On the Groundstate of Yang-Mills Quantum Mechanics

A M. Khvedelidze \textsuperscript{a} \textsuperscript{*} and H.-P. Pavel \textsuperscript{b}

\textsuperscript{a} Bogoliubov Theoretical Laboratory, Joint Institute for Nuclear Research, Dubna, Russia
\textsuperscript{b} Fachbereich Physik der Universität Rostock, D-18051 Rostock, Germany

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A systematic method to calculate the low energy spectrum of SU(2) Yang-Mills quantum mechanics with high precision is given and applied to obtain the energies of the groundstate and the first few excited states.

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The so-called Yang-Mills mechanics originates from Yang-Mills field theory under the supposition of the spatial homogeneity of the gauge fields. Since its introduction twenty years ago \cite{1} this model has been studied extensively from different points of view \cite{2,3,4,5,6}. The model is known to exhibit stochastic behaviour at the classical level. In particular it has been shown for a simplified two-dimensional version of the model that it is nonintegrable \cite{6}. How this reflects itself on the corresponding non-Abelian gauge field theory. With this point of view Yang-Mills quantum mechanics has been investigated in the small volume approximation \cite{6}, in the small coupling limit on the lattice using the semiclassical approximation \cite{6}, and to estimate the glueball spectrum \cite{13}. Furthermore it offers the possibility to develop methods generalizable to the study of the corresponding non-Abelian gauge theory. With this point of view Yang-Mills quantum mechanics has been investigated in the small volume approximation \cite{6}, in the small coupling limit on the lattice using the semiclassical approximation \cite{6}, and to estimate the glueball spectrum \cite{13}. Furthermore the question of the existence of normalizable zero-energy wave functions in supersymmetric matrix models \cite{14} as generalizations of Yang-Mills mechanics is under intensive investigation (see e.g. \cite{17} and references therein).

In the present work we would like to investigate the groundstate and the first few excited states of SU(2) Yang-Mills quantum mechanics using the variational approach. The quantum treatment of such models is confronted with the difficulties due to the existence of the non-Abelian Gauss law constraints and the presence of the unphysical degrees of freedom. In \cite{13} it has been shown that classical SU(2) Yang-Mills mechanics, after the elimination of all unphysical degrees of freedom, reduces to the equivalent unconstrained system described by the Hamiltonian

$$H = \frac{1}{2} \sum_{cyclic} \left[ p_i^2 + \xi_{i}^2 \frac{x_j^2 + x_k^2}{(x_j^2 - x_k^2)^2} + g^2 x_j^2 x_k^2 \right].$$

(1)

This Hamiltonian is defined on the phase space spanned by the three canonical pairs \((x_i, p_i)\) and the three \(SO(3)\) left-invariant Killing vectors \(\xi_i\) satisfying the Poisson bracket relations \(\{\xi_i, \xi_j\} = -\epsilon_{ijk}\xi_k\). Each of the three configuration space variables \(x_i\) is defined on the positive half line. The Hamiltonian \((1)\) has been obtained by writing the spatially homogeneous SU(2) gauge fields \(A_i^a(t)\) in the so-called polar representation \cite{18}

\[ A_{ai}(q, Q) = O_{ak}(q) Q_{ki}, \]

with the orthogonal \(3 \times 3\) matrix \(O\) parametrized by the three angles \(q\) and the positive definite \(3 \times 3\) symmetric matrix \(Q\). The three angles \(q\) are pure gauge degrees of freedom, which do not enter the Hamiltonian while their conjugated momenta are vanishing according to the Gauss law constraints.

The variables \(x_i\) appearing in the Hamiltonian \((1)\) are the eigenvalues of the positive definite symmetric matrix \(Q\)

\[ Q = R^T(\chi) D(x_1, x_2, x_3) R(\chi). \]

The angles \(\chi\) in the orthogonal matrix \(R(\chi)\) and their canonical momenta are combined in the Killing vectors \(\xi_k\). We emphasize that by definition of the polar decomposition the diagonal elements \(x_i\) are positive definite which has important consequences on the quantum level, as will be shown below.

The transition to the corresponding quantum Hamiltonian is free of operator ordering ambiguities. The operators \(J_i = R_{ij}^a \xi_j\) corresponding to the right-invariant \(SO(3)\) Killing vectors commute with the Hamilton operator. Its eigenstates can therefore be classified according to the quantum numbers \(J^a\) and \(M\) as eigenvalues of the total spin \(J^2\) and its projection \(J_3\). We shall consider here only the spin zero sector, \(J^2 = \xi^2 = 0\), for which the Schrödinger eigenvalue problem reduces to

\*Permanent address: Tbilisi Mathematical Institute, 380093, Tbilisi, Georgia
For the Hermiticity of the Hamiltonian $H_0$ defined in (3) the wave functions have to satisfy the boundary conditions

\[
\lim_{x_i \to 0} \Psi(x_1, x_2, x_3) = 0, \quad \lim_{x_i \to \infty} \Psi(x_1, x_2, x_3) = 0.
\]

The potential in (3) has three flat valleys of zero energy, $x_1 = x_2 = 0$ and $x_3$ arbitrary, and the two others obtained from this by cyclic permutation. Close to the bottom of the valleys the potential is that of a harmonic oscillator with a width narrowing down for larger values of $x_3$.

One of the main results known for such a problem is that it has been proven to have a discrete spectrum due to quantum fluctuations [4] [5], although the classical problem allows for scattering trajectories. Based on the well-known operator inequality 1

\[-\frac{\partial^2}{\partial x^2} + y^2 x^2 \geq 3|y|,\]

it follows that

\[H_0 \geq \frac{1}{4} \left(-\Delta + 3\sqrt{2}g(x_1 + x_2 + x_3)\right) =: \frac{1}{2}H'.\]

Since the Hamiltonian $H'$ is known 1 to have a discrete spectrum, this is true also for $H_0$. An important open question is at which energy the groundstate is. The well-known nonnormalizable zero energy solution $\Psi_{\text{sep}} = A \exp(-gx_1 x_2 x_3)$ [19], [20], does not satisfy the necessary boundary condition (3). The knowledge of the groundstate energy of $H'$ in inequality (3) would provide a lower bound for the groundstate 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) and (4) is

\[E_{\text{sep}} = 6|\xi_0|(3g/2)^{2/3} = 9.1924 \ g^{2/3},\]

where $\xi_0 = -2.3381$ is the first zero of the Airy function. We shall see in this letter that there exist nonseparable solutions which have an energy below [5].

To obtain an upper bound $\mathcal{E}$ for the groundstate energy $E_0$ of the Hamiltonian the most powerful tool is the Rayleigh-Ritz variational technique [21], based on the minimization of energy functional

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

Guided by the harmonic oscillator form of the valleys of the potential in (3) close to there bottom a simple first choice for a trial function compatible with the boundary conditions (3) and (4) is to use the lowest state of three harmonic quantum oscillators on the positive half line

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

The stationarity conditions for the energy functional of this state,

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

lead to the isotropic optimal choice

\[\omega := \omega_1 = \omega_2 = \omega_3 = 3^{1/3} g^{2/3}.\]

As a first upper bound for the groundstate energy of the Hamiltonian we therefore find

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

This upper bound is in agreement with the lower bound of the energy functional for separable functions

\[\mathcal{E}[\Psi_{\text{sep}}] \geq \frac{1}{2} E_{\text{sep}} = 4.5962 \ g^{2/3},\]

obtained from the operator inequality (3) and the lower bound (4) for separable solutions of $H'$.

In order to improve the upper bound for the groundstate energy of the Hamiltonian $H_0$ we extend the space of trial functions (8) and consider the Fock space of the orthonormal set of the products

\[\Psi_{n_1 n_2 n_3} := \prod_{i=1}^3 \Psi_{n_i}(\omega, x_i),\]

of the odd eigenfunctions of the harmonic oscillator

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

1The number 3 in r.h.s of the inequality originates from the positiveness of $x$. 
with the frequency fixed by \( \mathbf{1} \). 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 \( \mathbf{2} \). It is invariant under arbitrary permutations of any two of the variables \( P_{ij}x_i = x_jP_{ij}, P_{ij}p_i = p_jP_{ij} \) and under time reflections \( T x_i = x_i T, T p_i = -p_i T \).

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

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

\[
P_{123} \Psi(x_1, x_2, x_3) = \Psi(x_2, x_3, x_1),
\]

\[
P_{12} \Psi(x_1, x_2, x_3) = \Psi(x_2, x_1, x_3),
\]

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

and decompose the Fock space spanned by the functions \( \mathbf{1} \) into the irreducible sectors, the variational approach 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 \( \mathcal{E}[^{1/2}_{000}±] = 4.8676 \ g^{2/3}, \mathcal{E}[^{1/2}_{100}±] = 7.1915 \ g^{2/3}, \mathcal{E}[^{1/2}_{012}±] = 13.8817 \ g^{2/3}, \) and \( \mathcal{E}[^{3/2}_{012}±] = 15.6845 \ g^{2/3} \) 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 \( H_{\text{trunk}} \) 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 \( \mathbf{2} \) for the eigenvectors of \( H_{\text{trunk}} \) coincides with the \( H_{\text{trunk}} \) 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 \( S_1, S_2, S_3 \)

\[
\mathcal{E}[S_1] = 4.8070 \ g^{2/3}, \mathcal{E}[S_2] = 8.2639 \ g^{2/3}, \mathcal{E}[S_3] = 9.6298 \ g^{2/3},
\]

where the number in brackets show the corresponding result for 4 knots. The lowest state \( S_1 \) is very close to the state \( ^{1/2}_{000}± \):

\[
S_1 = 0.994562 ^{1/2}_{000}± + 0.0252533 ^{1/2}_{001}± + 0.0216617 ^{1/2}_{002}± - 0.0970056 ^{3/2}_{010}± + 0.0145832 ^{3/2}_{110}±.
\]

Similarly including all states in the doublet sector with up to 6(5) knots the following energy expectation values for the three lowest states \( D_1^{(±)} , D_2^{(±)} , D_3^{(±)} \)
\[ E[D_i^{(1\pm1)}] = 7.1682 \ g^{2/3}(7.1689 \ g^{2/3}), \\
E[D_2^{(1\pm1)}] = 9.6171 \ g^{2/3}(9.6394 \ g^{2/3}), \\
E[D_3^{(1\pm1)}] = 10.9903 \ g^{2/3}(10.9951 \ g^{2/3}), \] (15)

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 \( A_1, A_2, A_3 \)

\[ E[A_1] = 13.2235 \ g^{2/3}(13.2275 \ g^{2/3}), \\
E[A_2] = 16.6652 \ g^{2/3}(16.7333 \ g^{2/3}), \\
E[A_3] = 19.1470 \ g^{2/3}(19.3028 \ g^{2/3}). \] (16)

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 \( C_1^{(1\pm1)}, C_2^{(1\pm1)}, C_3^{(1\pm1)} \)

\[ E[C_1^{(1\pm1)}] = 14.8768 \ g^{2/3}(14.8796 \ g^{2/3}), \\
E[C_2^{(1\pm1)}] = 17.6648 \ g^{2/3}(17.6839 \ g^{2/3}), \\
E[C_3^{(1\pm1)}] = 19.9019 \ g^{2/3}(19.9914 \ g^{2/3}), \] (17)

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 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 4.8067 \ g^{2/3} with expected accuracy up to three digits after the dot. For comparison we remark that due to our boundary condition \( \frac{3}{2} \) all our spin-0 states correspond to the 0\(^{-}\) sector in the work of \[10\] 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 \[14\], using an analogy of \( SU(N) \) Yang-Mills quantum mechanics in the large \( N \) limit to membrane theory, obtain the energy values 6.4960 \ g^{2/3} and 19.8253 \ g^{2/3} for the groundstate and the first excited state.

Finally we remark that an analogous calculation shows that also the groundstate energy of the Hamiltonian \( H' \) in Eq. \( \text{(3)} \) is lower than the value \( E'_\text{sep} \) of \( \text{(4)} \) for the lowest separable solution.

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