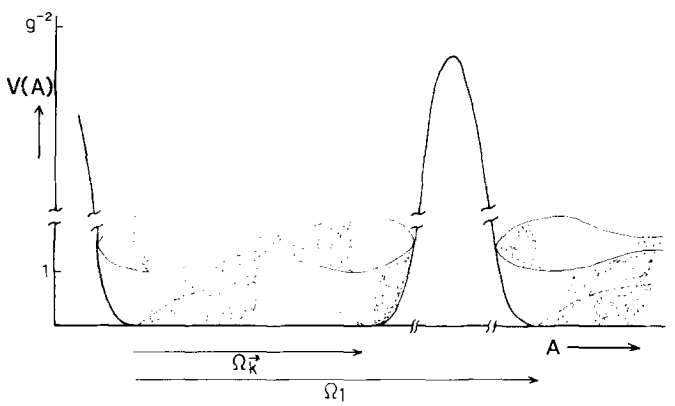


FIG. 1. An impressionistic graph of the potential $V(\mathbf{A})$, with the infinite-dimensional space of field configurations represented as two-dimensional. A classical vacuum valley lies at the minimum of the potential, but the squeezing of the potential in the transverse direction induces a quantum barrier (the dashed curve), causing the perturbative quantum vacua to occur where the potential is widest. Configurations with different winding number are separated by a classical barrier. Allowed gauge transformations Ω map one perturbative vacuum to another.

Note that for $\mathbf{C} = -2\pi\mathbf{n}$ there are modes with zero eigenvalues, which implies that the quadratic approximation fails for these modes. This is the well-known infrared problem, and it means that a naive perturbation expansion will fail. Much of this paper is devoted to treating these "quartic modes" correctly. It is a non-trivial problem to do this, and the same problem reappears in various guises at different places in the calculation. In the next section we will show how to deal with this.

Figure 1 is an attempt to show the shape of the potential $V(\mathbf{A})$. We have reduced the three-dimensional vacuum valley to one dimension, and shown only one of the infinitely many "transverse" directions. The transverse direction we have shown is one with quartic behaviour at $\mathbf{C} = 0$. Thus V is wide at this point, but "pinches" narrower at non-zero $\mathbf{C}$.

One might wonder if it is possible to remove these quartic modes by changing the metric of the torus. However, we see from Eq. (2.17) that the quartic modes are due to a zero eigenvalue for the Laplacian on T^3, and are thus related to the non-triviality of the De Rham cohomology. This depends only on the topology of the space, and not on the metric. For *zero* magnetic flux, there is no way out of the quartic-mode problem. What happens for non-zero magnetic flux is shown in [29].

3. A Toy Model

Let us first remind the reader of a toy model which was analysed in [14]:

$$H = -\frac{g^2}{2}\frac{\partial^2}{\partial x^2} - \frac{g^2}{2}\frac{\partial^2}{\partial y^2} + \frac{1}{2g^2}(x^2-1)^2 y^2. \tag{3.1}$$

This toy model shares with our full problem the feature of a vacuum valley and the breakdown of the quadratic expansion at $x = \pm 1$. However, there is a feature here that is different from the full problem. In [14] it was explained that one can use the one-loop effective potential $V_1(x)$ in the adiabatic approximation. The non-adiabatic corrections could be ignored: where they become important, near the points where the quadratic approximation breaks down, the information is contained in the perturbative wavefunction, which is matched to the non-perturbative part in a higher-dimensional WKB-type approximation, called the *path decomposition expansion.* In the full problem, we have an infinite number of transverse modes, each giving a non-adiabatic correction in the Lagrangian of order $\dot{x}^2$ to the leading order term $(1/g_0^2)\dot{x}^2$. Instead of ignoring this correction, it is imperative to note that it should actually give the proper renormalization of the coupling constant. We will come back to this later in a Lagrangian approach (Sect. 4).

Another difference between (3.1) and the full problem is that in (3.1) the breakdown of the quadratic approximation is caused by the same transverse variable y at both $x = \pm 1$. In the QCD problem, a mode which is quartic at $\mathbf{C} = \mathbf{0}$ is perfectly well behaved at $\mathbf{C} = 2\pi\mathbf{n}$. To understand what happens if the breakdown

of the quadratic approximation occurs due to different transverse modes, we have constructed another simple toy model,

$$H = -\frac{g^2}{2}\left(\frac{\partial^2}{\partial w^2}+\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+\frac{2}{g^2}\left((z-1)^2 y^2+(z+1)^2 x^2 + \left(\frac{z^2+3}{z^2+1}\right)^2 w^2\right)-4. \tag{3.2}$$

This exhibits the following symmetry:

$$\Pi(w, x, y, z) = (w, y, x, -z). \tag{3.3}$$

Note that Π^2 is the identity and hence wavefunctions are even or odd under Π. In particular, the twofold-degenerate ground state will be split into an even and an odd state, whose energy difference is determined by tunneling through the one-loop effective potential $V_1(z)$:

$$V_1(z) = \left(|z-1|+|z+1|+\frac{z^2+3}{z^2+1}\right)-4. \tag{3.4}$$

Note that the part of the Hamiltonian quadratic in w was added to ensure that $V_1(z)$ has isolated conical minima at $z = \pm 1$. Thus perturbation theory is obtained by expanding around $z = 1$, $x = y = w = 0$ (or $z = -1$, $x = y = w = 0$).

Much of this section is concerned with understanding the relationship between Bloch degenerate perturbation theory [15], and tunneling through an induced potential barrier as discussed in [14]. Given a set of states degenerate in the unperturbed theory, the Bloch approach provides one with an effective Hamiltonian describing the perturbative energies of these states. We will demonstrate that tunneling in the effective theory and in the full theory gives the same result for the energy splitting, in problems of the type we are concerned with.

We thus want to use this example to prove commutativity of the following diagram (BP = Bloch perturbation theory [15], PDX = path decomposition expansion [17]):

$$\begin{array}{ccc} H(x, y, z, w) & \xrightarrow{\text{PDX}} & \Delta E \\ & \searrow^{\text{BP}} \quad \nearrow_{\text{PDX}} & \\ & H'_+(y, z) & \\ & H'_-(x, z) & \end{array} \tag{3.5}$$

Here H' is the effective Hamiltonian in the non-quadratic variables (H'_+ is obtained by expanding around $z = 1$, where x and w are quadratic, whereas H'_- is obtained

by expanding around $z = -1$ making y and w behave quadratically). At the end we shall discuss how to combine H'_+ and H'_- into one effective Hamiltonian. For the gauge theory problem, this then implies that we can study the tunneling in a finite dimensional setting, because there is only a finite number of non-quadratic modes.

We will first review Bloch's method for degenerate perturbation theory [15], in a spirit similar to the way Lüscher used it for gauge theories [2]. First we rescale the coordinates via

$$w = g\hat{w}, \qquad x = g\hat{x}, \qquad y = g^{2/3}\hat{y}, \qquad z = 1 + g^{2/3}\hat{z}, \tag{3.6}$$

so that the hatted coordinates are $O(1)$ for low-lying perturbative states in the well region. We thus find the perturbative expansion (we suppress the suffix $+$)

$$\begin{aligned} H &= H_0 + g^{2/3} H_1, \\ H_1 &= \sum_{\nu=0}^{\infty} g^{2\nu/3} H_1^{(\nu)}, \end{aligned} \tag{3.7}$$

with the following explicit expressions (a_ν constants):

$$\begin{aligned} H_0 &= -\frac{1}{2}\left(\frac{\partial^2}{\partial \hat{w}^2} + \frac{\partial^2}{\partial \hat{x}^2}\right) + 8\hat{w}^2 + 8\hat{x}^2 - 4, \\ H_1^{(0)} &= -\frac{1}{2}\left(\frac{\partial^2}{\partial \hat{y}^2} + \frac{\partial^2}{\partial \hat{z}^2}\right) + 2\hat{y}^2\hat{z}^2 + 8\hat{z}(\hat{x}^2 - \hat{w}^2), \\ H_1^{(1)} &= \hat{z}^2(2\hat{x}^2 + \hat{w}^2), \qquad H_1^{(\nu+2)} = a_\nu \hat{z}^{\nu+3}\hat{w}^2. \end{aligned} \tag{3.8}$$

Hence the Hamiltonian separates naturally into an unperturbed piece involving only the quadratic variables, and a perturbation involving the non-quadratic variables. The lowest energy unperturbed wavefunctions are given by

$$\Psi(w, x, y, z) = \phi(y, z)\, \Psi_0(w, x), \tag{3.9}$$

with $\Psi_0(w, x)$ the groundstate wavefunction for H_0 with zero energy:

$$\Psi_0(w, x) = \frac{2}{g\sqrt{\pi}} \exp\left(\frac{-2(w^2 + x^2)}{g^2}\right), \tag{3.10}$$

and $\phi(y, z)$ any square-integrable function. The idea of Bloch perturbation theory is that when we turn on the perturbation, $\phi(y, z)$ becomes an eigenfunction of an effective Hamiltonian $H' = \sum_{\nu=0}^{\infty} g^{2(\nu+1)/3} H'_\nu$. In particular, to lowest order $\phi(y, z)$ is an eigenfunction of

$$H'_0 = \langle \Psi_0 |\, H_1^{(0)}\, | \Psi_0 \rangle = -\frac{1}{2}\left(\frac{\partial^2}{\partial \hat{y}^2} + \frac{\partial^2}{\partial \hat{z}^2}\right) + 2\hat{y}^2\hat{z}^2. \tag{3.11}$$

(By choosing the z-dependent w-frequency as in Eq. (3.2), we get an H_0' similar to that for Yang–Mills and to the toy model in Eq. (3.1).) Beyond lowest order, the energy eigenstates are no longer direct products as in (3.9), but from the discussion below we see that they are related to direct products by the operator U.

Later we will need to find the higher order terms in the expansion of the effective potential, so we will follow the discussions in [2, 15, 16]. Let P_0 be the projector onto the state (3.10):

$$P_0 \Psi(w, x, y, z) = \Psi_0(w, x) \int dw'\, dx'\, \Psi(w', x', y, z)\, \Psi_0(w', x'). \tag{3.12}$$

The eigenvalues E_α of H, with the property that $E_\alpha = O(g^{2/3})$ (one of which is the groundstate energy) are determined by constructing an operator R whose eigenvalues are E_α,

$$R\,|\alpha_0\rangle = E_\alpha\,|\alpha_0\rangle, \tag{3.13}$$

where we *define* R by

$$R = P_0 H U, \tag{3.14}$$

with U the operator that maps $|\alpha_0\rangle$ to the eigenstate $|\alpha\rangle$ of H with the same energy E_α (and $U\,|\Psi\rangle = 0$ for all $|\Psi\rangle$ with $P_0\,|\Psi\rangle = 0$).

$$U\,|\alpha_0\rangle = |\alpha\rangle, \qquad H\,|\alpha\rangle = E_\alpha\,|\alpha\rangle. \tag{3.15}$$

Therefore combining (3.13) and (3.14), we must have

$$P_0\,|\alpha\rangle = |\alpha_0\rangle, \tag{3.16}$$

and one derives from this [15, 16] the Schwinger–Dyson equation for U:

$$U = P_0 + g^{2/3} \frac{(1 - P_0)}{(E_0 - H_0)} (H_1 U - U H_1 U). \tag{3.17}$$

Note that R is not hermitian. To derive an effective Hamiltonian H' we observe that with P the projector onto the eigenstates $|\alpha>$ of H, one has the following hermiticity property (use $UP_0 = U$ and $PU = U$ [16]):

$$P_0 H U P_0 P P_0 = P_0 H P P_0 = P_0 P H P_0 = P_0 P P_0 U^\dagger H P_0. \tag{3.18}$$

Thus, define the operator $B: \Omega_0 \to \Omega_0$ (Ω_0 the set of eigenstates of H_0 with eigenvalue 0, i.e., square integrable functions of y and z) by

$$B = P_0 P P_0. \tag{3.19}$$

Since $B = P_0 + O(g^{2/3})$ it is positive definite on Ω_0 for small enough g, so that we can define H' by

$$H' = B^{-1/2} R B^{1/2}. \tag{3.20}$$

Note that this perturbation theory breaks down for the smallest value of g where B is not invertible.

The operator H' acts on Ω_0 and can hence be expressed as a Hamilton operator in the variables y and z acting on square integrable functions. To lowest order we found the result of Eq. (3.11).

Next we will describe the features of the PDX for the situation where a vacuum valley is present (the line $x = y = w = 0$). In [14], a recipe was given for applying the PDX to a tunneling problem with a vacuum valley. We solve for fixed-z eigenstates of H ($p_z = (1/i)(\partial/\partial z)$, and $n = 1$ labels the ground state),

$$H(p_z = 0)\, \chi^{(n)}_{[z]}(w, x, y) = V_n(z)\, \chi^{(n)}_{[z]}(w, x, y), \tag{3.21}$$

and expand a wavefunction $\Psi(w, x, y, z)$ as

$$\Psi(w, x, y, z) = \sum_n \varphi^{(n)}(z)\, \chi^{(n)}_{[z]}(w, x, y). \tag{3.22}$$

(In this simple example we can obtain the $\chi^{(n)}_{[z]}$ in closed form.) The Hamiltonian in this representation becomes

$$H_{nm} = -\frac{g^2}{2}\left(\delta_{nm}\frac{\partial}{\partial z} - A_{nm}(z)\right)^2 + \delta_{nm} V_n(z), \tag{3.23}$$

with the following definition of A_{nm}:

$$A_{nm}(z) = \langle \chi^{(m)}_{[z]} | \frac{\partial}{\partial z} | \chi^{(n)}_{[z]} \rangle. \tag{3.24}$$

The first ingredient in the recipe for the tunneling energy split is the potential $V_1(z)$, defined in Eq. (3.21) and given in Eq. (3.4). The second ingredient for the PDX as described in [14] is what was called the ground state $\Psi_0^{[0]}$ for the single-well potential $V_{[0]}$ or single-well Hamiltonian $H_{[0]}$. $H_{[0]}$ is H to the lowest order in perturbation theory where degeneracies are lifted. We obviously have

$$\begin{aligned} \Psi_0^{[0]}(w, x, y, z) &= \phi_0^{[0]}(y, z)\, \Psi_0(w, x), \\ H'_0 \phi_0^{[0]}(y, z) &= E_0^{[0]} \phi_0^{[0]}(y, z). \end{aligned} \tag{3.25}$$

The final ingredient is the single-well energy $E_0^{[0]}$. Observe, incidentally, that H'_0 is identical to the single-well Hamiltonian for Eq. (3.1), which was studied in detail in

[14]. The recipe now instructs one to expand $\Psi_0^{[0]}$ as in (3.22), and thus find the single-well approximation $\varphi_0^{[0]}$ for $\varphi_0^{(1)}(z)$, for z deep within the barrier. As shown in [14], the $n=1$ term dominates (3.22) in this region, so we find for $|z-1| \gg g^{2/3}$:

$$\phi_0^{[0]}(y, z) \simeq \varphi_0^{[0]}(z) \frac{1}{\sqrt{g}} \left(\frac{4|z-1|}{\pi}\right)^{1/4} \exp\left(-\frac{2|z-1|\, y^2}{g^2}\right). \tag{3.26}$$

The energy splitting between the even and odd ground states is now given in terms of what we will call the *tunneling data* $(V_1(z), E_0^{[0]}, \varphi_0^{[0]}(z))$ by [14]:

$$\begin{aligned} \Delta E(g) = 2g\, |\varphi_0^{[0]}(1-d)|^2 \sqrt{2(V_1(1-d) - E_0^{[0]})} \\ \times \exp\left(-\frac{1}{g}\int_d^{1-d} \sqrt{2(V_1(z) - E_0^{[0]})}\, dz\right). \end{aligned} \tag{3.27}$$

For $d \simeq g^{1/2}$ this determines $\Delta E(g)$ up to a relative error that vanishes as a positive power of g.

It is immediately clear from Eq. (3.25) that the tunneling data $E_0^{[0]}$ and $\varphi_0^{[0]}$ can equally well be obtained from the single-well ground state $\Psi_0^{[0]}$ of $H_{[0]}$ or from the single-well ground state $\phi_0^{[0]}$ of H_0'. We are now going to show an even stronger result: we can also derive $V_1(z)$ from the effective Hamiltonian H'. This is similar in spirit to the discussion in Appendix A of [5], where it was verified to the fourth order in the coordinates.

Since $V_1(z)$ comes from an infinite resummation of Bloch perturbation theory, we will rearrange things slightly. Instead of rescaling, we will stick to the original variables and write

$$\begin{aligned} H &= H_0 + H_0' + W, \\ H_0 &= -\frac{g^2}{2}\left(\frac{\partial^2}{\partial w^2} + \frac{\partial^2}{\partial x^2}\right) + \frac{8}{g^2}(w^2 + x^2) - 4, \\ H_0' &= -\frac{g^2}{2}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{2}{g^2} y^2 (z-1)^2, \\ W &= \frac{2}{g^2}[(z+1)^2 - 4]\, x^2 + \frac{2}{g^2}\left[\left(\frac{z^2+3}{z^2+1}\right) - 4\right] w^2. \end{aligned} \tag{3.28}$$

Equation (3.17) can now be rewritten in terms of

$$U(\mathbf{n}) = \langle \mathbf{n} |\, U\, | \mathbf{0} \rangle, \tag{3.29}$$

where $|\mathbf{n}\rangle$ is the set of eigenfunctions of H_0:

$$H_0\, |\mathbf{n}\rangle = E_{\mathbf{n}}\, |\mathbf{n}\rangle; \qquad E_{\mathbf{n}} = 4(n_1 + n_2), \tag{3.30}$$

and $\langle w, x \mid \mathbf{0} \rangle = \Psi_0(w, x)$ as given in Eq. (3.10). The reason that only the matrix element $U(\mathbf{n})$ enters is that $U = UP_0$ (see [16]). We find

$$\begin{aligned} &U(\mathbf{0}) = 1, \\ &U(\mathbf{n}) = \{ U(\mathbf{n}) \langle \mathbf{0} | W | \mathbf{m} \rangle U(\mathbf{m}) - \langle \mathbf{n} | W | \mathbf{m} \rangle U(\mathbf{m}) + [U(\mathbf{n}), H_0'] \}/E_{\mathbf{n}}, \end{aligned} \tag{3.31}$$

whereas the operator R is given by

$$R = H_0' + \langle \mathbf{0} | W | \mathbf{m} \rangle U(\mathbf{m}). \tag{3.32}$$

The matrix elements of W are easily computed explicitly,

$$\begin{aligned} \langle \mathbf{n} | W | \mathbf{m} \rangle &= \frac{1}{4}\left[\left(\frac{z^2+3}{z^2+1} \right)^2 - 4 \right] X_{n_1 m_1} + \frac{1}{4}[(z+1)^2 - 4] X_{n_2 m_2}, \\ X_{nm} &= \sqrt{n(n-1)}\, \delta_{n,m+2} + \sqrt{m(m-1)}\, \delta_{m,n+2} - (2n+1)\, \delta_{nm}, \end{aligned} \tag{3.33}$$

but the important point is that they are g-independent. If we next rescale y as

$$\tilde{y} = y/g, \tag{3.34}$$

dependence on g only enters in the term containing H_0' in Eq. (3.31), so we can expand $U(\mathbf{n})$ in powers of g,

$$U(\mathbf{n}) = U_0(\mathbf{n}) + g^2 U_1(\mathbf{n}), \tag{3.35}$$

where $U_0(\mathbf{n})$ satisfies the equation

$$\begin{aligned} U_0(\mathbf{n}) = \Big\{ &U_0(\mathbf{n}) \langle \mathbf{0} | W | \mathbf{m} \rangle U_0(\mathbf{m}) - \langle \mathbf{n} | W | \mathbf{m} \rangle U_0(\mathbf{m}) \\ &+ \left[U_0(\mathbf{n}), \frac{1}{2}\frac{\partial^2}{\partial \tilde{y}^2} + 2\tilde{y}(z^2-1) \right] \Big\} \Big/ E_{\mathbf{n}}. \end{aligned} \tag{3.36}$$

Since Eq. (3.36) is obtainable from Eq. (3.31) by ignoring $[\partial^2/\partial z^2, U(\mathbf{n})]$, it means we can compute things by deriving the effective Hamiltonian for $H(p_z = 0)$ and considering z as a fixed parameter.

Next, because $H(p_z = 0)$ separates we easily find

$$R - H_0' = |z+1| + \left(\frac{z^2+3}{z^2+1} \right) - 4 + g^2 R_1. \tag{3.37}$$

To obtain H' one observes that B in Eqs. (3.19) and (3.20) is only introduced to obtain a hermitian operator, and since R is hermitian to lowest order, we also obtain

$$H' = H_0' + |z+1| + \left(\frac{z^2+3}{z^2+1} \right) - 4 + g^2 \tilde{H}_1'. \tag{3.38}$$

We can now decompose H' in a similar way along the vacuum valley; we solve for the fixed-z eigenstates of $H'(p_z=0)$,

$$H'(p_z=0)\,\chi'^{(n)}_{[z]}(y) = V'_n(z)\,\chi'^{(n)}_{[z]}(y), \tag{3.39}$$

and expand the effective wavefunction $\phi(y, z)$ as

$$\phi(y, z) = \sum_n \varphi^{(n)}(z)\,\chi'^{(n)}_{[z]}(y). \tag{3.40}$$

One therefore finds

$$H'_{nm} = -\frac{g^2}{2}\left(\delta_{nm}\frac{\partial^2}{\partial z^2} - A'_{nm}(z)\right)^2 + \delta_{nm}V'_n(z) + g^2 T_{nm}(z), \tag{3.41}$$

with A'_{nm} defined as in Eq. (3.24) and

$$T_{nm} = \langle \chi'^{(m)}_{[z]} |\, \tilde{H}'_1 - \tilde{H}'_1(p_z=0)\,|\chi'^{(n)}_{[z]}\rangle.$$

One easily deduces (see Eq. (3.4))

$$V'_1(z) = V_1(z) + O(g^2), \tag{3.42}$$

which is what we set out to prove. The $O(g^2)$ correction in (3.42) and the one coming from T_{nm} can be shown to give negligible contributions to $\Delta E(g)$, as should be true for consistency.

In conclusion, one can obtain the tunneling data $\varphi_0^{[0]}(z)$, $E_0^{[0]}$ from H'_0 (which is the single-well approximation of H'), and $V_1(z)$ from the one-loop approximation for the effective potential along the vacuum valley, which can be computed in a variety of ways.

The above derivation of the one-loop effective potential was one example showing that H' makes sense beyond perturbation theory. We have two different expressions, $H'_\pm$, related to two different quartic modes. The symmetry Π (Eq. (3.3)) guarantees an intimate connection between these two expressions,

$$H'_+(u, z) = H'_-(u, -z), \tag{3.43}$$

and one easily verifies that the same holds for the operators R and B (as maps from Ω_0 into itself). We can then naturally combine H'_+ and H'_- into one effective Hamiltonian:

$$\begin{aligned} H'(u, z) &= H'_+(u, |z|) \\ &= H'_-(u, -|z|). \end{aligned} \tag{3.44}$$

Note that $H'_+(u, z)$ is ill-defined for $z \searrow -1$, but that we do not use it in that region. Now suppose that $\psi(x, y, z, w)$ is a simultaneous eigenvector of H and Π

with eigenvalues E and σ $(=\pm 1)$. The reduced wavefunctions $\psi_+(y, z)$ and $\psi_-(x, z)$ are then related by (use Eqs. (3.12) and (3.16))

$$\psi_+(u, z) = \sigma\psi_-(u, -z), \tag{3.45}$$

and one can show that $\psi_\pm(u, z)$ is an eigenfunction of $H'_\pm(u, z)$ with eigenvalue E. Let us define the wavefunction $\hat{\psi}(u, z)$ by

$$\hat{\psi}(u, z) = \begin{cases} \psi_+(u, z), & z \geqslant 0 \\ \psi_-(u, z), & z \leqslant 0. \end{cases} \tag{3.46}$$

It is clearly an eigenfunction of H' with eigenvalue E, and by Eq. (3.45) has the property

$$\hat{\psi}(u, z) = \sigma\hat{\psi}(u, -z). \tag{3.47}$$

However, we have to worry about continuity. For example, $\sigma = -1$ forces $\hat{\psi}(u, 0) = 0$ and thus $\psi_+(u, 0) = 0$, which is not automatically guaranteed by the general symmetry properties of ψ under Π. In general, we have

$$\psi(x, y, 0, w) = \sigma\psi(y, x, 0, w), \tag{3.48}$$

but one easily verifies that if $\psi(x, y, 0, w)$ is not even under interchanging x and y, ψ will correspond to an excited state, not degenerate with the ground state for vanishing coupling, and is hence outside Ω_0. To see this, consider the decomposition of the wavefunction in Eq. (3.22). We find in particular that if $\psi(x, y, 0, w)$ is odd under interchanging x and y, *and non-zero,* the wavefunction cannot couple to those modes for which $\chi^{(n)}_{[z]}(x, y, w)$ is even under interchange of x and y. But an analysis along the lines of [14] shows that the wavefunctions belonging to Ω_0 do couple to those modes. Thus if $\psi(x, y, 0, w)$ is non-zero and odd under interchanging x and y, then ψ is orthogonal to Ω_0. Consequently, $\hat{\psi}$ is properly defined as an $\mathscr{L}^2$ wavefunction on $\mathbf{R}^2$ with Hamiltonian H' as defined in Eq. (3.44).

We have therefore obtained an effective model in a smaller number of dimensions, allowing one (in principle) to compute the energy split between the even and odd ground states, beyond the semiclassical approximation, using H' as Hamiltonian.

This result carries over in a suitable generalization to our full problem of QCD on a torus, but we will leave the more extensive discussion that this issue deserves to the future, since this paper is restricted to the semiclassical analysis. (For a few additional remarks, see [3].)

4. The Effective Lagrangian

With the example of the previous section to guide us, we can now return to discussing $SU(2)$ Yang–Mills on T^3. The Bloch effective Hamiltonian H' has already

been calculated by Lüscher [2], and if we expand about $\mathbf{C}=\mathbf{0}$, then H' is a function of the spatially constant vector potentials ($\mathbf{k}=\mathbf{0}$ in Eq. (2.18)). To lowest order, it is just the Yang–Mills Hamiltonian in the gauge $\mathbf{A}_0=0$, restricted to these constant vector potentials, *with the coupling constant properly renormalized*,

$$H'_0 = -\frac{g^2}{2L}\frac{\partial^2}{\partial c_i^{a2}} - \frac{1}{2g^2 L}\operatorname{Tr}[c_i, c_j]^2, \tag{4.1}$$

where

$$A_i = \frac{c_i}{L} = \frac{c_i^a \sigma_a}{2L}, \qquad \partial_j c_i = 0 \quad \forall i, j. \tag{4.2}$$

A straightforward generalization of the arguments in the previous chapter tells us that the following Hamiltonian $\hat{H}$ can be used to calculate the lowest order energy splitting between the different electric flux sectors:

$$\hat{H} = H'_0(c_i^a) + V'_1(\mathbf{C}), \qquad |C_i| \leqslant \pi. \tag{4.3}$$

We extend $\hat{H}$ by periodicity to C values outside this range. Here $V'_1(\mathbf{C})$ is the one-loop effective potential along the vacuum valley, where the prime denotes that we have excluded the contribution from the constant modes:

$$\begin{aligned} V'_1(\mathbf{C}) &= V_1(\mathbf{C}) - \frac{2\,|\mathbf{C}|}{L}, \\ V_1(\mathbf{C}) &= \frac{4}{L\pi^2}\sum_{\mathbf{n}\neq\mathbf{0}} \frac{\sin^2(\mathbf{n}\cdot\mathbf{C}/2)}{(\mathbf{n}^2)^2}. \end{aligned} \tag{4.4}$$

We have used the fact that up to a constant, the sum of the ($\mathbf{C}$-dependent) eigenvalues of the quadratic fluctuations (see Eq. (2.18)), gives the effective potential

$$V_1(\mathbf{C}) = 2\sum_{\mathbf{k}\in Z^3} \lambda_{\mathbf{C}}^{+}(\mathbf{k})^{1/2}, \tag{4.5}$$

$$V'_1(\mathbf{C}) = V_1(\mathbf{C}) - 2\lambda_{\mathbf{C}}^{+}(\mathbf{0})^{1/2}. \tag{4.6}$$

In Appendix A we will show how to resum these expressions to obtain the more rapidly converging result

$$V_1(C\mathbf{e}^{(1)}) = \frac{4}{\pi L}\left[\frac{C}{2}\left(\pi - \frac{C}{2}\right) + 2\sum_{n=1}^{\infty} a_n \sin^2(nC/2)\right]. \tag{4.7}$$

The a_n decrease rapidly with n,

$$a_n < \frac{5\pi^2}{n} e^{-2\pi n}, \tag{4.8}$$

and the first few are

$$\begin{aligned} a_1 &= 2.7052746... \cdot 10^{-2} \\ a_2 &= 1.6048745... \cdot 10^{-5} \\ a_3 &= 1.6065690... \cdot 10^{-8} \\ a_4 &= 1.9385627... \cdot 10^{-11}. \end{aligned} \tag{4.9}$$

In [5] we explained how one could calculate κ_1, κ_3, and κ_4 in Lüscher's one-loop effective Hamiltonian:

$$\begin{aligned} LH' = (1 + g^2\kappa_2)\, LH'_0 + \kappa_1 c_k^a c_k^a + \kappa_3 (c_k^a c_k^a c_l^b c_l^b + 2 c_k^a c_l^a c_k^b c_l^b) \\ + \kappa_4 (5 c_k^a c_k^a c_k^b c_k^b - c_k^a c_k^a c_l^b c_l^b - 2 c_k^a c_l^a c_k^b c_l^b). \end{aligned} \tag{4.10}$$

We found

$$\begin{aligned} \kappa_1 &= \frac{1}{\pi}\left(-1 + 2 \sum_{n=1}^{\infty} n^2 a_n\right), \\ \kappa_4 + \frac{3}{2}\kappa_3 &= -\frac{1}{12\pi} \sum_{n=1}^{\infty} n^4 a_n, \\ \kappa_3 &= \frac{4}{45}(4\pi)^{-2}. \end{aligned} \tag{4.11}$$

This was part of a consistency check, analogous to the one we performed for the toy model in the previous section.

Before we continue to analyze $\hat{H}$ (Eq. (4.3)) in more detail, it is useful to show how these formulae can be derived using the Lagrangian approach. In this language, we are seeking an effective Lagrangian in the spatially constant vector potentials, obtained by integrating out all other degrees of freedom in the path integral. We start by introducing the projector P onto these states:

$$PA_\mu = \frac{1}{L^3} \int_{T^3} A_\mu. \tag{4.12}$$

A convenient gauge-fixing function for this procedure is then given by [3],

$$\chi = (1 - P)(\partial_\mu A_\mu + i[PA_\mu, A_\mu]) + L^{-1} PA_0, \tag{4.13}$$

so that if we define

$$B_\mu = PA_\mu, \qquad Q_\mu = (1 - P) A_\mu, \tag{4.14}$$

then $\chi = 0$ is equivalent to

$$B_0 = 0, \qquad \partial_\mu Q_\mu + i[B_\mu, Q_\mu] = 0. \tag{4.15}$$

This looks just like the background field gauge-fixing condition. However, there is an important difference from the standard background field approach, in that here B and Q are functions of A. This has consequences for the Faddeev–Popov ghost, as we will see. Also, because B is a dynamical variable, and is not invariant under gauge transformations, we need the first condition in Eq. (4.15) to fix the spatially constant but time varying gauge transformations. Clearly, $B_0 = 0$ is the most convenient choice of gauge for converting the effective Lagrangian to a Hamiltonian.

One can calculate the Faddeev–Popov determinant in the standard way. The variation of χ under an infinitesimal gauge transformation $\Omega = e^{i\in\Lambda}$ is

$$\begin{aligned}\delta_\Lambda \chi = (1-P)\{&D_\mu(PA)\, D_\mu(\mathbf{A})\, \Lambda + i[P(D_\mu(\mathbf{A})\, \Lambda), A_\mu]\} \\ &+ L^{-1}\partial_0 P\Lambda + iL^{-1}P[A_0, \Lambda],\end{aligned} \tag{4.16}$$

where $D_\mu(A)$ is the covariant derivative

$$D_\mu(\mathbf{A})\, \Lambda = \partial_\mu \Lambda + i[A_\mu, \Lambda]. \tag{4.17}$$

Splitting Λ into $P\Lambda$ and $(1-P)\,\Lambda = \Lambda'$, we find

$$\begin{aligned}\delta_\Lambda \chi = (1-P)\{&D_\mu(PA)\, D_\mu(\mathbf{A})\, \Lambda' - [P[A_\mu, \Lambda'], A_\mu]\} \\ &+ \frac{1}{L}\partial_0 P\Lambda + \frac{i}{L}P[A_0, \Lambda'] + i[\chi, P\Lambda].\end{aligned} \tag{4.18}$$

and introducing the operator $\mathscr{M}$ via

$$\mathscr{M}\Lambda = D_\mu(PA)\, D_\mu(\mathbf{A})\, \Lambda + [A_\mu, P[A_\mu, \Lambda]], \tag{4.19}$$

gives the Fadeev–Popov determinant

$$\begin{aligned}\Delta(\mathbf{A}) &= \left(\int \mathscr{D}\Omega\delta(\chi^\Omega)\right)^{-1} \\ &= \int \mathscr{D}'\Psi\mathscr{D}'\bar{\Psi}\, d\eta\, d\bar{\eta} \exp\left(\frac{-i}{g_0^2}\int 2\mathrm{Tr}(\bar{\Psi}\mathscr{M}\Psi) + 2\,\mathrm{Tr}\left(\bar{\eta}\partial_0\eta + \frac{i}{L}\bar{\eta}P[A_0, \Psi]\right)\right).\end{aligned} \tag{4.20}$$

The prime indicates that $P\Psi = P\bar{\Psi} = 0$. Here, η and $\bar{\eta}$ are spatially constant, and can be integrated out explicitly, giving an irrelevant constant. Continuing the standard arguments, we have $1 = \Delta(A^{\Omega_0})\int \mathscr{D}\Omega\delta(\chi^\Omega - E)$, where Ω_0 is defined by $\chi^{\Omega_0} = E$ (see e.g., [18, p. 581]). Inserting this into the generating functional, we get

$$\mathscr{Z} = \int \mathscr{D}A_\mu \mathscr{D}'\Psi\, \mathscr{D}'\Psi \exp\left(\frac{-i}{g_0^2}\int \frac{1}{2}\mathrm{Tr}(F_{\mu\nu}^2) - 2\,\mathrm{Tr}(\bar{\Psi}\mathscr{M}\Psi)\right)\delta(\chi - E), \tag{4.21}$$

which is independent of E. Integrating over E with $\int \mathscr{D}'E \exp((i/g_0^2)\int \mathrm{Tr}(E^2))$, where again the prime denotes $PE=0$), we find

$$\mathscr{Z} = \int \mathscr{D}B_k \int \mathscr{D}'Q_\mu \mathscr{D}'\Psi \mathscr{D}'\bar{\Psi} \exp\left[\frac{-i}{g_0^2}\int \frac{1}{2}\mathrm{Tr}(F_{\mu\nu}(B+Q)^2)\right.$$
$$\left. -\mathrm{Tr}((D_\mu(B)\,Q_\mu)^2) - 2\,\mathrm{Tr}(\bar{\Psi}D_\mu(B)\,D_\mu(B+Q)\,\Psi) - 2\,\mathrm{Tr}([Q_\mu, \Psi]\,P[Q_\mu, \bar{\Psi}])\right]. \tag{4.22}$$

One now easily extracts the effective Lagrangian for B, by writing this as

$$\mathscr{Z} \equiv \int \mathscr{D}B_k \exp\left(i\int dt\, \mathscr{L}_{\mathrm{eff}}(B)\right). \tag{4.23}$$

A peculiarity in our expression is the non-local interaction for the ghost, which is of course due to the non-local gauge fixing. In addition, we have a non-linear gauge, which normally needs a counterterm quartic in the ghosts [30]. However, because our non-linearity is only due to the constant modes, simple power counting shows that no quartic ghost divergences arise.

We wish to observe here that although Eq. (4.22) is renormalizable, in principle one needs to verify that gauge invariance is maintained at the quantum level, by using Ward identities. In this way, one could establish perturbative renormalizability *without ignoring infrared difficulties*. Here, we just assume that only one renormalized coupling constant has to be introduced. This assumption, incidentally, is made in the Hamiltonian approach too.

The one-loop calculation of $\mathscr{L}_{\mathrm{eff}}(B)$ is particularly simple, and confirms to that order the above assumption:

$$\exp\left(i\int \mathrm{dt}\, \mathscr{L}_{\mathrm{eff}}^{\text{1-loop}}(B)\right) = \int \mathscr{D}'Q_\mu \mathscr{D}'\Psi \mathscr{D}'\bar{\Psi} \exp\left[\frac{-i}{g_0^2}\int \frac{1}{2}\mathrm{Tr}(F_{\mu\nu}(B)^2)\right.$$
$$\left. + \mathrm{Tr}(Q_\mu \mathscr{M}_{\mu\nu}(B)\,Q_\nu) - 2\,\mathrm{Tr}(\bar{\Psi}D_\mu(B)^2\,\Psi)\right], \tag{4.24}$$

with

$$\mathscr{M}_{\mu\nu}Q_\nu = -D_\sigma(B)^2\,Q_\mu - 2i[F_{\mu\nu}(B), Q_\nu]. \tag{4.25}$$

This is precisely the expression one obtains in a standard background-field calculation, except that the integration over the gauge and ghost fields excludes the constant modes. We can thus follow 't Hooft's approach [19] and write (f_{abc} are the structure constants for the gauge group):

$$\begin{aligned} &\mathrm{Tr}(Q_\mu \mathscr{M}_{\mu\nu}(B)\,Q_\nu) = -\tfrac{1}{2}(\partial_\mu Q_\nu^a)^2 + Q_\alpha^a (N^\mu)_{\alpha\beta}^{ab}\,\partial_\mu Q_\beta^b + \tfrac{1}{2}Q_\mu^a M_{\mu\nu}^{ab} Q_\nu^b, \\ &-2\,\mathrm{Tr}(\bar{\Psi}D_\mu(B)^2\,\Psi) = -(\partial_\mu \bar{\Psi}^a)(\partial_\mu \Psi^a) + 2\bar{\Psi}^a (N_\mu)^{ab}\,\partial_\mu \Psi^b + \bar{\Psi}^a \mathscr{M}_0^{ab}\Psi^b, \end{aligned} \tag{4.26}$$

with

$$\begin{aligned}(N^\mu)^{ab}_{\alpha\beta} &= f_{abc} B^c_\mu \delta_{\alpha\beta},\\ M^{ab}_{\mu\nu} &= -2 f_{abc} F^c_{\mu\nu}(B) + (N_\sigma N^\sigma)^{ab}_{\mu\nu},\\ (\Lambda_\mu)^{ab} &= f_{abc} B^c_\mu,\\ \Lambda^{ab}_0 &= (\Lambda_\sigma \Lambda^\sigma)^{ab}.\end{aligned} \tag{4.27}$$

Note that $N_0 = \Lambda_0 = 0$, and that $f_{abc} A^c$ is just $i(\mathrm{ad}\, A)^{ab}$, the matrix for A in the adjoint representation. We now want to write down the most general possible one-loop effective action for B, compatible with the remaining symmetries, i.e., the cubic group $O(3, Z)$ and a global background gauge invariance. Clearly $\mathscr{L}_{\mathrm{eff}}^{\text{1-loop}}(B)$ must be a function of ad $\dot{B}_i$, ad B_i, and ad $F_{ij}(B)$. If we restrict ourselves to terms no more than quadratic in $\dot{B}$ and quartic in B, which is the order to which Lüscher works [2], we find

$$\begin{aligned}\mathscr{L}_{\mathrm{eff}}(B) = \frac{1}{2g_0^2}\,\mathrm{Tr}(F_{\mu\nu}(B)^2) - b_1(\dot{B}_i^a)^2 + b_2(B_i^a)^2 + b_3\,\mathrm{Tr}(F_{ij}(B)^2)\\ + b_4\,\mathrm{Tr}((\mathrm{ad}\, B_i)^4) + b_5 \sum_{i\neq j}^{3} \mathrm{Tr}(\mathrm{ad}\, B_i)^2(\mathrm{ad}\, B_j)^2).\end{aligned} \tag{4.28}$$

This can be put in a more convenient form (see [2] for some tools), which for $SU(2)$ is

$$\begin{aligned}\mathscr{L}_{\mathrm{eff}}(B) = \frac{1}{2g_0^2}\,\mathrm{Tr}(F_{\mu\nu}(B)^2) - b_1(\dot{B}_i^a)^2 + b_3'\,\mathrm{Tr}(F_{ij}(B)^2)\\ + b_2(B_i^a)^2 + b_4' B_i^a B_i^a B_i^b B_i^b + b_5'(B_i^a B_i^a B_j^b B_j^b + 2B_i^a B_j^a B_i^b B_j^b).\end{aligned} \tag{4.29}$$

Next we observe that when we calculate the *divergent* part of $\mathscr{L}_{\mathrm{eff}}$, the sum over the (non-zero) loop momenta can be replaced by an integral. Thus the divergent parts of the coefficients in Eq. (4.29) are exactly the same as in the infinite volume field theory calculation, i.e., the infinite parts of b_1 and b_3' are equal, and renormalize $(1/2g_0^2)\,\mathrm{Tr}(F_{\mu\nu}^2)$ to $(1/2g^2)\,\mathrm{Tr}(F_{\mu\nu}^2)$ in the usual way, whereas the other parameters (b_2, b_4', and b_5') are finite.

An alternative approach leading to the same conclusion is to use the quasi-classical expansion, as described for an arbitrary compact manifold in [20]. There one *always* gets the proper renormalization of the coupling constant, essentially because the small-scale behaviour is insensitive to the large-scale details of the smooth manifold on which we formulate our gauge theory.

We can actually get the finite coefficients in Eq. (4.29) without further work, by making some simple observations. First, if the finite parts of b_1 and b_3' are not equal, we can just rescale $B \to (1 + \alpha g^2)\, B$ to absorb those terms, without changing anything else at this order. Second, note that for $\dot{B} = 0$, $-\mathscr{L}_{\mathrm{eff}}$ is just the effective potential V', which we have already calculated to one loop for abelian B in

Eq. (4.4). A Taylor expansion of V_1' thus fixes the remaining constants, giving $b_2 = L\kappa_1$, $b_4' = 5L^3\kappa_4$, and $b_5' = L^3(\kappa_3 - \kappa_4)$. This argument is clearly the consistency requirement we discussed earlier.

Converting Eq. (4.29) to a Hamiltonian indeed reproduces Lüscher's Hamiltonian, Eq. (4.10), and using the effective potential for arbitrary $SU(N)$ derived in Appendix D, we can apply the same reasoning and reproduce his more general formula. In principle, the results of Appendix D will in this way give the effective Hamiltonian for any simple gauge group, but we have left this to the reader.

We also leave to the reader the task of explicitly doing the background field calculation in Eq. (4.24) [19]. We have found that after integrating over the contiuous energy, one is left with exactly those momentum sums encountered by Lüscher in his Hamiltonian approach. We believe that there is a general one-to-one correspondence between Bloch perturbation theory and this Lagrangian method. In particular, rescaling $B_i^a = g_0^{2/3} c_i^a / L$ and $t = L g_0^{-2/3} \tau$ leaves an expansion in powers of $g_0^{2/3}$, and the energy integral of the propagator is analogous to the fundamental operator in Bloch perturbation theory [15]:

$$\frac{i}{\pi} \int dk_0 \frac{(1 - \delta_{\mathbf{k},\mathbf{0}})}{k_0^2 - \mathbf{k}^2 - i\varepsilon} \Leftrightarrow \frac{1 - P_0}{H_0 - E_0}. \tag{4.30}$$

In all this, the non-local ghost interaction plays a subtle and intriguing role. A nice example of the necessity of this non-local interaction was recently observed in a two-loop calculation [29].

Although the above gauge fixing term allows us to verify Lüscher's results and test our understanding, it is not well suited to a non-perturbative analysis, since it breaks the symmetry which maps $\mathbf{C}$ into $\mathbf{C} + 2\pi\mathbf{n}$. As was noted before in [3], a better choice is to replace everywhere the projector P by the projector P_3:

$$P_3 A_\mu = \frac{1}{L^3} \int_{T^3} \mathrm{Tr}(A_\mu \sigma_3) \frac{\sigma_3}{2}. \tag{4.31}$$

This is invariant under the gauge transformation $\Omega^{(i)}(\mathbf{x})$ in Eq. (2.13). The explicit expression for the gauge-fixing function is then

$$\chi_3 = (1 - P_3)(\partial_\mu A_\mu + i[P_3 A_\mu, A_\mu]) + L^{-1} P_3 A_0, \tag{4.32}$$

and one easily verifies that all steps from Eq. (4.13) to before the one-loop evaluation can be repeated. Thus one can write

$$\begin{aligned} \mathscr{Z} = \int \mathscr{D}\tilde{B}_k \int \mathscr{D}'\tilde{Q}_\mu \mathscr{D}'\tilde{\Psi}\mathscr{D}'\tilde{\bar{\Psi}} \exp\Bigg[\frac{-i}{g_0^2} \int \frac{1}{2} \mathrm{Tr}(F_{\mu\nu}(\tilde{B} + \tilde{Q})^2) \\ - \mathrm{Tr}((D_\mu(\tilde{B})\, \tilde{Q}_\mu)^2) - 2\, \mathrm{Tr}(\tilde{\bar{\Psi}} D_\mu(\tilde{B})\, D_\mu(\tilde{B} + \tilde{Q})\, \tilde{\Psi}) \\ - 2\, \mathrm{Tr}([\tilde{Q}_\mu, \tilde{\Psi}]\, P_3[\tilde{Q}_\mu, \tilde{\bar{\Psi}}]) \Bigg], \end{aligned} \tag{4.33}$$

with

$$\tilde{B}_k = P_3 A_\mu, \qquad \tilde{Q}_\mu = (1 - P_3) A_\mu, \tag{4.34}$$

and the conditions

$$P_3 A_0 = P_3 \tilde{\Psi} = P_3 \tilde{\bar{\Psi}} = 0. \tag{4.35}$$

This rigorously defines an effective Lagrangian via the analogue of Eq. (4.23):

$$\mathcal{Z} = \int \mathcal{D}\tilde{B}_k \exp\left(i \int dt\, \tilde{\mathcal{L}}_{\text{eff}}(\tilde{B}) \right). \tag{4.36}$$

Setting as in Eq. (2.11)

$$\tilde{B}_k = \frac{C_k \sigma_3}{2L}, \tag{4.37}$$

we obtain an effective Lagrangian for $\mathbf{C}$ with the symmetries

$$\tilde{\mathcal{L}}_{\text{eff}}(\mathbf{C}) = \tilde{\mathcal{L}}_{\text{eff}}(-\mathbf{C}) = \tilde{\mathcal{L}}_{\text{eff}}(\mathbf{C} + 2\pi\mathbf{n}). \tag{4.38}$$

However, a Feynman graph expansion around $\mathbf{C} = \mathbf{0}$ (or any point gauge-equivalent to $\mathbf{0}$) is not well defined, because the quadratic approximation breaks down there. But one can certainly expand around $\mathbf{C} = \pi\mathbf{e}^{(i)}$, and from Eq. (4.38) one for example easily derives that $L(\mathbf{q}) = \tilde{\mathcal{L}}_{\text{eff}}(\pi\mathbf{e}^{(i)} + \mathbf{q})$ satisfies $L(\mathbf{q}) = L(-\mathbf{q})$ and $L(\mathbf{q} + 2\pi\mathbf{n}) = L(\mathbf{q})$. By arguments similar to those used in deriving $\mathcal{L}_{\text{eff}}$, we find

$$L(\mathbf{q}) = \frac{L\dot{\mathbf{q}}^2}{2g^2}(1 + g^2 a_1) - a_2\mathbf{q}^2 - a_3(\mathbf{q}^2)^2 - a_4 \sum_i q_i^4, \tag{4.39}$$

where we work to the same order as in Eq. (4.29). One can then calculate a_2, a_3, and a_4 indirectly as before by noting $L(\mathbf{q}, \dot{\mathbf{q}} = \mathbf{0}) = -V_1(\pi\mathbf{e}^{(i)} + \mathbf{q})$. In general in the classically forbidden region one has

$$\tilde{\mathcal{L}}_{\text{eff}}(\mathbf{C}) = \frac{L\dot{\mathbf{C}}^2}{2g^2} - V_1(\mathbf{C}), \tag{4.40}$$

but this breaks down near the points $\mathbf{C} = 2\pi\mathbf{n}$. As is clear from the toy models, which mimic the quartic mode problem and the V-shape of $V_1(\mathbf{C})$, this approximation is good for $\min_{\mathbf{n}} |\mathbf{C} - 2\pi\mathbf{n}| \gg g^{2/3}$. The path decomposition expansion tells us that we can deal separately with the clasically forbidden regions and the classically allowed regions. For $\mathbf{C} \to \mathbf{0}$ the dynamics is described by H_0', and, after proper rescaling, enters in the combination $g^{-2/3}\mathbf{C}$. In Appendix C we will show how this combination can be understood heuristically in a loop expansion for $\tilde{\mathcal{L}}_{\text{eff}}(\mathbf{C})$ by examining the leading infrared ($\mathbf{C} \to \mathbf{0}$) behaviour.

5. The Polar Decomposition of the Effective Hamiltonian

We now address the problem of eliminating the gauge degrees of freedom from Lüscher's effective Hamiltonian, since they complicate the calculations. The gauge-invariant parameter **C** is a natural coordinate for the vacuum valley, so we will aim for an expression involving **C** and some "transverse" coordinates. Let us first describe an attempt based on the standard Faddeev–Popov gauge-fixing procedure, which turns out to be a nice illustration of the notion of Gribov ambiguities [26].

In the Hamiltonian approach we fix the gauge by $\chi_3 = 0$, restricted to the constant vector potentials, i.e.,

$$\chi = -i[P_3 c_i, c_i] = 0. \tag{5.1}$$

One can easily verify the following expression for the variation of χ under an infinitesimal gauge transformation $\Omega = \exp(i \in \Lambda) = \exp(i \in \Lambda^a \sigma^a/2)$,

$$\delta_\Lambda \chi = \sum_{a,b=1}^{2} M_{ab} \Lambda^b \frac{\sigma^a}{2} - i\left[\frac{\sigma_3}{2}, \chi\right] \Lambda^3, \tag{5.2}$$

where M is the ghost propagator:

$$M_{ab} = \begin{pmatrix} -(\mathbf{c}^2)^2 + (\mathbf{c}^3)^2 & \mathbf{c}^1 \cdot \mathbf{c}^2 \\ \mathbf{c}^1 \cdot \mathbf{c}^2 & -(\mathbf{c}^1)^2 + (\mathbf{c}^3)^2 \end{pmatrix}, \tag{5.3}$$

with eigenvalues

$$\lambda_\pm(\mathbf{c}) = \tfrac{1}{2}\{3(\mathbf{c}^3)^2 - (c_i^a)^2 \pm \sqrt{((\mathbf{c}^1)^2 - (\mathbf{c}^2)^2)^2 + 4(\mathbf{c}^1 \cdot \mathbf{c}^2)^2}\}. \tag{5.4}$$

Hence Gribov copies are found at $\lambda_\pm(\mathbf{c}) = 0$ or

$$(\mathbf{c}^3)^2 = \tfrac{1}{2}\{(\mathbf{c}^1)^2 + (\mathbf{c}^2)^2 \pm \sqrt{((\mathbf{c}^1)^2 - (\mathbf{c}^2)^2)^2 + 4(\mathbf{c}^1 \cdot \mathbf{c}^2)^2}\} \geqslant 0. \tag{5.5}$$

A naive perturbation expansion around $\mathbf{c} = \mathbf{0}$ will thus encounter severe problems, because Gribov copies occur in any neighbourhood of that point. For $|\mathbf{c}^3|$ sufficiently large they can be avoided in perturbating around $(\mathbf{0}, \mathbf{0}, \mathbf{c}^3)$, but their presence is a cause for suspicion, so we will not use this approach.

Instead of using this gauge-fixing method, we will transform to gauge-invariant coordinates using the polar decomposition [12], and thus explicitly eliminate the gauge degrees of freedom. In a sense, Gribov ambiguities are still present, as zeros in a Jacobian. These zeros are related to fixed points under a subgroup of the gauge group. (An analog is spherical coordinates on $\mathbf{R}^3$, with symmetry group $SO(3)$: The origin is left fixed, and the Jacobian vanishes at that point.) However, such zeros do not lead to any singular behaviour, and there is no difficulty in dealing with them, as we will show.

The polar decomposition is given by [27]

$$c_i^a = \sum_{b=1}^{3} \xi^{ab} x_b \eta_{bi}, \tag{5.6}$$

with $\xi, \eta \in SO(3)$. The uniqueness of this decomposition is discussed in Appendix B. Clearly, ξ carries the gauge degrees of freedom and η the rotational degrees. The x_b label the gauge- and rotation-invariant degrees of freedom. Let us first consider gauge-invariant, rotationally-symmetric wavefunctions. Since H_0' is both gauge and rotation invariant, the equation for H_0' acting on such a wavefunction can be written in terms of the x_b only. The potential part is easy:

$$\begin{aligned} V_0'(c_i^a) &= -\tfrac{1}{2}\,\mathrm{Tr}[c_i, c_j]^2 = \tfrac{1}{4}[(c_i^a c_i^a)^2 - c_i^a c_j^a c_i^b c_j^b] \\ &= \tfrac{1}{2}(x_1^2 x_2^2 + x_1^2 x_3^2 + x_2^2 x_3^2). \end{aligned} \tag{5.7}$$

The kinetic part is a little harder. If we write ξ and η in terms of the $SO(3)$ generators $(L_i)_{jk} = \varepsilon_{ijk}$ as $\xi = \exp(i\mathbf{y}\cdot\mathbf{L})$ and $\eta = \exp(i\mathbf{z}\cdot\mathbf{L})$, and denote the nonet $(\mathbf{x}, \mathbf{y}, \mathbf{z})$ by u^μ, $\mu = 1,\ldots, 9$ we can write

$$\frac{\partial^2}{\partial c_i^{a2}} = \frac{1}{\mathscr{J}} \frac{\partial}{\partial u^\mu} g^{\mu\nu} \mathscr{J} \frac{\partial}{\partial u^\nu}, \tag{5.8}$$

and the metric $g_{\mu\nu}$ is determined by $(\dot{c}_i^a)^2 = g_{\mu\nu}\dot{u}_\mu \dot{u}_\nu$, with $\mathscr{J} = \sqrt{\det(g_{\mu\nu})}$. Using the orthogonality properties $\sum_a \xi^{ab}\xi^{ab} = \sum_a \eta_{ab}\dot{\eta}_{ab} = 0$ one easily verifies that $g_{\mu\nu}$ has the form

$$g_{\mu\nu} = \begin{pmatrix} \mathbf{1}_3 & 0 \\ 0 & \hat{g}_{\hat{\mu}\hat{\nu}} \end{pmatrix}, \tag{5.9}$$

where $\hat{g}_{\hat{\mu}\hat{\nu}}$ is a 6×6 symmetric matrix. Clearly the inverse of the metric, $g^{\mu\nu}$, is of the same form. Hence (5.8) acting on gauge-invariant rotation-invariant wavefunctions is of the form $(1/\hat{\mathscr{J}})(\partial/\partial x_i)\,\hat{\mathscr{J}}(\partial/\partial x_i)$. Since $\hat{\mathscr{J}}$ is invariant it can be evaluated at $\xi = \eta = \mathbf{1}$; a simple calculation using the explicit form of the $SO(3)$ generators yields

$$\hat{g}_{\hat{\mu}\hat{\nu}} = \begin{pmatrix} A & B \\ B & A \end{pmatrix},$$

$$A = \begin{pmatrix} x_2^2 + x_3^2 & 0 & 0 \\ 0 & x_1^2 + x_3^2 & 0 \\ 0 & 0 & x_1^2 + x_2^2 \end{pmatrix}, \qquad B = \begin{pmatrix} x_2 x_3 & 0 & 0 \\ 0 & x_1 x_3 & 0 \\ 0 & 0 & x_1 x_2 \end{pmatrix}, \tag{5.10}$$

and we find

$$\mathscr{J}^2 = \det(A^2 - B^2) = \prod_{i>j} (x_i^2 - x_j^2)^2. \tag{5.11}$$

Hence restricted to the gauge and rotation invariant sector we have:

$$H_0' = -\frac{g^2}{2}\left(\prod_{i>j}(x_i^2 - x_j^2)\right)^{-1} \frac{\partial}{\partial x_k} \prod_{i>j}(x_i^2 - x_j^2) \frac{\partial}{\partial x_k} + \frac{1}{2g^2}(x_1^2 x_2^2 + x_1^2 x_3^2 + x_3^2 x_2^2), \tag{5.12}$$

and the inner product of two such invariant wavefunctions is (up to a constant)

$$\langle \Psi \mid \Phi \rangle = \int d^3x \left| \prod_{i>j}(x_i^2 - x_j^2) \right| \bar{\Psi}(x)\, \Phi(x). \tag{5.13}$$

As remarked earlier, like when converting cartesian to polar coordinates we can understand the zeros of the Jacobian as being due to points which are fixed under combined rotations and gauge transformations. A point where some of the x_i are equal is clearly invariant under a nontrivial subgroup of $SO(3) \times SO(3)$.

From the invariance of $\det c_i^a = \prod_i x_i$ one sees that any permutation of the x_i or any simultaneous change of the sign of two of the x_i can be achieved by a combined rotation and gauge transformation. This implies we have a 6×4-fold covering of the gauge and rotation invariant configurations by $\mathbf{R}^3$, and it explains why vanishing of the Jacobian at $x_i = x_j$ implies its vanishing at $x_i = -x_j$. It also shows that the absolute value in (5.13) does not lead to singularities, because the wavefunction has a permutation symmetry. Equation (5.12) is hermitian with respect to (5.13) on the Hilbert space of wavefunctions satisfying

$$\psi(x_1, x_2, x_3) = \psi(\pm x_{\pi(1)}, \pm x_{\pi(2)}, \pm x_{\pi(3)}), \tag{5.14}$$

where π is any 3-permutation. Equivalently, we can restrict x_i as follows:

$$0 \leqslant x_2 \leqslant x_3, \qquad x_1^2 \leqslant x_2^2. \tag{5.15}$$

The potential V_0' (Eq. (5.7)) of H_0' is zero if and only if two of the three x_i are zero. With the restriction (5.15) this means $x_1 = x_2 = 0$. Hence the vacuum valley is specified by

$$C_i = x_3 \eta_{3i}. \tag{5.16}$$

Thus $x_3 = |\mathbf{C}|$ and the following parameterization of η is forced upon us:

$$\begin{aligned} \eta_{3i} &= C_i/|\mathbf{C}|, \\ \eta_{1i} &= a_i \cos\xi - b_i \sin\xi, \\ \eta_{2i} &= a_i \sin\xi + b_i \cos\xi, \end{aligned} \tag{5.17}$$

with **a**, **b**, and **C**/|**C**| mutually orthogonal unit vectors with positive orientation. Explicitly we can write

$$\begin{aligned} \mathbf{a} &= (\cos\varphi\cos\theta, \sin\varphi\cos\theta, -\sin\theta), \\ \mathbf{b} &= (-\sin\varphi, \cos\varphi, 0), \\ \mathbf{C}/|\mathbf{C}| &= (\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta), \end{aligned} \tag{5.18}$$

with

$$\theta \in [0, \pi], \qquad \varphi \in [0, 2\pi], \qquad \xi \in [0, 2\pi]. \tag{5.19}$$

Thus (x_3, θ, φ) is a spherical coordinate system for the vacuum valley, and $(x_1\ x_2, \xi)$ are the "transverse" coordinates.

The kinetic term in the general case of a gauge-invariant, but not necessarily rotationally invariant, wavefunction is derived in the appendix,

$$\frac{\partial^2}{\partial c_i^{a2}} = -\frac{1}{2}\left(\prod_{i>j}(x_i^2 - x_j^2)\right)^{-1} \frac{\partial}{\partial x_k}\prod_{i>j}(x_i^2 - x_j^2)\frac{\partial}{\partial x_k} - \frac{1}{4}\sum_{i\neq j\neq k}\frac{x_i^2 + x_j^2}{(x_i^2 - x_j^2)^2}\hat{L}_k^2, \tag{5.20}$$

where $\hat{L}_k$ are the generators for the representation of $SO(3)$ acting on the wavefunction $\psi(x_i, \theta, \varphi, \xi)$ with the inner product

$$\langle \Psi \mid \Phi \rangle = \int_{0\le x_1, x_2 \le x_3} d^3x\, d\theta\, d\varphi\, d\xi \sin\theta \left|\prod_{i>j}(x_i^2 - x_j^2)\right| \bar{\Psi}(c)\,\Phi(c). \tag{5.21}$$

Explicitly these generators are

$$\begin{aligned} \hat{L}_1 &= -i\left[\cot\theta\cos\xi\partial_\xi + \frac{\cos\xi}{\sin\theta}\partial_\varphi + \sin\xi\partial_\theta\right], \\ \hat{L}_2 &= -i\left[\cot\theta\sin\xi\partial_\xi + \frac{\sin\xi}{\sin\theta}\partial_\varphi - \cos\xi\partial_\theta\right], \\ \hat{L}_3 &= -i\partial_\xi, \end{aligned} \tag{5.22}$$

and a simple calculation shows that indeed $[\hat{L}_i, \hat{L}_j] = i\varepsilon_{ijk}\hat{L}_k$.

Let us finally transform the Jacobian away, by scaling the wavefunction according to

$$\tilde{\Psi} = \sqrt{|\mathscr{J}|}\,\Psi, \qquad \mathscr{J} = (x_2^2 - x_1^2)(x_3^2 - x_1^2)(x_3^2 - x_2^2). \tag{5.23}$$

Noting that $(\partial^2/\partial x_k^2)\,\mathscr{J} = 0$ and $((\partial/\partial x_k)\ln\mathscr{J})^2 = 2\sum_{i\neq j}((x_i^2 + x_j^2)/(x_i^2 - x_j^2)^2)$ we find

$$\tilde{H}_0' = -\frac{g^2}{2L}\frac{\partial^2}{\partial x_k^2} + \frac{g^2}{4L}\sum_{i\neq j\neq k}\frac{x_i^2 + x_j^2}{(x_i^2 - x_j^2)^2}(\hat{L}_k^2 - 1) + \frac{1}{2g^2 L}\sum_{i>j} x_i^2\, x_j^2. \tag{5.24}$$

Our next task is to define $\tilde{\hat{H}}$, which is obtained by applying the above transformation to the Hamiltonian $\hat{H}$ of Eq. (4.3). Thus we write

$$\tilde{\hat{H}} = \tilde{\hat{H}}_0' + V_1'(\mathbf{C}) = H(\mathbf{C}) + \tilde{H}_{[\mathbf{C}]}(x_1, x_2, \xi) + T, \tag{5.25}$$

with (it will become clear below why we make this split)

$$H(\mathbf{C}) = -\frac{g^2}{2L}\frac{\partial^2}{\partial |\mathbf{C}|^2} + \frac{4}{L\pi^2}\sum_{\mathbf{n}\neq 0}\frac{\sin^2(\mathbf{n}\cdot\mathbf{C}/2)}{(\mathbf{n}^2)^2} - \frac{g^2}{2L\mathbf{C}^2}(\sin^2\theta\partial_\varphi^2 + \partial_\theta^2), \tag{5.26}$$

$$\begin{aligned}\tilde{H}_{[\mathbf{C}]}(x_1, x_2, \xi) = &-\frac{g^2}{2L}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) - \frac{g^2}{2L}\left(\frac{x_1^2 + x_2^2}{(x_1^2 - x_2^2)^2}\right)(\partial_\xi^2 + 1) \\ &- \frac{g^2}{2L}\cot^2\theta\left[\cos^2\xi\,\frac{(\mathbf{C}^2 + x_1^2)}{(\mathbf{C}^2 - x_1^2)^2} + \sin^2\xi\,\frac{(\mathbf{C}^2 + x_2^2)}{(\mathbf{C}^2 - x_2^2)^2}\right]\partial_\xi^2 - \frac{g^2}{L\mathbf{C}^2} \\ &+ \frac{1}{2g^2L}(x_1^2 + x_2^2)\,\mathbf{C}^2 + \frac{1}{2g^2L}x_1^2 x_2^2 - \frac{2\,|\mathbf{C}|}{L}.\end{aligned} \tag{5.27}$$

One easily verifies that T, implicitly defined by the above three equations, vanishes when ∂_θ and ∂_φ vanish. The fixed-$\mathbf{C}$ eigenfunctions $\tilde{\chi}^{(n)}_{[\mathbf{C}]}(x_1, x_2, \xi)$ for $\tilde{H}_{[\mathbf{C}]}(x_1, x_2, \xi)$ satisfy vanishing boundary conditions for $x_1^2 = x_2^2$, $x_1^2 = \mathbf{C}^2$ and $x_2^2 = \mathbf{C}^2$.

The split in Eq. (5.25) of course anticipates that we want to derive an equation along the vacuum valley for the original Yang–Mills Hamiltonian, similar to (3.41) for the toy model; this will be done in the next section. Although in this case, we cannot solve exactly for $\chi^{(n)}_{[\mathbf{C}]}$, we can use perturbation theory [5]. To see what the expansion parameter is we scale x_1 and x_2 as

$$x_i = \frac{g y_i}{|\mathbf{C}|^{1/2}}. \tag{5.28}$$

The rescaled Hamiltonian becomes

$$\tilde{H}_{[\mathbf{C}]} = \frac{|\mathbf{C}|}{2L}\left\{-\frac{\partial^2}{\partial y_i^2} - \frac{y_1^2 + y_2^2}{(y_1^2 - y_2^2)^2} + y_1^2 + y_2^2 - 2 + K\hat{L}_3^2 + \frac{g^2}{|\mathbf{C}|^3}(y_1^2 y_2^2 - 2)\right\}, \tag{5.29}$$

with vanishing boundary conditions at $y_1^2 = y_2^2$, $y_1^2 = |\mathbf{C}|^3/g^2$, and $y_2^2 = |\mathbf{C}|^3/g^2$. K is positive definite and can be read off from Eq. (5.27). Comparing with (5.23) it is clear that we can also write

$$\tilde{\chi}^{(n)}_{[\mathbf{C}]} = \sqrt{|x_1^2 - x_2^2|}\,\chi^{(n)}_{[\mathbf{C}]}, \tag{5.30}$$

with $\tilde{H}_{[\mathbf{C}]}$ transformed to $H_{[\mathbf{C}]}$,

$$H_{[\mathbf{C}]}=\frac{|\mathbf{C}|}{2L}\left\{-\frac{1}{y_1^2-y_2^2}\frac{\partial}{\partial y_i}(y_1^2-y_2^2)\frac{\partial}{\partial y_i}+y_1^2+y_2^2-2+K\left(\frac{1}{i}\partial_\xi\right)^2\right.$$
$$\left.+\frac{g^2}{|\mathbf{C}|^3}(y_1^2y_2^2-2)\right\}, \tag{5.31}$$

where $\chi_{[\mathbf{C}]}$ only has vanishing boundary conditions at $y_1^2=|\mathbf{C}|^3/g^2$ and $y_2^2=|\mathbf{C}|^3/g^2$. The ground state is especially easy to determine; it is clearly independent of ξ, so that $g^2/|\mathbf{C}|^3$ will be the expansion parameter;

$$H_{[\mathbf{C}]}\chi^{(n)}_{[\mathbf{C}]}=W_n(\mathbf{C})\,\chi^{(n)}_{[\mathbf{C}]} \tag{5.32}$$

therefore has the property that the ground state $(\chi^{(1)}_{[\mathbf{C}]}, W_1(\mathbf{C}))$ only depends on $|\mathbf{C}|$, so $T_{11}\equiv 0$, where

$$T_{nm}=\frac{1}{g^2}\langle\chi^{(n)}_{[\mathbf{C}]}|\,T\,|\chi^{(m)}_{[\mathbf{C}]}\rangle. \tag{5.33}$$

Furthermore, ignoring the boundary conditions for the ground state would only lead to $O(\exp(-\text{const.}/g))$ corrections, so that these boundary conditions can be replaced by square integrability of $\chi^{(1)}_{[\mathbf{C}]}$, and we find $(\chi^{(1)}_{[\mathbf{C}]}$ does not depend on ξ, but "ξ-dependence" is present because of the normalization)

$$\chi^{(1)}_{[\mathbf{C}]}=\frac{|\mathbf{C}|}{\sqrt{4\pi}\,g^2}\exp\left(\frac{-|\mathbf{C}|\,(x_1^2+x_2^2)}{2g^2}\right)(1+O(g^2/|\mathbf{C}|^3)),$$
$$W_1(\mathbf{C})=-\frac{3}{4\pi L}\frac{g^2}{\mathbf{C}^2}+L^{-1}O(g^4/|\mathbf{C}|^5). \tag{5.34}$$

$\tilde{\chi}$ is normalized with respect to the standard inner product (cf. (5.21) and Appendix B).

The next section shows how the tunneling problem can be reduced to the tunneling problem for a simple potential (essentially $V_1(\mathbf{C})$) on a cubic lattice (lattice constant 2π) with the lattice momenta restricted to multiples of π.

6. The Reduction Formula

Combining the results of the previous sections we can write (we introduce the factor $|\mathbf{C}|$ to convert the measure to $d^3\mathbf{C}\,dx_1\,dx_2\,d\xi$)

$$\tilde{\Psi}_0(\mathbf{C}, x_1, x_2, \xi)=\sum_n |\mathbf{C}|\,\varphi_0^{(n)}(\mathbf{C})\,\tilde{\chi}^{(n)}_{|\mathbf{C}|}(x_1, x_2, \xi), \tag{6.1}$$

$$\int_{\substack{|x_1|\leqslant|\mathbf{C}|\\ |x_2|\leqslant|\mathbf{C}|}} d^3\mathbf{C}\,dx_1\,dx_2\,d\xi\,|\tilde{\Psi}_0(\mathbf{C}, x_1, x_2, \xi)/|\mathbf{C}||^2=1, \tag{6.2}$$

$$\hat{H}_{nm}(\mathbf{C})\,\varphi_0^{(m)}(\mathbf{C}) = \Big[-\frac{g^2}{2L}\Big(\delta_{nm}\frac{\partial}{\partial \mathbf{C}} - \mathbf{A}_{nm}(\mathbf{C})\Big)^2 + g^2 T_{nm}\Big(\mathbf{C}, \frac{\partial}{\partial \mathbf{C}}\Big) + (V_1(\mathbf{C}) + W_n(\mathbf{C}))\,\delta_{nm}\Big]\varphi_0^{(m)}(\mathbf{C}) = E_0\varphi_0^{(n)}(\mathbf{C}), \tag{6.3}$$

$$\mathbf{A}_{nm}(\mathbf{C}) = \Big\langle \tilde{\chi}^{(m)}_{[\mathbf{C}]} \Big| \frac{\partial}{\partial \mathbf{C}} \Big| \tilde{\chi}^{(n)}_{[\mathbf{C}]} \Big\rangle. \tag{6.4}$$

The single-well lowest order wavefunction $\Psi_0^{[0]}(x_i)$ is determined by

$$H_0'\Psi_0^{[0]}(x_i) = \Big(-\frac{g^2}{2L}\frac{1}{\mathscr{J}}\frac{\partial}{\partial x_i}\mathscr{J}\frac{\partial}{\partial x_i} + \frac{1}{2g^2 L}\sum_{i>j} x_i^2 x_j^2\Big)\Psi_0^{[0]}(x_i) = E_0^{[0]}\Psi_0^{[0]}(x_i), \tag{6.5}$$

$$8\pi^2 \int_{\substack{0 \leqslant |x_1| \leqslant x_3 \\ 0 \leqslant |x_2| \leqslant x_3}} dx_1\,dx_2\,dx_3\,|\mathscr{J}|\,|\Psi_0^{[0]}(x_i)|^2 = 1, \tag{6.6}$$

$$E_0^{[0]} = \frac{g^{2/3}}{L}\varepsilon, \qquad \varepsilon = 4.11672\ldots. \tag{6.7}$$

The value of ε was determined previously by Lüscher and Münster [13] using Rayleigh–Ritz perturbation theory. The associated expression for $\varphi_0^{(1)}(\mathbf{C})$ is in the single-well approximation given by

$$\varphi_0^{[0]}(\mathbf{C}) = \frac{1}{|\mathbf{C}|}\int dx_1\,dx_2\,d\xi\;\Psi_0^{[0]}(x_i)\,|\mathscr{J}|^{1/2}\,\tilde{\chi}^{(1)}_{[\mathbf{C}]}(x_1, x_2, \xi). \tag{6.8}$$

Using the approximation (Eq. (5.34)) of $\chi^{(1)}_{[\mathbf{C}]}(x_1, x_2)$ for $|\mathbf{C}| \gg g^{2/3}$ we find

$$\varphi_0^{[0]}(\mathbf{C}) \cong \frac{\sqrt{\pi}\,|\mathbf{C}|^2}{g^2}\int dx_1\,dx_2\,|x_1^2 - x_2^2|\;\Psi_0^{[0]}(x_i)\exp\Big(\frac{-|\mathbf{C}|\,(x_1^2 + x_2^2)}{2g^2}\Big). \tag{6.9}$$

This completes the construction of the tunneling data as described in Section 3, with the difference that z is replaced by a three-component vector $\mathbf{C}$.

We next apply the path decomposition expansion, as was described in detail for the toy-models [14]. For this we need to analyze the asymptotic behaviour of $\varphi_0^{[0]}(\mathbf{C})$. For $g^{2/3} \ll |\mathbf{C}| \ll 1$, $\varphi_0^{[0]}(\mathbf{C})$ satisfies the following effective Schrödinger equation:

$$\Big[-\frac{g^2}{2L}\frac{\partial}{\partial \mathbf{C}^2} + V_1^{[0]}(\mathbf{C})\Big]\varphi_0^{[0]}(\mathbf{C}) = E_0^{[0]}\varphi_0^{[0]}(\mathbf{C}), \tag{6.10}$$

$$V_1^{[0]}(\mathbf{C}) = \frac{2\,|\mathbf{C}|}{L} = \lim_{\lambda \to 0}\lambda^{-1}V_1(\lambda\mathbf{C}). \tag{6.11}$$

Using the spherical symmetry, the WKB approximation in $|\mathbf{C}|$ gives the asymptotics

$$\varphi_0^{[0]}(\mathbf{C}) \cong \frac{g^{-1/6}}{|\mathbf{C}|} B \frac{\exp(-(4|\mathbf{C}| - 2LE_0^{[0]})^{3/2}/6g)}{(4|\mathbf{C}| - 2LE_0^{[0]})^{1/4}}. \tag{6.12}$$

The following observations should make this result clear: Rescaling $x_i = g^{2/3} y_i$ and $\mathbf{C} = g^{2/3}\mathbf{W}$ gives $\Psi_0^{[0]}(x_i) = g^{-1}\hat{\Psi}_0^{[0]}(y_i)$ and $\varphi_0^{[0]}(\mathbf{C}) = g^{-1}\hat{\varphi}_0^{[0]}(\mathbf{W})$, where $\hat{\Psi}$ satisfies (6.6) with x_i replaced by y_i, and $\hat{\Psi}(y_i)$ is independent of g. Consequently $\hat{\varphi}_0^{[0]}(\mathbf{W})$ is also independent of g and it satisfies

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial \mathbf{W}^2} + 2|\mathbf{W}|\right)\hat{\varphi}_0^{[0]}(\mathbf{W}) = \varepsilon \hat{\varphi}_0^{[0]}(\mathbf{W}), \tag{6.13}$$

so that the WKB approximation gives

$$\hat{\varphi}_0^{[0]}(\mathbf{W}) \cong \frac{B}{|\mathbf{W}|} \frac{\exp(-\int_{\varepsilon/2}^{|\mathbf{W}|} \sqrt{2(2s-\varepsilon)}\, ds)}{(4|\mathbf{W}| - 2\varepsilon)^{1/4}}. \tag{6.14}$$

Substituting $\mathbf{W} = g^{-2/3}\mathbf{C}$ gives Eq. (6.12).

We would now like to construct a three-dimensional quantum mechanics problem completely equivalent (to this order) to the present problem. This can be done as follows: We replace $V_1(\mathbf{C})$ by $\tilde{V}_1(\mathbf{C})$, where

$$\begin{aligned} \tilde{V}_1(\mathbf{C}) &= LV_1'(\mathbf{C}) + 2g^{2/3}\delta, \qquad && |\mathbf{C} - 2\pi\mathbf{n}| \leqslant g^{2/3}\delta \\ \tilde{V}_1(\mathbf{C}) &= LV_1(\mathbf{C}), && \text{elsewhere.} \end{aligned} \tag{6.15}$$

The g-independent constant δ is chosen so that the lowest eigenvalue for the three-dimensional Hamiltonian with the potential

$$\begin{aligned} V_\delta(x) &= 2\delta, \qquad && |x| \leqslant \delta \\ &= 2|x|, && |x| > \delta \end{aligned} \tag{6.16}$$

is exactly equal to ε:

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V_\delta(|\mathbf{x}|)\right)\hat{\varphi}_\delta(x) = \varepsilon\hat{\varphi}_\delta(x). \tag{6.17}$$

$\hat{\varphi}_\delta(x)$ satisfies the asymptotic equation ($|\mathbf{x}| \gg 1$)

$$\hat{\varphi}_\sigma(\mathbf{x}) = \frac{B_\delta}{|\mathbf{x}|} \frac{\exp(-\int_{\varepsilon/2}^{|\mathbf{x}|} \sqrt{2(2s-\varepsilon)}\, ds)}{(4|\mathbf{x}| - 2\varepsilon)^{1/4}}, \tag{6.18}$$

which is purposely of the same form as Eq. (6.14).

Finally, consider the Hamiltonian

$$-\frac{g^2}{2}\frac{\partial^2}{\partial \mathbf{C}^2}+\tilde{V}_1(\mathbf{C}), \tag{6.19}$$

and restrict the wavefunctions to

$$\varphi_{\mathbf{e}}(\mathbf{C}+2\pi\mathbf{n})=(-1)^{\mathbf{e}\cdot\mathbf{n}}\varphi_{\mathbf{e}}(\mathbf{C}), \tag{6.20}$$

and let $E_\delta(\mathbf{e}, g)$ be the associated groundstate energies for each given $\mathbf{e}$. Then (up to relative errors vanishing as a positive power of $g(L)$) the energy of electric flux for $SU(2)$ on the hypertorus T^3 of size L^3 is given by

$$E(\mathbf{e}, L)=\frac{1}{L}\frac{|B|^2}{|B_\delta|^2}E_\delta(\mathbf{e}, g(L)), \tag{6.21}$$

with $g(L)$ the renormalized coupling constant at the scale L, i.e., to leading order

$$g(L)=\left[-\frac{11}{12\pi^2}\ln(\Lambda L)\right]^{-1/2}. \tag{6.22}$$

Hence we have reduced the problem to that of the calculation of the energy for a particle in a cubic lattice with potential $\tilde{V}_1(\mathbf{C})$. Furthermore, we are only interested in the lattice momenta $\mathbf{p}=\mathbf{e}\pi$ (because of the gauge invariance).

It will turn out that the actual value of δ is irrelevant, as it should be, since we introduced it only for a convenient formulation of the problem. We will therefore not specify the value of δ. The next section deals with the calculation of $E_\delta(\mathbf{e}, g)$, and it will be shown (as is obvious from the double-cone toy model in [14]) that $E_\delta(\mathbf{e}, g)$ is of the form $|B_\delta|^2$ times something independent of δ, so that indeed the δ-dependence drops out of Eq. (6.21).

7. The Tunneling Calculation

In the calculation of the energy as a function of the lattice momenta $\mathbf{p}$, for the Hamiltonian of Eq. (6.19) one can apply the tight binding limit of solid state quantum mechanics or the dilute gas picture for instantons. In both cases one finds

$$E_\delta(\mathbf{p}, g)=\left(\sum_{i=1}^{3}\sin^2\frac{p_i}{2}\right)\Delta(g), \tag{7.1}$$

where we normalize such that $E(\mathbf{0}, g)\equiv 0$. $\Delta(g)$ is the energy split between the even and odd wavefunctions, taking only tunneling between two nearest neighbour minima into account. In other words, $\Delta(g)$ is the energy split due to the single pinchon contribution, where we called the instanton for the Hamiltonian of

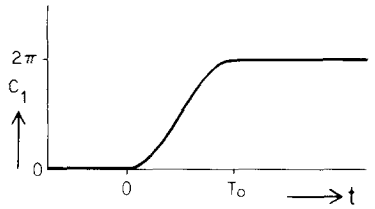


FIG. 2. The pinchon solution $C(t)$ in the approximation $V_1(C) = C(2\pi - C)/\pi$.

Eq. (6.19) a pinchon, because the effective potential $V_1(\mathbf{C})$ is quantum induced and provides a potential barrier due to the pinching of the full potential $V(\mathbf{A})$, between the two minima (cf. Fig. 1). In Fig. 2 we present this pinchon solution in the approximation $a_n = 0$ [3] and in Fig. 3 we sketch the electric field it generates.

Having reduced the problem to that of a double well, we can directly apply techniques developed in [14]. We focus on the domain $-\pi \leqslant C_1 \leqslant 3\pi$, $-\pi \leqslant C_2$, $C_3 \leqslant \pi$, containing two nearest neighbour minima at $\mathbf{C} = \mathbf{0}$ and $\mathbf{C} = 2\pi\mathbf{e}^{(1)}$. It is clear (shifting the origin to $\mathbf{C} = \pi\mathbf{e}^{(1)}$ and rescaling by π) that the conditions of [14] are satisfied for $\tilde{V}_1(\mathbf{C})$. Indeed, in the appendix we will show that $V_1(\mathbf{C}) \geqslant V_1(C_1\mathbf{e}^{(1)})$ for all C_2, C_3, so that the tunneling path is along the C_1 axis. Furthermore, the lowest order single-well potential $\tilde{V}_1^{[0]}(\mathbf{C}) = V_\delta(|\mathbf{C}|)$ is spherically symmetric and thus of the double-cone shape studied in [14]. Accordingly, we can copy the expression for $A(g)$ directly from these toy models ([14], Eq. (4.2)) ($d \gg g^{2/3}$),

$$A(g) = 2g\sqrt{2(\tilde{V}_1(d\mathbf{e}^{(1)}) - g^{2/3}\varepsilon)}\,|\varphi_\delta(d\mathbf{e}^{(1)})|^2 \times \exp\left(-\frac{1}{g}\int_d^{2\pi - d}\sqrt{2(\tilde{V}_1(s\mathbf{e}^{(1)}) - g^{2/3}\varepsilon)}\,ds\right) A(d), \tag{7.2}$$

where $\varphi_\delta(\mathbf{C}) = g^{-1}\hat{\varphi}_\delta(g^{-2/3}|\mathbf{C}|)$, (see Eq. (6.18)) and $A(d)$ is the contribution due to the transverse fluctuations. Hence,

$$A(g) = 2g^{2/3}d^{-2}A(d)\,|B_\delta|^2 \exp\left(-\frac{1}{g}\int_{g^{2/3}\varepsilon}^{2\pi - g^{2/3}\varepsilon}\sqrt{2(\tilde{V}_1(s\mathbf{e}^{(1)}) - g^{2/3}\varepsilon)}\,ds\right). \tag{7.3}$$

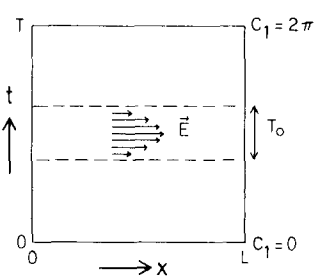


FIG. 3. The electric field $E = \dot{C}(t)$ from the pinchon in Fig. 2.

Thus we are left with the computation of $\Lambda(d)$ which is given by [14] ($\dot{} = d/dt$)

$$\Lambda(d) = 2\pi g[\dot{q}(T) + \phi_\perp''(d)\, q(T)]^{-1},$$
$$\phi_\perp''(d) = -g^2 \frac{\partial^2}{\partial C_2^2} \ln(|\varphi_S(\mathbf{C})|)\,|_{\mathbf{C}=d\mathbf{e}^{(1)}}. \tag{7.4}$$

The fluctuation $q(t)$ is a solution of

$$\ddot{q}(t) = \Omega^2(t)\, q(t),$$
$$q(0) = 1, \qquad \dot{q}(0) = \phi_\perp''(d), \tag{7.5}$$

where $\Omega^2(t)$ is the second-order variation of $\tilde{V}_1$ along the pinchon path $\mathbf{C}(t) = C(t)\,\mathbf{e}^{(1)}$,

$$\Omega^2(t) = \frac{\partial^2 \tilde{V}_1}{\partial C_2^2}(\mathbf{C}(t)), \tag{7.6}$$

and the pinchon is given by the equation

$$\dot{C}(t) = \sqrt{2(\tilde{V}_1(\mathbf{C}(t)) - g^{2/3}\varepsilon)}, \qquad C(0) = d, \qquad C(T) = 2\pi - d. \tag{7.7}$$

This equation also defines implicitly the tunneling time $T(d)$:

$$T(d) = \int_d^{2\pi - d} \frac{ds}{\sqrt{2(\tilde{V}_1(s\mathbf{e}^{(1)}) - g^{2/3}\varepsilon)}}. \tag{7.8}$$

As noted in [14] and proved further on, we have $\Lambda(d) = \lambda g d^2$, because of the spherical symmetry of $\tilde{V}_1^{[0]}(\mathbf{C})$. As for the double cone we have to calculate $\Lambda(d)$ explicitly to find the constant λ. Furthermore, $\tilde{V}_1$ can be replaced by LV_1 in Eqs. (7.3), (7.6), (7.7), and (7.8), since $d > \delta$ or $(0 < s < 2\pi)$:

$$\tilde{V}_1(s) \equiv \tilde{V}_1(s\mathbf{e}^{(1)}) = \frac{1}{\pi}\left[s(2\pi - s) + 8 \sum_{n=1}^{\infty} a_n \sin^2(ns/2) \right], \tag{7.9}$$

(cf. Eqs. (A.18), (4.7)). Taken together we have

$$\Lambda(g) = 2g^{5/3}\lambda\, |B_S|^2 \exp\left(-\frac{S}{g} + \frac{\varepsilon T}{g^{1/3}} \right), \tag{7.10}$$

where

$$S = \int_0^{2\pi} \sqrt{2\tilde{V}_1(s)}\, ds, \tag{7.11}$$

$$T = \int_0^{2\pi} \frac{1}{\sqrt{2\tilde{V}_1(s)}}\, ds. \tag{7.12}$$

We are thus left with the calculation of S, T, and λ. The first two can be calculated by explicitly substituting (7.9) in (7.11) and (7.12) and expanding the results in the coefficients a_n. We substitute

$$s=\pi(1-\sin\theta), \qquad \theta\in\left[-\frac{\pi}{2},\frac{\pi}{2}\right], \tag{7.13}$$

and find

$$\begin{aligned}\tilde{V}_1(\theta)&=\frac{1}{\pi}\left(\pi^2\cos^2\theta+8\sum_{n=1}^{\infty}a_n\sin^2\left(\frac{n\pi}{2}(1-\sin\theta)\right)\right)\\&=\frac{1}{\pi}\left(\pi^2\cos^2\theta+8a_1\cos^2\left(\frac{\pi}{2}\sin\theta\right)+8a_2\sin^2(\pi\sin\theta)+\cdots\right).\end{aligned} \tag{7.14}$$

A straigthforward but lengthy calculation yields

$$S=\frac{1}{2}\pi^2\sqrt{2\pi}\left[1+\frac{4a_1}{\pi^2}(1+J_0(\pi))+\frac{4a_2}{\pi^2}(1-J_0(2\pi))-\frac{4a_1^2}{\pi^3}(2J_1(\pi)+J_1(2\pi))+\cdots\right], \tag{7.15}$$

$$\begin{aligned}T=\frac{1}{2}\pi\sqrt{2\pi}\Bigg[1&-\frac{2a_1}{\pi}J_1(\pi)+\frac{4a_2}{\pi^2}J_1(2\pi))\\&+\frac{2a^2}{\pi^3}(4J_1(\pi)+2J_1(2\pi)-3\pi J_0(\pi)-\pi J_0(2\pi))+\cdots\Bigg].\end{aligned} \tag{7.16}$$

J_n is the Bessel function of order n. The numerical values are

$$\begin{aligned}S&=12.4637\ldots,\\T&=3.9186\ldots.\end{aligned} \tag{7.17}$$

We now attack the calculation of λ. As in the double cone problem of [14], we can ignore the $g^{2/3}\varepsilon$ terms in Eq. (7.7), because they yield corrections to λ of order $g^{2/3}$. Using the spherical symmetry for $d\ll 1$, we have

$$\phi_\perp''(d)=\frac{1}{d}\sqrt{2\tilde{V}_1(d)}=2d^{-1/2}, \tag{7.18}$$

with a relative error of $O(gd^{-3/2}+d^{1/2})$, which can be absorbed in the overall error (for $d=g^{1/2}$, $gd^{-3/2}=g^{1/4}$). Because of the isotropy of $\tilde{V}_1(\mathbf{C})$ orthogonal to the pinchon $\mathbf{C}(t)$ we have (Δ the three-dimensional Laplacian)

$$\Omega^2(t)=\frac{1}{2}\left(\Delta-\frac{\partial^2}{\partial C_1^2}\right)\tilde{V}_1\Big|_{\mathbf{C}(t)}, \tag{7.19}$$

and $\mathbf{C}(t) = C(t)\,\mathbf{e}^{(1)}$ now satisfies

$$\dot{C}(t) = \sqrt{2\tilde{V}_1(C(t))}, \qquad C(0) = d, \qquad C(T(d)) = 2\pi - d.$$

This allows us to eliminate the pinchon time t in favour of the pinchon coordinate C (from now on we write V for $\tilde{V}_1$, and the arguments apply to any potential with spherically symmetric $V^{[0]}$):

$$\dot{q}(t) = \sqrt{2V(C)}\,\frac{d}{dC}\,q(C) = \sqrt{2V(C)}\,q'(C). \tag{7.20}$$

Hence from Eq. (7.4),

$$\lambda = d^{\ 2}g^{\ 1}\Lambda(d) = 2\pi d^{\ 2}\left[\sqrt{2V(2\pi - d)}\,q'_d(2\pi - d) + \sqrt{2V(d)}\,d^{-1}q_d(2\pi - d)\right]^{\ 1}, \tag{7.21}$$

where $q_d(C)$ satisfies the equations

$$\begin{gathered}\sqrt{2V(C)}\,\frac{d}{dC}\sqrt{2V(C)}\,\frac{d}{dC}\,q_d(C) = \frac{1}{2}\left[\left(\Delta - \frac{\partial^2}{\partial C_1^2}\right)V\right](C)\,q_d(C) \\ q_d(d) = 1, \qquad q'_d(d) = d^{-1}.\end{gathered} \tag{7.22}$$

Note that (7.21) can be simplified due to the symmetry $V(2\pi - d) = V(d)$, and that $q_d(C)$ depends on d through its initial values. Furthermore, for $d \ll 1$, the spherical symmetry in that region gives $\Delta V = V'' + (2/d)\,V'$, so that $q''_d(d) = 0$. Next, differentiating (7.22) with respect to d shows that $(\partial/\partial d)\,q_d(s)$ satisfies the same differential equation as $q_d(s)$. The boundary conditions are obtained in the same way:

$$\begin{aligned}\frac{\partial}{\partial d}\,q_d(s)\bigg|_{s=d} &= -q'_d(d) = -\frac{1}{d}\,q_d(d), \\ \frac{\partial}{\partial d}\,q'_d(s)\bigg|_{s=d} &= -q''_d(d) - \frac{1}{d^2} = -\frac{1}{d}\,q'_d(d).\end{aligned} \tag{7.23}$$

Thus the boundary conditions for $(\partial/\partial d)\,q_d(s)$ are $-d^{-1}$ times those for $q_d(s)$, so we have for all s:

$$\frac{\partial}{\partial d}\,q_d(s) = -\frac{1}{d}\,q_d(s). \tag{7.24}$$

Hence,

$$\frac{\partial}{\partial d}\,\lambda^{-1} = \frac{V'(d)}{2V(d)}\,\lambda^{-1} - q''_d(2\pi - d)\,\frac{d^2\sqrt{2V(d)}}{2\pi}. \tag{7.25}$$

Using the equations of motion (7.22) and the spherical symmetry at $2\pi = d$ we obtain

$$q_d''(2\pi - d) = \frac{V'(d)}{2V(d)} \left(q_d'(2\pi - d) + d^{-1} q_d(2\pi - d)\right). \tag{7.26}$$

As promised, we find $\partial\lambda/\partial d \equiv 0$. (The relative error due to the breakdown of spherical symmetry is smaller than $O(d^2) = O(g)$ for $d = g^{1/2}$.)

We are finally ready to collect all our analytic results. Inserting the expression for the periodic potential $E_\delta(\mathbf{p}, g)$ (Eq. (7.1)) into the formula for energy of electric flux (Eq. (6.21)), we obtain the energy of electric flux in terms of the double-well energy splitting $\Delta(g)$ (Eq. (7.3)):

$$E(\mathbf{e}, L) = \sum_{i=1}^{3} \sin^2\left(\frac{\pi e_i}{2}\right) 2\lambda\, |B|^2 \frac{g^{5/3}(L)}{L} \exp\left(-\frac{S}{g(L)} + \frac{\varepsilon T}{g(L)^{1/3}}\right). \tag{7.27}$$

The tunneling action S and tunneling time T are given in (7.17), and the constant λ, which accounts for transverse fluctuations, is obtained from Eq. (7.21) by taking the limit $d \to 0$. This involves calculating the transverse fluctuations q_d using Eq. (7.22). Explicitly,

$$\begin{gathered} \lambda^{-1} = \lim_{d \to 0} \frac{d^{3/2}}{\pi} \left[dq_d'(2\pi - d) + q_d(2\pi - d)\right], \\ \sqrt{2V_1(C)}\left(\sqrt{2V_1(C)}\, q_d'(C)\right)' = \tfrac{1}{2} q_d(C)(\Delta V_1(C) - V_1''(C)), \\ q_d(d) = 1, \qquad q_d'(d) = d^{-1}. \end{gathered} \tag{7.28}$$

The constant B is determined by the asymptotics of the groundstate wave function $\varphi_0^{[0]}(\mathbf{C})$ in the direction of the vacuum valley, Eq. (6.12). This component of the groundstate wavefunction can be obtained from the single-well perturbative groundstate wavefunction $\Psi_0^{[0]}$ by projecting with the "transverse" wavefunction $\tilde{\chi}_{[\mathbf{C}]}^{[1]}$ using Eq. (6.8) or (6.9). Thus B is obtained by taking the following limit:

$$\begin{aligned} B = \lim_{x_3 \to \infty} \sqrt{8\pi}\, x_3^{3/4} \exp\left(\frac{(4x_3 - 2\varepsilon)^{3/2}}{6}\right) \int dx_1\, dx_2\, |x_1^2 - x_2^2|\, \Psi_0^{[0]}(\mathbf{x}) \\ \times \exp\left(-\frac{1}{2} x_3 (x_1^2 + x_2^2)\right), \end{aligned} \tag{7.29}$$

with $\Psi_0^{[0]}(\mathbf{x})$ the single-well eigenfunction

$$\left[-\frac{1}{2\mathscr{I}} \frac{\partial}{\partial x_i} \mathscr{I} \frac{\partial}{\partial x_i} + \frac{1}{2}(x_1^2 x_2^2 + x_1^2 x_3^2 + x_2^2 x_3^2)\right] \Psi_0^{[0]}(\mathbf{x}) = \varepsilon \Psi_0^{[0]}(\mathbf{x}), \tag{7.30}$$

normalized according to

$$8\pi^2 \int_{\substack{0 \leqslant |x_1| \leqslant x_3 \\ 0 \leqslant |x_2| \leqslant x_3}} d^3x \, |\mathscr{J}| \, |\Psi_0^{[0]}(\mathbf{x})|^2 = 1. \tag{7.31}$$

Using the fact that (see Appendix B) Eq. (7.31) equals $(2/\pi^2) \int d^9c \, |\Psi_0^{[0]}(\mathbf{x})|^2$, one can alternatively determine B by fitting the wavefunction $\Psi_0(\mathbf{x}) \equiv (2/\pi^2)^{1/2} \Psi_0^{[0]}(\mathbf{x})$, normalized as $\int d^9c \, |\Psi_0(\mathbf{x})|^2 = 1$, to the asymptotic form

$$\Psi_0(\mathbf{x}) \underset{\substack{x_3 \gg 1 \\ x_1, x_2 \ll x_3}}{=} \frac{\sqrt{2}\, B \exp(-(4x_3 - 2\varepsilon)^{3/2})/6)\, e^{-(1/2)x_3(x_1^2 + x_2^2)}}{2\pi^{3/2} x_3 (4x_3 - 2\varepsilon)^{1/4}}. \tag{7.32}$$

In the next section we will describe the numerical evaluation of the constants B and λ.

8. Calculating the Wave Function

8.1. *Introduction*

In previous sections we showed how the energy split due to tunneling through a potential barrier can be calculated. The g-dependence of the result was completely determined, and we must now find the overall coefficient. It depends on two contributions: a factor λ, accounting for the effect of transverse fluctuations along the tunneling path, and a factor $|B|^2$, representing the amount of penetration of the wavefunction into the barrier. More precisely, we found

$$\Delta E = 2\lambda \, |B|^2 \, g^{5/3} \exp(-Sg^{-1} + T\varepsilon g^{-1/3}), \tag{8.1}$$

where λ is determined from the stability equation by (see Sect. 7)

$$\lambda^{-1} = \lim_{d \to 0} \frac{d^{3/2}}{\pi} [dq_d'(2\pi - d) + q_d(2\pi - d)], \tag{8.2}$$

and B is the coefficient in the asymptotic form of the single-well wave function deep within the barrier.

The evaluation of λ presents no real problem, amounting to the integration of an ordinary differential equation. We discuss this in Section 8.5, and turn first to calculating B.

At first sight, this is quite an easy calculation, because the single-well Hamiltonian is so simple, being just the kinetic term plus the lowest power term in the potential. Indeed, in many cases the lowest power in the potential is the quadratic one, and we find the familiar harmonic oscillator wavefunction, whose

asymptotic form is known exactly. This is the class of tunneling problems that instanton methods can handle. However, if the lowest power in the potential is not quadratic, the problem can be much more complicated. A non-quadratic Hamiltonian cannot in general be separated to give non-interacting normal modes, and we are faced with a true higher dimensional quantum mechnics problem. This is the case in our present problem: we cannot obtain the wavefunction in closed form, and a Raleigh–Ritz approach is necessary.

In Section (8.2) we discuss the single-well Hamiltonian, its transformation to convenient coordinates, and its integrability properties. Section (8.3) considers the choice of basis vectors for our Rayleigh–Ritz calculation, which we will see requires some care. The following section discusses the numerical calculation, and how to extract the coefficient B. Then we return to calculating λ, and put everything together to get the final formula for ΔE.

8.2. *The Single-Well Hamiltonian*

Our single-well Hamiltonian has been examined in other contexts by various authors, because it is interesting in its own right. The Lagrangian for the single well was shown in Section 4 to be the usual Yang–Mills Lagrangian, in the $A_0 = 0$ gauge, with a renormalized coupling constant and spatially constant fields. We can make the following discussion self-contained by simply imposing these conditions.

Begin with the standard Yang–Mills action per unit time for $SU(2)$:

$$\mathscr{L} = -\frac{1}{4\pi g^2}\int_{T^3} d^3x\, F^a_{\mu\nu}F^{\mu\nu a}. \tag{8.3}$$

If we now work in the gauge $A_0 = 0$, and make the simplifying assumption that the remaining fields have no space dependence, then we find

$$\frac{g^2}{L^3}\mathscr{L} = \frac{1}{2}\left(\frac{d}{dt}c_i^a\right)^2 + \frac{1}{4}(c_i^a c_j^a)(c_i^b c_j^b) - \frac{1}{4}(c_i^a c_i^a)^2, \tag{8.4}$$

where L^3 is the volume of the box, and

$$A_i^a(\mathbf{x}, t) = c_i^a(t), \qquad A_0^a(\mathbf{x}, t) = 0. \tag{8.5}$$

$\mathscr{L}$ is invariant under spatial rotations and parity, $c_i^a \to c_j^a R_i^j$ $(R \in O(3))$, and also exhibits a remnant of the global gauge invariance, being invariant under $c_i^a \to S_b^a c_i^b$ $(S \in SO(3))$. It is useful to thus think of c_i^a as a square matrix, transforming by $c \to ScR$. In Section 5 we have used the polar decomposition to diagonalize c:

$$\begin{aligned} c_i^a &= \eta_b^a \Lambda_j^b \xi_i^j, & \xi, \eta &\in SO(3), \\ \Lambda_j^b &= \mathrm{diag}(x_1, x_2, x_3), & x_3 &\geqslant x_2 \geqslant |x_i| \geqslant 0. \end{aligned} \tag{8.6}$$

Under parity, $x_1 \to -x_1$. Here we find it convenient to use a different set of invariant coordinates, (s, x, y), related to (x_1, x_2, x_3) by

$$\begin{aligned} s &\equiv x_1^2 + x_2^2 + x_3^2 \\ s^2 x &= x_1^2 x_2^2 + x_1^2 x_3^2 + x_2^2 x_3^2 \\ s^3 y &= x_1^2 x_2^2 x_3^2. \end{aligned} \tag{8.7}$$

A simple motivation for this choice is to note that the function $f(\lambda) = \det(c^{\mathrm{T}} c + \lambda \mathrm{I})$ is invariant under $c \to ScR$, so the coefficients of the power of λ are invariants of c. Expanding the determinant gives

$$f(\lambda) = \det(c^{\mathrm{T}} c + \lambda \mathrm{I}) = \lambda^3 + s\lambda^2 + s^2 x\lambda + s^3 y. \tag{8.8}$$

We have scaled out appropriate powers of s in the definitions of x and y, so that if we consider the c_i^a as coordinates in a nine-dimensional Euclidean space, then s is a "radial" coordinate,

$$s = \mathrm{Tr}(c^{\mathrm{T}} c) = c_i^a c_i^a = \sum_{i,a} (c_i^a)^2, \tag{8.9}$$

and x and y are "angles." The utility of our new coordinates is that the potential in Eq. (8.4) takes a very simple form:

$$-V(c_i^a) = \tfrac{1}{4}(c_i^a c_j^a)(c_i^b c_j^b) - \tfrac{1}{4}(c_i^a c_i^a)^2 = -\tfrac{1}{2} s^2 x. \tag{8.10}$$

Before converting to Hamiltonian form, we can scale out the g^3/L^2 dependence: just choose the length scale such that $L = g^{2/3}$, and remember that c has units of mass. Then the quantum Hamiltonian is

$$H = -\frac{1}{2} \frac{\partial^2}{(\partial c_i^a)^2} + V(c_i^a) = -\frac{1}{2} \nabla^2 + V, \tag{8.11}$$

where ∇^2 is the nine-dimensional Laplacian. Savvidy [12] has recently shown that this Hamiltonian is non-integrable, which means that there is no operator that commutes with H, other than the known symmetry generators. It is thus impossible to obtain the energy eigenfunctions in closed form, and we *have* to use a numerical method, such as Rayleigh–Ritz perturbation theory [13]. However, let us simplify the problem as much as possible before resorting to such an approach.

We are interested in solutions of

$$H\Psi = E\Psi \tag{8.12}$$

invariant under $c_i^a \to S_b^a c_i^b$, because physical wave functions must be gauge invariant. Also, we will restrict ourselves to the zero angular momentum sector,

with positive parity, so that wave functions are also invariant under $c_i^a \to c_j^a R_i^j$ ($R \in O(3)$). It follows then that Ψ is a function of s, x, and y only. The Laplacian ∇^2 can now be written in terms of (s, x, y) as

$$\nabla^2 \Psi(s, x, y) = \left(4s \frac{\partial^2}{\partial s^2} + 18 \frac{\partial}{\partial s} + \frac{1}{s} \tilde{\nabla}^2 \right) \Psi(s, x, y), \tag{8.13}$$

where $\tilde{\nabla}^2$ is the Laplacian on the two-dimensional surface parameterized by the angular variables (x, y):

$$\begin{aligned} \tilde{\nabla}^2 = {} & (12y + 4x - 16x^2) \frac{\partial^2}{\partial x^2} + 2(8y - 24xy) \frac{\partial^2}{\partial x \partial y} + (4xy - 36y^2) \frac{\partial^2}{\partial y^2} \\ & + (8 - 44x) \frac{\partial}{\partial x} + (2x - 78y) \frac{\partial}{\partial y}. \end{aligned} \tag{8.14}$$

It is clear from the form of V in Eq. (8.10) that H is not separable in our coordinate system, and the statement that H is non-integrable implies that it is not separable in *any* coordinate system. On the other hand, if V were purely a function of s, then the eigenfunction problem would indeed separate into a radial part and an angular part. We are going to use this fact in the next section, when we pick a basis for the Rayleigh–Ritz procedure, so we conclude this section by examining the operator $\tilde{\nabla}^2$ of Eq. (8.14) in detail.

Although $\tilde{\nabla}^2$ is not separable (and possibly non-integrable), we can still solve for the eigenfunctions because they must be polynomials in x and y. To see this, note first that $\tilde{\nabla}^2$ transforms polynomials into polynomials. Now suppose we have a polynomial P containing all powers $x^i y^j$ such that $ai + jb \leqslant N$ for some positive integers a, b, N. All powers in $\tilde{\nabla}^2 P$ will also have $ai + jb \leqslant N$, except possibly for terms coming from $y(\partial^2/\partial x^2) P$ and $x(\partial^2/\partial y^2) P$, which change $x^i y^j$ into $x^{i-2} y^{j+1}$ and $x^{i+1} y^{j-1}$, respectively. But both these also satisfy the constraint provided $2a \geqslant b \geqslant a$. Thus for fixed N, $\tilde{\nabla}^2$ is a Hermitian operator on a finite set of polynomials and can be diagonalized. It turns out that the correct choice is $a = 2$, $b = 3$. Let

$$P_{\alpha\beta}(x, y) = x^\alpha y^\beta + \sum_{2\gamma + 3\delta < 2\alpha + 3\beta} C_{\gamma\delta} x^\gamma y^\delta, \tag{8.15}$$

for integer α, β, and some coefficients $C_{\gamma\delta}$. Then

$$\tilde{\nabla}^2 P_{\alpha\beta}(x, y) = -(4\alpha + 6\beta)(4\alpha + 6\beta + 7)\, x^\alpha y^\beta + \sum_{2\gamma + 3\delta < 2\alpha + 3\beta} C'_{\gamma\delta} x^\gamma y^\delta.$$

The $C'_{\gamma\delta}$ are linear combinations of the $C_{\gamma\delta}$, plus some pieces from $\tilde{\nabla}^2 x^\alpha y^\beta$, so we can solve the equations

$$C'_{\gamma\delta} = -(4\alpha + 6\beta)(4\alpha + 6\beta + 7)\, C_{\gamma\delta}$$

to obtain an eigenfunction $P_{\alpha\beta}(x, y)$ of $\tilde{\nabla}^2$:

$$\tilde{\nabla}^2 P_{\alpha\beta}(x, y) = -(4\alpha + 6\beta)(4\alpha + 6\beta + 7)\, P_{\alpha\beta}(x, y). \tag{8.16}$$

In this way, we can construct a complete set of polynomial eigenfunctions of $\tilde{\nabla}^2$. Clearly, all $P_{\alpha\beta}$ with the same value of $q \equiv 2\alpha + 3\beta$ are degenerate. The combination $2\alpha + 3\beta$ occurs because $s^{2\alpha+3\beta} P_{\alpha\beta}$ is a polynomial in (x_1, x_2, x_3), by Eqs. (8.7), (8.8), and (8.15).

Finally, we must decide how to normalize $P_{\alpha\beta}$. Introduce an integration measure $d\Omega$ such that integrals in the nine-dimensional Euclidean space are given by $\int d^9c = \int r^8\, dr \int d\Omega$, where we can identify $r = (c_i^a c_i^a)^{1/2} = \sqrt{s}$. It is easy to show that $\int d\Omega\, \tilde{\nabla}^2 x^i y^j = 0$. (For instance, by using $\int d^9c \nabla^2 (e^{-r^2} x^i y^j) = 0$). If we use Eq. (8.14) for $\tilde{\nabla}^2$, this gives a recursion relation for

$$\mathscr{I}_{ij} = \int d\Omega\, x^i y^j, \tag{8.17}$$

which relates $\mathscr{I}_{ij}$ with $2i + 3j \equiv q$ to $\mathscr{I}_{i'j'}$ with $2i' + 3j' < q$:

$$\mathscr{I}_{ij} = \frac{1}{2q(2q+7)} [4(1 + i + 4j)\, \mathscr{I}_{i-1,j} + 12i(i-1)\, \mathscr{I}_{i-2,j+1} + 2j(2j-1)\, \mathscr{I}_{i+1,j-1}]. \tag{8.18}$$

We can finally evaluate $\mathscr{I}_{00}$ explicitly, since

$$\int d^9c\, e^{-r^2} = \pi^{9/2} = \int r^8\, dr\, e^{-r^2} \int d\Omega = \tfrac{105}{32} \sqrt{\pi} \int d\Omega,$$

i.e.,

$$\mathscr{I}_{00} = \tfrac{32}{105} \pi^4. \tag{8.19}$$

Thus the $\mathscr{I}$ can be calculated recursively, and this allows one to calculate the inner products $\int d\Omega\, P^*_{\alpha\beta} P_{\gamma\delta}$.

8.3. *Preparing for a Rayleigh–Ritz Calculation*

We have seen that the single-well Hamiltonian is non-integrable, and must be attacked with numerical methods. This problem has been examined by Lüscher and Münster [13], who have found the lowest energy eigenstates and eigenvalues. They used the Rayleigh–Ritz algorithm, which is:

> Given a Hermitian operator H on Hilbert space, and a complete orthonormal set of basis vectors $|n\rangle$, consider the matrix
>
> $$H^{(N)}_{nm} = \langle n|\, H\, |m\rangle \quad n, m \leqslant N.$$

Find the eigenvalues $\lambda_\alpha^{(N)}$ and eigenvectors $v_{\alpha i}^{(N)}$ of this matrix. Then $\lambda_\alpha^{(N)}$ is an approximaton for an eigenvalue λ_α of H, and $|\psi_\alpha^{(N)}\rangle = v_{\alpha i}^{(N)} |i\rangle$ is an approximation for the associated eigenvector $|\psi_\alpha\rangle$ of H. As $N \to \infty$, $\lambda_\alpha^{(N)}$ converges monotonically to λ_α, and $|\psi_\alpha^{(N)}\rangle \to |\psi_\alpha\rangle$ in the Hilbert space norm.

In practice, this method works well, but it is very difficult to put any theoretical bounds on the error in one's answers, because a bad choice of basis vectors could cause very slow convergence. The usual approach is to decide on a particular accuracy, and then methodically increase N until the answers are constant to this accuracy.

For us the problem of errors is quite crucial, because we are interested in the magnitude of the wavefunction in a region where it is decaying exponentially. Because the wavefunction only converges in the $\mathscr{L}^2$ sense as $N \to \infty$, relative errors can be large in regions where the wavefunction is small. We need to take N to very large values to achieve reasonable accuracy, and the method of Lüscher and Münster begins to suffer from rounding inaccuracy before we can reach these values. Lüscher and Münster were well aware of this problem, and to reach $N = 100$ they did sensitive parts of their calculation using extended precision. Let us review the problem.

The authors of [13] start out with an obviously complete but non-orthonormal basis, in our notation

$$\hat{\Psi}^{\omega}_{abc} = e^{-\omega s/2} s^a x^b y^c. \tag{8.20}$$

The number ω is adjusted to optimize the Rayleigh–Ritz convergence, and is in the range $1 \sim 2$. There is a canonical way to order such a basis: by smallest a, then by smallest $2b + 3c$, then by smallest b. A recursion relation for $\int e^{-\omega s} s^a x^b y^c$ can be found, and the inner product calculated. An orthonormal basis is then constructed by the Gram–Schmidt procedure. The reason for the instability is that for large N, the basis Eq. (8.20) becomes almost degenerate, with

$$\frac{\langle \hat{\Psi}_{abc} \mid \hat{\Psi}_{a'b'c'} \rangle}{|\hat{\Psi}_{abc}|\,|\hat{\Psi}_{a'b'c'}|} \sim 1. \tag{8.21}$$

The Gram–Schmidt procedure then involves subtracting almost-equal numbers, which produces rounding error in a computer. In our case, this would propagate through the "diagonalization" and "wavefunction reconstruction" steps, to produce large errors in the sensitive part of the wavefunction that we are interested in.

The solution is to orthonormalize to a much greater (preferably infinite) precision. For values of $N \sim 200$, however, orthonormalizing the basis (8.20) to sufficient accuracy as Lüscher and Münster did for $N \sim 100$, would take an enormous amount of computer time and space, so we have taken a slightly different route, which we now describe.

We noted in the previous subsection that the angular Laplacian $\tilde{\nabla}^2$ could be

block diagonalized to give sets of degenerate eigenfuctions $P_{\alpha\beta}$ with eigenvalues $-(4\alpha+6\beta)(4\alpha+6\beta+7)$. The size of the blocks is quite small: for $q=2\alpha+3\beta\leqslant 16$ we have at most a triple degeneracy. Moreover, the $P_{\alpha\beta}$ are only two-variable polynomials, so an algebraic manipulation program can perform the orthonormalization quite readily.

We now need to take combinations of the $P_{\alpha\beta}$ with orthonormal functions of s to produce a complete basis. A conceptually simple way of doing this is to use the eigenfunctions of the nine-dimensional harmonic oscillator. Thus, replace the potential $V(c)$ in Eqs. (8.4) and (8.10) by

$$V_\omega(c_i^a)=\tfrac{1}{2}\omega^2 c_i^a c_i^a=\tfrac{1}{2}\omega^2 s. \tag{8.22}$$

The eigenvalues equation in the sector we are interested in becomes a separable one:

$$\left[-\frac{1}{2}\left(4s\frac{\partial^2}{\partial s^2}+18\frac{\partial}{\partial s}+\frac{1}{s}\tilde{\nabla}^2\right)+\frac{1}{2}\omega^2 s-E_\omega\right]\Psi^\omega(s,x,y)=0. \tag{8.23}$$

Putting

$$\Psi^\omega(s,x,y)=X_q^\omega(s)\,P_{\alpha\beta}(x,y)\qquad(q=2\alpha+3\beta) \tag{8.24}$$

therefore gives us a radial equation

$$\left(-2s\frac{\partial^2}{\partial s^2}-9\frac{\partial}{\partial s}+\frac{q(2q+7)}{s}+\frac{\omega^2}{2}s\right)X_q^\omega=E_\omega X_q^\omega, \tag{8.25}$$

the solution to which involves half-integer-order Laguerre polynomials [22]:

$$X_{n,q}^{\omega=1}(s)=\hat{N}(n,q)\,e^{-(1/2)s}s^q L_n^{2q+7/2}(s). \tag{8.26}$$

The new quantum number n is related to the eigenvalue $E_{\omega=1}$ by

$$E_{\omega=1}=2n+2q+\tfrac{9}{2}, \tag{8.27}$$

and $N(n,q)$ is chosen so that

$$\int s^4 d(\sqrt{s})\,(X_{n,q}^{\omega=1}(s))^2=1, \tag{8.28}$$

$$\hat{N}(n,q)=\left[\frac{2n!}{\Gamma(n+2q+9/2)}\right]^{1/2}. \tag{8.29}$$

For general ω,

$$E_\omega=\omega E_{\omega=1},\qquad X_{n,q}^\omega(s)=\omega^{9/4}X_{n,q}^{\omega=1}(\omega s). \tag{8.30}$$

TABLE I

Orthogonal Eigenfunctions of $\tilde{V}^2$

$$\hat{P}_{0,0} = 1$$

$$\hat{P}_{1,0} = -\frac{2}{11} + x$$

$$\hat{P}_{0,1} = \frac{4}{663} - \frac{1}{17}x + y$$

$$\hat{P}_{2,0} = \frac{8}{399} - \frac{40}{133}x - \frac{4}{7}y + x^2$$

$$\hat{P}_{1,1} = -\frac{16}{29325} + \frac{4}{345}x - \frac{144}{575}y - \frac{1}{25}x^2 - xy$$

$$\hat{P}_{0,2} = \frac{256}{8554275} - \frac{128}{150075}x + \frac{212}{6525}y + \frac{1}{261}x^2 - \frac{6}{29}xy - y^2$$

$$\hat{P}_{3,0} = -\frac{80}{44511} + \frac{760}{14837}x + \frac{4432}{14837}y - \frac{6196}{14837}x^2 - \frac{21504}{14837}xy + \frac{14914}{14837}y^2 + x^3$$

$$\hat{P}_{2,1} = \frac{32}{741675} - \frac{392}{247225}x + \frac{424}{9889}y - \frac{128}{9889}x^2 - \frac{136}{341}xy - \frac{4}{11}y^2 - \frac{1}{33}x^3 + x^2y$$

$$\hat{P}_{1,2} = -\frac{128}{58908775} + \frac{256}{2561251}x - \frac{65288}{12806255}y - \frac{414}{441595}x^2 + \frac{864}{14245}xy - \frac{334}{1295}y^2 + \frac{3}{1295}x^3 - \frac{6}{37}x^2y + xy^2$$

$$\hat{P}_{4,0} = \frac{128}{875195} - \frac{5888}{875195}x - \frac{482688}{6126365}y - \frac{119328}{1225273}x^2 - \frac{1047168}{1225273}xy - \frac{251952}{1225273}y^2 - \frac{660160}{1225273}x^3 - \frac{399960}{175039}x^2y + \frac{365952}{175039}xy^2 + x^4$$

$$\hat{P}_{0,3} = \frac{256}{1861563795} - \frac{960}{124104253}x + \frac{2256}{4279457}y + \frac{12}{138047}x^2 - \frac{1140}{138047}xy + \frac{1240}{19721}y^2 - \frac{5}{19721}x^3 + \frac{15}{533}x^2y - \frac{15}{41}xy^2 + y^3$$

$$\hat{P}_{3,1} = -\frac{1792}{588740115} + \frac{6720}{39249341}x - \frac{1047936}{196246705}y - \frac{481072}{196246705}x^2 + \frac{3344816}{39249341}xy - \frac{10576720}{39249341}y^2 + \frac{1566320}{117748023}x^3 - \frac{531400}{1060793}x^2y - \frac{1267666}{1060793}xy^2 - \frac{22416}{25873}y^3 - \frac{1}{41}x^4 + x^3y$$

$$\hat{P}_{2,2} = \frac{2048}{13801248825} - \frac{9216}{920083255}x + \frac{92224}{148400525}y + \frac{9872}{63600225}x^2 - \frac{164144}{12720045}xy - \frac{3232}{68757}y^2 - \frac{176}{206271}x^3 + \frac{376}{5289}x^2y - \frac{88}{215}xy^2 - \frac{4}{15}y^3 - \frac{1}{645}x^4 - \frac{2}{15}x^3y + x^2y^2$$

$$\hat{P}_{5,0} = -\frac{256}{22756637} + \frac{1920}{2526293}x - \frac{10240}{688989}y - \frac{1280}{75537}x^2 - \frac{874240}{3248091}xy - \frac{338080}{3248091}y^2 + \frac{141280}{885843}x^3 - \frac{6182640}{3248091}x^2y - \frac{14320}{98427}xy^2 - \frac{62096}{75537}y^3 - \frac{2149870}{3248091}x^4 - \frac{232480}{75537}x^3y - \frac{77620}{25179}x^2y^2 + x^5$$

$$N^2(0,0) = \frac{105}{32}\pi^4 \qquad N^2(1,0) = \frac{945}{64}\pi^4 \qquad N^2(0,1) = \frac{1395}{128}\pi^4$$

$$N^2(2,0) = \frac{1395}{256}\pi^4 \qquad N^2(1,1) = \frac{135135}{256}\pi^4 \qquad N^2(0,2) = \frac{2027025}{512}\pi^4$$

$$N^2(3,0) = \frac{45045}{512}\pi^4 \qquad N^2(2,1) = \frac{2027025}{1024}\pi^4 \qquad N^2(1,2) = \frac{34459425}{1024}\pi^4$$

$$N^2(4,0) = \frac{675675}{4096}\pi^4 \qquad N^2(0,3) = \frac{654729075}{2048}\pi^4 \qquad N^2(3,1) = \frac{11486475}{2048}\pi^4$$

$$N^2(2,2) = \frac{654729075}{4096}\pi^4 \qquad N^2(5,0) = \frac{2297295}{8192}\pi^4$$

If we call the orthonormalized $P_{\alpha\beta}$, "$\hat{P}_{\alpha\beta}$" then the complete set of harmonic oscillator eigenfunctions in this sector is

$$\Psi_{n\alpha\beta}(s, x, y) = X_{n,q}(s)\,\hat{P}_{\alpha\beta}(x, y). \tag{8.31}$$

The unnormalized $\hat{P}_{\alpha\beta}$ and their norms $N(\alpha, \beta)$ for $2\alpha + 3\beta \leqslant 10$ are given in Table I.

We are now in a position to evaluate the matrix elements of the Hamiltonian (8.11) exactly in this basis. We can write

$$\begin{aligned} H &= (-\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}\omega^2 s) - \tfrac{1}{2}\omega^2 s + \tfrac{1}{2}s^2 x \\ &= H_\omega - \tfrac{1}{2}\omega^2 s + \tfrac{1}{2}s^2 x, \end{aligned} \tag{8.32}$$

and it merely remains to evaluate the two kinds of matrix elements $\langle \Psi_{n\alpha\beta}|\, s\, |\Psi_{n'\alpha'\beta'}\rangle$ and $\langle \Psi_{n\alpha\beta}|\, s^2 x\, |\Psi_{n'\alpha'\beta'}\rangle$, since H_ω is diagonal in this basis, with

$$\langle \Psi_{n\alpha\beta}|\, H_\omega\, |\Psi_{n'\alpha'\beta'}\rangle = (2n + 4\alpha + 6\beta + \tfrac{9}{2})\, \omega \delta_{nn'} \delta_{\alpha\alpha'} \delta_{\beta\beta'}. \tag{8.33}$$

The quantities $\langle \alpha\beta|\, x\, |\alpha'\beta'\rangle \equiv \int d\Omega\, \hat{P}_{\alpha\beta} x \hat{P}_{\alpha'\beta'}$ can be calculated exactly because the $\hat{P}_{\alpha\beta}$ are polynomials in x and y, and we know $\int d\Omega\, x^i y^j = \mathscr{I}_{ij}$. Moreover, by using the generating function for Laguerre polynomials, one can calculate

$$\begin{aligned}\langle n, q|\, s\, |n', q'\rangle &\equiv \int s^4 d\sqrt{s}\, X_{n,q}(s)\, s X_{n',q'}(s) \\ &= (2n + 2q + \tfrac{9}{2})\, \delta_{nn'} - \sqrt{n+1}\, \sqrt{n + 2q + \tfrac{9}{2}}\, \delta_{n,n'-1} \\ &\quad - \sqrt{n}\, \sqrt{n + 2q + \tfrac{7}{2}}\, \delta_{n,n'+1},\end{aligned} \tag{8.34}$$

and

$$\begin{aligned}\langle n, q|\, s^2\, |n', q'\rangle &\equiv \int s^4 d(\sqrt{s})\, X_{n,q}(s)\, s^2 X_{n',q'}(s) \\ &= \frac{\sqrt{\pi}}{2^{q+q'+6}} (-1)^{n+n'} \\ &\quad \times \sum_{t=t_{\min}}^{t=t_{\max}} \binom{q'-q+2}{n-t} \binom{m-m'+2}{n'-t} \frac{(2(t+q+q')+11)!!}{2^t t!},\end{aligned} \tag{8.35}$$

where $t_{\max} = \min(n, n')$ and $t_{\min} = \max(n - q' + q - 2,\ n' - m + m' - 2, 0)$. The obvious requirement $t_{\min} \leqslant t_{\max}$ then implies the matrix elements are zero unless

$$-2 - q + q' \leqslant n' - n \leqslant 2 - q + q', \tag{8.36}$$

and the sum in Eq. (8.35) runs over at most 5 values of t. Equations (8.33) – (8.35) are sufficient to evaluate all matrix elements $\langle n\alpha\beta|\, H\, |n'\alpha'\beta'\rangle$ exactly. Reinstating the ω dependence gives

$$\begin{aligned}\langle n\alpha\beta|\, H\, |n'\alpha'\beta'\rangle &= \delta_{nn'} \delta_{\alpha\alpha'} \delta_{\beta\beta'} E_\omega - \tfrac{1}{2}\omega \delta_{\alpha\alpha'} \delta_{\beta\beta'} \langle nq|\, s\, |n'q'\rangle \\ &\quad + \frac{1}{2\omega^2} \langle nq|\, s^2\, |n'q'\rangle \langle \alpha\beta|\, x\, |\alpha'\beta'\rangle.\end{aligned} \tag{8.37}$$

One needs to decide on an order for the $|n\alpha\beta\rangle$. We order first by lowest $n + 2\alpha + 3\beta$, then by lowest n, then by lowest α. This choice can be understood as an ordering in increasing powers of the variables s, x, y: $|n\alpha\beta\rangle \sim e^{-(1/2)s} s^{n+2\alpha+3\beta} x^\alpha y^\beta$. In our calculation we have chosen the bound $n + 2\alpha + 3\beta \leqslant 16$, which allows 204 orthonormal basis vectors. Increasing the bound to say 17 would only increase this to 237, and not change the result significantly.

8.4. *The Wavefunction in the Barrier Region*

Once a suitable basis is chosen, the Rayleigh–Ritz algorithm can be applied, using readily available computer programs for matrix diagonalization. We list here the various steps in our calculation. The algebraic manipulation was done using the program SMP [28], and floating point calculations used routines in the IMSL library.

(1) The angular eigenfunctions $P_{\alpha\beta}$ for $q = 2\alpha + 3\beta \leqslant 16$ were found by explicitly solving Eq. (8.16) with the ansatz Eq. (8.15). The result was a set of polynomials in (x, y) with rational coefficients.

(2) The integrals $\int d\Omega\, x^i y^j = \mathcal{I}_{ij}$ were calculated exactly from the recursion relation Eq. (8.18), and the initial condition Eq. (8.19). We need all $\mathcal{I}_{ij}$ for $2i + 3j \leqslant 34$.

(3) In each subspace of fixed $q = 2\alpha + 3\beta$, the Gram–Schmidt orthonormalization procedure was applied to the functions $P_{\alpha\beta}$. Because the degeneracy was at most triple ($q = 12, 14, 15, 16$), it was feasible to do this exactly using algebraic manipulation. The lowest order orthogonal $\hat{P}_{\alpha\beta}$ and the squares of their norms are given in Table I. Note that after orthogonalization, there is no significance to how we label the degenerate $\hat{P}_{\alpha\beta}$ for a given $2\alpha + 3\beta$.

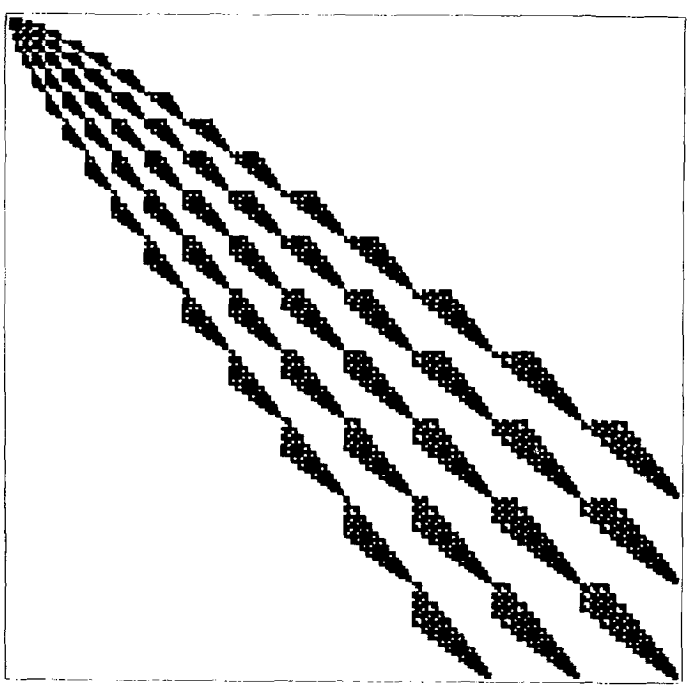


FIG. 4. Non-zero matrix elements $\langle n\alpha\beta | xs^2 | n'\alpha'\beta' \rangle$ are shown as black squares. The 204 vectors $|n\alpha\beta\rangle$ are canonically ordered as described in the text. The large scale structure can be understood from the derivation in the text, but the many zeros within the black "islands" are a mystery.

(4) The Laguerre polynomials $L_n^{2q+7/2}(s)$ were constructed for $n+q \leqslant 16$, using their explicit definition [22].

(5) The reduced matrix elements $\langle \alpha\beta | x | \alpha'\beta' \rangle$, $\langle nq | s | n'q' \rangle$, and $\langle nq | s^2 | n'q' \rangle$ were evaluated. Many of these are zero, so only those expected to be non-zero were calculated.

(6) The full matrix elements $\langle n\alpha\beta | s^2 x | n'\alpha'\beta' \rangle$ were formed. In Fig. 4 we have plotted the positions of all non-zero elements as black squares, where the vectors are ordered canonically.

(7) The matrix elements were converted to 64-bit floating-point numbers and stored.

(8) The wave functions $\Psi_{n\alpha\beta}$ were calculated, and the coefficients in the polynomial part (i.e., in $e^{s/2}\Psi_{n\alpha\beta}$) were converted to floating point and stored.

(9) A program using IMSL routines (and written in the language C) read in the matrix elements and wavefunction coefficients.

(10) For any given ω, and number of basis vectors N, the Hamiltonian was constructed and the lowest eigenvalues and eigenvectors found. (Figure 5 is a plot of the groundstate wavefunction.)

(11) Using the basis wavefunction coefficients from step (8), the eigenvectors were converted to polynomial functions of (s, x, y) with floating-point coefficients.

(12) The value of B was extracted from the wavefunction in various ways, as will be described later in this section.

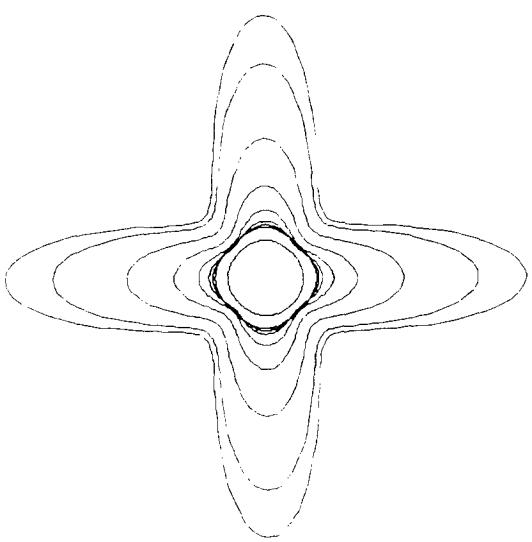


FIG. 5. Plot showing the single-well wavefuction $\Psi_0^{[0]}(x_1, x_2, x_3)$. We have taken a spherical coordinate system for (x_1, x_2, x_3) and plotted the probability per unit solid angle as a function of φ, for θ in steps of 10°. The outermost contour is $\theta = 90°$. It is instructive to compare with the three-dimensional plots of the energy surface in [12].

The total amount of computer time exceeded 50 h on a Ridge 32 (comparable in speed to a VAX 11/780). To insure reliability of our results, we made the following consistency checks at each stage:

(1) Each $P_{\alpha\beta}$ satisfies Eq. (8.16) identically.

(2) $\int d\Omega\, P_{\alpha\beta}=0$ if $\alpha\neq 0$ or $\beta\neq 0$ checks the $\mathcal{X}_{ij}$, as does $\int P_{\alpha\beta}P_{\alpha'\beta'}=0$ if $2\alpha+3\beta\neq 2\alpha'+3\beta'$.

(3) The 30 $\hat{P}_{\alpha\beta}$ are orthogonal after application of the Gram-Schmidt procedure.

(4) All Laguerre polynomials satisfy the defining equations identically.

(5) $xs^2\,|n\alpha\beta\rangle=\sum_{n'\alpha'\beta'}|n'\alpha'\beta'\rangle\langle n'\alpha'\beta'|\,xs^2\,|n\alpha\beta\rangle$ checks the accuracy of the matrix elements. This test is limited to the first ~ 140 vectors, because beyond that point matrix elements involving vectors outside the set of 204 that we work with are required for the completeness relation (see Fig. 4).

(6) Converting to floating point at earlier points in the calculation produces consistent results.

(7) Results scale correctly with ω, and accuracy improves with increasing N.

We therefore believe our result is trustworthy.

One finds that the results are fairly insensitive to the value of ω if $\omega\sim 1.5$–1.6. Any ω in this range gives results consistent with the error bars we quote.

We must now compare the asymptotic form of the Rayleigh–Ritz eigenfunction with the predicted asymptotic form. We are interested in the properties of the eigenfunction along the vacuum valley, which is the direction $x=y=0$. However, we will find it convenient to work for a while in the polar decomposition variables (x_1, x_2, x_3) of Eqs. (8.6) and (8.7), where the vacuum valley is along $x_1=x_2=0$.

Recall that in Section 6 we derived the following "adiabatic decomposition" of a spherically symmetric wavefunction

$$\Psi(x_1, x_2, x_3)=[(x_3^2-x_1^2)(x_3^2-x_2^2)]^{1/2}\sum_{n=1}^{\infty}\Phi^{(n)}(x_3)\,\chi^{(n)}_{[x_3]}(x_1, x_2), \qquad (8.38)$$

where here $\Phi^{(n)}(|\mathbf{C}|)=|\mathbf{C}|\,\varphi^{(n)}(\mathbf{C})$ of Section 6. This expression is useful because the $\Phi^{(n)}$ are known to be exponentially decaying functions of x_3. As was shown in some detail for the toy models in [14], the asymptotic form of the wavefunction for large x_3 is given by the $n=1$ term. The $\chi^{(n)}_{[x_3]}$ are otrhonormal eigenfunctions of a Hamiltonian in which x_3 is regarded as an adiabatic parameter.

Now the forms of $\Phi^{(1)}$ and $\chi^{(1)}_{[x_3]}$ are both known for large x_3. $\chi^{(1)}_{[x_3]}$ is known to be normalized for any value of the "parameter" x_3, but what is not known, and what this whole section is trying to find, is the normalization of $\Phi^{(1)}$. From Eq. (5.34), we have to first order in $1/x_3^3$,

$$\chi^{(1)}_{[x_3]}=\frac{1}{\sqrt{2}}x_3\left(1-\frac{[2x_1^2x_2^2x_3^2+x_3(x_1^2+x_2^2)-3]}{16x_3^3}\right)e^{-x_3(x_1^2+x_2^2)/2}. \qquad (8.39)$$

Here we adopt the simpler normalization conventions of [5], which differ by a factor of $\sqrt{2\pi}$ in $\chi^{(1)}_{[x_3]}$ and Ψ (because we drop ξ in the measure for the spherical sector). Thus $\chi^{(1)}_{[x_3]}(x_1, x_2) = \sqrt{2\pi}\, \chi^{(1)}_{[x_3]}(x_1, x_2, \xi)$ and $\Psi(x_1, x_2, x_3) = \sqrt{2\pi}\, \Psi^{[0]}_0(x_1, x_2, x_3)$. Let ε be the true energy eigenvalue of $\Psi(x_1, x_2, x_3)$. Then, as shown in Section 6 and [5], $\Phi^{(1)}$ is known to satisfy

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x_3^2} + 2x_3 - \frac{1}{2x_3^2} + O(x_3^{-5}) \right) \Phi^{(1)}(x_3) = \varepsilon \Phi^{(1)}(x_3). \tag{8.40}$$

This equation determines the asymptotic behaviour of $\Phi^{(1)}(x_3)$. If for convenience we relable $x_3 = r$, then we find from Eq. (6.12)

$$\Phi^{(1)}(r) \to B(4r - 2\varepsilon)^{-1/4} \exp\left(-\frac{(4r - 2\varepsilon)^{3/2}}{6} \right) \quad \text{as} \quad r \to \infty \tag{8.41}$$

(where only the lowest order term $(2x_3)$ in Eq. (8.40) has been used so far). This is the *definition* of B. The simplest way, therefore, to extract B from the wavefunction $\Psi(x_1, x_2, x_3)$ is to take the limit of (cf. Eq. (7.32))

$$B(r) = (4r - 2\varepsilon)^{1/4} \exp\left(\frac{(4r - 2\varepsilon)^{3/2}}{6} \right) \frac{\Psi(r, 0, 0)}{r^2 \chi^{(1)}_{[r]}(0, 0)} \tag{8.42}$$

as $r \to \infty$.

It turns out, though, that this approach is too simplistic. In Fig. 6, we plot the function on the right of Eq. (8.42), for the lowest energy wave function Ψ, calculated using $\omega = 1.5$ and $N = 204$ in the Rayleigh–Ritz program. It obviously does not have a non-zero limit as $r \to \infty$, but we cannot expect it to have a meaningful limit: all our basis functions are polynomials times $e^{-\omega r^2/2}$, and a finite sum of such terms can never accurately reproduce the different exponential behaviour of Eq. (8.41). Thus there is a limitation on the Rayleigh–Ritz method's ability to reproduce asymptotic behaviour correctly. The problem therefore is to extract B without taking the limit in Eq. (8.42).

Suppose, therefore, that we look at $B(r)$ for some finite value of r, where the Rayleigh–Ritz wave function is accurate (say $r \leqslant r_{\max}$). $B(r)$ may not be constant for $r < r_{\max}$, for two reasons. First, $\Phi^{(1)}(r)$ may not yet have attained its asymptotic form, Eq. (8.41). Second, for finite r, terms involving $\Phi^{(2)}$, $\Phi^{(3)}$, etc. are still contributing to the wavefunction Ψ, by Eq. (8.38). Nevertheless, we do expect $B(r)$ to be approximately constant for r large enough, where these effects are small, say in a region $r_{\min} \leqslant r \leqslant r_{\max}$. Clearly, $r_{\min}$ is intrinsic to our problem, but $r_{\max}$ depends on how many basis vectors we use in the Rayleigh–Ritz calculation. Looking at Fig. 6 shows that $r_{\max} \sim 6$, and since the plateau in $B(r)$ is not very flat, we deduce that the asymptotic form of Ψ has not been attained very accurately yet. This uncertainty in the precise height of the plateau is the dominant contribution to our error in the determination of B.

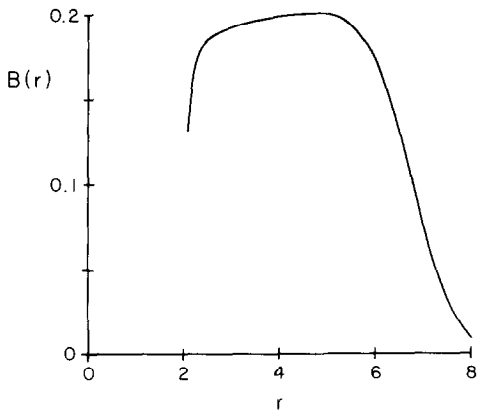


FIG. 6. $B(r)$ extracted from the wavefunction using the naive definition Eq. (8.42). There is no flat plateau.

The fact that the plateau in Fig. 6 has a definite slope suggests that a systematic correction could be made to improve our accuracy. We have found two ways to do this. First, one can find the leading correction to the asymptotic form of $\Phi^{(1)}(r)$, and divide that into $B(r)$. Second, one can use the orthogonality of the $\chi^{(n)}_{[r]}(x_1, x_2)$ for different n to project out the $\Phi^{(1)}$ contribution to Ψ in Eq. (8.38).

For the correction to the asymptotic form of $\Phi^{(1)}(r)$, we just use Eq. (8.40), but now with the $-1/2x_3^2$ term included. (Note that this is an $O(r^{-3})$ correction relative to the $2x_3$ term.) In practice, we made the ansatz

$$\Phi(r) = Bf(r)(4r-2\varepsilon)^{-1/4}\exp\left(-\frac{(4r-2\varepsilon)^{3/2}}{6}\right),$$
$$f(\infty)=1, \tag{8.43}$$

and numerically integrated Eq. (8.40) back from $r\sim 100$ to get $f(r)$. The integration is stable all the way down to $r\sim 2.1$.

Projection with the $\chi^{(1)}_{[r]}$ term also has to be carried out to order r^{-3}, and for this we use Eq. (8.39). Taking into account the normalization of the $\chi^{(n)}_{[x_3]}$, we can thus project out $\Phi^{(1)}$ from Eq. (8.38) (cf. Eq. (6.8) and [5, Eq. (23)] with $N=\pi^{-3/2}$):

$$\Phi^{(1)}(x_3) = \int_{-x_3}^{x_3} dx_1 \int_{-x_3}^{x_3} dx_2\, |x_1^2 - x_2^2|\, [(x_3^2-x_1^2)(x_3^2-x_2^2)]^{1/2}$$
$$\times\ \Psi(x_1, x_2, x_3)\, \chi^{(1)}_{[x_3]}(x_1, x_2). \tag{8.44}$$

In Fig. 7 we have plotted two curves. The curve labeled (I) is $B(r)$ improved by both methods. That labeled (II) is just the $B(r)$ of Fig. 6 divided by $f(r)$ of Eq. (8.43), i.e., $B(r)$ improved only by the first method.

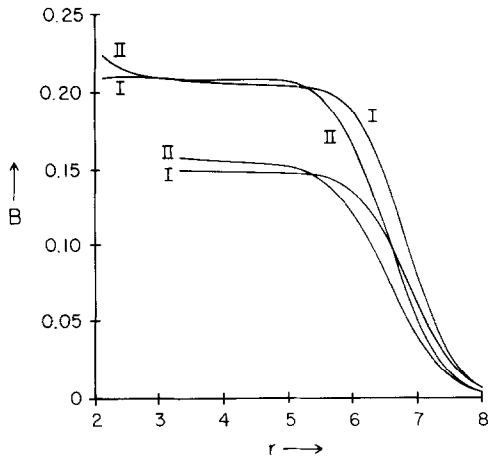


FIG. 7. Improved $B(r)$ for the ground state (upper two curves) and 0^+ state (lower two curves). Curves labelled I are improved by both methods discussed in the text. Those labeled II have been improved only by the first method.

We have included in the computer program code to use either or both of these methods, and have examined results for various numbers of basis vectors and values of ω. Some of these curves $B(r)$ are shown in Fig. 8. We calculated the integral in Eq. (8.44) by expanding the square root to the appropriate order in x_3^{-3}. The type (I) curves were obtained by integrating this correction explicitly. The curves merging into the middle curve of Fig. 8 were instead obtained by approximating the square root by its weighted average (i.e., the right hand side of (8.44) with Ψ replaced by $\chi^{(1)}_{[x_3]}$). In general, the curves coincide between $r \sim 2.9$ and $r \sim 3.5$, and

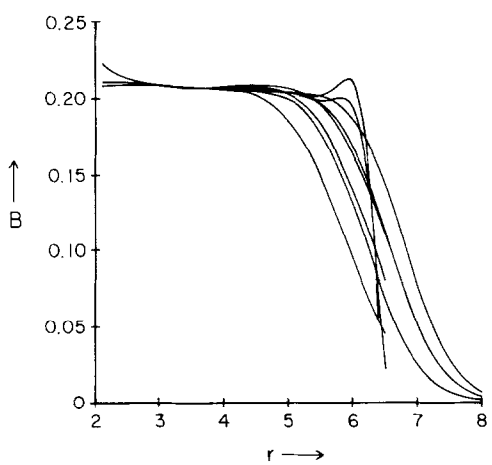


FIG. 8. $B(r)$ for the ground state, for a variety of values of N ($100 \leqslant N \leqslant 204$) and ω ($1.5 \leqslant \omega \leqslant 1.6$), showing that curves overlap between $r = 2.9$ and $r = 3.5$.

differ slightly for larger r. It is clear that the Rayleigh–Ritz wavefunction is inaccurate beyond $r \sim 5$, whereas for $r \leqslant 2.9$ curves only coincide within each class of corrections, showing that for small x_3, $\Phi^{(n)}(x_3)$ $(n>1)$ gives a significant contribution to Ψ. We thus measure B between $r=2.9$ and $r=3.5$.

From the curves in Fig. 7, we can thus extract the following values for the lowest energy state and the first excited state:

$$\begin{aligned} (1) \quad & \varepsilon = 4.116719735 \pm 1 \times 10^{-9} \\ & B = 0.2063 \pm 8 \cdot 10^{-4} \end{aligned} \tag{8.45}$$

$$\begin{aligned} (2) \quad & \varepsilon' = 6.3863588 \pm 1 \times 10^{-7} \\ & B' = 0.1480 \pm 8 \cdot 10^{-4}. \end{aligned} \tag{8.46}$$

The energies were obtained directly from the Rayleigh–Ritz calculation. The errors in ε are estimated from the variation in ε as the number of basis vectors is changed, and the error in B is the uncertainty in the height of the plateau between $r=2.9$ and $r=3.5$. For the first excited state, correcting by just the first method is inadequate for any value of r, because a much larger fraction of the wavefunction is contained in $\Phi^{(n)}$ $(n>1)$; therefore we *must* project out the $\Phi^{(1)}$ term first, via Eq. (8.44).

In summary, we saw that the Rayleigh–Ritz method became inaccurate before we reached the asymptotic region, but by including corrections we could understand the wavefunction in the non-asymptotic region, and still determine the constant B. It was nevertheless imperative that we used at least 200 basis vectors.

8.5. *Calculation of* λ

In Section 7, we defined the constant λ through the stability equation

$$\lambda^{-1} = \lim_{d \to 0} \frac{d^{3/2}}{\pi} [dq'_d(2\pi - d) + q_d(2\pi - d)], \tag{8.47}$$

where $q_d(s)$ satisfies the differential equation

$$W(s)(W(s)\, q'_d(s))' = q_d(s)\, U(s), \tag{8.48}$$

$$q_d(d) = 1, \qquad q'_d(d) = \frac{1}{d}. \tag{8.49}$$

U and W are known functions of s, given by Eqs. (7.28), (A.18), and (A.30).

The only difficulty in evaluating λ is that $q_d(2\pi - d)$ diverges as $d \to 0$. We have numerically integrated Eq. (8.48) from d to $2\pi - d$ for various values of d, using a fourth-order Runge–Kutta algorithm. We plot the results for $\lambda(d)$ in Fig. 9. The limit $d \to 0$ is now easily obtained by extrapolation or, equivalently, by linear regression. Thus we find

$$\lambda = 0.69970 \pm 0.00001. \tag{8.50}$$

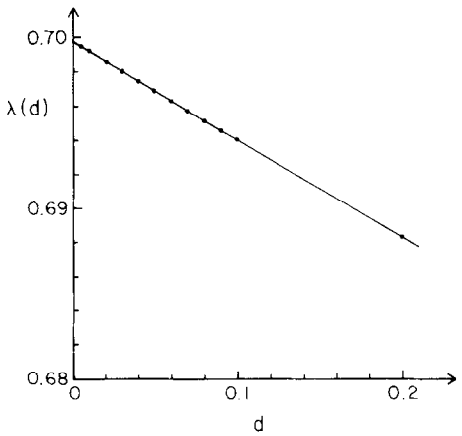


FIG. 9. Evaluation of the constant $\lambda = \lim_{d \to 0} \lambda(d) = 0.69970 \pm 0.00001$. Because it is defined as the difference of two divergent functions, $\lambda(0)$ cannot be evaluated directly. Points marked were evaluated using numerical integration.

Inserting the values for λ, ε, and B into Eq. (8.1) thus gives the final answer for ΔE for the two states we have considered [5]:

$$(1) \qquad \varepsilon = 4.116719735 \pm 1 \times 10^{-9}$$

$$\Delta E = 0.05956 g^{5/3} L^{-1} \exp(-12.4637 g^{-1} + 16.132 g^{-1/3}) \tag{8.51}$$

$$(2) \qquad \varepsilon = 6.3863588 \pm 1 \times 10^{-7}$$

$$\Delta E = 0.03065 g^{5/3} L^{-1} \exp(-12.4637 g^{-1} + 25.026 g^{1/3}). \tag{8.52}$$

These are the semi-classical expressions for the tunneling energy splits. In the next section we will discuss these results, but for a more complete discussion of the physics involved, we refer the reader to [5], where we used them without a detailed derivation.

9. Discussion and Conclusion

The expression for the energy of electric flux in terms of L and $g(L)$ in general depends on the renormalization scheme used, although to the order displayed in Eq. (8.51) it is actually scheme independent. To compare analytic and numerical calculations it is convenient to derive an expression in terms of scheme-independent parameters. Pure QCD in a box has only two free parameters: the box size L, and a mass scale Λ. Thus the theory is completely fixed by specifying some energy (say the mass of the 0^+ glueball, $M_L(0^+)$), plus the box size in those units:

$z = L \cdot M_L(0^+)$. There are of course other choices of parameterization, but this is the one used by Lüscher [4], and we adopt it here. Note that our definitions in no way require $M_L(0^+)$ to be the mass gap (i.e., the *lowest* mass state). In perturbation theory, z has been calculated by Lüscher and Münster [13]:

$$z = 2.2696390 \cdot g^{2/3} - 0.7975278 \cdot g^{4/3} + O(g^2) \tag{9.1}$$

If we now eliminate g from our expressions in favour of z, and express all energies in units of $M_L(0^+)$, we obtain physical, renormalization-scheme-independent functions. Not only are these functions physically meaningful, but, as emphasized in previous work [5], we expect these functions of z to have a smoother behaviour than functions of g as we go from small to large box size, for the following reason. As L gets large, $g(L)$ gets large, and higher order terms in the β-function start to affect the behaviour of g. Therefore g can vary rapidly, and its behaviour is highly renormalization-scheme-dependent. Thus any physical quantity, expressed as a function of g or L, could acquire a complicated behaviour just to compensate for this irregular g behaviour.

Rewriting Eq. (8.51) in terms of the renormalization-scheme-independent parameters gives

$$\mathscr{E}(z) \equiv \frac{\Delta E}{M_L(0^+)} = 0.00767 \cdot z^{3/2} \cdot \exp(-42.6169 \cdot z^{-3/2} + 34.2001 \cdot z^{-1/2}). \tag{9.2}$$

We have discussed the implications of this result in detail in another paper [5]. Note that $\mathscr{E}(z)$ increases suddenly by several orders of magnitude at $z \sim 1.2$. Thus for $z < 1.2$, the energy of electric flux is exponentially small, because the box is so small that all interactions are weak. However, as we increase the size of the box, stronger interactions can take place, and tunneling between the degenerate vacua occurs. The effect of tunneling becomes sizeable at around $z \simeq 1.2$. For boxes with $z \geqslant 1.2$, the degeneracy between states with different electric flux is lifted completely. We wish to emphasize, however, that this transition is smooth, and is thus *not* a phase transition. In particular, it should not be confused with the deconfining phase transition in finite-temperature QCD. It is a smooth but rapid transition associated with the restoration of the Z_2 symmetry of the vacuum.

Because $\mathscr{E}(z)$ is a physical function, it is possible to relate our results to those obtained in other ways, such as from Monte Carlo calculations on a lattice. In particular, by taking recent Monte Carlo results [6, 7], and assuming that they are in a region where lattice artifacts are small, we can obtain an estimate of $\mathscr{E}(z)$ for $z \geqslant 1.5$ [5]. On the other hand, from the discussion in the previous paragraph, it is clear that our analytic result is valid for z values up to about 1.2. At that point, where the tunneling becomes important, the assumptions inherent in our semiclassical approximation break down. Taking our analytic result and the Monte Carlo data together thus provides a description of $\mathscr{E}(z)$ over an almost continuous

range, from $z=0$ to $z\sim 8$, and the remarkably simple picture which emerges is described in [5]. The dominant feature in $\mathscr{E}(z)$ appears to be the onset of the tunneling that we have just calculated, and *no other rapid transitions seem to occur.* We also noted in [5] that string formation appears to set in around $z=5$, so that only beyond $z=5$ will $\mathscr{E}(z)$ approach its asymptotic value. There could be variables which are more sensitive to an expected transition around $z=5$, such as the expectation value of the absolute value of spatial Polyakov loop in the fundamental representation. For a further discussion of this important issue, see [29].

It is our conjecture that we will be able to calculate $\mathscr{E}(z)$ for z values up to ~ 2 by going beyond the semiclassical approximation. This would completely bridge the gap between our present analytic calculation and the Monte Carlo data, and even provide some overlap, which would be a very significant advance.

Instead of repeating discussions contained in [5], we will conclude by describing in this article a classic textbook tunneling example (see, e.g., [31]), the double harmonic oscillator. The Hamiltonian is given by

$$H=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}|x^2-a^2|. \tag{9.3}$$

Here, the quantity analogous to the electric flux is the energy difference between the even and odd ground states Δv; the first excited state in the even sector, with energy v_1 above the ground state, is analogous to the 0^+ glueball in QCD. The parameter a is adjustable: when $a\gg 1$ the wells are far apart and tunneling is suppressed, but as a decreases, the tunneling sets in. Thus $1/a$ is analogous to L. In Fig. 10 we plot $\mathscr{E}(z)=\Delta v/v_1$ vs. $z=v_1(a)/(\sqrt{2}\,a)$ for this simple model, using data from the exact solution of [31]. The reader is invited to compare Fig. 10 with Fig. 2 of [5], the energy of electric flux for $SU(2)$ QCD on the hypertorus. If we could show that Fig. 2 of [5] is asymptotically linear while Fig. 10 is asymptotically constant, we would be explaining confinement.

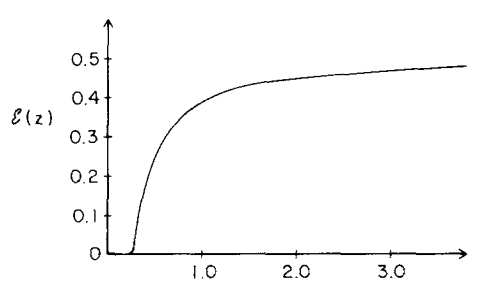


FIG. 10. The analog of $\mathscr{E}(z)$ for the double harmonic oscillator. This should be compared with Fig. 2a of [5].

APPENDIX A

In this appendix we will derive some of the properties of the one-loop effective potential $V_1(\mathbf{C})$. Here we will put $L \equiv 1$ and hence study

$$V_1(\mathbf{C}) = \frac{4}{\pi^2} \sum_{\mathbf{n} \neq 0} \frac{\sin^2(\mathbf{n} \cdot \mathbf{C}/2)}{(\mathbf{n}^2)^2}. \tag{A.1}$$

We will first discuss the use of lattice sums [21] to express $V_1(\mathbf{C})$ in rapidly converging sums, valid for all $\mathbf{C}$. After that we construct more efficient expressions when restricting (A.1) to one of the coordinate axes. Finally the extremal properties of $V_1(\mathbf{C})$ are discussed.

The lattice sum technique is based on splitting $\sum f(\mathbf{n})$ into $\sum f(\mathbf{n}) g(\mathbf{n})$ and $\sum f(\mathbf{n})(1 - g(\mathbf{n}))$. Here $g(\mathbf{n})$ is a rapidly decreasing auxiliary function such that $f(\mathbf{x})(1 - g(\mathbf{x}))$ behaves very smoothly for $|\mathbf{x}| \to 0$. So if $f(\mathbf{n})$ is some more slowly decreasing series, $f(\mathbf{n}) g(\mathbf{n})$ becomes rapidly decreasing, whereas the second part behaves similarly after Poisson resummation. One obtains the result [21]

$$\begin{aligned}
&\sum_{\mathbf{n} \neq 0} \frac{e^{2\pi i \mathbf{X} \cdot \mathbf{r}(\mathbf{n})}}{|\mathbf{r}(\mathbf{n}) - \mathbf{R}|^{2p}} \\
&\quad = \frac{1}{\Gamma(p)} \left\{ \sum_{\mathbf{n} \neq 0} \frac{\Gamma(p, \pi |\mathbf{r}(\mathbf{n}) - \mathbf{R}|^2)}{|\mathbf{r}(\mathbf{n}) - \mathbf{R}|^{2p}} e^{2\pi i \mathbf{X} \cdot \mathbf{r}(\mathbf{n})} - \frac{\gamma(p, \pi \mathbf{R}^2)}{\mathbf{R}^{2p}} \right. \\
&\qquad \left. + \frac{\pi^{2p - 3/2}}{V_a} \sum_{\mathbf{n}} |\mathbf{x}(\mathbf{n}) - \mathbf{X}|^{2p - 3} \Gamma\left(\frac{3}{2} - p, \pi |\mathbf{x}(\mathbf{n}) - \mathbf{X}|^2\right) e^{2\pi i (\mathbf{x}(\mathbf{n}) - \mathbf{X}) \cdot \mathbf{R}} \right\},
\end{aligned} \tag{A.2}$$

with $\mathbf{r}(\mathbf{n})$ running over the lattice spanned by $\mathbf{a}_i$, $\mathbf{x}(\mathbf{n})$ running over the dual lattice, $\gamma(p, x)$ and $\Gamma(p, x)$ the incomplete gamma function [22, p. 260]:

$$\begin{aligned}
&\mathbf{r}(\mathbf{n}) = \sum n_i \mathbf{a}_i, \qquad \mathbf{x}(\mathbf{n}) = \sum n_i \mathbf{b}_i, \\
&\mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij}, \qquad V_a = \mathbf{a}_1 \cdot (\mathbf{a}_2 \wedge \mathbf{a}_3),
\end{aligned} \tag{A.4}$$

$$\begin{aligned}
\Gamma(p, x) &= \int_x^\infty e^{-t} t^{p-1} \, dt, \\
\gamma(p, x) &= \Gamma(p) - \Gamma(p, x).
\end{aligned} \tag{A.5}$$

To compute $V_1(\mathbf{C})$ we take the limit $\mathbf{R} \to 0$, $\mathbf{X} = \mathbf{C}/2\pi$, $\mathbf{a}_i = \mathbf{b}_i = \mathbf{e}^{(i)}$ (hence $V_a = 1$) and substitute $p = 2$:

$$\begin{aligned}
V_1(\mathbf{C}) = 4 &\sum_{\mathbf{n} \neq 0} \left[\frac{1 + \pi \mathbf{n}^2}{(\pi \mathbf{n}^2)^2} + 2 \right] e^{-\pi \mathbf{n}^2} \sin^2(\mathbf{n} \cdot \mathbf{C}/2) \\
&- 4\pi \sum_{\mathbf{n}} \left[|\mathbf{n}| \operatorname{erfc}(\sqrt{\pi} |\mathbf{n}|) - |\mathbf{n} - \mathbf{C}/2\pi| \operatorname{erfc}(\sqrt{\pi} (|\mathbf{n} - \mathbf{C}/2\pi|)) \right],
\end{aligned} \tag{A.6}$$

with

$$\operatorname{erfc}(x)=\frac{1}{\sqrt{\pi}}\Gamma(\tfrac{1}{2},x^2)=\frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}\,dt. \tag{A.7}$$

In going from (A.2) to (A.6) we applied the Poisson resummation formula:

$$\sum_{\mathbf{n}}\left[e^{-\pi\mathbf{n}^2}-e^{-\pi(\mathbf{n}-\mathbf{C}/2\pi)^2}\right]=2\sum_{\mathbf{n}\neq\mathbf{0}}\sin^2\left(\frac{\mathbf{n}\cdot\mathbf{C}}{2}\right)e^{-\pi\mathbf{n}^2}. \tag{A.8}$$

Similarly we compute the Laplacian of the one-loop effective potential

$$\Delta V_1(\mathbf{C})=\frac{2}{\pi^2}\sum_{\mathbf{n}\neq\mathbf{0}}\frac{\cos(\mathbf{n}\cdot\mathbf{C})}{\mathbf{n}^2}, \tag{A.9}$$

in which case we substitute $p=1$ in Eq. (A.2),

$$\Delta V_1(\mathbf{C})=\frac{2}{\pi}\left[-1+\sum_{\mathbf{n}\neq\mathbf{0}}\frac{e^{-\pi\mathbf{n}^2}}{\pi\mathbf{n}^2}\cos(\mathbf{n}\cdot\mathbf{C})+\sum_{\mathbf{n}}\frac{\operatorname{erfc}(\sqrt{\pi}\,|\mathbf{n}-\mathbf{C}/2\pi|)}{|\mathbf{n}-\mathbf{C}/2\pi|}\right], \tag{A.10}$$

or we can apply the Laplacian directly to Eq. (A.6).

A special role is played by the restriction of $V_1(\mathbf{C})$ and $\Delta V_1(\mathbf{C})$ to $C_2=C_3=0$, for which (A.6) and (A.10) are a bit clumsy. We can write ($\mathbf{C}=C\mathbf{e}^{(1)}$):

$$V_1(\mathbf{C})=\frac{4}{\pi^2}\sum_{n=1}^{\infty}b_n\sin^2(nC/2), \tag{A.11}$$

$$b_n=\sum_{\mathbf{k}\in Z^2}\frac{2}{(\mathbf{k}^2+n^2)^2}. \tag{A.12}$$

To compute b_n we note that

$$g_n(\mathbf{y})=\sum_{\mathbf{k}\in Z^2}\frac{e^{i\mathbf{y}\cdot\mathbf{k}}}{n^2+\mathbf{k}^2} \tag{A.13}$$

satisfies the equation

$$\left[-\frac{\partial^2}{\partial y^2}+n^2\right]g_n(\mathbf{y})=(2\pi)^2\sum_{\mathbf{k}}\delta(\mathbf{y}-2\pi\mathbf{k}), \tag{A.14}$$

which is solved by the modified Bessel function [22, p. 374],

$$g_n(\mathbf{y})=2\pi\sum_{\mathbf{k}}K_0(n\,|\mathbf{y}-2\pi\mathbf{k}|), \tag{A.15}$$

and we find

$$b_n = \lim_{\mathbf{y}\to 0} -\frac{1}{n}\frac{d}{dn} g_n(\mathbf{y}) = \frac{2\pi}{n^2} + \frac{(2\pi)^2}{n} \sum_{\mathbf{k}\neq \mathbf{0}} |\mathbf{k}|\, K_1(2\pi n\, |\mathbf{k}|). \tag{A.16}$$

We can exactly calculate the slowly converging part

$$\sum_{n=1}^{\infty} \frac{2\pi}{n^2} \sin^2(nC/2) = \pi C(2\pi - C)/4, \qquad C \in [0, 2\pi], \tag{A.17}$$

periodically extended outside the interval $[0, 2\pi]$ ($\partial^2/\partial C^2$ of the left- and right-hand sides of (A.17) are identical). Hence

$$V_1(C\mathbf{e}^{(1)}) = \frac{C(2\pi - C)}{\pi} + \frac{8}{\pi} \sum_{n=1}^{\infty} a_n \sin^2(nC/2), \tag{A.18}$$

$$a_n = \frac{2\pi}{n} \sum_{\mathbf{k}\neq \mathbf{0}} |\mathbf{k}|\, K_1(2\pi n\, |\mathbf{k}|). \tag{A.19}$$

The a_n form a very rapidly decreasing series, and one easily shows that $a_n < 5\pi^2 n^{-1} e^{-2\pi n}$. The values of the first four a_n are

$$\begin{aligned} a_1 &= 2.7052746... \times 10^{-2} \\ a_2 &= 1.6048745... \times 10^{-5} \\ a_3 &= 1.6065690... \times 10^{-8} \\ a_4 &= 1.9385627... \times 10^{-11}. \end{aligned} \tag{A.20}$$

Similar arguments show that we can write ($\mathbf{C} = (C, y_1, y_2)$):

$$\Delta V_1(\mathbf{C}) = \frac{8}{\pi} \sum_{n=1}^{\infty} c_n \cos(nC) + \frac{8}{\pi} \sum_{n=1}^{\infty} \cos(nC)\, K_0(2\pi n\, |\mathbf{y}|) + \frac{2}{\pi} \sum_{\mathbf{k}\neq \mathbf{0}} \frac{e^{i\mathbf{k}\cdot\mathbf{y}}}{\mathbf{k}^2}, \tag{A.21}$$

$$c_n = \sum_{\mathbf{k}\neq \mathbf{0}} K_0(2\pi n\, |\mathbf{k}|). \tag{A.22}$$

Now the limit $\mathbf{y}\to\mathbf{0}$ is not easily taken because of logarithmic singularities. However, for $|\mathbf{y}| < \pi$, applying the Laplacian to the last two terms in (A.21) is easily seen to give a sum of δ-functions at $\mathbf{C} = 2\pi n\mathbf{e}^{(1)}$, and this is sufficient to show that

$$(\Delta V_1)(C\mathbf{e}^{(1)}) = -\frac{16}{\pi} \sum_{n=1}^{\infty} c_n \sin^2(nC/2) + \sum_{n=-\infty}^{\infty} \frac{4}{|C - 2\pi n|} + Q, \tag{A.23}$$

where Q is an infinite constant. Introducing the logarithmic derivative of the Gamma function

$$\psi(C)=\frac{d}{dC}(\ln \Gamma(C)) \tag{A.24}$$

which satisfies [22]

$$-\psi(x+1)=\gamma+\sum_{n=1}^{\infty}\left[\frac{1}{n+x}-\frac{1}{n}\right], \tag{A.25}$$

we can write (A.23) for $C\in[0, 2\pi]$ as

$$\begin{aligned}(\Delta V_1)(C\mathbf{e}^{(1)})=&-\frac{16}{\pi}\sum_{n=1}^{\infty}c_n\sin^2(nC/2)+\frac{4}{C}\\&-\frac{2}{\pi}\left[\psi\left(1+\frac{C}{2\pi}\right)+\psi\left(1-\frac{C}{2\pi}\right)\right]+Q'.\end{aligned} \tag{A.26}$$

Q' is now a finite constant and it can be fixed by comparing (A.26) with (A.10) or with the expansion of $V_1(\mathbf{C})$ to fourth order in $\mathbf{C}$ in terms of a_n (Eqs. (4.10) and (4.11)) which gives

$$(\Delta V_1)(\mathbf{C})=\frac{4}{|\mathbf{C}|}+6\kappa_1+60\kappa_3\mathbf{C}^2+O(\mathbf{C}^4). \tag{A.27}$$

Combining this with the expansion of $\psi(1+x)$,

$$-\psi(1+x)=\gamma+\sum_{n=1}^{\infty}\zeta(n+1)(-x)^n, \tag{A.28}$$

we find ($\gamma=0.57721566...$, Euler's constant):

$$Q'=6\kappa_1-\frac{4\gamma}{\pi}=-\frac{6}{\pi}-\frac{4\gamma}{\pi}+\frac{12}{\pi}\sum_{n=1}^{\infty}n^2a_n. \tag{A.29}$$

Exhibiting explicitly the pole terms we can write

$$\begin{aligned}(\Delta V_1)(C\mathbf{e}^{(1)})=&\frac{4}{C}+\frac{4}{2\pi-C}-\frac{8}{\pi}+\frac{12}{\pi}\sum_{n=1}^{\infty}n^2a_n-\frac{16}{\pi}\sum_{n=1}^{\infty}c_n\sin^2(nC/2)\\&-\frac{2}{\pi}\left[\psi\left(1+\frac{C}{2\pi}\right)-\psi(1)+\psi\left(2-\frac{C}{2\pi}\right)-\psi(2)\right]\qquad C\in[0, 2\pi],\end{aligned} \tag{A.30}$$

and periodically extended outside the interval $[0, 2\pi]$. The first four coefficients for c_n (Eq. (A.22)) are given by

$$\begin{aligned} c_1 &= 3.9029359... \times 10^{-3} \\ c_2 &= 4.9074404... \times 10^{-6} \\ c_3 &= 7.4739898... \times 10^{-9} \\ c_4 &= 1.2102679... \times 10^{-11}. \end{aligned} \tag{A.31}$$

They satisfy the same upperbound as the coefficients a_n.

Note that the function in square brackets in Eq. (A.30) is symmetric about $C=\pi$ and vanishes at $C=0$ and $C=2\pi$. It can therefore be written as $\sum_{n=1}^{\infty} \frac{1}{8} d_n \sin^2(nC/2)$, with

$$d_n = -\frac{32}{\pi} \int_0^{2\pi} \cos(nC)\, \psi\left(1+\frac{C}{2\pi}\right) dC = -64Ci(2\pi n), \tag{A.32}$$

($Ci(2\pi n) = -g(2\pi n) \sim 1/(2\pi n)^2$, see [22]) and thus

$$(\Delta V_1)(C\mathbf{e}^{(1)}) = \frac{8\pi}{C(2\pi - C)} + \frac{12}{\pi} \sum_{n=1}^{\infty} n^2 a_n - \frac{8}{\pi} - \frac{16}{\pi} \sum_{n=1}^{\infty} (c_n + d_n) \sin^2(nC/2), \tag{A.33}$$

or (one can sum the slowly converging part of d_n using Eq. (A.17))

$$\begin{aligned} \Omega^2 &= \frac{1}{2}\left(\Delta - \frac{\partial^2}{\partial C^2}\right) V_1(C\mathbf{e}^{(1)}) \\ &= \frac{4\pi}{C(2\pi - C)} - \frac{3}{\pi} + \frac{2}{\pi} \sum_{n=1}^{\infty} n^2 a_n + 4 \sum_{n=1}^{\infty} (n^2 a_n - 2c_n - 2d_n) \sin^2(nC/2). \end{aligned} \tag{A.34}$$

We finally address the properties of $V_1(\mathbf{C}) - V_1(C_1\mathbf{e}^{(1)})$ which can be written as ($\mathbf{C} = (C, y_1, y_2)$, $\mathbf{n} = (n, k_1, k_2)$):

$$V_1(\mathbf{C}) - V_1(C\mathbf{e}^{(1)}) = \frac{4}{\pi} \sum_{\mathbf{n} \neq \mathbf{0}} \frac{\cos(nC) \sin^2(\mathbf{k} \cdot \mathbf{y}/2)}{(\mathbf{n}^2)^2}. \tag{A.35}$$

In this case we find the sum over n to be

$$\begin{aligned} \frac{4}{\pi^2} \sum_n \frac{\cos(nC)}{(n^2 + \mathbf{k}^2)^2} &= -\frac{2}{\pi^2 |\mathbf{k}|} \frac{d}{dx} \left[\sum_n \frac{\cos(nC)}{n^2 + x^2} \right]_{x = |\mathbf{k}|} \\ &= -\frac{2}{\pi^2 |\mathbf{k}|} \frac{d}{dx} \left[\frac{\pi}{x} \frac{\cosh(x(\pi - C))}{\sinh(\pi x)} \right]_{x = |\mathbf{k}|}, \qquad C \in [0, 2\pi]. \end{aligned} \tag{A.36}$$

The result is

$$V_1(\mathbf{C}) = V_1(C\mathbf{e}^{(1)}) + \sum_{\mathbf{k}\neq\mathbf{0}} f_{|\mathbf{k}|}(C)\sin^2(\mathbf{k}\cdot\mathbf{y}/2), \tag{A.37}$$

with $f_{|\mathbf{k}|}(2\pi - C) = f_{|\mathbf{k}|}(C)$ and periodically extended outside the interval $[0, 2\pi]$. Explicitly $f_x(C)$ can be written as

$$f_x(C) = \frac{2}{\pi x^3}\frac{\cosh(x(\pi - C)) + xC\sinh(x(\pi - C))}{\sinh(x\pi)} + \frac{2\cosh(xC)}{x^2\sinh^2(x\pi)}, \tag{A.38}$$

which is positive definite. Hence $V_1(\mathbf{C}) \geqslant V_1(C_1\mathbf{e}^{(1)})$ for all $\mathbf{C}$, and equal iff $C_2 = C_3 = 0 \bmod 2\pi$.

Consequently for fixed C_1, $C_2 = C_3 = 0 \bmod 2\pi$ are minima. This is in accordance with

$$\left.\frac{\partial V_1(\mathbf{C})}{\partial C_i}\right|_{C_i = 0 \bmod \pi} = 0, \qquad \mathbf{C} \neq \mathbf{0} \bmod 2\pi, \tag{A.39}$$

which can be derived from the symmetries of $V_1(\mathbf{C})$: $V_1(\mathbf{C} + 2\pi\mathbf{n}) = V_1(-\mathbf{C}) = V_1(\mathbf{C})$. The extrema of V_1 are hence given by $\mathbf{C} = \mathbf{0} \bmod \pi$, where $\mathbf{C} = \mathbf{0} \bmod 2\pi$ are absolute minima ($V_1(\mathbf{C}) = 2|\mathbf{C}| + O(\mathbf{C}^2)$), $\mathbf{C} = \pi(1, 1, 1) \bmod 2\pi$ are maxima and the other extrema are saddle points. Except for the cone-shaped minima, $V_1(\mathbf{C})$ is C^1. In Fig. 11 we sketch the behaviour of $V_1(\mathbf{C})$ in one eighth of the unit cell (i.e., $[0, \pi]^3$).

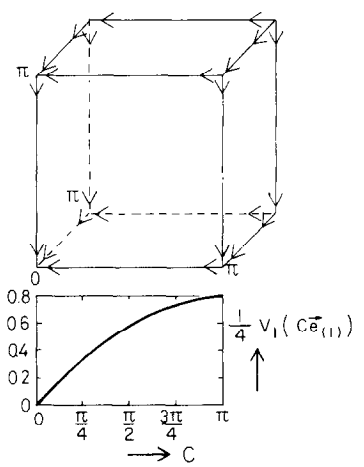


FIG. 11. Picture showing the behaviour of $V_1(\mathbf{C})$. The corners are extrema and arrows give the direction of decrease of the potential. The behaviour of V_1 along the C_1 axis is plotted.

APPENDIX B

Here we will derive the polar decomposition retaining gauge and rotational degrees of freedom. (There is some overlap with [27], and we choose our definitions so as to reproduce the standard commutation relations in Eq. (B.26).) To keep the algebra simple, we parameterize ξ and η by their S_3 coordinates of $SU(2)$ after steriographic projection (giving a double covering for both $SO(3)$ factors)

$$\xi^{ab} = \tfrac{1}{2}\,\mathrm{Tr}(R\sigma^a R^\dagger \sigma^b) \tag{B.1}$$

$$\eta_{ij} = \tfrac{1}{2}\,\mathrm{Tr}(S^\dagger \sigma_i S \sigma_j) \tag{B.2}$$

$$R = ((1-\mathbf{r}^2) + 2i\mathbf{r}\cdot\sigma)/(1+\mathbf{r}^2), \qquad \mathbf{r}\in R^3 \tag{B.3}$$

$$S = ((1-\mathbf{s}^2) + 2i\mathbf{s}\cdot\sigma)/(1+\mathbf{s}^2), \qquad \mathbf{s}\in R^3. \tag{B.4}$$

The S_3 coordinates are given by

$$\hat r_0 = (1-\mathbf{r}^2)/(1+\mathbf{r}^2), \qquad \hat{\mathbf{r}} = 2\mathbf{r}/(1+\mathbf{r}^2), \tag{B.5}$$

$$\hat s_0 = (1-\mathbf{s}^2)/(1+\mathbf{s}^2), \qquad \hat{\mathbf{s}} = 2\mathbf{s}/(1+\mathbf{s}^2), \tag{B.6}$$

in terms of which we can write

$$\xi^{ab} = (\hat r_0^2 - \hat{\mathbf{r}}^2)\,\delta_{ab} + 2\hat r_a \hat r_b - 2\hat r_0 \hat r_k \varepsilon_{kab}, \tag{B.7}$$

$$\eta_{ij} = (\hat s_0^2 - \hat{\mathbf{s}}^2)\,\delta_{ij} + 2\hat s_i \hat s_j - 2\hat s_0 \hat s_k \varepsilon_{kij}. \tag{B.8}$$

The next step is to calculate $\dot c_i^a \dot c_i^a$ for $c_i^a = \sum_{b=1}^3 \xi^{ab} x_b \eta_{bi}$ to deduce the metric $g_{\mu\nu}$, where we label $x^\mu = (\mathbf{x}, \mathbf{r}, \mathbf{s})$, and a dot denotes differentiation w.r.t. the geodesic parameter. So

$$\dot x^\mu g_{\mu\nu} \dot x^\nu = \sum_{b=1}^3 \dot x_b \dot x_b + 2 \sum_{b,c=1}^3 \dot\xi^{ab} x_b \eta_{bi} \xi^{ac} x_c \dot\eta_{ci} + \sum_{b=1}^3 [(\dot\xi^{ab})^2 + (\dot\eta_{ib})^2]\, x_b^2. \tag{B.9}$$

We have

$$\begin{aligned}\dot\xi^{ab}\xi^{ac} &= \tfrac{1}{4}\,\mathrm{Tr}(\sigma^a(R^\dagger\sigma^b\dot R + \dot R^\dagger\sigma^b R))\,\mathrm{Tr}(\sigma^a R^\dagger \sigma^c R)\\ &= \tfrac{1}{2}\,\mathrm{Tr}((R^\dagger\sigma^b\dot R + \dot R^\dagger\sigma^b R)\,R^\dagger\sigma^c R)\\ &= -i\,\mathrm{Tr}(\dot R R^\dagger \sigma^a)\,\varepsilon_{abc},\end{aligned} \tag{B.10}$$

and, similarly,

$$\eta_{ik}\dot\eta_{jk} = i\,\mathrm{Tr}(\dot S S^\dagger \sigma_k)\,\varepsilon_{kij}. \tag{B.11}$$

Introducing the $SO(3)$ matrices U and V by

$$U_{ia} = -\frac{i}{4}(1+\mathbf{r}^2)\,\mathrm{Tr}\left(\frac{\partial R}{\partial r_i}R^{\dagger}\sigma_a\right), \tag{B.12}$$

$$V_{ia} = \frac{i}{4}(1+\mathbf{s}^2)\,\mathrm{Tr}\left(\frac{\partial S}{\partial s_i}S^{\dagger}\sigma_a\right), \tag{B.13}$$

we can write

$$g_{\mu\nu} = \begin{pmatrix} 1_3 & 0 & 0 \\ 0 & A & B \\ 0 & B^{\dagger} & C \end{pmatrix}, \tag{B.14}$$

with

$$A_{ij} = \frac{16}{(1+\mathbf{r}^2)^2}\sum_{b=1}^{3} U_{ib}U_{jb}(\mathbf{x}^2 - x_b^2), \tag{B.15}$$

$$B_{ij} = \frac{16}{(1+\mathbf{r}^2)(1+\mathbf{s}^2)}\sum_{b=1}^{3}\frac{U_{ib}V_{jb}}{x_b}\cdot 2x_1x_2x_3, \tag{B.16}$$

$$C_{ij} = \frac{16}{(1+\mathbf{s}^2)^2}\sum_{k=1}^{3} V_{ik}V_{jk}(\mathbf{x}^2 - x_k^2). \tag{B.17}$$

Hence $g = \det g_{\mu\nu} = \det A \det(C - B^{\dagger}A^{-1}B)$ and because $U, V \in SO(3)$ they drop out of the expression for g:

$$g = \left(\frac{16}{(1+\mathbf{r}^2)(1+\mathbf{s}^2)}\right)^6 \prod_{i>j}(x_i^2 - x_j^2)^2. \tag{B.18}$$

Also $g^{\mu\nu}$ is easily determined:

$$g^{\mu\nu} = \begin{pmatrix} 1_3 & 0 & 0 \\ 0 & E & F \\ 0 & F^{\dagger} & G \end{pmatrix}. \tag{B.19}$$

If we introduce the shorthand notation,

$$W_b = \tfrac{1}{2}\sum_{i,j=1}^{3}\varepsilon_{bij}^2(x_i^2 - x_j^2)^2, \tag{B.20}$$

we can write

$$E_{ij}=\frac{(1+\mathbf{r}^2)^2}{16}\sum_{h=1}^{3}U_{ih}U_{jh}\frac{(\mathbf{x}^2-x_h^2)}{W_h}, \tag{B.21}$$

$$F_{ij}=-\frac{(1+\mathbf{r}^2)(1+\mathbf{s}^2)}{16}\sum_{h=1}^{3}\frac{U_{ih}V_{jh}}{x_hW_h}\cdot 2x_1x_2x_3, \tag{B.22}$$

$$G_{ij}=\frac{(1+\mathbf{s}^2)^2}{16}\sum_{k=1}^{3}V_{ik}V_{jk}\frac{(\mathbf{x}^2-x_k^2)}{W_h}. \tag{B.23}$$

Using $(\partial/\partial r_i)((1+\mathbf{r}^2)^{-2}U_{ih})=(\partial/\partial s_i)((1+\mathbf{s}^2)^{-2}V_{ih})=0$ we finally find

$$\begin{aligned}\frac{\partial^2}{\partial c_i^a\,\partial c_i^a}&=\frac{1}{\sqrt{g}}\frac{\partial}{\partial x_\mu}\sqrt{g}\,g^{\mu\nu}\frac{\partial}{\partial x_\nu}\\&=\frac{1}{\mathscr{J}}\frac{\partial}{\partial x_i}\mathscr{J}\frac{\partial}{\partial x_i}-\sum_{h=1}^{3}\frac{(\mathbf{x}^2-x_h^2)}{W_h}(\hat{T}_h^2+\hat{L}_h^2)-\sum_{h=1}^{3}\frac{4x_1x_2x_3}{x_hW_h}\hat{T}_h\hat{L}_h,\end{aligned} \tag{B.24}$$

with $\mathscr{J}=\prod_{i>j}(x_i^2-x_j^2)$ and

$$\hat{T}_h=i\frac{(1+\mathbf{r}^2)}{4}U_{jh}\frac{\partial}{\partial r_j},\qquad \hat{L}_h=-i\frac{(1+\mathbf{s}^2)}{4}V_{jh}\frac{\partial}{\partial s_j}, \tag{B.25}$$

which are easily seen to be representations of $SO(3)$:

$$[\hat{L}_i,\hat{L}_j]=i\varepsilon_{ijk}\hat{L}_k,\qquad [\hat{T}_i,\hat{T}_j]=i\varepsilon_{ijk}\hat{T}_k,\qquad [\hat{L}_i,\hat{T}_j]=0. \tag{B.26}$$

We can rewrite (B.24) in the elegant form

$$\frac{\partial^2}{\partial c_i^a\,\partial c_i^a}=\frac{1}{\mathscr{J}}\frac{\partial}{\partial x_i}\mathscr{J}\frac{\partial}{\partial x_i}-\frac{1}{4}\sum_{i\neq j\neq k}\left[\left(\frac{\hat{L}_k+\hat{T}_k}{x_i-x_j}\right)^2+\left(\frac{\hat{L}_k-\hat{T}_k}{x_i+x_j}\right)^2\right], \tag{B.27}$$

and the normalization of the wave function is related by

$$\begin{aligned}\int d^9c\,|\psi(c)|^2&=\frac{1}{v}\int d^3x\,d^3r\,d^3s\,\sqrt{g}\,|\psi(\mathbf{x},\mathbf{r},\mathbf{s})|^2\\&=\frac{16^3}{384}\int\frac{d^3r}{(1+\mathbf{r}^2)^3}\int\frac{d^3s}{(1+\mathbf{s}^2)^3}\int d^3x\,|\mathscr{J}|\,|\psi(\mathbf{x},\mathbf{r},\mathbf{s})|^2.\end{aligned} \tag{B.28}$$

$v=384$ is the degree of the map $(\mathbf{x},\mathbf{r},\mathbf{s})\mapsto c_i^a=\xi_{ab}x_b\eta_{bi}$ decomposed as follows: a factor 2 for each $SU(2)$ (covering $SO(3)$ twice), a factor 4 for the set (ξ,η) leaving $\mathbf{x}$ fixed (hence ξ and η are equal and diagonal with ±1 on the diagonal), a factor 6 for the pairs (ξ,η) which permute the x_b, and a factor 4 for the pairs (ξ,η) which change the signs of x_b ($\det c=\prod_{i=1}^3x_i$; thus sign changes occur in pairs). In total $v=2\cdot2\cdot4\cdot6\cdot4=384$ (one easily verifies, e.g., that Eq. (B.28) is satisfied for $\psi(c)=1$ (0) for $c^2<1$ (>1)). These symmetries will be needed to show the gauge and rotational invariance of (B.27) (i.e., to show explicitly that $[\partial^2/\partial c_i^a\,\partial c_i^a,\hat{L}_k]=$

$[\partial^2/\partial c_i^a\,\partial c_i^a, \hat{T}_k]=0$). We will not discuss this, or the interesting consequences for the spectrum at non-zero angular momentum. (For example, in [2] it was shown that gauge invariant wave functions with $J=1$ do not exist.)

Finally, we discuss the explicit parameterization of η_{ij} (Eqs, (5.17) and (5.18)). This parameterization is equivalent to the following one for S^3:

$$\hat{s}_\mu = \left(\cos\left(\frac{\theta}{2}\right)\cos\left(\frac{1}{2}(\varphi-\xi)\right), -\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{1}{2}(\xi+\varphi)\right), \sin\left(\frac{\theta}{2}\right)\cos\left(\frac{1}{2}(\xi+\varphi)\right), \cos\left(\frac{\theta}{2}\right)\cos\left(\frac{1}{2}(\varphi-\xi)\right)\right). \tag{B.29}$$

Using (B.4), (B.6), (B.13), and (B.25) we find

$$\hat{L}_b = \frac{i}{2}\left[\hat{s}_0\frac{\partial}{\partial \hat{s}_0} + \hat{s}_k\varepsilon_{kbi}\frac{\partial}{\partial \hat{s}_i}\right], \tag{B.30}$$

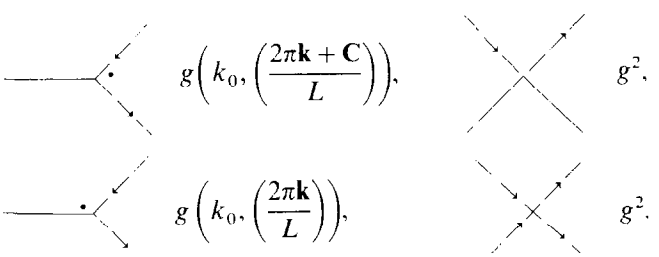
which after some calculation yields (5.22).

Appendix C

In this appendix we will give a heuristic derivation of the contribution to the effective potential along the vacuum valley due to the leading infrared behaviour in a multiloop expansion for the effective Lagrangian introduced in Eq. (4.36). Hence we take **C** to be constant in time. One can easily specify the Feynman rules in terms of **C** and there is no need to expand in powers of the background field. If we call σ_3 the neutral component and $(\sigma_1 \pm \sigma_2)/\sqrt{2}$ the charge components, we have two types of propagators:

$$\text{———} = \frac{1}{k_0^2 - ((2\pi\mathbf{k})/L)^2}, \qquad \mathbf{k}\neq\mathbf{0};$$
$$\text{———}\!\!\rightarrow\!\!\text{———} = \frac{1}{k_0^2 - ((2\pi\mathbf{k}+\mathbf{C})/L)^2}, \tag{C.1}$$

where we suppress factors of i, 2π and spacetime indices. We also make no distinction between vector and ghost particles. The vertices are of the following type:



(C.2)

We are now interested in the leading infrared behaviour and will only consider the part of the diagram with $\mathbf{k}=\mathbf{0}$, hence only the last (four-point) vertex in (C.2) will occur. Let us point out that this is precisely what one would obtain if an effective Lagrangian in $\mathbf{C}$ were derived from the Yang–Mills Lagrangian in the sector of spatially constant vector potentials, and indeed one easily verifies that in this sector no three-point vertices are present.

If we next rescale k_0 by $|\mathbf{C}|/L$, each propagator has a factor $L^2/\mathbf{C}^2$ and each loop integration a factor $|\mathbf{C}|/L^4$. A vacuum graph with V_4 vertices, P propagators and l loops therefore contributes

$$\mathcal{G}(V_4, P, l) \propto L^3 g^{2V_4} \left(\frac{|\mathbf{C}|}{L}\right)^{l-2P} L^{-3l} \tag{C.3}$$

to the effective potential. Using the well-known relations

$$P = 2V_4, \qquad l = 1 + P - V_4, \tag{C.4}$$

one finds

$$\mathcal{G}(V_4, P, l) = L^{-1} g^{2/3} (g^{-2/3}|\mathbf{C}|)^{1-3V_4}. \tag{C.5}$$

One indeed recognizes the one-loop result $L^{-1}|\mathbf{C}|$ ($V_1(\mathbf{C}) = 2L^{-1}|\mathbf{C}|$ for $|\mathbf{C}| \ll 1$) and a two-loop contribution behaves as $g^2 L^{-1} |\mathbf{C}|^{-2}$. In conclusion, the leading infrared behaviour of the effective potential to all loop orders yields a contribution of the form

$$V_{\text{eff}} = g^{2/3} L^{-1} f(|\mathbf{C}|\, g^{-2/3}), \tag{C.6}$$

and it is no accident that W_1 in Eq. (5.34) is exactly of this form.

Appendix D

In this appendix we discuss the generalization to $SU(N)$ for zero magnetic flux $\mathbf{m}$ in such a way that the generalization to any simple, simply connected group is obvious.

The vector potential is again chosen periodic, and the remaining gauge invariance is specified by a gauge function, periodic up to an element of the center:

$$\Omega(\mathbf{x} + L\mathbf{e}^{(j)}) = \exp(2\pi i k_j/N)\, \Omega(\mathbf{x}), \tag{D.1}$$

where $\mathbf{k} \in \mathbf{Z}_N^3$ and $P \in \mathbf{Z}$ (Eq. (2.3)) specify the homotopy type, with conjugate variables $\mathbf{e}$ (integer mod N) and θ (mod 2π). $\mathbf{e}$ and θ label the physical state vectors

$$[\Omega]\, |\mathbf{e}, \theta\rangle = e^{2\pi i \mathbf{k}\cdot\mathbf{e}/N + i\theta P} |\mathbf{e}, \theta\rangle. \tag{D.2}$$

The classical vacuum is again given by the curvature-free connections (Ω *not* periodic)

$$A_k(\mathbf{x}) = -i\Omega(\mathbf{x})\,\partial_k \Omega^{-1}(\mathbf{x}). \tag{D.3}$$

Imposing periodicity on $\mathbf{A}$ is easily seen to imply that the

$$\Omega_j(\mathbf{x}) \equiv \Omega^{-1}(\mathbf{x} + L\mathbf{e}^{(j)})\,\Omega(\mathbf{x}) \tag{D.4}$$

are independent of $\mathbf{x}$ and mutually commute

$$\Omega_j \Omega_k = \Omega^{-1}(\mathbf{x} + L\mathbf{e}^{(j)} + L\mathbf{e}^{(k)})\,\Omega(\mathbf{x}) = \Omega_k \Omega_j. \tag{D.5}$$

Therefore, we can simultaneously diagonalize Ω_k, $k = 1, 2, 3$ by a constant gauge transformation U,

$$\Omega_k = U \exp(i\Phi_k)\, U^{-1}, \tag{D.6}$$

where Φ_k is real, traceless, and diagonal. Using Eq. (D.4) this is seen to imply that

$$\tilde{\Omega}(\mathbf{x}) = \Omega(\mathbf{x})\, U \exp\left(i \sum_k x_k \Phi_k / L \right) \tag{D.7}$$

is a periodic gauge function, such that A_k is gauge equivalent to Φ_k/L:

$$A_k(\mathbf{x}) = \tilde{\Omega}(\mathbf{x})(\Phi_k/L)\,\tilde{\Omega}(\mathbf{x})^{-1} - i\tilde{\Omega}(\mathbf{x})\,\partial_k \tilde{\Omega}(\mathbf{x})^{-1}. \tag{D.8}$$

Again as in Section 2, the gauge invariance of Φ can be established by considering the Wilson loop

$$W(\mathscr{C}) = \mathrm{Tr}\left(\prod_k \exp(i\Phi_k)^{n_k} \right), \tag{D.9}$$

where n_l are the winding numbers of the curve $\mathscr{C}$, but apart from these, $\mathscr{C}$ is arbitrary. $W(\mathscr{C})$ is invariant under: (i) $\Phi_k \to \Phi_k + 2\pi$ and (ii) permutations of the eigenvalues of Φ_k (for all k simultaneously). The associated gauge transformations are easily written down. Including invariance of $W(\mathscr{C})$ up to an element of the center of the gauge group, we also have invariance under the gauge transformation

$$\Omega_{\mathbf{k}}(\mathbf{x}) = \mathrm{diag}(e^{2\pi i \mathbf{k}\cdot\mathbf{x}N/L}, \ldots, e^{2\pi i \mathbf{k}\cdot\mathbf{x}N/L}, e^{2\pi i(1-N)\mathbf{k}\cdot\mathbf{x}N/L}), \tag{D.10}$$

which leaves Φ_j diagonal. Hence Φ_j is to be identified with $\Phi_j + 2\pi\Theta_j$ whenever

$$\exp(2\pi i \Theta_j) \in \mathbf{Z}_N \tag{D.11}$$

($\mathbf{Z}_n$ the center of $SU(N)$). This condition on Θ is well known from monopoles [23], and is solved by elements of the dual weight lattice of $SU(N)$.

To be more precise, we consider the canonical (complex) basis for the Lie algebra (l is the rank and m the dimension of the group (resp. $N-1$ and N^2-1 for $SU(N)$), $r=\frac{1}{2}(m-l)$):

$$T_1, T_2, \ldots, T_l, E_{\pm\alpha^{(1)}}, \ldots, E_{\pm\alpha^{(r)}}, \tag{D.12}$$

$$[T_i, E_\alpha] = \alpha_i E_\alpha. \tag{D.13}$$

The T_i span the Cartan sub-algebra and can be chosen diagonal, hermitian, and traceless; they generate the maximal torus which contains the center of the gauge group and we can consequently expand

$$\mathbf{\Phi} = \mathbf{c}^a T_a; \qquad \mathbf{\Theta} = \mathbf{t}^a T_a. \tag{D.14}$$

Note $\exp(2\pi i\Theta_k) \in \mathbf{Z}_N$ if and only if it commutes with all group elements or, iff for all α

$$\exp(2\pi i\Theta_k)\, E_\alpha \exp(-2\pi i\Theta_k) = E_\alpha. \tag{D.15}$$

The α form an l-dimensional root system. The metric on the Euclidean space spanned by these roots is $((\alpha, \beta) \equiv \alpha_i g^{ij} \beta_j, g^{ij} = g_{ij}^{-1})$:

$$g_{ij} = \mathrm{Tr}_{\mathrm{ad}}(T_i T_j). \tag{D.16}$$

Let $\Delta = \{\alpha^{(1)}, \alpha^{(2)}, \ldots, \alpha^{(l)}\}$ be a basis [24] for the root lattice. The associated *dual* weight lattice (i.e., the weight lattice for the dual root lattice spanned by $\alpha^v = 2\alpha/(\alpha, \alpha)$) is defined by its basis $\{\tilde{\lambda}^{(1)}, \tilde{\lambda}^{(2)}, \ldots, \tilde{\lambda}^{(l)}\}$ such that

$$(\tilde{\lambda}^{(a)}, \alpha^{(b)}) = \tilde{\lambda}_i^{(a)} g^{ij} \alpha_j^{(b)} = \delta_{ab}. \tag{D.17}$$

Since Eq. (D.15) is easily seen to imply that $\exp(2\pi i t_k^a \alpha_a) = 1$ for each root α we find that $\mathbf{t}_a$ is an element of the dual weight lattice:

$$\mathbf{t}^b = g^{ba} \mathbf{t}_a; \qquad \mathbf{t}_a = \mathbf{n}^{(i)} \tilde{\lambda}_a^{(i)}, \quad n_k^{(i)} \in \mathbf{Z}. \tag{D.18}$$

If we express $\mathbf{c}^a$ in terms of the basis for the dual weight lattice,

$$\mathbf{\Phi} = \mathbf{c}^a T_a = \mathbf{z}^{(i)} g^{ab} \tilde{\lambda}_b^{(i)} T_a = \mathbf{z}^{(i)} (\tilde{\lambda}^{(i)}, T), \tag{D.19}$$

then the gauge transformation (D.10) corresponds to shifting $\mathbf{z}^{(i)}$ over multiples of 2π, whereas the gauge transformations which permute the eigenvalues of $\mathbf{\Phi}$ correspond to the action of the Weyl group (see also [10]). Let us remind the reader that the Weyl group is generated by the Weyl reflections (α a root)

$$\sigma_\alpha(\beta) = \beta - \frac{2(\beta, \alpha)}{(\beta, \beta)} \alpha, \tag{D.20}$$

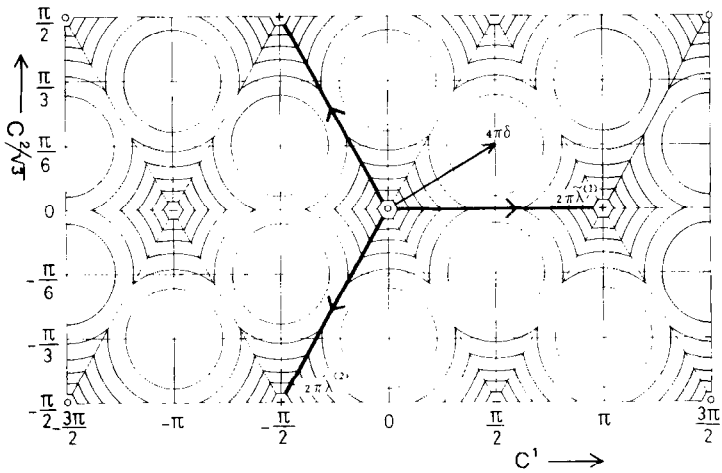


FIG. 12. Equipotential lines for the $SU(3)$ one-loop potential V_1 restricted to one dimension ($\mathbf{c}^a = c^a \mathbf{e}^{(1)}$). The homotopically nontrivial gauge transformations $\Omega_{\mathbf{k}}$ with $\mathbf{k} = \pm \mathbf{e}^{(1)} \bmod 3$ connecting minima of type 0 and type $\pm$ correspond to translations over $2\pi\tilde{\lambda}^{(1)}$ and $2\pi\tilde{\lambda}^{(2)}$, respectively. The broad lines correspond to the pinchons connecting type **0** and type + vacua. The point $4\pi\delta$ corresponds to the maximum M of V_1, and equipotentials are plotted in steps of $M/7$.

and that an element of the Weyl group is an automorphism of the root system. The above-mentioned gauge transformations form the normalizer $N_{\mathcal{G}}(H)$ of the Cartan subalgebra H (the span $\{T_i\}_{i=1,\ldots,l}$) *in* $\mathcal{G}$:

$$N_{\mathcal{G}}(H) = \{ g \in \mathcal{G} \mid ghg^{-1} \in H, \forall h \in H \}. \tag{D.21}$$

Note that the normalizer contains the centralizer $C_{\mathcal{G}}(H)$ of H in $\mathcal{G}$ which leaves $\mathbf{\Phi}$ invariant.

$$C_{\mathcal{G}}(H) = \{ g \in \mathcal{G} \mid ghg^{-1} = h, \forall h \in H \}. \tag{D.22}$$

Hence (see [25, Theorem 4.9.1]) we have an isomorphism between the Weyl group and $N_{\mathcal{G}}(H)/C_{\mathcal{G}}(H)$ generated by the map $g \mapsto \mathrm{Ad}(g)\,|_H$, with $\mathrm{Ad}(g)\,h = ghg^{-1}$.

There exists an elegant description for the action of the Weyl group. Recall that the fundamental Weyl chamber (w.r.t. the basis Δ) is defined by y such that $(y, \alpha^{(i)}) > 0$ for all i, or $y_i > 0$ for all i, where y_i are the components of y w.r.t. the basis for the dual weight lattice ($y = y_i \tilde{\lambda}^{(i)}$). Any y can be written as an element of the Weyl group acting on the closure of the fundamental Weyl chamber. For $SU(3)$ this is sketched in Fig. 12, to which we will return in a while.

As for $SU(2)$, the one-loop effective potential is given by

$$V_1(\mathbf{\Phi}) = \mathrm{Tr}((-D_i^2(\mathbf{\Phi}))^{1/2}), \tag{D.23}$$

with

$$D_k(\mathbf{\Phi}) = \partial_k + i\,\mathrm{ad}(\Phi_k/L). \tag{D.24}$$

The spectrum of $-D_i^2(\mathbf{\Phi})$ is explicitly given by

$$\begin{aligned} -D_i^2(\mathbf{\Phi})\, e^{2\pi i \mathbf{k}\cdot\mathbf{x}/L} T_a &= \left(\frac{2\pi \mathbf{k}}{L}\right)^2 e^{2\pi i \mathbf{k}\cdot\mathbf{x}/L} T_a \\ -D_i^2(\mathbf{\Phi})\, e^{2\pi i \mathbf{k}\cdot\mathbf{x}/L} E_\alpha &= \left(\frac{2\pi \mathbf{k} + \mathbf{c}^a \alpha_a}{L}\right)^2 e^{2\pi i \mathbf{k}\cdot\mathbf{x}/L} E_\alpha, \end{aligned} \tag{D.25}$$

and we can copy the result for $V_1(\mathbf{\Phi})$ directly from $SU(2)$:

$$\begin{aligned} V_1(\mathbf{\Phi}) &= \frac{2}{\pi^2 L} \sum_\alpha \sum_{\mathbf{n}\neq \mathbf{0}} \frac{\sin^2((1/2)\,\mathbf{n}\cdot\mathbf{c}^a\alpha_a)}{(\mathbf{n}^2)^2} \\ &= \frac{2}{\pi^2 L} \sum_\alpha \sum_{\mathbf{n}\neq \mathbf{0}} \frac{\sin^2((1/2)\,\mathbf{n}\cdot\mathbf{z}^{(i)}(\vec{\lambda}^{(i)}, \alpha))}{(\mathbf{n}^2)^2}. \end{aligned} \tag{D.26}$$

We can explicitly verify the invariance of $V_1(\mathbf{\Phi})$ under Weyl transformations W using $\{W\alpha\} = \{\alpha\}$, and under translations of $z_k^{(i)}$ over 2π, because a basis Δ for a root lattice is defined such that for any root α we have $\alpha = \sum_{i=1}^{l} k_i \alpha^{(i)}$ with k_i all positive (or all negative) integers.

As for $SU(2)$ we have that the quadratic approximation breaks down for those $\mathbf{z}^{(i)}$ where $-D_i^2(\mathbf{\Phi})$ has a vanishing eigenvalue. Since this vanishing eigenvalue for $SU(2)$ causes $V_1(\mathbf{z})$ to behave as $2\,|\mathbf{z}|/L$ we see that for general gauge group this breakdown occurs at $\mathbf{z}^{(i)} = 0 \pmod{2\pi}$ for one or more values of i. This corresponds precisely to the boundaries of the Weyl chambers. This is obvious since boundaries of Weyl chambers are associated with points left invariant by one or more elements of the Weyl group. This is equivalent to the fact that the associated value of $\mathbf{\Phi}$ has a smaller holonomy group than those $\mathbf{\Phi}$ not related to the boundary. As we discussed in detail this leads to the breakdown of the quadratic approximations, and extra zeros in the Faddeev–Popov determinant. For $SU(2)$ these singularities were isolated, but in general they are of codimension 3. Although of zero measure, they strongly dominate the quantum behaviour, as caustics do in optics.

Away from these singularities the effective one-loop Lagrangian is given by

$$\mathscr{L} = \frac{1}{g(L)^2} \operatorname{Tr}(\dot{\mathbf{\Phi}}^2) - V_1(\mathbf{\Phi}). \tag{D.27}$$

It should be plausible, but we will give no proof, that in *lowest* order the energy splitting due to electric flux is determined by the Lagrangian in (D.27). The situation is more complicated than for $SU(2)$; it will turn out that the pinchon solution is contained in the set of singular points. Still, one can show that $V_1(\mathbf{\Phi})$ can be regularized by $O(g^{2/3})$ corrections by taking the quartic interactions into account. This, however, leaves the leading result unaltered.

Before specializing to $SU(N)$ we first derive a few general properties of $V_1(\mathbf{\Phi})$. $V_1(\mathbf{\Phi}) \geq V_1(\Phi_1 \mathbf{e}^{(1)})$ follows because $V_1(\mathbf{\Phi})$ is related to the $SU(2)$ potential. It

means that pinchon solutions are again obtained by "dimensional reduction." Restricted to one dimension we find[1]:

$$V_1(\Phi \mathbf{e}^{(1)}) = \frac{1}{\pi L} \sum_{\alpha > 0} \left[z_\alpha (2\pi - z_\alpha) + 8 \sum_{n=1}^{\infty} a_n \sin^2(n z_\alpha / 2) \right], \tag{D.28}$$

$$z_\alpha = c^a \alpha_a = z^{(i)}(\vec{\lambda}^{(i)}, \alpha) \in [0, 2\pi], \tag{D.29}$$

extended periodically in z_α with periods 2π in the obvious way. If we introduce the so-called maximal weight δ

$$\delta = \tfrac{1}{2} \sum_{\alpha > 0} \alpha = \sum_{i=1}^{l} \lambda^{(i)} \tag{D.30}$$

where $\lambda^{(i)}$, $i = 1, \ldots, l$ form the basis of the weight lattice defined by

$$\langle \lambda^{(i)}, \alpha^{(j)} \rangle = \delta_{ij}, \tag{D.31}$$

with (for α, β roots always integer)

$$\langle \alpha, \beta \rangle = 2 \frac{(\alpha, \beta)}{(\beta, \beta)}, \tag{D.32}$$

and if we use the "completeness" relation

$$\sum_{\alpha} \alpha_i \alpha_j = g_{ij} \tag{D.33}$$

(the sum is over all roots), then for $z_\alpha \in [0, 2\pi]$,

$$V_1(\Phi \mathbf{e}^{(1)}) = \frac{1}{2\pi L} ((4\pi\delta)^2 - (c - 4\pi\delta)^2) + \frac{8}{\pi L} \sum_{n=1}^{\infty} \sum_{\alpha > 0} a_n \sin^2(n z_\alpha / 2). \tag{D.34}$$

This, in the approximation $a_n \equiv 0$, is indeed a very simple expression. Also, the kinetic part is simple since

$$\mathrm{Tr}(\dot{\Phi}^2) = \dot{\mathbf{c}}^a \dot{\mathbf{c}}^b \, \mathrm{Tr}(T_a T_b) = \dot{\mathbf{c}}^a \dot{\mathbf{c}}^b K g_{ab}. \tag{D.35}$$

The constant K only depends on the group and g_{ab} can always be chosen proportional to δ_{ab}.

We will now specialize to $SU(N)$ for which $K = 2N$. The associated algebra is of type A_N [24]. All roots are of equal length $(\alpha, \alpha) = N^{-1}$ and for $\alpha > 0$ are given by $\alpha^{(i)}$ and $\alpha^{(i)} + \alpha^{(j)}$, $i \neq j$. It hence follows that

$$\vec{\lambda}^{(i)} = 2N \lambda^{(i)}, \qquad \delta = \frac{1}{2N} \sum_{i=1}^{N-1} \vec{\lambda}^{(i)} \tag{D.36}$$

[1] Any root can be written as $\sum n_i \alpha^{(i)}$ with all n_i positive ($\alpha > 0$) or negative ($\alpha < 0$).

and

$$\mathscr{L} = \frac{L\dot{\mathbf{z}}^{(i)}(A_N^{-1})_{ij}\dot{\mathbf{z}}^{(j)}}{g^2(L)} - \sum_{i=1}^{N-1} V_1(\mathbf{z}^{(i)}) - \sum_{i>j=1}^{N-1} V_1(\mathbf{z}^{(i)} + \mathbf{z}^{(j)}), \tag{D.37}$$

where $(A_N)_{ij} = \langle \alpha^{(i)}, \alpha^{(j)} \rangle$ is the Cartan matrix with 2 on the diagonal and -1 on both subdiagonals, and $V_1(\mathbf{z})$ is the $SU(2)$ potential. Note that $(\tilde{\lambda}^{(i)}, \tilde{\lambda}^{(j)}) = (2N)^2(\lambda^{(i)}, \lambda^{(j)})$ and $\alpha^{(i)} = \langle \alpha^{(i)}, \alpha^{(j)} \rangle \lambda^{(j)} = (A_N)_{ij}\lambda^{(j)}$, which leads to $(\tilde{\lambda}^{(i)}, \tilde{\lambda}^{(j)}) = 2N(A_N^{-1})_{ij}$. This proves the expression for the kinetic part, whereas the potential part follows from the above-mentioned explicit form of the roots α. In Fig. 12 we exhibit the potential for $SU(3)$ by choosing units according to:

$$\Phi = \operatorname{diag}\left(\frac{2c^1}{3} + \frac{2c^2}{\sqrt{3}}, \frac{2c^1}{3} - \frac{2c^2}{\sqrt{3}}, -\frac{4c^1}{3}\right). \tag{D.38}$$

From this it is obvious that the pinchon has one and only one pair (i, k) such that $z_k^{(i)} \neq 0$. This is easily seen to generalize to arbitrary N (with a little imagination). The energy splitting due to electric flux can therefore be computed by restricting $\mathscr{L}$ as

$$\mathscr{L} = \frac{L\dot{z}^2(A_N^{-1})_{11}}{g^2(L)} - (N-1)\, V_1(z\mathbf{e}^{(1)}). \tag{D.39}$$

With $(A_N^{-1})_{11} = \det(A_{N-1})/\det(A_N) = (N-1)/N$ we find

$$E(\mathbf{e}, L) = \frac{1}{L}\sum_{i=1}^{3} \sin^2\left(\frac{\pi e_i}{N}\right) \exp\left(-\left(\frac{2(N-1)^2}{Ng^2(L)}\right)^{1/2} S + O(g^{-1/3})\right), \tag{D.40}$$

with S the $SU(2)$ pinchon action.

Note that we expect $O(g^{2/3})$ corrections to V_1 in Eq. (D.39), and hence the $O(g^{-1/3})$ is expected to have contributions from this modification. Equation (D.40) would also imply that the effect does not survive in the $N \to \infty$ limit.

Acknowledgments

We would like to thank Martin Lüscher for his interest and providing his notes on the Rayleigh–Ritz analysis. We are also grateful to Fred Goldhaber for moral support. This work was supported in part by NSF grants PHY-85-07627 and DMS-84-05661.

Note added in proof. Recently the $SU(3)$ effective Hamiltonian of Lüscher [2] was numerically analysed by Weisz and Ziemann [33], giving results similar to those found by Lüscher and Münster [13] for $SU(2)$. We also extended our result for arbitrary $SU(N)$ (Eq. (D.40)) beyond the leading order, predicting for $SU(3)$ the onset of tunneling at $z \sim 1.6$ [34]. Reference 34 also contains a further discussion of an expected crossover at $z \sim 5$. It is only beyond this value of z that one can expect formation of flux tubes and the glueball to behave as a particle state.

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