Variational calculations in gauge theories with approximate projection on gauge invariant states

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Abstract

Variational calculations using Gaussian wave functionals combined with an approximate projection on gauge invariant states are presented. We find that the energy exhibits a minimum for a wave functional centered around a non vanishing background magnetic field. We show that divergences can be removed by a renormalization of the coupling constant. The resulting expectation value of the gluon condensate is found to be in qualitative agreement with phenomenological estimates.

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The application of the variational method to gauge theories is generally plagued by the difficulty to implement in a calculable way the requirement of gauge invariance of physical states [2, 1, 3]. In the present letter we propose to use an approximate projection method developed in 1962 by Thouless and Valatin [5]. This method deals with the restoration of rotational invariance when deformed solutions are obtained in nuclear Hartree-Fock calculations.

In the case of gauge theories this formalism allows one to explore a class of invariant trial vacuum functionals for which closed expressions can be obtained. This class is generated by projecting Gaussian wave functionals onto the subspace of gauge invariant states. This class of trial functionals has already been explored by Kogan and Kovner [3], and Brown and Kogan [4]. Since these authors use different approximation schemes their approach and ours appear complementary.

We consider the functional Schrödinger description of the SU($N$) Yang-Mills theory. In the temporal gauge $A^0_a = 0$, the canonical coordinates are the vector potentials $A^i_a(x)$ and the electric fields $E^i_a(x)$, which we shall often write as color matrices in the adjoint representation: e.g., $A^i ≡ A^i_b T^b$ (the color indices $a, b, \ldots$ run from 1 to $M ≡ N^2 − 1$).

The Hamiltonian density reads
\[ H(x) = \frac{1}{2} \left\{ E^i_a E^i_a(x) + B^i_a B^i_a(x) \right\}, \]
(2)
with the color magnetic fields $B^i_a ≡ -\epsilon^{ijk} F^j_a / 2$, and $F^{ij}_a ≡ \partial^i A^j_a - \partial^j A^i_a + g f_{abc} A^i_b A^j_c$ ($g$ denotes the coupling constant). By also introducing the covariant derivative $D^i ≡ \partial^i - ig A^i$, we can rewrite the previous formulae in matrix form: e.g., $F^{ij} ≡ F^{ij}_a T^a = [D^i, D^j]/(ig).

In the Schrödinger representation, the states are represented by functionals of $A^i_a(x)$, $\Psi[A]$, and the electric field is acting on such states by functional differentiation:
\[ E^i_a(x) \Psi[A] = i \frac{\delta}{\delta A^i_a(x)} \Psi[A]. \] (3)
The hamiltonian $H$ commutes with the generator $\mathcal{G}$ of time-independent gauge transformations,
\[ \mathcal{G}(x) ≡ \nabla \cdot \mathbf{E}(x) + ig[A^i, E^i], \] (4)
so it is possible to diagonalize $H$ and $\mathcal{G}$ simultaneously. We are here interested only in those eigenstates $\Psi$ of $H$ which are gauge invariant, i.e.,
\[ \mathcal{G}(x) \Psi[A] = 0, \] (5)
or in superpositions of them, to be referred to as physical states.

The variational principle consists in the inequality

\[ \langle H \rangle \equiv \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_{\text{vac}}, \]  

(6)

which holds for any functional \( \Psi[A] \) from the physical Hilbert space. In this equation, \( E_{\text{vac}} \) is the ground state energy, assumed to be non-degenerate. In practice, however, one has to restrict oneself to Gaussian wave functionals, the only ones which allow for the analytical computation of \( \langle H \rangle \). These have the form

\[ \Psi[A] = \exp \left\{ -\frac{1}{4} \int d^3x d^3y \left[ A^i_a(x) - \bar{A}^i_a(x) \right] \left( G^{-1} \right)^{ab}_{ij}(x,y) \left[ A^j_b(y) - \bar{A}^j_b(y) \right] \right\}, \]  

(7)

where the background field \( \bar{A}^i_a(x) \) and the kernel \( G^{-1} \) (with matrix elements \( (G^{-1})^{ab}_{ij}(x,y) \)) are the variational parameters.

The expectation value of the Hamiltonian density in the Gaussian state \( \Psi \) is

\[ \langle \Psi | \mathcal{H}(x) | \Psi \rangle = \frac{1}{2} \bar{B} \cdot \bar{B}(x) + \frac{1}{8} \text{Tr} \langle x | G^{-1} | x \rangle + \frac{1}{2} \text{Tr} \langle x | KG | x \rangle \]

\[ + \frac{2^2}{8} (\text{Tr} \{ S^i T^a(x | G(x) \})^2 \]

\[ + \frac{2^2}{4} \text{Tr} \{ S^i T^a(x | G(x) S^i T^a(x | G(x) \}. \]

(8)

In this equation \( \bar{B} \) is the magnetic field associated to the center \( \bar{A} \) and \( S^i \) is the spin one matrix whose elements \( (j, k) \) are given by \( i\varepsilon_{ijk} \). The notation \( \text{Tr} \) in equation (8) implies a summation over both the color and the spacial indices. For instance, \( \text{Tr} \langle x | G^{-1} | x \rangle = \sum_{i,a} (G^{-1})^{aa}_{ii}(x, x) \). Finally, the operator \( K \) is the second derivative of the classical energy with respect to the center \( \bar{A}^i_a \). It is given by

\[ K = (-iS \cdot \mathcal{D})^2 - S \cdot B, \]

(9)

where

\[ \mathcal{D}^i \equiv \partial^i - ig\bar{A}^i \]

(10)

denotes the covariant derivative defined by the background field \( \bar{A}^i_a \equiv \bar{A}^i_a T^a \).

In the case of non-Abelian gauge theories, however, the Gaussian functionals suffer from a major drawback: they do not satisfy the requirement of gauge invariance (5). It is thus necessary to project them onto the subspace of gauge invariant states. This is achieved by means of the formula

\[ \Psi_0[A] = \frac{1}{\mathcal{N}} \int \mathcal{D}[U(x)] \Psi[U[A]], \]

(11)
where the functional integration is performed over the unitary \( N \times N \) matrix field \( U(x) \), with the adequate group invariant measure, and \( \mathcal{N} \) is a normalization factor. The integrand in eq. (11) is the gauge-transform of \( \Psi[A] \):

\[
\Psi_U[A] = \Psi[U\mathbf{A} U^+ + \frac{i}{g} \mathbf{U} \nabla U^+].
\]

The expectation value \( E_P \) of the energy in the projected state is given by the following formula

\[
E_P = \frac{\int \mathcal{D}[U(x)] < \Psi | H | \Psi_U >}{\int \mathcal{D}[U(x)] < \Psi | \Psi_U >},
\]

which should replace eq. (8) in practical calculations. Unfortunately, eq. (12) cannot be evaluated in closed form because the functional integral over the group is not Gaussian [3].

In what follows, we shall propose an approximation to eq. (12) which is inspired from techniques used in nuclear physics to calculate the zero point rotational energy of deformed nuclei. The starting point is the formula for the collective rotational energy of a classical rotating rigid body

\[
E = \frac{1}{2} \mathcal{I}_{ij} \omega_i \omega_j,
\]

where \( \mathcal{I}_{ij} \) is the inertia tensor and \( \omega_i \) the angular velocity along the i-th axis. When deformed solutions are obtained in solving the nuclear Hartree-Fock equations, the Thouless-Valatin formalism provides a quantum extension of this formula. It gives the energy gain when projecting on zero angular momentum states as [5, 6]

\[
\Delta E = \frac{< J_x^2 >}{2I_x} + \frac{< J_y^2 >}{2I_y} + \frac{< J_z^2 >}{2I_z}.
\]

(13)

In this formula \( J_x \) is the angular momentum operator along the x axis and \( I_x \) the corresponding moment of inertia. This quantity is the polarizability

\[
\mathcal{I}_x = \lim_{\omega \to 0} \frac{< J_x >}{\omega_x}
\]

of the system in the presence of an external constraint \( \omega_x J_x \). Equation (13) is an approximate expression valid in the limit of a large fluctuation in the angular momentum \( < J^2 > \gg 1 \) [6].

In the case of gauge theories it is straightforward to generalize the above formula (see [3] for more details). The moment of inertia is now a matrix in color and position in space defined as the polarization tensor

\[
\mathcal{T}^{ab}(x, y) = \frac{\delta < \mathcal{G}^a(x) >}{\delta \omega^b(y)}|_{\omega=0},
\]

(15)
in the presence of an external constraint

\[ H_{\text{ext}} = \int d^3y \, \omega^b(y) G^b(y). \]  

(16)

In the equations above, \( G \) is the generator of time-independent gauge transformations (cf. eq. (13)). The gain in energy when projecting a wave functional \( \Psi[A] \) onto the subspace of gauge invariant states reads, in analogy to eq. (13),

\[ \Delta E = \int d^3x d^3y \langle \Psi | \bar{G}^a(x) G^b(y) | \Psi \rangle \langle a, x| \frac{1}{2L} | b, y \rangle. \]  

(17)

The expectation values in eqs. (15) and (17) are all Gaussian and can be exactly computed. Nevertheless, the ensuing calculation of the moment of inertia is extremely tedious, which invites us to look for a convenient approximation. Namely, we shall assume in what follows that the condensate is large enough so that we can replace the field operator \( A \) by its mean value \( \bar{A} \) in the expression (4) for the gauge generator. We thus define:

\[ \bar{G}(x) \equiv \nabla \cdot E(x) + ig[A^i, E^i]. \]  

(18)

It is then straightforward [7] to obtain the corresponding, approximate form of the inertial moment:

\[ \langle a, x| | b, y \rangle \approx \frac{\delta \langle \bar{G}^a(x) \rangle}{\delta \omega^b(y)} |_{\omega=0} = \langle a, x| \Pi^2 | b, y \rangle \]  

(19)

where \( \Pi^2 \) denotes the square of the kinetic momentum \( \Pi_j \equiv iD_j = i\partial_j + g\bar{A}_j \). Furthermore, from eq. (7) and (18), one readily obtains:

\[ \langle \Psi | \bar{G}^a(x) G^b(y) | \Psi \rangle = \frac{1}{4} \langle a, x| \Pi_i G^{-1}_{ij} \Pi_j | b, y \rangle, \]  

(20)

so that the projection energy (17) can be written as:

\[ \Delta E = \frac{1}{8} \int d^3x \langle a, x| \left( \Pi_i \frac{1}{\Pi^2} \Pi_j \right) G^{-1}_{ij} | a, x \rangle. \]  

(21)

The Thouless-Valatin correction thus changes the term \( \text{Tr}(1/8G) \) of equation (8) into \( \text{Tr}(Q/8G) \) where

\[ Q_{ij} \equiv \delta_{ij} - \Pi_i \frac{1}{\Pi^2} \Pi_j. \]  

(22)

It is easily checked that \( Q^2=Q \) and that the action of \( Q \) on a transverse vector field \( A^i_0(x) \) (i.e., such that \( \Pi_i A_i=0 \)) gives back \( A^i_0 \). We will refer to \( Q \) as projector on transverse fields. We conclude that the Thouless-Valatin correction makes the kinetical part of the energy transverse with respect to the mean-field covariant derivative \( D_i \).

Further note that the operator \( K \) is transverse as well. In fact, eq. (2) can be rewritten as

\[ K_{ij} = \Pi^2 \delta_{ij} - \Pi_i \Pi_j + 2[\Pi_i, \Pi_j]. \]  

(23)
which is manifestly transverse: \( \Pi_i K_{ij} = 0 \). Then, by minimizing the projected energy \( E - \Delta E \) with respect to \( G \), we immediately find that the kernel \( G^{-1} \) must be transverse,

\[
\mathcal{D}^i G^{-1}_{ij} = 0. \tag{24}
\]

This condition has a simple interpretation: it is equivalent to \( \bar{G}(x) \Psi[A] = 0 \), showing that the Gauss law (3) is approximately satisfied by the Gaussian (6).

Eq. (24) requires the operator \( G^{-1} \) to be a functional of the background field \( \bar{A}_i \). A specific Ansatz for \( G^{-1} \) can be obtained from the variational equation for the projected energy \( E - \Delta E \). To this aim, we write \( G^{-1}_T \equiv Q G^{-1} Q \) (and similarly \( G_T \equiv Q G Q \)), and consider the gap equation for \( G_T \). In order to exploit this equation, we consider a restricted variational space defined by the following background field:

\[
\bar{A}_x = 0, \quad \bar{A}_y = x T^3 B, \quad \bar{A}_z = 0. \tag{25}
\]

This corresponds to a constant magnetic field in the z-direction and in the third color with a strength \( B \) which is a variational parameter. For such a background, one can show \[7\] that the most general kernel \( G_T \) which is consistent with the gap equation is of the form

\[
\frac{1}{4 G^2_T} = K + \beta Q S \cdot B Q = Q (\Pi^2 + \alpha S \cdot B) Q, \tag{26}
\]

where the dimensionless coefficient \( \beta = 2 + \alpha \) is a new variational parameter. The acceptable range of values of \( \beta \) is \( \beta \geq 1 \) \[7\]. Indeed, for \( \beta < 1 \) the previous equation is undefined because of the occurrence of negative modes in the right hand side \[8, 9, 10\].

The expression of the energy density involves quantities such as \( \langle x \vert G_T \vert x \rangle \) and \( \langle x \vert G^{-1}_T \vert x \rangle \). A proper definition of these quantities requires a regularization scheme. A convenient one in the present context is Schwinger’s proper time representation which gives \[11, 12\]

\[
\langle x \vert G_T \vert x \rangle = \frac{1}{\sqrt{\pi}} \int_{1/\Lambda^2}^{\infty} \frac{dt}{\sqrt{t}} \langle x \vert e^{-t(K + \beta Q S \cdot B Q)} \vert x \rangle, \tag{27}
\]

and

\[
\langle x \vert G^{-1}_T \vert x \rangle = \frac{1}{\sqrt{\pi}} \int_{1/\Lambda^2}^{\infty} \frac{dt}{t^{3/2}} \langle x \vert 1 - e^{-t(K + \beta Q S \cdot B Q)} \vert x \rangle. \tag{28}
\]

Integrations for small values of the proper time \( t \) have been regularized by the introduction of a cutoff \( \Lambda \). In the limit of a large cutoff one derives

\[
\text{Tr}(G^{-1}_T) = \frac{1}{8 \pi^2} \left\{ 2 \Lambda^4 - c_N \left( \frac{11}{3} - 2 \beta + \frac{\beta^2}{3} \right) g^2 B^2 \ln \frac{\Lambda^2}{B} + \ldots \right\}, \tag{29}
\]
and
\[ \langle x|G_T|x \rangle = \frac{1}{16\pi^2} \left\{ \frac{2}{3} \Lambda^2 + (1 - \frac{\beta}{3}) S \cdot B \ln \frac{\Lambda^2}{B} + \langle x|G_F|x \rangle + \mathcal{O}(\frac{1}{\Lambda^2}) \right\}. \] (30)

In this last equation \( G_F \) is the finite part of \( G_T \) in the limit of a large cutoff. An approximate closed formula for this term can be obtained by ignoring the projection on transverse states in the Ansatz (26) for the kernel of the Gaussian. In this case one finds indeed \[ \langle x|G_F|x \rangle = \frac{1}{16\pi^2} \int_0^\infty ds \frac{eBs}{\sinh eBs} \left( e^{eBs} - e\alpha S \cdot B \right) - 1 \]. (31)

The resulting energy density reads
\[ \langle \Psi|H(x)|\Psi \rangle = \frac{1}{32\pi^2} \Lambda^4 + \frac{1}{4} B^2 - \frac{1}{32\pi^2} c_N \left\{ \frac{11}{3} - \frac{\beta^2}{3} \right\} g^2 B^2 \ln \frac{\Lambda^2}{B} \]
\[ + \frac{\alpha^2}{(32\pi^2)^2} c_N^2 B^2 (1 - \frac{\beta^2}{3}) g^4 \ln^2 \frac{\Lambda^2}{B} + \left( \frac{g^2}{32\pi^2} \right)^2 c_N \Lambda^2 \text{Tr} \langle x|G_F|x \rangle, \] (32)

where \( c_N = \text{Tr}(T(3)T(3)) = N \) for the group SU(N). Ignoring the \( B \)-independent divergent piece \( \sim \Lambda^4 \), the remaining expression in eq. (32) should become finite after the renormalization of the coupling constant: that is, \( \langle \Psi|H(x)|\Psi \rangle \) must become finite after sending the bare coupling strength to zero logarithmically in the limit of a large cutoff. But obviously this procedure cannot work for the last term in eq. (32), which involves a quadratic ultraviolet divergence. We conclude that the renormalizability of \( \langle \Psi|H(x)|\Psi \rangle \) requires the trace of the finite part of the kernel to vanish identically, which then gives a condition on the variational parameter \( \beta = 2 + \alpha \). Using the approximate expression (31), this condition reads:
\[ \int_0^\infty ds \frac{\sinh eBs}{s^2} \left\{ \frac{eBs}{\sinh eBs} (1 + 2 \cosh \alpha eBs) - 3 \right\} = 0. \] (33)

An approximate solution of this equation (with non-vanishing \( B \)) can be found by expanding the hyperbolic functions to second order. One thus obtains:
\[ \alpha^2 \simeq \frac{1}{2}, \quad \text{i.e.} \quad \beta \simeq 2 \pm \frac{1}{\sqrt{2}}. \] (34)

Remarkably, these values of \( \beta \) guarantee that, in the present calculation, there is no problem with the negative modes \[ \] (recall that, for \( \beta = 0 \), one faces infrared divergences at large proper times \[ \] ; see, e.g., eq. (31)). The minimum in the energy density can be seen to correspond to the value \( \beta = 2 - 1/\sqrt{2} \). For this value of \( \beta \), the energy density is, in the case of the SU(3) gauge group,
\[ \langle \mathcal{H} \rangle = \frac{1}{2} B^2 - \frac{1}{192\pi^2} (13 + 4\sqrt{2}) c_3 g^2 B^2 \ln \frac{\Lambda^2}{B} + \frac{g^4}{12(16\pi^2)^2} (3 + 2\sqrt{2}) c_3^2 B^2 \ln^2 \frac{\Lambda^2}{B}, \] (35)
where only the \( B \)-dependent terms have been kept. The minimum in the energy density occurs for \( B = B_{\text{min}} \) with

\[
B_{\text{min}} = \Lambda^2 \exp(-\frac{16\pi^2}{g^2c_3}X_{\text{min}}),
\]

(36)

and

\[
X_{\text{min}} \simeq 0.363 + \frac{g^2}{32\pi^2}c_3 + \mathcal{O}(g^4).
\]

(37)

The value of the energy at the minimum is

\[
<\mathcal{H}>_{\text{min}} = \frac{B_{\text{min}}^2}{2}\left\{\left(\frac{3}{2} + \sqrt{2}\right)X_{\text{min}} - \frac{13}{4} - \sqrt{2}\right\}\frac{g^2c_3}{16\pi^2} < 0.
\]

(38)

In order to obtain a finite value of the magnetic field at the minimum when the cutoff \( \Lambda \) is sent to infinity, namely \( B_{\text{min}} = \mu^2/\sqrt{\varepsilon} \), the coupling constant \( g \) must run with the cutoff according to

\[
\frac{g^2c_3}{16\pi^2} \ln \frac{\Lambda^2}{\mu^2} = 0.363.
\]

(39)

We can now define the effective coupling constant for a given scale \( \mu \) by looking at the coefficient of \( B^2 \) in the expression of the energy density and by writing the quantity \( \ln(\Lambda^2/B) \) as \( \ln(\Lambda^2/\mu^2) + \ln(\mu^2/B) \). The result is

\[
\frac{1}{g_R^3(\mu^2)} = \frac{1}{g^2} - \frac{1}{96\pi^2}(13 + 4\sqrt{2})c_3 \ln \frac{\Lambda^2}{\mu^2} + \frac{g^2}{6(8\pi^2)^2}(3 + 2\sqrt{2})c_3^2 \ln^2 \frac{\Lambda^2}{\mu^2}.
\]

(40)

From this equation we obtain the beta function

\[
\beta(g_R(\mu)) \equiv \mu \frac{\partial g_R}{\partial \mu} = -g_R^3\frac{1}{48\pi^2}c_3\sqrt{52.05},
\]

(41)

in the limit \( g_R^2/g^2 \to 0 \). It differs from the perturbative one loop result

\[
\beta_P(g) = -g^3\frac{1}{16\pi^2}c_3\frac{11}{3}.
\]

(42)

This is not unexpected in view of the fact that our vacuum state exhibits a non vanishing value of the condensate and a kernel which largely differs from the perturbative one. In fact the perturbative result can be recovered in our approach by simply ignoring the term \( \beta S_z T^{(3)} \) in the trial Gaussian kernel. This is however not legitimate in the variational context because \( \beta = 0 \) belongs to a region where the kernel exhibits unstable modes. Our result also differs from that of Kogan and Kovner [3] who use a variational Ansatz which does not include the possibility of a condensate.
By looking at the energy expression at the minimum we find that the quantity \( \langle \mathcal{H} \rangle_{\text{min}} / g^2 \) has a limit

\[
\frac{\langle \mathcal{H} \rangle_{\text{min}}}{g^2} \simeq -4.2 \times 10^{-3} \mu^4
\]

when the cutoff goes to infinity, i.e. is a renormalization group invariant quantity. We can compare this result to the value of the energy density in the bag model \( \varepsilon = -B \) where \( B \) is now the bag constant [14]. With \( B = (240 \text{ MeV})^4 \), the bag model leads to \( \varepsilon = -3.3 \times 10^{-3} \text{ GeV}^4 \). This gives \( \mu = 0.941 \text{ GeV} \).

Our approximate solution for the vacuum functional, it is easy to calculate the value of the gluon condensate:

\[
\langle F^a_{\mu\nu} F^a_{\mu\nu} \rangle = -2 \langle E^a_i E^a_i - B^a_i B^a_i \rangle.
\]

At the minimum, we obtain for this quantity a \textit{finite} value

\[
\langle F^a_{\mu\nu} F^a_{\mu\nu} \rangle = \frac{1}{3} (7 + \sqrt{2}) B^2_{\text{min}} X_{\text{min}},
\]

which gives

\[
\langle F^a_{\mu\nu} F^a_{\mu\nu} \rangle \simeq 0.37 \mu^4,
\]

where \( \mu \simeq 1 \text{ GeV} \). This result is in qualitative agreement with the phenomenological value 0.5 GeV\(^4\) of the gluon condensate [15].

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