Unconstrained SU(2) Yang-Mills quantum mechanics with the theta angle

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The unconstrained classical system equivalent to spatially homogeneous SU(2) Yang-Mills theory with the theta angle is obtained and canonically quantized. The Schrödinger eigenvalue problem is solved approximately for the low lying states using variational calculation. The properties of the ground state are discussed, in particular its electric and magnetic properties, and the value of the ''gluon condensate'' is calculated. Furthermore it is shown that the energy spectrum of SU(2) Yang-Mills quantum mechanics is independent of the theta angle. Explicit evaluation of the Witten formula for the topological susceptibility gives strong support for the consistency of the variational results obtained.

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I. INTRODUCTION

One of the central problems in the investigation of non-Abelian gauge theories is a gauge invariant description of the vacuum and the low-lying excited states. In the standard approach to the quantization of gauge theories the physical states have to satisfy not only the Schrödinger equation but additionally be annihilated by the Gauss law operator to implement gauge invariance at the quantum level [1]. However, it is well known that there exist states which satisfy the Gauss law but are not invariant under the so-called homotopically nontrivial gauge transformations, leading to the appearance of the theta angle [2,3]. A well-elaborated semiclassical approach to the theta structure of the ground state has been given in the ''instanton picture,'' where the theta angle is interpreted [1] in analogy to the Bloch momentum in solid state physics. The instantons, which are self-dual solutions of the Euclidean classical equations of motion with finite action, correspond to semiclassical quantum mechanical tunneling paths in Minkowski space between the infinite sequence of degenerate zero-energy Yang-Mills vacua of different homotopy classes of the gauge potential. The semiclassical instanton picture of the theta vacuum however is of course reliable only for weak coupling. For a complete investigation of the theta structure of the vacuum of Yang-Mills quantum theory a rigorous treatment at strong coupling is necessary. The effect of the theta angle for arbitrary coupling constant can be taken into account by adding the Pontryagin density to the Yang-Mills Lagrangian [1]. Although the extra theta dependent CP-violating term is only a total divergence and therefore has no meaning classically, it can have a physical meaning at the quantum level as is still under lively discussion [4–6].

As a first step towards a full investigation of Yang-Mills theory in the strong coupling limit the toy model of SU(2) Yang-Mills mechanics of spatially homogeneous fields has been considered on the classical [7–11] as well as on the quantum level [12–21]. In the present paper we will analyze the model of SU(2) Yang-Mills mechanics of spatially homogeneous fields for arbitrary theta angle. In order to obtain the equivalent unconstrained classical system in terms of gauge invariant variables only [22–35], we apply the method of Hamiltonian reduction (Ref. [35], and references therein) in the framework of the Dirac constraint formalism [36–38]. As in our recent work [11] the elimination of the pure gauge degrees of freedom is achieved by using the polar representation for the gauge potential, which trivializes the Abelianization of the Gauss law constraints, and finally projecting onto the constraint shell. The obtained unconstrained system then describes the dynamics of a symmetrical second rank tensor under spatial rotations. The main-axis transformation of this symmetric tensor allows us to separate the gauge invariant variables into scalars under ordinary space rotations and into ''rotational'' degrees of freedom. In this final form the physical Hamiltonian and the topological operator can be quantized without operator ordering ambiguities. We study the residual symmetries of the resulting unconstrained quantum theory with arbitrary theta angle and reduce the eigenvalue problem of the Hamiltonian to the corresponding problem with zero theta angle. The energy spectrum is found to be independent of the theta angle by construction of the explicit transformation relating the Hamiltonians with different theta parameter. Using the variational approach we calculate the low energy spectrum with rather high accuracy. In particular we find the energy eigenvalue and the magnetic and electric properties of the ground state, as well as the corresponding value of the ''gluon condensate.'' Explicit calculation of the Witten formula for the topological susceptibility using our variational results for the ground state and the low lying excitations gives strong support for the consistency of our results.

Our paper is organized as follows. In Sec. II the Hamiltonian reduction of SU(2) Yang-Mills mechanics for arbitrary theta angle is carried out and the corresponding unconstrained system put into a form where the rotational and the scalar degrees of freedom are maximally separated. In Sec. III the obtained unconstrained classical Hamiltonian is quantized, its residual symmetries, the necessary boundary condi-

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tions for the wave functions, and the relevance of the theta angle on the quantum level discussed. In Sec. IV the eigenvalue problem of the unconstrained Hamiltonian with vanishing theta angle is solved approximately in the low energy region using the variational approach. In Sec. V the Witten formula for the topological susceptibility is evaluated using the obtained variational results. Section VI finally gives our conclusions. Appendixes A–C state several results and additional discussions relevant to the main text.

II. UNCONSTRAINED CLASSICAL SU(2) YANG-MILLS MECHANICS WITH THE THETA ANGLE

A. Hamiltonian formulation

It is well known [1] that the theta angle can be included already at the level of the classical action

$$S[A]:=-\frac{1}{4}\int d^4x\left(F^a_{\mu\nu}F^{a\mu\nu}-\frac{\alpha_s\theta}{2\pi}F^a_{\mu\nu}\tilde{F}^{a\mu\nu}\right), \quad (2.1)$$

with the SU(2) Yang-Mills field strengths $F^a_{\mu\nu}:=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu+g\epsilon^{abc}A^b_\mu A^c_\nu$, $(a=1,2,3)$, the dual $\tilde{F}^a{}_{\mu\nu}:=1/2\,\epsilon_{\mu\nu\sigma\rho}F^{a\sigma\rho}$ and $\alpha_s=g^2/4\pi$. For the special case of spatially homogeneous fields the Lagrangian in Eq. (2.1) reduces to[1]

$$L=\frac{1}{2}(\dot{A}_{ai}-g\epsilon_{abc}A_{b0}A_{ci})^2-\frac{1}{2}B^2_{ai}-\frac{\alpha_s\theta}{2\pi}(\dot{A}_{ai}-g\epsilon_{abc}A_{b0}A_{ci})B_{ai}, \quad (2.2)$$

with the magnetic field $B_{ai}=(1/2)g\epsilon_{abc}\epsilon_{ijk}A_{bj}A_{ck}$. After the supposition of spatial homogeneity of the fields the SU(2) gauge invariance of the Yang-Mills action Eq. (2.1) reduces to the symmetry under the SO(3) local transformations

$$A_{a0}(t)\to A^\omega_{a0}(t)=O[\omega(t)]_{ab}A_{b0}(t)-\frac{1}{2g}\epsilon_{abc}\{O[\omega(t)]\dot{O}[\omega(t)]\}_{bc},$$

$$A_{ai}(t)\to A^\omega_{ai}(t)=O[\omega(t)]_{ab}A_{bi}(t), \quad (2.3)$$

and as a result the Lagrangian (2.2) is degenerate. From the calculation of the canonical momenta

$$P_a:=\partial L/\partial(\partial_0A_{a0})=0,$$

$$\Pi_{ai}:=\partial L/\partial(\partial_0A_{ai})=\dot{A}_{ai}-g\epsilon_{abc}A_{b0}A_{ci}-\frac{\alpha_s\theta}{2\pi}B_{ai}, \quad (2.4)$$

one finds that the phase space spanned by the variables (A_{a0},P_a) and (A_{ai},Π_{ai}) is restricted by the primary constraints $P_a=0$. The evolution of the system is governed by the total Hamiltonian [36] with three arbitrary functions $\lambda_a(t)$

$$H_T:=\frac{1}{2}\Pi^2_{ai}+\frac{1}{2}\left[1+\left(\frac{\alpha_s\theta}{2\pi}\right)^2\right]B^2_{ai}(A)+\theta Q(\Pi,A)-gA_{a0}\epsilon_{abc}A_{bi}\Pi_{ci}+\lambda_aP_a, \quad (2.5)$$

where the topological charge has been introduced

$$Q:=-\frac{\alpha_s}{2\pi}\Pi_{ai}B_{ai}. \quad (2.6)$$

Apart from the primary constraints $P^a=0$ the phase space is restricted also by the non-Abelian Gauss law, the secondary constraints

$$\Phi_a:=g\epsilon_{abc}A_{ci}\Pi_{bi}=0,\ \{\Phi_a,\Phi_b\}=g\epsilon_{abc}\Phi_c, \quad (2.7)$$

which follow from the maintenance of the primary constraints in time.

To overcome the problems of the existence of these constraints and the nonunique character of the dynamics governed by the total Hamiltonian (2.5) we will follow the method of Hamiltonian reduction to construct the unconstrained system with uniquely predictable dynamics. As in the recent paper [11] we shall use a special set of coordinates which is very suitable for the implementation of Gauss law constraints and the derivation of the physically relevant theory equivalent to the initial degenerate theory. This will be the subject of the following subsection.

B. Canonical transformation to adapted coordinates and projection to Gauss law constraint

The local symmetry transformation (2.3) of the gauge potentials A_{ai} prompts us with the set of coordinates in terms of which the separation of the gauge degrees of freedom occurs. As in Ref. [11] we use the polar decomposition for arbitrary 3×3 quadratic matrices [39]

$$A_{ai}(\chi,S)=O_{ak}(\chi)S_{ki}, \quad (2.8)$$

with the orthogonal matrix $O(\chi)$, parametrized by the three angles χ_i and the positive definite 3×3 symmetric matrix S. The representation (2.8) can be regarded as transformation from the gauge potentials A_{ai} to the set of coordinates χ_i and S_{ik}. The corresponding canonical conjugate momenta (p_{χ_i},P_{ik}) can be obtained using the generating function

$$F(\Pi;\chi,S)=\sum_{a,i}^{3}\Pi_{ai}A_{ai}(\chi,S)=\mathrm{tr}[\Pi^TO(\chi)S] \quad (2.9)$$

as

$$p_{\chi_j}=\frac{\partial F}{\partial\chi_j}=\sum_{a,s,i}^{3}\Pi_{ai}\frac{\partial O_{as}}{\partial\chi_j}S_{si}=\mathrm{tr}\left[\Pi^T\frac{\partial O}{\partial\chi_j}S\right], \quad (2.10)$$

[1]Everywhere in the paper we put the spatial volume $V=1$. As a result the coupling constant g becomes dimensionful with $g^{2/3}$ having the dimension of energy. The volume dependence can be restored in the final results by replacing g^2 by g^2/V.

$$P_{ik}=\frac{\partial F}{\partial S_{ik}}=\frac{1}{2}(O\Pi^T+\Pi O^T)_{ik}. \tag{2.11}$$

A straightforward calculation [11] yields the following expressions for the field strengths Π_{ai} in terms of the new canonical variables:

$$\Pi_{ai}=O_{ak}(\chi)\{P_{ki}+\epsilon_{kli}(s^{-1})_{lj}[(\Omega^{-1}(\chi)p_\chi)_j - \epsilon_{mjn}(PS)_{mn}]\}, \tag{2.12}$$

with

$$\Omega_{ij}(\chi):=\frac{1}{2}\epsilon_{\min}\left[\frac{\partial O^T(\chi)}{\partial\chi_j}O(\chi)\right]_{mn}, \tag{2.13}$$

and

$$s_{ik}:=S_{ik}-\delta_{ik}\mathrm{tr}\,S. \tag{2.14}$$

Using the representations (2.8) and (2.12) one can easily convince oneself that the variables S and P make no contribution to the Gauss law constraints (2.7)

$$\Phi_a:=O_{as}(\chi)\Omega^{-1}_{sj}(\chi)p_{\chi_j}=0. \tag{2.15}$$

Hence, assuming the invertibility of the matrix Ω, the non-Abelian Gauss law constraints are equivalent to the set of Abelian constraints

$$p_{\chi_a}=0. \tag{2.16}$$

After having rewritten the model in terms of adapted canonical pairs and after Abelianization of the Gauss law constraints (2.7) the construction of the unconstrained Hamiltonian system can be obtained as follows. The physical unconstrained Hamiltonian, defined as

$$H_\theta(S,P):=H_T|_{p_{\chi_a}=0},$$

takes the form

$$H_\theta=\frac{1}{2}\mathrm{tr}(\mathcal{E}^2)+\frac{g^2}{4}\left(1+\frac{\alpha_s^2}{4\pi^2}\theta^2\right)[\mathrm{tr}^2(S)^2-\mathrm{tr}(S)^4] + \theta Q(S,P), \tag{2.17}$$

where the ''physical'' electric field strengths $\mathcal{E}_{ai}$ are

$$\Pi_{ai}|_{\pi_a=0}=:O_{ak}(q)\mathcal{E}_{ki}(S,P), \tag{2.18}$$

and the topological charge

$$Q(S,P)=-\frac{\alpha_s}{2\pi}\mathrm{tr}(PS). \tag{2.19}$$

Using the representation (2.12) for the electric field one can express the $\mathcal{E}_{ai}$ in terms of the physical variables P and S

$$\mathcal{E}_{ki}(S,P)=P_{ik}+\frac{1}{\det s}(s\mathcal{M}s)_{ik}, \tag{2.20}$$

where $\mathcal{M}$ denotes the spin part of the angular momentum tensor of the initial gauge field

$$\mathcal{M}_{mn}:=(SP-PS)_{mn}. \tag{2.21}$$

Using Eq. (2.20) the unconstrained Yang-Mills Hamiltonian reads

$$H_\theta(S,P)=\frac{1}{2}\mathrm{tr}(P)^2+\frac{1}{2\det^2 s}\mathrm{tr}(s\mathcal{M}s)^2+\frac{g^2}{4}\left(1+\frac{\alpha_s^2}{4\pi^2}\theta^2\right) \times[\mathrm{tr}^2(S)^2-\mathrm{tr}(S)^4]+\theta Q(S,P). \tag{2.22}$$

C. Unconstrained Hamiltonian in terms of rotational and scalar degrees of freedom

In order to achieve a more transparent form for the reduced Yang-Mills system (2.22) it is convenient to decompose the positive definite symmetric matrix S as

$$S=R^T(\alpha,\beta,\gamma)D(x_1,x_2,x_3)R(\alpha,\beta,\gamma), \tag{2.23}$$

with the SO(3) matrix R parametrized by the three Euler angles (α,β,γ), and the diagonal matrix

$$D:=\mathrm{diag}(x_1,x_2,x_3). \tag{2.24}$$

Using the x_i and the Euler angles (α,β,γ) and the corresponding canonical momenta p_i and $p_\alpha,p_\beta,p_\gamma$ as the new set of canonical variables on the unconstrained phase space we get the following physical Hamiltonian:

$$H_\theta(x_i,p_i;\xi_i)=\frac{1}{2}\sum_{\mathrm{cyclic}}^{3}\left[p_i^2+\xi_i^2\frac{x_j^2+x_k^2}{(x_j^2-x_k^2)^2} + g^2\left(1+\frac{\alpha_s^2}{4\pi^2}\theta^2\right)x_j^2x_k^2\right]+\theta Q(p,x). \tag{2.25}$$

In Eq. (2.25) all rotational variables are combined into the quantities ξ_i

$$\xi_1:=\frac{\sin\gamma}{\sin\beta}p_\alpha+\cos\gamma p_\beta-\sin\gamma\cot\beta p_\gamma, \tag{2.26}$$

$$\xi_2:=-\frac{\cos\gamma}{\sin\beta}p_\alpha+\sin\gamma p_\beta+\cos\gamma\cot\beta p_\gamma, \tag{2.27}$$

$$\xi_3:=p_\gamma, \tag{2.28}$$

representing the SO(3) invariant Killing vectors with the Poisson brackets algebra

$$\{\xi_i,\xi_j\}=-\epsilon_{ijk}\xi_k. \tag{2.29}$$

The topological charge Q is independent of the rotational degrees of freedom and depends on the diagonal canonical pairs in the particularly simple cyclic form

$$Q=-g\frac{\alpha_s}{2\pi}(x_1x_2p_3+x_2x_3p_1+x_3x_1p_2). \tag{2.30}$$

This completes our reduction of the spatially homogeneous constrained Yang-Mills system with theta angle to the equivalent unconstrained system describing the dynamics of the physical degrees of freedom.

If we would restrict our consideration only to the classical level, the above generalization to arbitrary theta angle would be unnecessary, because the theta dependence enters the initial Lagrangian in the form of a total time derivative and thus the value of the theta angle has no influence on the classical equations of motion. In the Hamiltonian formulation one can easily verify that the theta dependence can be removed from the Hamiltonian H_θ by the canonical transformation to the new variables

$$\tilde{p}_i := p_i - g\frac{\alpha_s\theta}{2\pi}x_jx_k, \quad i,j,k \text{ cyclic},$$

$$\tilde{x}_i := x_i. \tag{2.31}$$

However, the transition to the quantum level requires a more careful treatment of the problem. It is necessary to clarify whether the operator corresponding to Eq. (2.31) acting on the quantum states is unitary. In subsequent sections we shall consider the quantum treatment of the obtained classical system and shall discuss the theta dependence of the vacuum in this model.

III. QUANTIZATION, SYMMETRIES AND BOUNDARY CONDITIONS

The Hamilton operator corresponding to Eq. (2.25) is obtained in the Schrödinger configuration representation by the conventional representation for the canonical momenta $p_k = -i\partial/\partial x_k$

$$H_\theta := \frac{1}{2}\sum_{\text{cyclic}}^{3}\left[-\frac{\partial^2}{\partial x_i^2}+\xi_i^2\frac{x_j^2+x_k^2}{(x_j^2-x_k^2)^2}+g^2\left(1+\frac{\alpha_s^2}{4\pi^2}\theta^2\right)x_j^2x_k^2\right] + \theta Q, \tag{3.1}$$

with the topological charge operator

$$Q = ig\frac{\alpha_s}{2\pi}\sum_{\text{cyclic}}^{3}x_ix_j\frac{\partial}{\partial x_k}, \tag{3.2}$$

and the intrinsic angular momenta ξ obeying the commutation relations

$$[\xi_i,\xi_j] = -i\epsilon_{ijk}\xi_k. \tag{3.3}$$

The transition to the quantum system in this adapted basis is free from operator ordering ambiguities.

As already mentioned in the last section the parameter theta is unphysical on the classical level, since it can be removed from Hamiltonian H_θ by the canonical transformation (2.31). One can easily convince oneself that the quantum Hamiltonians H_θ and $H_{\theta=0}$ can be related to each other via the transformation

$$H_\theta = U(\theta)H_{\theta=0}U^{-1}(\theta), \tag{3.4}$$

with

$$U(\theta) = \exp\left[ig\frac{\alpha_s}{2\pi}\theta x_1x_2x_3\right]. \tag{3.5}$$

The question is whether this operator is unitary in the domain of definition of the Hamiltonians H_θ and $H_{\theta=0}$, which is determined by their respective symmetries and the boundary conditions to be imposed on the corresponding wave functions.

A. Boundary conditions

Due to the positivity of the coordinates x_i in the polar decomposition (2.8) the configuration space is R_3^+ after the elimination of the pure gauge degrees of freedom. Thus the implementation of the canonical rules of quantization to the unconstrained classical system requires the specification of the boundary conditions both at positive infinity and on the three boundary planes $x_i=0$, $i=1,2,3$. The requirement of Hermiticity of the Hamiltonian H_θ (3.1) leads to the condition

$$\left(\Psi_\theta^*\partial_k\Phi_\theta-\partial_k\Psi_\theta^*\Phi_\theta+2ig\frac{\alpha_s}{2\pi}\theta x_ix_j\Psi_\theta^*\Phi_\theta\right)\Big|_{x_k=0}=0, \quad i,j,k \text{ cyclic}. \tag{3.6}$$

Using the relation $\Psi_\theta = U(\theta)\Psi_{\theta=0}$ with $U(\theta)$ given in Eq. (3.5), this reduces to the corresponding requirement of Hermiticity of $H_{\theta=0}$

$$(\Psi_{\theta=0}^*\partial_k\Phi_{\theta=0}-\partial_k\Psi_{\theta=0}^*\Phi_{\theta=0})|_{x_k=0}=0, \quad i,j,k \text{ cyclic}. \tag{3.7}$$

It is satisfied for (κ arbitrary c number)

$$(\partial_k\Psi_{\theta=0}+\kappa\Psi_{\theta=0})|_{x_k=0}=0, \quad k=1,2,3, \tag{3.8}$$

which includes the two limiting cases of vanishing wave function ($\kappa\to\infty$) or vanishing derivative of the wave function ($\kappa=0$) at the boundary. The requirement of the Hermiticity of the momentum operators in the Schrödinger configuration representation $p_i := -i\partial/\partial x_i$ on R_3^+ requires the wave function to obey the boundary conditions

$$\Psi_{\theta=0}|_{x_i=0}=0, \quad i=1,2,3, \tag{3.9}$$

$$\Psi_{\theta=0}|_{x_i\to\infty}=0, \quad i=1,2,3. \tag{3.10}$$

In particular, they also imply the Hermiticity and the existence of a real eigenspectrum of the topological charge operator Q. Its eigenstates, however, given explicitly in Appendix A, do not satisfy the boundary conditions (3.9) and

(3.10), similar to the eigenstates of the momentum operator $-i\partial/\partial x_i$. Furthermore, it is interesting to note that the characteristics of the Q operator coincide with the Euclidean self-(anti)dual zero-energy solutions of the classical equations of motion. They are the analogues of the instanton solutions, but do not correspond to quantum tunneling between different vacua (see Appendix A).

B. Symmetries of the Hamiltonians H_θ and $H_{\theta=0}$

As a relic of the rotational invariance of the initial gauge field theory the Hamiltonian (3.1) possesses the symmetry

$$[H_\theta, J_k]=0, \tag{3.11}$$

where $J_i=R_{ij}\xi_j$ are the spin part of the generators of the angular momentum of Yang-Mills fields satisfying the so(3) algebra

$$[J_i, J_j]=i\epsilon_{ijk}J_k, \tag{3.12}$$

and commuting with the intrinsic angular momenta, $[J_i, \xi_j]=0$. Hence the eigenstates can be classified according to the quantum numbers J and M as the eigenvalues of the spin $\vec{J}^2=J_1^2+J_2^2+J_3^2$ and J_3. The Hilbert spaces of states with different spin J are each invariant subspaces under the action of all generators J_i and can therefore be considered as separate eigenvalue problems.

Apart from this continuous rotational symmetry the Hamiltonians H_θ and $H_{\theta=0}$ possess the following discrete symmetries. Both $H_{\theta=0}$ and Q are invariant under arbitrary permutations of any two of the variables $\sigma_{ij}x_i=x_j\sigma_{ij}$, $\sigma_{ij}p_i=p_j\sigma_{ij}$

$$[H_{\theta=0}, \sigma_{ij}]=0, \quad [Q, \sigma_{ij}]=0. \tag{3.13}$$

However, under time reflections $Tx_i=x_iT$, $Tp_i=-p_iT$, as well as under parity reflections $\mathcal{P}x_i=-x_i\mathcal{P}$, $\mathcal{P}p_i=-p_i\mathcal{P}$, $H_{\theta=0}$ commutes with T and $\mathcal{P}$,

$$[H_{\theta=0}, T]=0, \quad [H_{\theta=0}, \mathcal{P}]=0, \tag{3.14}$$

but Q anticommutes with T and $\mathcal{P}$,

$$QT=-TQ, \quad Q\mathcal{P}=-\mathcal{P}Q. \tag{3.15}$$

Hence for the $H_{\theta=0}$ Schrödinger eigenvalue problem we can restrict to the Hilbert space of real and parity odd wave functions which automatically satisfy the boundary conditions (3.9). Observe that the transformation (3.5) leads out of the corresponding Hilbert space and is therefore not unitary.

C. Independence of the energy spectrum of the theta angle

Due to the relation (3.4) between the Hamiltonians H_θ, and $H_{\theta=0}$ and the corresponding compatibility of the boundary conditions discussed above the energy spectrum should be independent of the theta angle. In particular the topological susceptibility of the vacuum should vanish. Using the Witten formula [40,41], the topological susceptibility can be represented as the sum of a propagator term involving the transition matrix elements of the topological operator Q and a contact term proportional to the vacuum expectation value of the square of the magnetic field. Independence of the ground state energy of the theta angle and hence vanishing topological susceptibility should therefore imply

$$\left.\frac{d^2E_0(\theta)}{d\theta^2}\right|_{\theta=0} = -2\sum_n \frac{\langle 0|Q|n\rangle|^2}{E_n-E_0} + \langle 0|\left(\frac{\alpha_s}{2\pi}\right)^2 B^2|0\rangle = 0, \tag{3.16}$$

where $|n\rangle$ are eigenstates of the Hamiltonian $H_{\theta=0}$ with energy eigenvalues E_n. As we shall see below, our calculation of the low energy part of the spectrum of $H_{\theta=0}$ using the variational technique is in full accordance with Eq. (3.16).

IV. SCHRÖDINGER EIGENVALUE PROBLEM FOR VANISHING THETA

A. Low energy spin-0 spectrum from variational calculation

The Hilbert space of states with zero spin $\vec{J}^2=0$ is an invariant subspace under the action of all generators J_i and one can consider the eigenvalue problem separately from states characterized by higher spin value. Thus in the sector of zero spin $\vec{J}^2=\vec{\xi}^2=0$ the Schrödinger eigenvalue problem (3.1) reduces to

$$H_0\Psi_E \equiv \frac{1}{2}\sum_{\text{cyclic}}^{3}\left[-\frac{\partial^2}{\partial x_i^2}+g^2x_j^2x_k^2\right]\Psi_E=E\Psi_E. \tag{4.1}$$

We shall use the boundary conditions (3.9) and (3.10). Already a long time ago it has been proven by Rellich [42] that Hamiltonians of the type (4.1) have a discrete spectrum due to quantum fluctuations, although the classical problem allows for scattering trajectories (see discussion in Ref. [12]). Related and simplified versions of the eigenvalue problem (4.1) have been studied extensively by many authors using different methods [12–20]. In particular, in Refs. [14,15] the eigenstates and eigenvalues have been found in the semiclassical approximation for the special two dimensional case $x_3=0$.[2]

To obtain the approximate low energy spectrum of the Hamiltonian in the spin-0 sector we will use the Rayleigh-Ritz variational method [46] based on the minimization of the energy functional

[2]It is interesting that for the three-dimensional case one can write the potential term in Eq. (4.1) in the form $V=\Sigma_{i=1}^3(\partial_i W)^2$ with the ''superpotential'' $W(x_1,x_2,x_3)=x_1x_2x_3$. Note that in the simplified two-dimensional case there is no such superpotential. The two-dimensional superpotential $W^{(2)}=xy$ corresponds to the two-dimensional harmonic oscillator $V^{(2)}=x^2+y^2$. From the form of the superpotential it follows that the wave function $\Psi_0=\exp[-gW]$ solves the Schrödinger eigenvalue problem with energy eigenvalue $E=0$. It is the unconstrained, strong coupling form of the well-known exact but non-normalizable zero-energy solution [43] of the Schrödinger equation of Yang-Mills field theory. Obviously it is also not satisfying the boundary conditions (3.9), (3.10) and has to be disregarded as a false ground state.

$$\mathcal{E}[\Psi] := \frac{\langle\Psi|H_0|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{4.2}$$

The key moment in all variational calculations is the choice of the trial functions. Guided by the harmonic oscillator form of the valleys of the potential in Eq. (4.1) close to the bottom a simple first choice for a trial function compatible with the boundary conditions (3.9) and (3.10) is to use [21] the lowest state of three harmonic quantum oscillators on the positive half line

$$\Psi_{000} = 8\prod_{i=1}^{3}\left(\frac{\omega_i}{\pi}\right)^{1/4}\sqrt{\omega_i}x_i e^{-\omega_i x_i^2/2}. \tag{4.3}$$

The stationarity conditions for the energy functional of this state,

$$\mathcal{E}[\Psi_{000}] = \sum_{\text{cyclic}}^{3}\left(\frac{3}{4}\omega_i + \frac{9}{8}g^2\frac{1}{\omega_j\omega_k}\right),$$

lead to the isotropic optimal choice

$$\omega := \omega_1 = \omega_2 = \omega_3 = 3^{1/3}g^{2/3}. \tag{4.4}$$

As a first upper bound for the ground-state energy of the Hamiltonian we therefore find

$$E_0 \leqslant \mathcal{E}[\Psi_{000}] = \frac{27}{8}3^{1/3}g^{2/3} = 4.8676\ g^{2/3}. \tag{4.5}$$

The upper bound (4.5) is in agreement with the lower bound of the energy functional for separable functions

$$\mathcal{E}[\Psi_{\text{sep}}] \geqslant 4.5962\ g^{2/3}, \tag{4.6}$$

derived in Appendix B.

In order to improve the upper bound for the ground-state energy of the Hamiltonian H_0 we extend the space of trial functions (4.3) and consider the Fock space of the orthonormal set of products

$$\Psi_{n_1n_2n_3} := \prod_{i=1}^{3}\Psi_{n_i}(\omega, x_i), \tag{4.7}$$

of the odd eigenfunctions of the harmonic oscillator

$$\Psi_n(\omega,x) := \frac{(\omega/\pi)^{1/4}}{\sqrt{2^{2n}(2n+1)!}}e^{-\omega x^2/2}H_{2n+1}(\sqrt{\omega}x),$$

with the frequency fixed by Eq. (4.4).

Furthermore the variational procedure becomes much more effective, if the space of trial functions is decomposed into the irreducible representations of the residual discrete symmetries of the Hamiltonian (4.1). As has been discussed in Sec. III B, it is invariant under arbitrary permutations of any two of the variables $\sigma_{ij}x_i = x_j\sigma_{ij}$, $\sigma_{ij}p_i = p_j\sigma_{ij}$ and under time reflections $Tx_i = x_iT$, $Tp_i = -p_iT$,

$$[H_0, \sigma_{ij}] = 0, \quad [H_0, T] = 0.$$

We shall represent these by the permutation operator σ_{12}, the cyclic permutation operator σ_{123} and the time reflection operator T, whose action on the states is

$$\sigma_{123}\Psi(x_1,x_2,x_3) = \Psi(x_2,x_3,x_1),$$

$$\sigma_{12}\Psi(x_1,x_2,x_3) = \Psi(x_2,x_1,x_3),$$

$$T\Psi(x_1,x_2,x_3) = \Psi^*(x_1,x_2,x_3),$$

and decompose the Fock space spanned by the functions (4.7) into the irreducible representations of the permutation group and time reflection T. For given (n_1,n_2,n_3) we define

$$\Psi^{(0)+}_{nnn} := \Psi_{nnn}, \tag{4.8}$$

if all three indices are equal (type I), the three states ($m = -1,0,1$)

$$\Psi^{(m)+}_{nns} := \frac{1}{\sqrt{3}}\sum_{k=0}^{2} e^{-2km\pi i/3}(\sigma_{123})^k\Psi_{nns}, \tag{4.9}$$

when two indices are equal (type II), and the two sets of three states ($m = -1,0,1$)

$$\Psi^{(m)\pm}_{n_1n_2n_3} := \frac{1}{\sqrt{6}}\sum_{k=0}^{2} e^{-2km\pi i/3}(\sigma_{123})^k(1\pm\sigma_{12})\Psi_{n_1n_2n_3}, \tag{4.10}$$

if all (n_1,n_2,n_3) are different (type III). In this new orthonormal set of irreducible basis states $\Psi^{(m)\alpha}_{\mathbf{N}}$, the Fock representation of the Hamiltonian H_0 reads

$$H_0 = \sum |\Psi^{(m)\alpha}_{\mathbf{M}}\rangle\langle\Psi^{(m)\alpha}_{\mathbf{M}}|H_0|\Psi^{(m)\alpha}_{\mathbf{N}}\rangle\langle\Psi^{(m)\alpha}_{\mathbf{N}}|.$$

The basis states $\Psi^{(m)\alpha}_{\mathbf{N}}$ are eigenfunctions of σ_{123} and $\sigma_{12}T$

$$\sigma_{123}\Psi^{(m)\pm}_{\mathbf{N}} = e^{2m\pi i/3}\Psi^{(m)\pm}_{\mathbf{N}},$$

$$\sigma_{12}T\Psi^{(m)\pm}_{\mathbf{N}} = \pm\Psi^{(m)\pm}_{\mathbf{N}}. \tag{4.11}$$

Under σ_{12} and T separately, however, they transform into each other

$$\sigma_{12}\Psi^{(m)\pm}_{\mathbf{N}} = \pm\Psi^{(-m)\pm}_{\mathbf{N}},$$

$$T\Psi^{(m)\pm}_{\mathbf{N}} = \Psi^{(-m)\pm}_{\mathbf{N}}.$$

We therefore have the following irreducible representations. The singlet states $\Psi^{(0)+}$, the ''axial'' singlet states $\Psi^{(0)-}$, the doublets $(\Psi^{(+1)+};\Psi^{(-1)+})$ and the ''axial'' doublets $(\Psi^{(+1)-};\Psi^{(-1)-})$. Since the partner states of the doublets transform into each other under the symmetry operations σ_{12} or T, the corresponding values of the energy functional are equal.

The energy matrix elements of the irreducible states can then be expressed in terms of the basic matrix elements as given in Appendix C. Because of this decomposition of the Fock space into the irreducible sectors, the variational ap-

proach allows us to give upper bounds for states in each sector. The values of the energy functional for the states in each irreducible sector with the smallest number of knots $\mathcal{E}[\Psi_{000}^{(0)+}]=4.8676\ g^{2/3}$, $\mathcal{E}[\Psi_{100}^{(\pm1)+}]=7.1915\ g^{2/3}$, $\mathcal{E}[\Psi_{012}^{(0)-}]=13.8817\ g^{2/3}$, and $\mathcal{E}[\Psi_{012}^{(\pm1)-}]=15.6845\ g^{2/3}$ give first upper bounds for the lowest energy eigenvalues of the singlet, the doublet, the axial singlet, and the axial doublet states.

In order to improve the upper bounds for each irreducible sector, we truncate the Fock space at a certain number of knots of the wave functions and search for the corresponding states in the truncated space with the lowest value of the energy functional. We achieve this by diagonalizing the corresponding truncated Hamiltonian $H_{\rm trunk}$ to find its eigenvalues and eigenstates. Due to the orthogonality of the truncated space to the remaining part of Fock space the value of the energy functional (4.2) for the eigenvectors of $H_{\rm trunk}$ coincides with the $H_{\rm trunk}$ eigenvalues.

Including all states in the singlet sector with up to 5 knots we find rapid convergence to the following energy expectation values for the three lowest states S_1, S_2, S_3:

$$\mathcal{E}[S_1]=4.8067\ g^{2/3}(4.8070\ g^{2/3}),$$
$$\mathcal{E}[S_2]=8.2515\ g^{2/3}(8.2639\ g^{2/3}),$$
$$\mathcal{E}[S_3]=9.5735\ g^{2/3}(9.6298\ g^{2/3}), \tag{4.12}$$

where the numbers in brackets show the corresponding result when including only states up to 4 knots into the variational calculation. The lowest state S_1, given explicitly as

$$\begin{aligned} S_1 = {} & 0.9946\Psi_{000}^{(0)+} + 0.0253\Psi_{001}^{(0)+} - 0.0217\Psi_{002}^{(0)+} \\ & - 0.0970\Psi_{110}^{(0)+} - 0.0005\Psi_{003}^{(0)+} - 0.0033\Psi_{012}^{(0)+} \\ & - 0.0146\Psi_{111}^{(0)+} - 0.0005\Psi_{004}^{(0)+} + 0.0040\Psi_{013}^{(0)+} \\ & - 0.0080\Psi_{220}^{(0)+} - 0.0038\Psi_{112}^{(0)+} + 0.0001\Psi_{005}^{(0)+} \\ & - 0.0004\Psi_{014}^{(0)+} + 0.0011\Psi_{023}^{(0)+} - 0.0004\Psi_{113}^{(0)+} \\ & + 0.0031\Psi_{221}^{(0)+}, \end{aligned} \tag{4.13}$$

nearly coincides with the state $\Psi_{000}^{(0)+}$, the contributions of the other states are quite small. Similarly including all states in the doublet sector with up to 6(5) knots the following energy expectation values for the three lowest states $D_1^{(\pm1)}, D_2^{(\pm1)}, D_3^{(\pm1)}$

$$\mathcal{E}[D_1^{(\pm1)}]=7.1682\ g^{2/3}(7.1689\ g^{2/3}),$$
$$\mathcal{E}[D_2^{(\pm1)}]=9.6171\ g^{2/3}(9.6394\ g^{2/3}),$$
$$\mathcal{E}[D_3^{(\pm1)}]=10.9903\ g^{2/3}(10.9951\ g^{2/3}) \tag{4.14}$$

have been obtained. Including all states in the axial singlet sector with up to 8(7) knots we find the following energy expectation values for the three lowest states A_1, A_2, A_3

$$\mathcal{E}[A_1]=13.2235\ g^{2/3}(13.2275\ g^{2/3}),$$
$$\mathcal{E}[A_2]=16.6652\ g^{2/3}(16.7333\ g^{2/3}),$$
$$\mathcal{E}[A_3]=19.1470\ g^{2/3}(19.3028\ g^{2/3}). \tag{4.15}$$

Finally taking into account all states in the axial doublet sector with up to 8(7) knots we find the following energy expectation values for the three lowest states $C_1^{(\pm1)}, C_2^{(\pm1)}, C_3^{(\pm1)}$

$$\mathcal{E}[C_1^{(\pm1)}]=14.8768\ g^{2/3}(14.8796\ g^{2/3}),$$
$$\mathcal{E}[C_2^{(\pm1)}]=17.6648\ g^{2/3}(17.6839\ g^{2/3}),$$
$$\mathcal{E}[C_3^{(\pm1)}]=19.9019\ g^{2/3}(19.9914\ g^{2/3}). \tag{4.16}$$

We therefore obtain rather good estimates for the energies of the lowest states in the spin-0 sector. Extending to higher and higher numbers of knots in each sector we should be able to obtain the low energy spectrum in the spin-zero sector to arbitrarily high numerical accuracy.

In summary comparing our results for the first few states in all sectors, we find that the lowest state appears in the singlet sector with energy

$$E_0=4.8067\ g^{2/3}, \tag{4.17}$$

with expected accuracy up to three digits after the dot. Its explicit form is given in Eq. (4.13) to the accuracy considered. For comparison with other work we remark that due to our boundary condition (3.9) all our spin-0 states correspond to the 0^- sector in the work of Ref. [16] where a different gauge invariant representation of Yang-Mills mechanics has been used. Their state of lowest energy in this sector is $9.52\ g^{2/3}$. Furthermore in Ref. [20], using an analogy of SU(N) Yang-Mills quantum mechanics in the large N limit to membrane theory, obtain the energy values $6.4690\ g^{2/3}$ and $19.8253\ g^{2/3}$ for the ground state and the first excited state.

The expectation values for the squares of the electric and the magnetic fields for the ground state (4.13) are found to be

$$\langle 0|E^2|0\rangle=6.4234\ g^{2/3},\ \ \langle 0|B^2|0\rangle=3.1900\ g^{2/3}, \tag{4.18}$$

and the value for the ''gluon condensate'' is therefore

$$\langle 0|G^2|0\rangle := 2(\langle 0|B^2|0\rangle - \langle 0|E^2|0\rangle) = -6.4669\ g^{2/3}. \tag{4.19}$$

These results are expected to be accurate up to three digits after the dot. Hence the variational calculation shows that the vacuum is not self-(anti)dual and that a nonperturbative ''gluon condensate'' appears.

B. Higher spin states

For the discussion of the eigenstates of the Hamiltonian $H_{\theta=0}$ with arbitrary spin we write

$$H_{\theta=0}=H_0+H_{\rm spin} \tag{4.20}$$

with the spin-0 Hamiltonian (4.1) discussed in the last subsection and the spin dependent part

$$H_{\rm spin}=\frac{1}{2}\sum_{i=1}^{3}\xi_i^2 V_i,\quad V_i:=\frac{x_j^2+x_k^2}{(x_j^2-x_k^2)^2},\quad i,j,k \text{ cyclic}. \tag{4.21}$$

Introducing the lowering and raising operators $\xi_\pm:=\xi_1\pm i\xi_2$, the spin dependent part $H_{\rm spin}$ of the Hamiltonian (4.20) can be written in the form

$$H_{\rm spin}=\frac{1}{8}(\xi_+^2+\xi_-^2)(V_1-V_2)+\frac{1}{8}(\xi_+\xi_-+\xi_-\xi_+)(V_1+V_2)+\frac{1}{2}\xi_3^2 V_3. \tag{4.22}$$

Since the Hamiltonian (4.20) commutes with $\vec{J}^2$ and J_3, the energy eigenfunctions Ψ_{JM} can be characterized by the two quantum numbers J and M. Furthermore we shall expand the wave function Ψ_{JM} in the basis of the well-known D functions [44], which are the common eigenstates of the operators $\vec{J}^2=\vec{\xi}^2$, J_3, and ξ_3 with the eigenvalues J, M, and k, respectively,

$$\Psi_{JM}(x_1,x_2,x_3;\alpha,\beta,\gamma)=\sum_{k=-J}^{J} i^J\sqrt{\frac{2J+1}{8\pi^2}}\times\Psi_{JMk}(x_1,x_2,x_3)D^{(J)}_{kM}(\alpha,\beta,\gamma), \tag{4.23}$$

where (α,β,γ) are the Euler angles. We have the relations

$$\xi_3 D^{(J)}_{kM}=kD^{(J)}_{kM},\quad \xi_\pm D^{(J)}_{kM}=\sqrt{(J\pm k+1)(J\mp k)}D^{(J)}_{k\pm 1\,M}. \tag{4.24}$$

The task to find the spectrum of the Hamiltonian (4.20) then reduces to the following eigenvalue problem for the expansion coefficients Ψ_{JMk} for fixed values of J and M

$$\sum_{k=-J}^{J}\left[(H_0-E)\delta_{k',k}+(-1)^J(2J+1)\times\int\frac{\sin\beta\, d\alpha\, d\beta\, d\gamma}{8\pi^2}D^{(J)*}_{k'M}(\alpha,\beta,\gamma)H_{\rm spin}D^{(J)}_{kM}(\alpha,\beta,\gamma)\right]\times\Psi_{JMk}=0. \tag{4.25}$$

Since the spin part $H_{\rm spin}$ of the Hamiltonian does not commute with ξ_3, nondiagonal terms arise, coupling different values of k. We shall in the following limit ourselves to the case of spin-1. Using the linear combinations [45]

$$\Psi_1(x_1,x_2,x_3):=\frac{1}{\sqrt{2}}[\Psi_{J=1,M,k=1}(x_1,x_2,x_3)-\Psi_{J=1,M,k=-1}(x_1,x_2,x_3)], \tag{4.26}$$

$$\Psi_2(x_1,x_2,x_3):=\frac{1}{\sqrt{2}}[\Psi_{J=1,M,k=1}(x_1,x_2,x_3)+\Psi_{J=1,M,k=-1}(x_1,x_2,x_3)], \tag{4.27}$$

$$\Psi_3(x_1,x_2,x_3):=\Psi_{J=1,M,k=0}(x_1,x_2,x_3), \tag{4.28}$$

the corresponding eigenvalue problem (4.25) for spin-1 decouples to the following three Schrödinger equations for the wave functions $\Psi_a(x_1,x_2,x_3)$:

$$\left[-\frac{1}{2}\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2}+\frac{g^2}{2}\sum_{i<j}x_i^2x_k^2+V_a^{\rm eff}(x_1,x_2,x_3)\right]\Psi_a(x)=E\Psi_a(x),\quad a=1,2,3, \tag{4.29}$$

with the effective potential

$$V_a^{\rm eff}(x_1,x_2,x_3):=\frac{1}{2}(V_b+V_c)=\frac{1}{2}\left(\frac{x_a^2+x_c^2}{(x_a^2-x_c^2)^2}+\frac{x_a^2+x_b^2}{(x_a^2-x_b^2)^2}\right),\quad a,b,c \text{ cyclic}. \tag{4.30}$$

In the spin-1 sector we have therefore succeeded to reduce the Schrödinger equation to three effective Schrödinger equations for the scalar degrees of freedom with an additional effective potential induced by the rotational degrees of freedom. Since the effective potentials $V_i^{\rm eff}$ are related via cyclic permutation

$$\sigma_{123}V_1^{\rm eff}=V_2^{\rm eff}\sigma_{123},\quad \sigma_{123}V_2^{\rm eff}=V_3^{\rm eff}\sigma_{123},\quad \sigma_{123}V_3^{\rm eff}=V_1^{\rm eff}\sigma_{123}, \tag{4.31}$$

all energy levels in the spin-1 sector are threefold degenerate.

As in the spin-0 sector we may use the variational approach to obtain an upper bound for the lowest spin-1 state. The variational ansatz

$$\Psi_a(x_1,x_2,x_3):=(x_a^2-x_b^2)(x_a^2-x_c^2)\prod_{i=1}^{3}\Psi_0(\omega_i^{(a)},x_i) \tag{4.32}$$

satisfies both the boundary conditions (3.9) and (3.10) and vanishes at the singularities of the additional effective spin-1 potential $V_{\rm eff}$. For the optimal values

$$\omega_i^{(a)}=1.1814\ g^{2/3},\quad \omega_b^{(a)}=\omega_c^{(a)}=2.34945\ g^{2/3}, \tag{4.33}$$

we obtain the energy minimum

$$E_{\rm spin-1}=8.6044\ g^{2/3}. \tag{4.34}$$

Analogous treatments of higher spin states can be carried out correspondingly. Using the linear combinations [45]

$$\Psi^{\pm}_{J|k|}(x_1,x_2,x_3) := \frac{1}{\sqrt{2}}[\Psi_{J,M,k}(x_1,x_2,x_3) \pm \Psi_{J,M,-k}(x_1,x_2,x_3)], \quad k \neq 0, \tag{4.35}$$

$$\Psi_{J0}(x_1,x_2,x_3) := \Psi_{J,M,k=0}(x_1,x_2,x_3), \tag{4.36}$$

and noting that there are no transitions between the states $\Psi^{\pm}_{J|k|}$ with even and odd k, and with $+$ and $-$ index, the corresponding eigenvalue problem (4.25) for spin J decouples into four separate Schrödinger eigenvalue problems. For spin-2 one finds one cyclic triplet of degenerate eigenstates and two singlets under cyclic permutation, for spin-3 two cyclic triplets each consisting of three degenerate states and one singlet, and so on. The corresponding reduction on the classical level using the integrals of motion (3.11) has been done in Ref. [11].

We conclude this subsection by pointing out that our variational result (4.34) shows that the higher spin states appear already at rather low energies and therefore have to be taken into account in calculations of the low energy spectrum of Yang-Mills theories.

V. CALCULATION OF THE TOPOLOGICAL SUSCEPTIBILITY

The explicit evaluation of the Witten formula (3.16) for the topological susceptibility allows us to check the consistency of the results for the low energy spectrum obtained in Sec. IV using the variational approach.

Using the ground state S_1 in Eq. (4.13), obtained from minimization of the energy functional in the singlet sector including irreducible states with up to 5 knots, and the expressions for the matrix elements of B^2 in the basis of irreducible states given in Appendix C, we obtain

$$\left.\frac{d^2E_0(\theta)}{d\theta^2}\right|^{\text{contact}}_{\theta=0} = +\left\langle 0\left|\left(\frac{\alpha_s}{2\pi}\right)^2 B^2\right|0\right\rangle = +0.0005117\, g^{14/3}(+0.0005119\, g^{14/3}) \tag{5.1}$$

for the contact term in the Witten formula. The number in brackets gives the corresponding result for up to 4 knots.

Since the Q operator is a spin-0 operator and symmetric under cyclic permutations, the propagator term involves only the singlet states in the spin-0 sector. Using the formula for the matrix elements of the topological operator Q stated in Appendix C and including the lowest fifteen (ten) excitations $S_2,\ldots,S_{16}$ $(S_2,\ldots,S_{11})$ obtained approximately in the variational calculation as eigenvectors of the truncated Fock space including irreducible singlet states up to 5 knots (4 knots), we obtain[3]

$$\left.\frac{d^2E_0(\theta)}{d\theta^2}\right|^{\text{prop}}_{\theta=0} = -2\sum_n \frac{\langle 0|Q|n\rangle|^2}{E_n - E_0} = -0.0004819\, g^{14/3}\ (-0.0004622\, g^{14/3}). \tag{5.2}$$

We see that the sum of the contact contribution (5.1) and the propagator contribution (5.2) seem to tend to zero when extending the variational calculation to Fock states of higher and higher number of knots. For comparison we point out that using the irreducible singlet states $\Psi^{(0)+}_{000}, \Psi^{(0)+}_{001}, \ldots,$ up to 5 knots (4 knots) in Eqs. (4.8)–(4.10) directly, instead of the eigenstates $S_1,S_2,\ldots,S_{16}$ $(S_1,S_2,\ldots,S_{11})$, we get $-0.0005205\, g^{14/3}$ for the contact contribution (5.1) and $-0.0003808\, g^{14/3}$ $(-0.0003761\, g^{14/3})$ for the propagator contribution (5.2). We herewith find strong support that our variational results are in accordance with vanishing topological susceptibility (3.16).

VI. CONCLUDING REMARKS

In this paper we have analyzed the quantum mechanics of spatially homogeneous gauge invariant SU(2) gluon fields with theta angle. We have reduced the eigenvalue problem of the Hamiltonian of this toy model for arbitrary theta angle to the corresponding problem with zero theta angle. The energy spectrum has been found to be independent of the theta angle by construction of the explicit transformation relating the Hamiltonians with different theta parameter. The ground state, its energy eigenvalue, its magnetic and electric properties, as well as the corresponding value of the ''gluon condensate'' and the lowest excitations have been obtained with high accuracy using the variational approach. Furthermore it has been shown that higher spin states become already relevant at rather low energy. Explicit calculation of the Witten formula for the topological susceptibility using our variational results for the ground state and the low lying excitations gives strong support for the consistency of our results. We have found a continuous spectrum and the corresponding eigenstates of the topological operator in this approximation and shown that its characteristics coincide with the Euclidean self-(anti)dual zero-energy solutions of the classical equations of motion. They are the analogues of the instanton solutions, but do not correspond to quantum tunneling be-

[3]Here the lowest six excitations $S_2,\ldots,S_7$ are found to give the contributions $-103.3\times10^{-6}\, g^{14/3}$ $(-107.7\times10^{-6}\, g^{14/3})$, $-201.6\times10^{-6}\, g^{14/3}$ $(-205.3\times10^{-6}\, g^{14/3})$, $-124.1\times10^{-6}\, g^{14/3}$ $(-120.4\times10^{-6}\, g^{14/3})$, $-8.8\times10^{-6}\, g^{14/3}$ $(-9.3\times10^{-6}\, g^{14/3})$, $-27.3\times10^{-6}\, g^{14/3}$ $(-18.4\times10^{-6}\, g^{14/3})$, and $-0.16\times10^{-6}\, g^{14/3}$ $(-4.1\times10^{-6}\, g^{14/3})$, respectively. The contributions from the remaining higher excitations $S_8,\ldots,S_{16}$ $(S_8,\ldots,S_{11}$ for up to 4 knots) are of the order of 5×10^{-6} or less and form a series which is rapidly decreasing with the number of knots.

tween different vacua. The generalization of these investigations to SU(2) field theory following Ref. [34] is under present investigation.

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APPENDIX A: TOPOLOGICAL CHARGE OPERATOR, ZERO-ENERGY SOLUTIONS OF THE CLASSICAL EUCLIDEAN EQUATIONS OF MOTION AND TUNNELING AMPLITUDES

In this appendix the solution of the eigenvalue problem for the topological charge operator is described and the relation between its characteristics and the Euclidean zero energy trajectories of the unconstrained Hamiltonian (2.25) discussed. We shall also discuss the role of these Euclidean zero energy solutions of the classical equations of motion to tunneling from one valley to another.

1. The eigenvalue problem for the Q operator

The eigenvalue problem for the topological charge operator

$$Q|\Psi(t)\rangle_\lambda=\lambda|\Psi(t)\rangle_\lambda \tag{A1}$$

in the Schrödinger representation reduces to the solution for the following linear partial differential equation:

$$x_1x_2\frac{\partial}{\partial x_3}\Psi_\lambda(x_1,x_2,x_3)+x_2x_3\frac{\partial}{\partial x_1}\Psi_\lambda(x_1,x_2,x_3)+x_3x_1\frac{\partial}{\partial x_2}\Psi_\lambda(x_1,x_2,x_3)=-i\frac{8\pi^2}{g^3}\lambda\Psi_\lambda(x_1,x_2,x_3). \tag{A2}$$

The conventional method of characteristics relates this problem to the solution of the set of ordinary differential equations

$$\frac{dx_1}{x_2x_3}=\frac{dx_2}{x_3x_1}=\frac{dx_3}{x_2x_1}. \tag{A3}$$

The integral curves corresponding to Eq. (A3) can be written in the form

$$I_1=x_2^2-x_1^2,\quad I_2=x_3^2-x_1^2. \tag{A4}$$

These integral curves prompts us with the introduction of the new adapted coordinates (ζ,η,ρ)

$$\zeta:=x_1,\quad \eta:=x_2^2-x_1^2,\quad \rho:=x_3^2-x_1^2. \tag{A5}$$

Such functions can be used as suitable coordinates on the subset

$$0<x_1<x_2<x_3<\infty \tag{A6}$$

of the whole configuration space R_3^+. The subset (A6) corresponds to the domain $0<\zeta<\sqrt{\eta+\zeta^2}<\sqrt{\rho+\zeta^2}$. Because of the symmetry of the Q operator under arbitrary permutations of the canonical pairs x_i,p_i the results can be extended to the whole R_3^+.

Writing the wave function in terms of new variables

$$\Psi_\lambda(x_1,x_2,x_3)=:W_\lambda(\zeta,\eta,\rho) \tag{A7}$$

the partial differential equation (A2) reduces to the following ordinary differential equation:

$$\sqrt{\zeta^2+\eta}\sqrt{\zeta^2+\rho}\,\frac{\partial}{\partial\zeta}W_\lambda(\zeta,\eta,\rho)=-i\lambda\frac{8\pi^2}{g^3}W_\lambda(\zeta,\eta,\rho). \tag{A8}$$

The general solution of this equation can be written in the form

$$W_\lambda(\zeta,\eta,\rho)=\Psi_0(\eta,\rho)\times\exp\left\{i\lambda\frac{8\pi^2}{g^3\sqrt{\rho}}F\left[\arctan\left(\frac{\zeta}{\sqrt{\eta}}\right),\sqrt{\frac{\rho-\eta}{\rho}}\right]\right\} \tag{A9}$$

with the arbitrary function $\Psi_0(\eta,\rho)$ and the Jacobi elliptic integrals $F(z,k)$ of the first kind [48]. In terms of the original coordinates (x_1,x_2,x_3) the eigenfunctions for the topological charge operator in the sector $x_1<x_2<x_3$ therefore have the form

$$\Psi_\lambda(x_1,x_2,x_3)=\Psi_0(x_2^2-x_1^2,x_3^2-x_1^2)\times\exp\left\{i\lambda\frac{8\pi^2}{g^3\sqrt{x_3^2-x_1^2}}\times F\left[\arctan\left(\frac{x_1}{\sqrt{x_2^2-x_1^2}}\right),\sqrt{\frac{x_3^2-x_2^2}{x_3^2-x_1^2}}\right]\right\}. \tag{A10}$$

In the other sectors the corresponding wave function is obtained from Eq. (A10) by cyclic permutation. Note that the eigenfunctions (A10), which constitute the most general solution of the eigenvalue problem (A1) for the Q operator, do not satisfy the boundary conditions (3.9) and (3.10) necessary for the Hermiticity of the Q operator. In the next section we will show that the characteristics of the topological

charge operator (A3) coincide with the equations which determine the zero-energy solutions of the Euclidean classical equations of motion.

2. Euclidean zero energy trajectories in Yang-Mills mechanics

The Euclidean action

$$S^{\mathrm{Eucl}}=\int d\tau\left[\frac{1}{2}\left(\frac{dx}{d\tau}\right)^2+V(x)\right] \tag{A11}$$

is obtained from the corresponding action in Minkowski space by inverting the potential $V(x)\rightarrow -V(x)$. In the one dimensional case the solutions of equation

$$\frac{dx}{d\tau}=\pm\sqrt{2V(x)}, \tag{A12}$$

corresponds to trajectories with zero Euclidean energy

$$E^{\mathrm{Eucl}}=\frac{1}{2}\dot{x}^2-V(x) \tag{A13}$$

and the same time satisfies the classical Euclidean equations of motion

$$\frac{d^2x}{d\tau^2}=\frac{dV}{dx}. \tag{A14}$$

Such a type of trajectory plays an important role in the description of quantum mechanical tunneling phenomena [47]. In the case that the potential $V(x)$ has at least two local minima, say at $x=-a$ and $x=+a$, with $V=0$, the Euclidean zero energy trajectories starting at $-a$ and ending at a correspond to quantum tunneling into the classically forbidden region. The Euclidean action for these classical $E^{Eucl}=0$ trajectories

$$S^{\mathrm{Eucl}}\big|_{E=0}=\int dt\left(\frac{dx}{dt}\right)^2=\int_{-a}^{a}dx\sqrt{2V(x)}, \tag{A15}$$

determine in the semiclassical limit the WKB amplitude for a particle to tunnel from $x=-a$ to $x=+a$

$$|T(E=0)|=\exp\left[-\frac{1}{\hbar}\int_{-a}^{a}dx\sqrt{2V(x)}\right][1+O(\hbar)]. \tag{A16}$$

The potential of the unconstrained system considered in the present article has three valleys. The question is whether there exist the trajectories corresponding to tunneling between the valleys. To answer the question let us rescale the coordinates $x_i\rightarrow g^{-1}x_i$ and write down the Euclidean action of the model in the form

$$S^{\mathrm{Eucl}}=\frac{1}{2g^2}\int d\tau\sum_{\mathrm{cycl}}(\dot{x}_i^2+x_j^2x_k^2). \tag{A17}$$

The equations of motion then read

$$\ddot{x}_i=x_i(x_j^2+x_k^2);\quad i,j,k \text{ cyclic.} \tag{A18}$$

The class of trajectories with zero energy

$$E^{\mathrm{Eucl}}=\frac{1}{2g^2}\sum_{\mathrm{cycl}}(\dot{x}_i^2-x_j^2x_k^2), \tag{A19}$$

can be chosen as the solutions of the following system of first order equations:

$$\dot{x}_1=\pm x_2x_3,\quad \dot{x}_2=\pm x_3x_1,\quad \dot{x}_3=\pm x_1x_2. \tag{A20}$$

If we fix one and the same sign on the RHS of Eqs. (A20), then they completely coincide with the characteristic equations (A3) of the Q operator. Furthermore from Eq. (A4) we see that the zero energy Euclidean solutions admit no trajectories from one $V=0$ minimum to another and they have no relation to the quantum tunneling phenomena.

3. Q operator and self-dual states

The commutator of the Hamiltonian H_0 of Eq. (4.1) in the spin-0 sector and the topological charge Q

$$[H_0,Q]=-i\frac{g^3}{4\pi^2}[(p_1p_2x_3+p_2p_3x_1+p_3p_1x_2) -gx_1x_2x_3(x_1^2+x_2^2+x_3^2)] \tag{A21}$$

vanishes only in the subspace of states $|\Psi\rangle$ which satisfy the Euclidean self-(anti)duality conditions

$$p_i|\Psi\rangle=\pm gx_jx_k|\Psi\rangle,\quad i,j,k \text{ cyclic}, \tag{A22}$$

which are the quantum analogues of the Euclidean $E=0$ constraints (A20) discussed before. Rewriting the Hamiltonian H_0 in Eq. (4.1) in the form

$$H_0=\frac{1}{2}\sum_{i,j,k\ \mathrm{cycl}}(p_i^2+g^2x_j^2x_k^2)=\sum_{i,j,k\ \mathrm{cycl}}(p_i\pm gx_jx_k)^2\pm\frac{8\pi}{g^2}Q, \tag{A23}$$

we see that the Hamiltonian H_0 and the topological operator Q coincide on the subspace of the Euclidean self-(anti)dual states (A22)

$$H_0|\Psi\rangle=\mp\frac{8\pi}{g^2}Q|\Psi\rangle. \tag{A24}$$

Comparing this discussion with the corresponding original situation $H=(1/2)(\Pi_i^{a2}+B_i^{a2})$ and $Q=-(\alpha_S/2\pi)\Pi_i^aB_i^a$ in terms of the constrained fields Π_i^a and A_i^a, where $H_0=\mp(8\pi/g^2)Q$ only in the Euclidean self-(anti)dual case $\Pi_i^a=B_i^a$, we see that Eq. (A22) corresponds to the unconstrained analogues of the self-(anti)dual configurations in Euclidean space. The question arises whether there are any self-(anti)dual states (A22) which are both eigenstates of Q and H. The solution

$$\Psi_{\mathrm{SD}}^{\pm}:=\exp[\mp igx_1x_2x_3], \tag{A25}$$

of the self-(anti)duality conditions (A22) in Euclidean space is neither eigenfunction of H_0 nor of Q

$$H_0\Psi^{\pm}_{\rm SD}=\mp\frac{8\pi}{g^2}Q\Psi^{\pm}_{\rm SD}=\pm 2V\Psi^{\pm}_{\rm SD}. \tag{A26}$$

The well-known exact non-normalizable zero-energy solution of the spin-0 Schrödinger equation (4.1)

$$\Psi^{\pm}_0=A\exp[\mp gx_1x_2x_3], \tag{A27}$$

which differs from functional $\Psi_{\rm SD}$ up to a factor of i in the exponent, actually satisfies the self-(anti)duality conditions in Minkowski space

$$-i\frac{\partial}{\partial x_i}\Psi^{\pm}_0=\pm igx_jx_k\Psi^{\pm}_0;\quad i,j,k \text{ cyclic} \tag{A28}$$

(corresponding to $\Pi^a_i=\pm iB^a_i$), but is not an eigenfunction of the topological operator Q

$$-\frac{8\pi}{g^2}Q\Psi^{\pm}_0=\pm ig^2(x_1^2x_2^2+x_2^2x_3^2+x_3^2x_1^2)\Psi^{\pm}_0$$
$$=\pm 2iV(x_1,x_2,x_3)\Psi^{\pm}_0. \tag{A29}$$

Finally we point out that the (approximate) ground-state wave function (4.13) obtained in the variational approach is not self-(anti)dual.

APPENDIX B: LOWER BOUND FOR THE SPIN-0 HAMILTONIAN H_0

In this appendix we would like to derive a lower bound for the spin-0 Hamiltonian H_0 in Eq. (4.1) along the line of Ref. [12]. Using the boundary conditions (3.9) and (3.10) and based on the well-known operator inequality for oscillator on positive half line

$$-\frac{\partial^2}{\partial x^2}+y^2x^2\geqslant 3|y|,$$

it follows that

$$H_0\geqslant\frac{1}{4}[-\Delta+3\sqrt{2}g(x_1+x_2+x_3)]=:\frac{1}{2}H'. \tag{B1}$$

Since the Hamiltonian H' is known [12] to have a discrete spectrum, this is true also for H_0. An important open question is at which energy the ground state is. The knowledge of the ground-state energy of H' in inequality (B1) would provide a lower bound for the ground-state energy of H_0. Due to the additive structure of the potential term in H' one can make a separable ansatz for the solution of the corresponding eigenvalue problem. The energy of the lowest such separable H' eigenstate satisfying the above boundary conditions (3.9) and (3.10) is

$$E'_{\rm sep}=6|\xi_0|(3g/2)^{2/3}=9.1924\ g^{2/3}, \tag{B2}$$

where $\xi_0=-2.3381$ is the first zero of the Airy function. From the operator inequality (B1) and the lower bound (B2) for separable solutions of H' we therefore obtain the lower bound of the energy functional for separable functions

$$\mathcal{E}[\Psi_{\rm sep}]\geqslant\frac{1}{2}E'_{\rm sep}=4.5962\ g^{2/3}. \tag{B3}$$

Finally we remark, as has been pointed out already in Ref. [21], that an analogous variational calculation for H' shows that also the ground-state energy of the Hamiltonian H' in Eq. (B1) is lower than the value $E'_{\rm sep}$ of Eq. (B2) for the lowest separable solution.

APPENDIX C: MATRIX ELEMENTS

For the evaluation of the energy functional, the calculation of the value of the ''gluon condensate'' of the ground state, as well as the propagator term in the Witten formula we need the matrix elements of E^2, B^2, and Q with respect to the irreducible Fock space states (4.8)–(4.10) built from the basic Fock space states (4.7).

1. Basic matrix elements for Hamiltonian and topological charge

The matrix elements of E^2 and B^2 with respect to the basic Fock space states (4.7) with ($\omega_1=\omega_2=\omega_3=3^{1/3}\ g^{2/3}$) are given by

$$\langle\Psi_{m_1;m_2;m_3}|E^2|\Psi_{n_1;n_2;n_3}\rangle=3^{1/3}g^{2/3}\sum_{\rm cyclic}\mathcal{H}^-_{m_in_i}\delta_{m_jn_j}\delta_{m_kn_k} \tag{C1}$$

and

$$\langle\Psi_{m_1;m_2;m_3}|B^2|\Psi_{n_1;n_2;n_3}\rangle=3^{1/3}g^{2/3}\sum_{\rm cyclic}\frac{1}{3}\delta_{m_in_i}\mathcal{H}^+_{m_jn_j}\mathcal{H}^+_{m_kn_k}, \tag{C2}$$

where

$$\mathcal{H}^{\pm}_{mn}:=\delta_{mn}(2n+3/2)\pm\delta_{m(n+1)}\sqrt{n+3/2}\sqrt{n+1}$$
$$\pm\delta_{(m+1)n}\sqrt{n+1/2}\sqrt{n}. \tag{C3}$$

For the topological operator Q we have

$$\langle\Psi_{m_1;m_2;m_3}|Q|\Psi_{n_1;n_2;n_3}\rangle=\frac{2ig^{8/3}}{\pi^{7/2}3^{1/6}}\sum_{\rm cyclic}\mathcal{Q}^-_{m_in_i}\mathcal{Q}^+_{m_jn_j}\mathcal{Q}^+_{m_kn_k}, \tag{C4}$$

where

$$\mathcal{Q}^+_{mn}:=\frac{1}{1-4(m-n)^2}\frac{(-1)^{m+n}(2m+1)!!(2n+1)!!}{\sqrt{(2m+1)!(2n+1)!}}, \tag{C5}$$

$$\mathcal{Q}^{-}_{mn} := \frac{m-n}{1-4(m-n)^2} \frac{(-1)^{m+n}(2m+1)!!(2n+1)!!}{\sqrt{(2m+1)!(2n+1)!}}. \tag{C6}$$

2. The irreducible matrix elements in terms of the basic ones

For any operator O invariant under the permutations σ_{ij}, such as E^2, B^2, the Hamiltonian H_0 and the topological operator Q,

$$[O, \sigma_{ij}] = 0, \tag{C7}$$

the matrix elements of the irreducible states $\langle \Psi^{(k)\pm}_M | O | \Psi^{(k)\pm}_N \rangle$ of type I (4.8), type II (4.9), and type III (4.10) can then be expressed in terms of the basic matrix elements

$$\mathcal{M}^{m_1 m_2 m_3}_{n_1 n_2 n_3} := \langle \Psi_{m_1;m_2;m_3} | O | \Psi_{n_1;n_2;n_3} \rangle \tag{C8}$$

as follows. For the type I, II, and III singlet states we have

$$\langle \Psi^{(0)+}_{mmm} | O | \Psi^{(0)+}_{nnn} \rangle = \mathcal{M}^{mmm}_{nnn}, \tag{C9}$$

$$\langle \Psi^{(0)+}_{mmr} | O | \Psi^{(0)+}_{nns} \rangle = \mathcal{M}^{mmr}_{nns} + 2\mathcal{M}^{mmr}_{nsn}, \tag{C10}$$

and

$$\begin{aligned} \langle \Psi^{(0)+}_{m_1 m_2 m_3} | O | \Psi^{(0)+}_{n_1 n_2 n_3} \rangle = {} & \mathcal{M}^{m_1 m_2 m_3}_{n_1 n_2 n_3} + \mathcal{M}^{m_1 m_2 m_3}_{n_3 n_1 n_2} + \mathcal{M}^{m_1 m_2 m_3}_{n_2 n_3 n_1} \\ & + \mathcal{M}^{m_1 m_2 m_3}_{n_2 n_1 n_3} + \mathcal{M}^{m_1 m_2 m_3}_{n_3 n_2 n_1} \\ & + \mathcal{M}^{m_1 m_2 m_3}_{n_1 n_3 n_2}, \end{aligned} \tag{C11}$$

respectively. The transition elements between the type I, II, and III singlets are

$$\langle \Psi^{(0)+}_{mmm} | O | \Psi^{(0)+}_{nns} \rangle = \sqrt{3}\mathcal{M}^{mmm}_{nns}, \tag{C12}$$

$$\langle \Psi^{(0)+}_{mmm} | O | \Psi^{(0)+}_{n_1 n_2 n_3} \rangle = \sqrt{6}\mathcal{M}^{mmm}_{n_1 n_2 n_3}, \tag{C13}$$

and

$$\begin{aligned} \langle \Psi^{(0)+}_{mmr} | O | \Psi^{(0)+}_{n_1 n_2 n_3} \rangle = {} & \sqrt{2}\mathcal{M}^{mmr}_{n_1 n_2 n_3} + \sqrt{2}\mathcal{M}^{mmr}_{n_3 n_1 n_2} \\ & + \sqrt{2}\mathcal{M}^{mmr}_{n_2 n_3 n_1}. \end{aligned} \tag{C14}$$

For the doublets, which exist only for type II and III states, we have

$$\langle \Psi^{(1,2)+}_{mmr} | O | \Psi^{(1,2)+}_{nns} \rangle = \mathcal{M}^{mmr}_{nns} - \mathcal{M}^{mmr}_{nsn} \tag{C15}$$

and

$$\begin{aligned} \langle \Psi^{(1,2)+}_{m_1 m_2 m_3} | O | \Psi^{(1,2)+}_{n_1 n_2 n_3} \rangle = {} & \mathcal{M}^{m_1 m_2 m_3}_{n_1 n_2 n_3} - (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_3 n_1 n_2} \\ & - (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_2 n_3 n_1} + \mathcal{M}^{m_1 m_2 m_3}_{n_2 n_1 n_3} \\ & - (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_3 n_2 n_1} - (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_1 n_3 n_2} \end{aligned} \tag{C16}$$

for the type III doublets. Their transition elements are

$$\begin{aligned} & \langle \Psi^{(1,2)+}_{mmr} | O | \Psi^{(1,2)+}_{n_1 n_2 n_3} \rangle \\ & \quad = \sqrt{2}\mathcal{M}^{mmr}_{n_1 n_2 n_3} - (\mathcal{M}^{mmr}_{n_3 n_1 n_2} + \mathcal{M}^{mmr}_{n_2 n_3 n_1})/\sqrt{2}. \end{aligned} \tag{C17}$$

For the axial singlets we have

$$\begin{aligned} \langle \Psi^{(0)-}_{m_1 m_2 m_3} | O | \Psi^{(0)-}_{n_1 n_2 n_3} \rangle = {} & \mathcal{M}^{m_1 m_2 m_3}_{n_1 n_2 n_3} + \mathcal{M}^{m_1 m_2 m_3}_{n_3 n_1 n_2} + \mathcal{M}^{m_1 m_2 m_3}_{n_2 n_3 n_1} \\ & - \mathcal{M}^{m_1 m_2 m_3}_{n_2 n_1 n_3} - \mathcal{M}^{m_1 m_2 m_3}_{n_3 n_2 n_1} \\ & - \mathcal{M}^{m_1 m_2 m_3}_{n_1 n_3 n_2}. \end{aligned} \tag{C18}$$

For the axial doublets we have

$$\begin{aligned} \langle \Psi^{(1,2)-}_{m_1 m_2 m_3} | O | \Psi^{(1,2)-}_{n_1 n_2 n_3} \rangle = {} & \mathcal{M}^{m_1 m_2 m_3}_{n_1 n_2 n_3} - (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_3 n_1 n_2} \\ & - (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_2 n_3 n_1} - \mathcal{M}^{m_1 m_2 m_3}_{n_2 n_1 n_3} \\ & + (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_3 n_2 n_1} + (1/2)\mathcal{M}^{m_1 m_2 m_3}_{n_1 n_3 n_2}. \end{aligned} \tag{C19}$$

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