Variational approach to Yang-Mills theory at finite temperatures

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We study the finite-temperature phase of a gluon ensemble in a variational approximation to QCD in the Coulomb gauge. We derive and numerically solve the underlying Dyson-Schwinger equations up to one-loop order. Assuming the subcritical solution at $T = 0$, we find a sharp transition in the infrared value of the gluon energy at a critical temperature.

I. INTRODUCTION

The determination of the phases of hadronic matter plays a major role in understanding the mechanisms of confinement and dynamical symmetry breaking in Quantum Chromodynamics (QCD). The methods available to investigate these phase transitions are the following: There are lattice simulations, which have been successful in mapping out the deconfinement transition of the QCD phase diagram as a function of temperature for near zero chemical potential [1–5], and phenomenological models, that in addition can cover the high-density regime [6–10]. Finally, in the asymptotically large temperature or density limit, due to asymptotic freedom, the weak interactions between quarks and gluons are expected to determine the properties of the quark-gluon plasma [11–15].

In this paper we investigate the thermal properties of the low-density phase using a set of tools that bridge QCD and phenomenology. In particular, we formulate the problem in the physical, Coulomb gauge, canonical Hamiltonian framework of the pure gauge theory. While there have been numerous studies of QCD based on Dyson-Schwinger resummation techniques [16–19], renormalization group flow equations [20], and lattice simulations [21–23] in covariant gauges, the few that exist in physical gauges are rather loosely related to the underlying QCD interactions [24–29], with a recent attempt at a self-consistent calculation at finite density [30].

The advantages of physical gauges for phenomenology and for developing physical intuition are clear, and we summarize them here. The degrees of freedom of the pure Yang-Mills (YM) theory are transverse gluons, and thermal excitations connect color singlet states of arbitrary number of gluons. Transverse gluons are expected to be effective only at high temperatures, while at low temperatures it would be more effective to compute the partition function in terms of the ground state glueballs [34, 35]. The underlying interactions in Coulomb gauge are dominated by the instantaneous Coulomb potential acting between color charges. In the non-Abelian theory, the potential not only couples charges but it also depends on the gluon distribution of the state in which it is calculated. At zero temperature, in the vacuum state this distribution is such that the Coulomb potential becomes confining, i.e., proportional to the distance $R$ between the external color charges, $V(R) = \sigma_c R$ [36, 37]. Using various approximate, variational models for the ground state YM wave functional, it has been possible to obtain a potential which is confining [38] or almost confining, i.e., $V(R) \propto R^{1-\epsilon}$ with $\epsilon \approx O(10\%)$ [39–41]. The Coulomb string tension $\sigma_c$ is larger than the string tension computed from the temporal Wilson loop. This is because the Coulomb potential represents the energy of a static quark-antiquark pair submersed in the QCD vacuum, while the Wilson loop measures the energy of the exact $QQ$ state in which the gluon distribution is squeezed by closed vortex lines. Since the Coulomb potential is an instantaneous observable, one might expect that it remains confining even in the high-temperature limit [37]: At high temperatures the integration over transverse fields becomes even less restricted than in the vacuum, and, according to the Gribov-Zwanziger confinement scenario [42, 43], Coulomb confinement originates from large field configurations near the the Gribov horizon.

In the following, we investigate the finite temperature properties of Coulomb gauge Yang-Mills theory with focus on the aspects of deconfinement at finite temperature. We extend the variational approach of Refs. [38, 40, 41] to finite temperature. In particular, the variational Gaussian ansatz for the vacuum wave functional is extended to include single particle, quasi-gluon excitations. In Sections II and III we present the general setting for the finite temperature, canonical Coulomb gauge problem. In Section IV we discuss the details of the variational approximation. In Section V we give details of the numerical computations and results. Our summary and outlook are given in Section VI.

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1 At zero temperature and density, Dyson-Schwinger studies in Coulomb gauge have been performed in Refs. [31–33].
II. HAMILTONIAN APPROACH AT FINITE TEMPERATURES

After resolving Gauss’s law in Coulomb gauge, the Yang-Mills Hamiltonian reads

\[ H_{YM} = \frac{1}{2} \int \! d^3x \left( J^{-1}[A] \Pi J[A] \Pi + B^2 \right) + H_c \]
\[ \equiv H_K + H_B + H_c, \]

\[ H_c = \frac{g^2}{2} \int \! d^3x \, d^3y \, J^{-1}[A] \rho^a(x) J[A] F_A^{ab}(x, y) \rho^b(y), \]

where \( \Pi^a(x) = -i \delta / \delta A^a(x) \) is the canonical momentum (electric field) operator, and

\[ J[A] = \text{Det}(-D \nabla) \]

is the Faddeev-Popov determinant with

\[ D = \nabla + g \hat{A}, \quad \hat{A}^{ab} = \hat{T}_c A^c, \quad (\hat{T}_c)^{ab} = f^{abc} \]

being the covariant derivative in the adjoint representation. Furthermore,

\[ \rho^a(x) = -f^{abc} A^b \cdot \Pi^c \]

is the color charge density of the gluons and

\[ F_A^{ab}(x, y) = \langle x, a|(-D \nabla)^{-1} (-\nabla^2)^{-1} |y, b \rangle \]

is the so-called Coulomb kernel. Its vacuum expectation value \( \langle F_A^{ab}(x, y) \rangle \) represents the static non-Abelian color Coulomb potential.

The gauge fixed Hamiltonian Eq. (1) is highly non-local due to Coulomb kernel \( F_A(x, y) \), Eq. (6), and due to the Faddeev-Popov determinant \( J[A] \), Eq. (3). In addition, the latter also occurs in the functional integration measure of the scalar product of the Coulomb gauge wave functionals

\[ \langle \psi_1|O|\psi_2 \rangle = \int \! DA J[A] \psi_1^\dagger[A] O \psi_2[A], \]

In Ref. [40] the Yang-Mills Schrödinger equation was solved by the variational principle using the following ansatz for the vacuum wave functional

\[ \langle A|0 \rangle = \frac{1}{\sqrt{J[A]}} \langle A|\tilde{0} \rangle, \]
\[ \langle A|\tilde{0} \rangle = \mathcal{N} \exp \left( -\frac{1}{2} \int \! dk \, A(-k) \omega(k) A(k) \right), \]

where

\[ \int \! dk = \frac{d^3k}{(2\pi)^3}. \]

The pre-exponential factor removes the Faddeev-Popov determinant from the scalar product Eq. (7). The kernel \( \omega(k) \) was determined by minimizing the vacuum energy \( \langle H_{YM} \rangle \), which yields an \( \omega(k) \) which can be well fitted by Gribov’s formula

\[ \omega(k) = \sqrt{k^2 + \frac{M^4}{k^2}} \]

and which is in satisfactory agreement with the lattice data [44], with \( M \approx 860 \text{ MeV} \).

The present paper is devoted to study Yang-Mills theory at finite temperatures, which is defined by the density operator

\[ D = Z^{-1} \exp(-\beta H_{YM}), \]

where \( \beta = 1/T \) is the inverse temperature and

\[ Z = \text{Tr} e^{-\beta H_{YM}} \]

is the partition function.

To calculate the trace in the thermal averages

\[ \langle O \rangle = \text{Tr}(OD) \]

we need a suitable basis in the gluonic Fock space, which we choose as follows: Let \( a^a_i(k) \) be the operator which annihilates the vacuum state \( |\tilde{0} \rangle \) [Eq. (8)], i.e.,

\[ a^a_i(k)|\tilde{0} \rangle = 0. \]

Then a complete basis in the gluonic Fock space is given by

\[ \{ |\tilde{n} \rangle \} = \{ |\tilde{0} \rangle, a^a_i(k)|\tilde{0} \rangle, a^a_i(k)a^b_j(k)|\tilde{0} \rangle, \ldots \}. \]

Following Ref. [40] we choose the basis states of the gluonic Fock space in the form (cf. Eq. (8))

\[ \{ |n \rangle \} = \{ J^{-1/2}[A]|\tilde{n} \rangle \}. \]

The thermal expectation value Eq. (13) can then be expressed as

\[ \langle O \rangle = \overline{\text{Tr}}(\tilde{D}\tilde{O}), \]

where the operation ‘\( \sim \)’ is defined by

\[ \tilde{D} = J^{1/2}[A]OJ^{-1/2}[A], \]

and ‘\( \overline{\text{Tr}} \)’ means that the trace is evaluated in the basis of the states \( \{ |\tilde{n} \rangle \} \) [Eq. (15)]. The transformed density operator reads explicitly

\[ \tilde{D} = Z^{-1} \exp(-\beta \tilde{H}_{YM}), \quad Z = \overline{\text{Tr}} e^{-\beta \tilde{H}_{YM}}. \]

This operator is too difficult to handle in semi-analytical calculations. In analogy to the zero-temperature case, where the Gaussian vacuum wave functional Eq. (8) was assumed, we will replace the exact (transformed according to Eq. (18)) Yang-Mills Hamiltonian \( \tilde{H}_{YM} \) by a single-particle operator

\[ \hat{h} = \int \! dk \, \Omega(k) a_{i}^{b_j}(k) a_{i}^{a}(k), \]
where the kernel $\Omega(k)$ will be determined by minimizing the free energy

$$\mathcal{F} = \langle H_{\text{elm}} \rangle - TS. \quad (21)$$

Here $S$ is the entropy, which is defined by

$$S = -\tilde{\text{Tr}} \tilde{D} \ln \tilde{D}. \quad (22)$$

By straightforward manipulations the expression for the entropy Eq. (22) can be cast into the form

$$S = \ln Z - \beta \frac{\partial \ln Z}{\partial \beta}, \quad (23)$$

which will be convenient in later calculations.

## III. COLOR PROJECTION

### A. Exact projection

By definition the trace in the thermal averages Eq. (17) should be taken in the physical Hilbert space. Before gauge fixing the physical Hilbert space is given by all gauge invariant states. After resolving Gauss’ law in Coulomb gauge, the physical Hilbert space is defined by a complete set of wave functionals of the transversal gauge field that are invariant under global gauge transformations (the latter is not fixed by the Coulomb gauge condition). These states are annihilated by the total color charge operator.

$$Q^a = \int d^3x \rho^a(x). \quad (24)$$

However, an individual basis state of the set Eq. (15) will, in general, carry a non-zero color charge, and the use of the basis Eq. (16) will lead to a colored statistical ensemble. Therefore we project these states onto color singlet states using the projector

$$\mathcal{P} = \int d\mu(\theta) \exp[i\theta_aQ^a], \quad (25)$$

where $d\mu(\theta)$ denotes the Haar measure of the gauge group parametrized in terms of the color angles $\theta_a$. The thermal average projected onto zero-color states reads

$$\langle O \rangle = \tilde{\text{Tr}}(\tilde{D} \tilde{\mathcal{P}}), \quad (26)$$

where $\tilde{D}$ is given by Eq. (19) with $\hat{H}_{\text{elm}}$ replaced by $\hat{h}$ [Eq. (20)]:

$$\tilde{D} = Z^{-1} e^{-\beta \hat{h}}, \quad Z = \tilde{\text{Tr}}(e^{-\beta \hat{h}} \mathcal{P}). \quad (27)$$

The density operator $\tilde{D}$ [Eq. (27)] is color singlet and hence commutes with the total color charge operator $Q^a$ [Eq. (24)], which in terms of the creation and annihilation operators reads

$$Q^a = if^{abc} k \int dk \, a_i^b(k) a_c^c(k). \quad (28)$$

With the explicit form of the projector Eq. (25) we have

$$\tilde{D}\mathcal{P} = \int d\mu(\theta) D_\theta, \quad (29)$$

where

$$D_\theta = e^{i\theta Q} \tilde{D} = e^{-\beta \hat{h} + i\theta Q} \quad (30)$$

is the density operator in the presence of an external color field $-i\theta_aQ^a/\beta$, i.e., for fixed color angle $\theta_a$. Due to the presence of the external color field $-i\theta_aQ^a/\beta$, this density matrix is non-diagonal in color space. However, since the total charge operator $Q_a$ is hermitian and $\hat{h}$ is color singlet, we can diagonalize $D_\theta$. For simplicity, we consider the gauge group $SU(2)$. Then we may write

$$D_\theta = \mathcal{U}(\theta) D_0 \mathcal{U}(\theta)^\dagger, \quad (31)$$

where $\mathcal{U}(\theta)$ lives in the coset $SU(2)/U(1)$ and

$$D_0 = \exp(-\beta \hat{h} + i\theta Q^3) \quad (32)$$

lives in the Abelian subgroup. In a parametrization of the gauge group $SU(2)$ corresponding to the coset decomposition Eq. (31) the Haar measure reads

$$\int_{S^2} d\mu(\theta) = \int d\mu(\theta) \int_{S^2} d\mu(\theta), \quad \int d\mu(\theta) = \frac{1}{\pi} \int_{-\pi}^{\pi} d\theta \, \sin^2 \frac{\theta}{2}, \quad (33)$$

where $d\mu(\theta)$ denotes the measure for the integration over the coset’s $SU(2)/U(1) \simeq S^2$ degrees of freedom.

In the thermal averages [Eq. (26)] of colorless operators $O$ the unitary matrix $\mathcal{U}(\theta)$ drops out. Since the density matrix $D_\theta$ does not depend on the coset degrees of freedom $\theta$, the corresponding integral can then be trivially carried out

$$\int_{S^2} d\mu(\theta) = 4\pi, \quad (34)$$

and we obtain for the projected thermal averages

$$\langle O \rangle = \frac{1}{Z} \int d\mu(\theta) \, Z(\theta) \langle O \rangle_\theta, \quad Z = \int d\mu(\theta) Z(\theta), \quad (35)$$

where

$$\langle O \rangle_\theta = \frac{1}{Z(\theta)} \tilde{\text{Tr}}(D_\theta \tilde{O}), \quad Z(\theta) = \tilde{\text{Tr}} D_\theta \quad (36)$$

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2 Also in the functional integral formulation after fixing to Coulomb gauge a careful treatment of the zero modes of the Faddeev-Popov operator related to the global gauge transformations constrains the ensemble of transversal gauge fields to those with vanishing total color charge [45].
Since the basic contraction is obtained as $D^3$ in three dimensions. Furthermore, for the partition function using Wick’s theorem. In the standard fashion one finds the non-Abelian color Coulomb potential. This quantity is known from the lattice and also from continuum studies to have the infrared behavior. Accordingly, the integrand in Eq. (44c) becomes divergent for $p = q$. Furthermore, the last term in Eq. (44c) is manifestly divergent. However, one easily shows that

\[
\langle a_i^\dagger(k) a_j^\beta(q) \rangle = \delta^{ij} t_{ij}(k) (2\pi)^3 \delta(k - q) n_{\alpha}(k, \theta).
\] (42)

Expressing the gauge field in terms of the creation and annihilation operators one finds from Eq. (42) for the gluon propagator

\[
\langle A^\alpha_\mu(p) A^\beta_\mu(q) \rangle = \delta^{\alpha\beta} t_{ij}(p) (2\pi)^3 \delta(p + q) \frac{1 + 2n_\alpha(p, \theta)}{2\omega(p)}.
\] (43)

With these relations it is straightforward to calculate the thermal expectation value of the Hamiltonian using the same approximation as at zero temperature in Ref. [40], i.e., assuming a bare ghost-gluon vertex and calculating the energy up to two loops.

To work out the effect of the color projection on the energy, let us for the moment ignore the Faddeev-Popov determinant in the Hamiltonian. We will later fully include $J[A]$. Using the explicit form of the thermal gluon propagator, Eq. (43), and the same approximation as in Ref. [40] but putting $J[A] = 1$, one finds for the various pieces of the energy

\[
\begin{align}
\langle H_K \rangle &= \frac{V}{4} \int dq \omega(q) \left[ 3 + 2 \sum_{\alpha} n_{\alpha}(q) \right], \\
\langle H_B \rangle &= \frac{V}{2} \int dq \frac{q^2}{\omega(q)} \left[ 3 + 2 \sum_{\alpha} n_{\alpha}(q) \right] \\
&\quad + \frac{V g^2 N_c}{16} \int dq dp \frac{3 - (q \cdot p)^2}{\omega(q) \omega(p)} \times \left[ 3 + 2 \sum_{\alpha} (n_{\alpha}(p) + n_{\alpha}(q)) + 2 \sum_{\alpha, \beta} n_{\alpha}(p) n_{\beta}(q) \\
&\quad - \sum_{\alpha} n_{\alpha}(p)(n_{\alpha}(q) + n_{-\alpha}(q)) \right].
\end{align}
\] (44b)

To simplify the notation, we have omitted the $\theta$-dependence of the occupation numbers Eq. (41). In Eq. (44c)

\[
F(x, y) = \langle F_A(x, y) \rangle
\] (45)

is the non-Abelian color Coulomb potential.
these divergent terms disappear after color projection. For this purpose, we note that if one replaces in the Coulomb Hamiltonian $H_C$ [Eq. (2)] the Coulomb kernel $F_A$ by

$$\frac{g^2}{2} F_A^{ab}(x,y) \to \delta^{ab}(x-y), \quad (47)$$

the Coulomb Hamiltonian becomes the square of the total charge

$$H_C \to Q^a Q^a. \quad (48)$$

This equivalence holds even when the Faddeev-Popov determinant is included, since $J[A]$, being invariant under global color rotations, commutes with the total color charge operator $Q^a$. In momentum space the replacement Eq. (47) corresponds to

$$\frac{g^2}{2} F(k) \to (2\pi)^3 \delta(k). \quad (49)$$

It follows that the singular $p = q$ contributions to the double integral in $\langle H_C \rangle_\theta$ [Eq. (44c)] are proportional to $\langle Q^a Q^a \rangle_\theta$. However, this quantity has to vanish after color projection

$$\langle Q^a Q^a \rangle = \frac{1}{Z} \int d\Omega(\theta) Z(\theta) \langle Q^a Q^a \rangle_\theta = 0. \quad (50)$$

Therefore, the singular contributions that occur from the $p = q$ part of the integrand vanish after color projection. We can explicitly eliminate these singularities by replacing the Coulomb potential $F(k)$ by

$$\tilde{F}(k) = F(k) - F(0) V^{-1} (2\pi)^3 \delta(k)$$

$$= F(k) (1 - V^{-1} (2\pi)^3 \delta(k)). \quad (51)$$

This replacement will, in particular, remove the last term of Eq. (44c). The kernel $\tilde{F}$ and thus the color-projected Coulomb energy $\langle H_C \rangle_\theta$ is invariant with respect to a shift of the Coulomb kernel by a constant

$$F(x,y) \to F(x,y) + C. \quad (52)$$

This shift implies in momentum space

$$F(k) \to F(k) + C(2\pi)^3 \delta(k), \quad (53)$$

which obviously leaves $\tilde{F}(k)$ [Eq. (51)] unchanged.

### B. Color projection in the thermodynamic limit

The partition function Eq. (40) depends via the finite-temperature occupation numbers $n_\theta(k)$ [Eq. (41)] on the color angle $\theta$. The $\theta$-dependence can be explicitly separated yielding

$$Z(\theta) = Z(0) \exp(-V f(\theta)), \quad (54)$$

where

$$Z(0) = \exp\left\{2(N_c^2 - 1)V \int dk \ln[1 + n(k)]\right\} \quad (55)$$

is the partition function for vanishing “external” color field ($\theta = 0$), with

$$n(k) = n_\theta(k)_{\theta=0} = n_{\alpha=0}(k) = \left( e^{i\Omega(k)\theta} - 1 \right)^{-1} \quad (56)$$

being the corresponding thermal occupation numbers. The $\theta$-dependence is entirely contained in the exponent of Eq. (54), which is given by

$$f(\theta) = 2 \int dk \ln[1 + 2(1 - \cos\theta) n(k)(1 + n(k))]. \quad (57)$$

Note that the partition function is an even function in $\theta$. This property holds for the expectation value $\langle O \rangle_\theta$ of any color singlet operator $O$.

Consider now the total partition function $Z$, Eq. (35). In the integration domain $\theta \in [-\pi, \pi]$ the function $f(\theta)$ [Eq. (57)] takes its minimum at $\theta = 0$, where it vanishes

$$f(\theta = 0) = 0. \quad (58)$$

Due to the presence of the volume factor $V$, in the thermodynamic limit $V \to \infty$ only small $\theta$ values contribute to the integral Eq. (57). Therefore it suffices to expand the function $f(\theta)$ to leading order in $\theta$ yielding

$$Z(\theta) = Z(0) e^{-\frac{1}{2} C \theta^2}, \quad (59)$$

where

$$C = V f''(0), \quad f''(0) = 2 \int dk \ln[1 + (1 + n(k))]. \quad (60)$$

With this representation for $Z(\theta)$, the thermal expectation value Eq. (35) of an observable $O$ becomes

$$\langle O \rangle = \frac{Z(0)}{Z} \int d\mu(\theta) \langle O \rangle_\theta e^{-\frac{1}{2} C \theta^2} \quad (61)$$

with

$$Z = Z(0) \int d\mu(\theta) e^{-\frac{1}{2} C \theta^2}. \quad (62)$$

Due to the presence of the Gaussian, only small $\theta$ values contribute significantly to the integrals. Therefore it suffices to expand $\langle O \rangle_\theta$ up to leading order in $\theta$

$$\langle O \rangle_\theta = \langle O \rangle_{\theta=0} + O^{(2)} \theta^2 + \cdots \quad (63)$$

Defining

$$I_n = \frac{1}{Z(0)} \int d\mu(\theta) Z(\theta) \theta^{2(n-1)} \quad (64)$$

3 The same expansion was used in Ref. [46] for the quark partition function.
and using
\[ Z = Z(0)I_1, \]
we obtain
\[ \langle O \rangle = \langle O \rangle_{\theta=0} + \frac{I_2}{I_1} O^{(2)}. \]

Along the same lines, we can also expand the integration measure \( d\mu(\theta) \) [Eq. (33)] to leading order in \( \theta \) and put the upper integration limit to \( \infty \). This yields for the integrals Eq. (64)
\[ I_n = \frac{1}{2\pi} \int_0^\infty d\theta \theta^{2n} e^{-\frac{1}{4}C\theta^2} = \frac{1}{\sqrt{8\pi C}} \frac{(2n-1)!!}{C^n}. \]

Since \( I_2/I_1 \sim 1/V \) in the thermodynamic limit \( V \to \infty \), the second term in Eq. (66) can be omitted and we find
\[ \langle O \rangle = \langle O \rangle_{\theta=0}. \]

This shows that in leading order in the thermodynamic limit the effect of the color projection can be ignored. In the following we will skip the subscript \( \theta = 0 \) and \( \langle O \rangle \) means \( \langle O \rangle_{\theta=0} \), which is the unprojected thermal average.

To include the Faddeev-Popov determinant we use the representation [47]
\[ J[A] = \exp \left( -\frac{1}{2} \int dk A(-k)\chi(k)A(k) \right), \]

where
\[ \chi(p) = \frac{N_c}{4} \int dp \left( 1 - (\hat{p} \cdot \hat{q})^2 \right) \frac{d(p - q) d(q)}{(p - q)^2} \]
is the ghost loop (curvature) and \( d(p) \) is the ghost form factor defined by
\[ \langle (-D\partial)^{-1} \rangle = \frac{1}{g} \frac{d(-\Delta)}{-\Delta}, \]

which satisfies the following Dyson-Schwinger equation
\[ d^{-1}(p) = \frac{1}{g} - I_d(p), \]
\[ I_d(p) = \frac{N_c}{2} \int dq \left[ 1 - (\hat{p} \cdot \hat{q})^2 \right] \frac{d(p - q) 1 + 2n(q)}{(p - q)^2 \omega(q)}, \]

where a bare ghost-ghost vertex has been assumed. This equation differs from the zero-temperature case only by the replacement of the gluon propagator by its finite temperature counterpart Eq. (43). The representation Eq. (69) is valid up to two loops in the energy, which is the order considered in the present paper.

With the inclusion of the Faddeev-Popov determinant, the thermal expectation value of the Hamiltonian \( \langle H_{\text{YM}} \rangle \) given by Eqs. (44) simplifies for \( \theta = 0 \) to
\[ \langle H_{\text{YM}} \rangle = (N_c^2 - 1) \cdot 2 \cdot V e, \quad e = e_K + e_B + e_c, \]

where
\[ e_K = \frac{1}{4} \int dq \left\{ [\omega^2(q) + \chi^2(q)] \frac{1 + 2n(q)}{\omega(q)} - 2\chi(q) \right\} \]

are the energy densities per degree of freedom.

**IV. FINITE TEMPERATURE VARIATIONAL PRINCIPLE**

Our ansatz for the density operator [Eqs. (20) and (27)] contains a so far arbitrary kernel \( \Omega(k) \), which we determine now by minimizing the free energy \( F \), Eq. (21). Instead of varying \( F \) with respect to \( \Omega(k) \), it is more convenient to take the variation with respect to the finite-temperature occupation number \( n(k) \) [Eq. (56)], which is a monotonic function of \( \Omega(k) \) for \( \Omega(k) > 0 \). Variation of \( F \) with respect to \( n(k) \) yields
\[ \Omega(k) = \frac{\delta e[n]}{\delta n(k)}, \]

which identifies \( \Omega(k) \) as the quasi-gluon energy.

So far, the kernel \( \omega(k) \), which defines the vacuum wave functional Eq. (8) and thus our basis of the Fock space, is completely arbitrary and, in principle, we could use any positive-definite kernel \( \omega(k) \). As long as we include the
complete set of states and do not introduce any approximation, the thermal expectation values will be independent of \(\omega(k)\). However, due to approximations necessary as, for example, the restriction to two loops, the thermal averages will depend on the \(\omega(k)\) chosen and the optimal choice is obtained by extremizing the free energy Eq. (21) with respect to \(\omega(k)\)

\[
\frac{\delta F}{\delta \omega(k)} = 0, \tag{76}
\]

which yields the finite temperature gap equation

\[\omega(k) = k^2 + \chi^2(k) + I^{(0)} + I(k), \tag{77}\]

where

\[I^{(0)} = \frac{g^2 N_c}{4} \int dq \frac{3 - (\hat{k} \cdot \hat{q})^2}{\omega(q)} [1 + 2n(q)],\]

\[I(k) = \frac{g^2 N_c}{4} \int dq \frac{1 + (\hat{k} \cdot \hat{q})^2}{\omega(q)} \left\{ [1 + 2n(q)] \left[ \omega^2(q) - \omega^2(k) + (\chi(q) - \chi(k))^2 \right] - 2\omega(q) [\chi(q) - \chi(k)] \right\}. \tag{78}\]

These loop integrals, as well as the ones of the curvature [Eq. (70)] and of the ghost Dyson-Schwinger equation [Eq. (72)], are ultraviolet divergent and need to be regularized and eventually renormalized.

Inserting the explicit expressions Eqs. (74) for the energy densities \(e\) into Eq. (75) and using the gap equation (71), one finds

\[
\Omega(k) = \omega(k) [1 + I_\Omega(k)],
\]

\[I_\Omega(k) = \frac{g^2 N_c}{4} \int dq \frac{1 + (\hat{k} \cdot \hat{q})^2}{\omega(q)} [1 + 2n(q)]. \tag{79}\]

To carry out the renormalization we will have to deal with both finite- and zero-temperature solutions. To avoid confusion, in the following we will explicitly indicate the temperature dependence by writing \(\omega(k, T), d(k, T), \ldots\) instead of \(\omega(k), d(k), \ldots\)

At very large momenta \(|k| \gg T\) the temperature should become irrelevant. Indeed, the temperature dependence of the loop integrals (which is due to the finite-temperature occupation numbers \(n(k)\)) does not give rise to additional UV singularities. Therefore the zero-temperature counterterms are sufficient to eliminate all UV singularities.

Adding the zero-temperature counterterms, see Ref. [41], and carrying out the renormalization as described in Ref. [48], one arrives at the following renormalized gap equation

\[\omega^2(k, T) = k^2 + \chi^2(k, T) + \Delta I^{(2)}(k, T) + c_0 + \bar{I}^{(0)}(T) + 2\bar{\chi}(k, T) \Delta I^{(1)}(k, T) + c_1 + \bar{I}(k, T), \tag{80}\]

where we have introduced the abbreviations

\[\bar{\chi}(k, T) = \chi(k, T) - \chi(\mu, T = 0),\]

\[\bar{I}^{(0)}(T) = I^{(0)}(T) - I^{(0)}(T = 0),\]

\[\Delta I^{(1)}(k, T) = I^{(1)}(k, T) - I^{(1)}(\mu, T = 0), \tag{81}\]

and defined the following loop integrals

\[
I^{(1)}(k, T) = \frac{g^2 N_c}{4} \int dq \frac{1 + (\hat{k} \cdot \hat{q})^2}{\omega(q, T)} \left\{ [\omega(q, T) - \bar{\chi}(q, T)] I - [\omega(k, T) - \bar{\chi}(k, T)] I \right\}, \tag{82}\]

\[I(k, T) = \frac{g^2 N_c}{4} \int dq \frac{1 + (\hat{k} \cdot \hat{q})^2}{\omega(q, T)} 2n(q) \left\{ \omega^2(q, T) - \omega^2(k, T) + [\bar{\chi}(q, T) - \bar{\chi}(k, T)]^2 \right\}. \tag{83}\]

In addition, the renormalized equation (72) for the ghost form factor reads

\[
\frac{1}{d(k, T)} = \left[ \frac{1}{d(\mu, T = 0)} + I_d(\mu_d, T = 0) \right] - I_d(k, T). \tag{84}\]

The renormalized Dyson-Schwinger equations (80) and (84) contain the finite renormalization scales, \(\mu_t = \mu_\chi, \mu_\omega, \mu_d, \) and the renormalization constants \(g(\mu_t), \chi(\mu_t), c_0(\mu_t), \) and \(c_1(\mu_t). \) The last two originate from the counterterms in the Hamiltonian and \(\chi(\mu_t)\) from the renormalization of the Faddeev-Popov determinant. In particular, in Ref. [48] it was shown that for \(\mu_\omega = \mu_d = 0\) the value \(c_1 = 0\) is required in order that the 't Hooft loop obeys a perimeter law and is also favored by the variational principle. It was also found that the parameter \(c_0\) has no influence on the IR- or UV-behavior of the resulting solutions and influences only the mid-momentum regime of \(\omega(k)\). The choice of renormalization conditions for our study at finite temperature will be discussed in Sec. V.
The Gribov-Zwanziger confinement scenario assumes that \( d^{-1}(0, T = 0) = 0 \). For practical reasons, in the present paper we will assume a small but finite \( d^{-1}(0, T) \), which results in a massive gluon propagator, referred to as subcritical solution in Ref. [41]. This solution does not provide a confining Coulomb potential, but for phenomenological purposes may be as useful as the critical confining solution \( d^{-1}(0) = 0 \) (see Ref. [41] for further discussions). One can give arguments that a \( d^{-1}(0) \) \( \neq 0 \) is the result of an improper treatment of the Gribov problem [33, 49]. In fact, it was explicitly demonstrated in 1 + 1 dimensions [50], and also arguments were given for 3 + 1 lattice gauge theory in Landau gauge [49], that extending the functional integral over the transverse gauge field to higher Gribov regions reduces the infrared strength of the ghost form factor, pushing \( d^{-1}(0) \) to higher values. Based on this observation, it was argued in Refs. [33] and [49] that choosing different values of \( d^{-1}(0) \) corresponds to different “gauge fixings”. (After all, a complete gauge fixing implies also the restriction to the fundamental modular region, which is a subset of the first Gribov region.) Presumably, in more than 1 + 1 dimensions the restriction to the fundamental modular region requires \( d^{-1}(0) = 0 \). In any case this value is required for a linearly rising Coulomb potential, which is a necessary condition for confinement in the Gribov-Zwanziger confinement scenario [42, 43]. Thus, if \( d^{-1}(0) \) is kept finite for technical reasons, it has to be kept small to stay close to the physical confining limit \( d^{-1}(0) = 0 \).

V. NUMERICAL RESULTS

As shown in Sec. III A, the color projection removes the zero mode from the Coulomb potential, see Eq. (51). In the continuum it is replaced by

\[
g^2 F(k) = \lim_{\epsilon \to 0} \frac{d^2(k)}{k^2 + \epsilon^2} \left[ 1 - \exp(-k^2/\epsilon^2) \right],
\]

were we used the approximation [cf. Eq. (6)] [40]

\[
\langle F^{ab}_A(x,y) \rangle = \sum_c \int d^3z \langle \langle x, a|(-D^2)^{-1}|c, z \rangle \rangle \langle (-D^2)^{-1}
\]

\[\langle \langle x, c|(-D^2)^{-1}|y, b \rangle \rangle \rangle,
\]

with the external \( \langle \cdots \rangle \) referring to the thermal average. In the confining limit

\[
g^2 F(k) = \frac{d^2(k)}{k^2} \text{ as } k \to 0 \frac{8\pi\sigma_c}{k^4} \text{ (87)}
\]

and the single, quasi-gluon energy in Eq. (79) is infinite at all temperatures, which is certainly an artifact of our approximation, since at least for large \( |k| \) the quasi-gluon energy should be finite due to asymptotic freedom. For infinite \( \Omega(k) \) the finite-temperature occupation numbers \( n(k) \) [Eq. (56)] vanish at all temperatures and there is no finite-temperature phase transition. Thus the presently used approximations are inappropriate for the strictly confining solution. As discussed in Ref. [41], without the approximation of Eq. (86) there are no strictly confining solutions in the sense of Eq. (87) in the variational approximation, and in this case the \( \Omega(k) \) are finite (for finite \( k \)) and at finite temperature a non-trivial solution with \( n(k) \neq 0 \) is expected. In this case we solve the set of finite-temperature Dyson-Schwinger equations numerically on a momentum grid. The non-confining solutions depend on the renormalized coupling or, alternatively, the value of \( d(k = 0, T) \) [cf. Eq. (72)]. As discussed in Sec. IV, the Dyson-Schwinger equations are renormalized by subtraction at zero temperature to account for temperature-independent counterterms. In the numerical computation, however, it is very difficult to solve these equations at fixed \( T \) unless subtracted at the same value of \( T \). Thus, in the numerical results that follow all subtractions will be done at finite \( T \). In particular, when

![FIG. 1. Low momentum (IR) behavior for \( \beta = 0.5, \epsilon = 0.01 \), and \( d^{-1}_0 = 0.0005, 0.0040 \) of solutions for gap equation for \( \omega \). In the limit \( \epsilon \to 0 \) and/or \( \beta \to \infty \) the solutions do not change qualitatively. The critical solution corresponds to \( d^{-1}_0 = 0 \), and the solution with \( d^{-1}_0 = 0.0005 \) is close to critical. The IR limit is weakened as \( d^{-1}_0 \) increases and the ghost propagator becomes massive.](image1)

![FIG. 2. Same as Fig. 1 for the ghost form factor \( d \).](image2)
solving for \( d(k, T) \) [see Eq. (72)] we use

\[
\frac{1}{d(k, T)} = \left[ \frac{1}{d(\mu_d, T)} + I_d(\mu_d, T) \right] - I_d(k, T). \tag{88}
\]

Comparing this with Eq. (84) we have

\[
d_0^{-1} = \frac{1}{d(\mu_d, T)} = \frac{1}{d(\mu_d, 0)} + I_d(\mu_d, 0) - I_d(\mu_d, T), \tag{89}
\]

with \( \mu_d \) chosen to be the lowest point on the momentum grid, which corresponds to \( \mu_d = 0 \) in the infinite volume limit. In other words, we fix \( d_0^{-1} \) with the temperature: At each temperature we thus control the distance to the confining limit of the color Coulomb potential. This implies that the mass scale which enters \( I_d(\mu_d \sim 0, T) \) on the r.h.s. of Eq. (89) depends on \( T \). Similarly, the numerical stability of the solution of the gap equation for \( \omega(k, T) \) [Eq. (80)] requires that we use temperature-dependent renormalization constants, i.e., in Eq. (81) instead of subtracting at \( T = 0 \) we subtract at finite \( T \), so that \( \mu_x = \mu_x(T) \) and \( \mu_\omega = \mu_\omega(T) \). In particular, we use a single renormalization scale and set \( \mu(T) = \mu_\omega(T) = \mu_x(T) \). This implies that we renormalize the gap equation at a finite momentum \( \mu_x \neq 0 \). By renormalizing at \( \mu_x = 0 \), one would be enforcing a particular IR limit of the solution of the gap equation, which could turn out to be incompatible with the finite-temperature equation. Instead, by choosing \( \mu_\omega \) away from the IR limit the value obtained from solving numerically for \( \omega(0) \equiv \omega(k = 0, T) \) will serve to illustrate the onset of a phase transition.

To search for the phase transition we proceed as follows. We start with a small but finite IR regulator \( \epsilon \) [see Eq. (85)], and at given, small \( T \) (large \( \beta \)) we choose a solution close to a critical one. A typical case is shown in Figs. 1 and 2. In all figures, physical, dimensional quantities are plotted in units of \( \mu(T) \). With fixed \( \epsilon \) and \( d_0 \) we increase \( T \) (decrease \( \beta \)) and study both \( \omega \) and \( d \). A series of computations of \( \omega(0) \) as function of \( \beta \) for \( \epsilon = 0.01 \) and \( d_0^{-1} \) in the range \([0.0005, 0.0060]\) is shown in Fig. 3. As \( d_0^{-1} \) increases, the solution becomes less critical, i.e., less IR enhanced, and the Coulomb potential moves away from the confining limit of Eq. (87). In this phase, as shown in Fig. 3, there is an abrupt change in the gap function \( \omega(0) \) at a critical temperature which decreases as the solution become weaker in the IR. Please note that the results shown for different values of \( d_0^{-1} \) correspond to different physical scales. We also studied the dependence on \( \epsilon \), as the limit \( \epsilon \to 0 \) should be taken to approach the infinite volume. Starting from a massive solution at zero temperature, e.g., with \( d_0^{-1} = 0.060 \), we increase the temperature and decrease \( \epsilon \). In particular, we solve the equations for \( \epsilon = 0.0001 \) and \( \epsilon = 0 \). The latter choice is possible, since with an IR finite ghost dressing function \( (d_0^{-1} \neq 0) \) the Coulomb potential in Eq. (87) does not lead to an IR singularity in the integrals. The results are shown in Figs. 4 and 5. Even though, in numerical simulations with a finite momentum grid, one cannot reach the exact critical limit of \( \epsilon = 0 \), \( d_0^{-1} = 0 \)

FIG. 3. \( \omega(0) \) as a function of temperature for \( \epsilon = 0.01 \) and \( d_0^{-1} = \{0.0060, 0.0040, 0.0029, 0.0015, 0.0005\} \). The phase transition is clearly visible and becomes stronger and moves to lower temperatures as \( d_0^{-1} \) increases. For \( d_0^{-1} \to 0 \) the phase transition disappears, i.e., moves to infinite temperatures.

FIG. 4. \( \omega(0) \) as a function of temperature for \( d_0^{-1} = 0.0060 \) and \( d_0^{-1} = \{0.0001, 0.0015\} \) compared with with solutions for \( \epsilon = 0.0001 \) and \( \epsilon = 0 \).

FIG. 5. Same as in Fig. 4 for \( d_0^{-1} = 0.0029 \).
Strictly speaking, the variational Coulomb gauge model which leads to $d_0^{-1} \neq 0$ is not confining and thus only loosely related to QCD. The Gribov-Zwanzinger confinement scenario is reached in the $d_0^{-1} \to 0$ (and $\epsilon \to 0$) limit. We find it amusing, however, that the quasi-gluons which for $d_0^{-1} \neq 0$ are deconfined at all temperatures behave similar to the physical gluons both below and above $T_c$. We have found that quasi-particle, gluonic excitations built on top of such a subcritical vacuum lead to a sharp transition in the above correlations functions. To solve the Dyson-Schwinger equations we used temperature dependent renormalization conditions. This results in the phase transition point in Fig. 3 moving with $d_0^{-1}$. By fixing the critical temperature to a physical value, if known, this variation could be used to determine the function $\mu(T)$ and, ultimately, the temperature dependence of these correlation functions. As one tunes the zero-temperature solution to approach the critical limit, $d_0^{-1} \to 0$, the phase transition moves to infinite temperatures. Even though thermal excitations are restricted to color single states, contribution to the partition function from two gluons is $O(1/V)$ compared to that of a glueball. The former are thus expected to make negligible contribution in the thermodynamical limit, which explains why a confining Coulomb potential at zero temperature remains confining at finite temperatures [37]. However, the confining potential can bind gluons into color-singlet glueballs and a phase transition could be observed, for example in a change of the radius of the glueball wave function. We will consider such a mixed glueball/quasi-gluon phase in the forthcoming work.

VI. SUMMARY AND OUTLOOK

We studied the temperature dependence of QCD correlation functions with a variational ansatz for the gluon density matrix in the Coulomb gauge. The resulting one-loop Dyson-Schwinger equations for the gluon propagator and ghost form factor $d(k)$ were solved numerically, assuming a subcritical behavior, i.e., $d^{-1}(0) \neq 0$, which, however, was chosen close to the critical one, $d^{-1}(0) = 0$.

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