A VARIATIONAL LOOK AT QCD

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I discuss the applicability of variational methods to the study of non-perturbative aspects of QCD. An illustration of the capabilities of the method pioneered by Kogan and Kovner is given through the analysis of the deconfinement phase transition in gluodynamics in 3+1 dimensions.

1. Introduction

There is very little doubt that Quantum Chromodynamics (QCD) is the correct theory of the strong interactions. Understanding the properties of the vacuum sector of QCD – phenomena such as confinement and chiral symmetry breaking – remains, in spite of years of attempts, one of the main problems in modern quantum field theory.

Amongst the variety of approaches used to tackle these problems, there have been several attempts to apply versions of the variational Rayleigh-Ritz method [1]. The crux of my argument is that such methods, in particular Kogan and Kovner’s version [1, 2], offer a possibility to analytically obtain non-perturbative dynamical information directly from QCD. Although this information is partial and incomplete, the variational approach provides significant qualitative understanding, and, to a limited extent, quantitative estimates.

When attempting to apply the variational principle to quantum field theory (QFT) one is faced with the discussed by Feynman [3]. In what follows I will describe the construction of a variational trial state which, to a certain extent, overcomes these difficulties, and then illustrate the variational approach’s capabilities by discussing its application to the study

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of the deconfining phase transition in gluodynamics in 3+1 dimensions [4,5].

2. The variational Ansatz

The first criterion to be considered when constructing a trial variational state is that the trial state ought to be general enough to allow, through variation of its parameters, the relevant physics to be spanned.

Then there is the problem of calculability. In QFT, our ability to evaluate path integrals is, to say the least, limited. The requirement of calculability almost unavoidably restricts the possible form of the trial state to a Gaussian.

Another serious problem is that of “ultraviolet modes”. The main motivation of a variational calculation in a strongly interacting theory is to learn about the distribution of the low momentum modes of the field in the vacuum wave functional. However, the VEV of the energy (and all other intensive quantities) is dominated by contributions of high momentum fluctuations, for the simple reason that there are infinitely more ultraviolet modes than modes with low momentum. Therefore, even if one has a clear idea of how the WF at low momenta should look, if the ultraviolet part of the trial state is even slightly incorrect the minimization of energy may lead to absurd results. Due to the interaction between the high and low momentum modes, there is a good chance that the infrared (IR) variational parameters will be driven to values which minimize the interaction energy, and have nothing to do with the dynamics of the low momentum modes themselves.

Finally, in gauge theories there is the additional complication of gauge invariance. Allowable wave functionals must be invariant under the time independent gauge transformations. If one does not impose the Gauss’ law on the states exactly, one is not solving the right problem. The QCD Hamiltonian is only defined on the gauge invariant states, and its action on non gauge invariant states can be modified at will. Thus, by minimizing a particularly chosen Hamiltonian without properly restricting the set of allowed states, one is taking the risk of finding a “vacuum” which has nothing to do with the physical one, but is only picked due to a specific form of the action of the Hamiltonian outside the physical subspace.

The trial variational state proposed by Kogan and Kovner [2] explicitly satisfies Gauss’ law, has the correct UV behaviour built-in, and allows for analytical calculations – yielding non-perturbative results – to be carried out.
In order to illustrate the capabilities of this variational method, I now turn to the analysis of the deconfinement transition in gluodynamics.

3. Deconfinement phase transition

In the almost 25 years since the pioneering work of Polyakov [6] and Susskind [7] much effort has been devoted to attempts to understand both the basic physics and quantitative features of the deconfining phase transition of QCD.

The high temperature phase is becoming well understood, and is widely believed to resemble a plasma of almost free quarks and gluons. However, the transition region, \( T_c < T < 2T_c \), is very poorly understood. This region is the most interesting since it is there that the transition between ‘hadronic’ and ‘partonic’ degrees of freedom occurs.

The study of the transition region is a complicated and inherently non-perturbative problem which has mostly evaded treatment by analytical methods. Recently, the method introduced by Kogan and Kovner [2] was applied to the study of the phase transition in \( SU(N) \) gluodynamics [4, 5]. Following [4, 5], we minimize the relevant thermodynamic potential at finite temperature, i.e. the Helmholtz free energy, on a set of suitably chosen trial density matrix functionals. We consider density matrices which, in the field basis, have Gaussian matrix elements and where gauge invariance is explicitly imposed by projection onto the gauge-invariant sector of the Hilbert space

\[
\rho[A, A'] = \int DU \exp \left\{ -\frac{1}{2} \int_{x,y} \left[ A_i^a(x) G^{-1}_{ij} a^{ab}(x, y) A_j^b(y) 
+ A_i^a(x) G^{-1}_{ij} a^{ab}(x, y) A_j^{Ua}(y) - 2 A_i^a(x) H_{ij}^{ab}(x, y) A_j^{Ub}(y) \right] \right\}, 
\]

(1)

where \( \int_{x,y} = \int d^3x d^3y \), \( DU \) is the \( SU(N) \) group-invariant measure, and under an \( SU(N) \) gauge transformation \( U \)

\[
A_i^a(x) \rightarrow A_i^{Ua}(x) = S^{ab}(x) A_i^b(x) + \lambda_i^a(x), 
\]

(2)

with

\[
S^{ab} = \frac{1}{2} \text{tr}(\tau^a \tau^b U), \quad \lambda_i^a = \frac{i}{g} \text{tr}(\tau^a U^\dagger \partial_i U), 
\]

(3)

and \( \tau^a \) form an \( N \times N \) Hermitian representation of \( SU(N) \): \([\tau^a, \tau^b] = if^{abc} \frac{\tau^c}{2} \) with normalization \( \text{tr}(\tau^a \tau^b) = 2 \delta^{ab} \).
We take the variational functions diagonal in both colour and Lorentz indices, and translationally invariant
\[
G_{ij}^{ab}(x, y) = \delta^{ab}\delta_{ij}G^{-1}(x - y), \quad H_{ij}^{ab}(x, y) = \delta^{ab}\delta_{ij}H(x - y).
\]

Further, we split the momenta into high and low modes with \( k \lesssim M \) and restrict the kernels \( G^{-1} \) and \( H \) to the one parameter momentum space forms
\[
G^{-1}(k) = \begin{cases} M, & k < M \\ k, & k > M \end{cases}, \quad H(k) = \begin{cases} H, & k < M \\ 0, & k > M \end{cases}.
\]

The logic behind this choice of ansatz is the following. At finite temperature we expect \( H(k) \) to be roughly proportional to the Boltzmann factor \( \exp\{ -E(k)\beta \} \). In our ansatz, the role of one particle energy is played by the variational function \( G^{-1}(k) \) and its form is motivated by the propagator of a massive scalar field, i.e. \( (k^2 + M^2)^{1/2} \). We will be interested only in temperatures close to the phase transition, and those we anticipate to be small, \( T_c \leq M \). For those temperatures one particle modes with momenta \( k \geq M \) are not populated, and we thus put \( H(k) = 0 \). For \( k \leq M \) the Boltzmann factor is non-vanishing, but small. Further, it depends only very weakly on the value of the momentum. With the above restrictions on the kernels, only two variational parameters, \( M \) and \( H \), remain.

Importantly, the density matrix functional in eq. (1) describes, for \( H = 0 \), a pure state \( \rho = |\Psi[A]\rangle <\Psi[A]| \) where \( \Psi[A] \) are Gaussian wave functionals. For \( H \neq 0 \), eq. (1) describes a mixed state with \( |H| \) proportional to the entropy of the trial density matrix.

The expectation value of a gauge invariant operator in the variational state eq. (1) is then given by
\[
\langle O \rangle_{A,U} = Z^{-1} \text{Tr}(\rho O) = Z^{-1} \int DU DA \mathcal{O}(A, A') \cdot \exp \left\{ -\frac{1}{2} \left[ AG^{-1}A + A^U G^{-1}A^U - 2AH A^U \right] \right\} \bigg|_{A' = A},
\]

where \( Z \) is the normalization of the trial density matrix \( \rho \), i.e.
\[
Z = \text{Tr} \rho = \int DU DA \exp \left\{ -\frac{1}{2} \left[ AG^{-1}A + A^U G^{-1}A^U - 2AH A^U \right] \right\}
\]

To evaluate the above expressions we first perform, for fixed \( U(x) \), the Gaussian integration over the vector potential \( A \). For \( Z \) we get, in leading
order in $H$,

$$Z = \int \mathcal{D}U \exp \left\{ -\frac{1}{2} \lambda \left( \frac{G^{-1}}{2} + \frac{H}{4}(S + S^T) \right) \lambda + \frac{3}{4} H G \text{tr}(S + S^T) \right\}. \quad (8)$$

We now integrate out the high momentum, $k^2 > M^2$, modes of $U$ perturbatively to one-loop order. This effects a renormalization group transformation on the low modes, replacing the bare coupling $g^2$ by the running coupling $g^2(M)$ \cite{2,9}. To one-loop accuracy, the coupling $g^2(M)$ runs identically to the Yang-Mills coupling \cite{9}.

The normalization $Z$ can be then interpreted as the generating functional

$$Z = \text{Tr} \rho = \int \mathcal{D}U e^{-S(U)} \quad (9)$$

for an effective non-linear $\sigma$-model for the low momentum modes ($k^2 < M^2$) defined by the action

$$S(U) = \frac{M}{2g^2} \text{tr}(\partial U \partial U^\dagger) - \frac{H}{8g^2} \text{tr}\left[ (U^\dagger \partial U - \partial U^\dagger U)(\partial U U^\dagger - U \partial U^\dagger) \right] - \frac{1}{4\pi^2} H M^2 \text{tr} U^\dagger \text{tr} U, \quad (10)$$

where $U$ independent pieces have been dropped.

The matrix $U$ plays the same role as Polyakov’s loop $P$ at finite temperature — the functional integration over $U$ projects out the physical subspace of the large Hilbert space on which the Hamiltonian of gluodynamics is defined.

This $\sigma$-model has a phase transition \cite{2} at the critical point (for $\Lambda_{QCD} = 150$MeV, $N = 3$ and with the one-loop Yang-Mills $\beta$ function)

$$M_c = \Lambda_{QCD} e^{\frac{22}{11}} = 8.86\Lambda_{QCD} = 1.33\text{Gev}. \quad (11)$$

For $M < M_c$, the $\sigma$-model is in a disordered, $SU(N)_L \otimes SU(N)_R$ symmetric, phase with massive excitations and where $\langle U \rangle = 0$. Since $U$ is the Polyakov loop, this corresponds to a confined state. When $M > M_c$, the $\sigma$-model is in an ordered, $SU(N)_V$ symmetric, phase with massless Goldstone bosons for which $\langle U \rangle \neq 0$, corresponding to a deconfined state. With this analysis we have established a correspondence between the $\sigma$-model phase transition and the deconfinement transition in $SU(N)$ gluodynamics.

In fact, this correspondence can be argued in rather general terms. Let us ask ourselves what would happen if we did not restrict $H$ to be small, and more generally did not restrict the functional forms of $G(k)$ and $H(k)$
in our variational ansatz. We could still carry on our calculation for a while. Namely we would be able to integrate over the vector potentials in all averages, and would reduce the calculation to a consideration of some non-linear $\sigma$-model of the $U$-field. This $\sigma$-model quite generally will have a symmetry breaking phase transition as the variational functions $G(k)$ and $H(k)$ are varied. Since at this transition the Polyakov loop $U$ changes its behavior, the disordered phase of the $\sigma$-model corresponds to the confining phase of the Yang-Mills theory, while the ordered phase of the $\sigma$-model represents the deconfined phase. Thus, in order to study deconfinement in the $SU(N)$ Yang-Mills theory, we should analyze the physics of each $\sigma$-model phase as accurately as possible and calculate the transition scale $M_c$ (or rather $G_c(k)$). We then calculate the free energy of the $\sigma$-model in each phase at temperature $T$ and extract the minimal free energy. The deconfinement transition occurs at the temperature for which the free energies calculated in the ordered and disordered phases of the sigma model coincide.

The Helmholtz free energy $F$ of the density matrix $\rho$ is given by

$$F = \langle H \rangle - T \langle S \rangle,$$

where $H$ is the standard Yang-Mills Hamiltonian

$$H = \int d^3 x \left[ \frac{1}{2} E_i^2 + \frac{1}{2} B_i^2 \right],$$

with

$$E_i^a(x) = i \frac{\delta}{\delta A_i^a(x)},$$

$$B_i^a(x) = \frac{1}{2} \epsilon_{ijk} \{ \partial_j A_k^a(x) - \partial_k A_j^a(x) + g f^{abc} A_j^b(x) A_k^c(x) \},$$

$S$ is the entropy, and $T$ is the temperature.

Thus

$$F = \frac{1}{2} \left( \text{Tr}(E^2 \varrho) + \text{Tr}(B^2 \varrho) \right) + T \cdot \text{Tr}(\varrho \ln \varrho).$$

In the disordered phase, no progress seems possible without restricting the arbitrary kernels. Following [4], we adopt the forms eq. (5). For small $H$, we consider only the first non-trivial order in $H$, that is a term of $o(H \ln H)$ in the entropy. This term can be written as a product of left $SU(N)$ and right $SU(N)$ currents and does, therefore, vanish in the disordered, $SU(N)_L \otimes SU(N)_R$ symmetric, phase [4]. The remaining contribution to the free energy, the average of the Hamiltonian, is evaluated
in the mean field approximation [2]. The free energy is minimized for
\[ M = M_c \simeq 1.33 \text{GeV} \]

\[ F_{\text{dis}} = -\frac{N^2 M^4_c}{30 \pi^2}. \]  \hspace{1cm} (16)

The simplest option to evaluate the free energy in the disordered phase
is to use perturbation theory. Perturbation theory is certainly appropriate
for large enough values of \( M \), where the expectation value of the \( U \) field is
close to unity. From numerical studies [10] it is known that the transition
occurs when the expectation value of \( U \) is greater than 0.5. We can thus
expect perturbation theory to be qualitatively reliable down to the transi-
tion point. In the leading order perturbation theory approximation to the
ordered phase of the \( \sigma \)-model, however, minimisation with respect to arbi-
trary kernels \( G^{-1} \) and \( H \) for both high and low modes is possible. Further,
the analysis can be carried out to all orders in the thermal disorder kernel
\( H \).

In this approximation, the \( U \) matrices can be parameterized in the stan-
dard exponential form and expanded in the coupling \( g \)
\[ U = \exp \left\{ ig \varphi^a \frac{\tau^a}{2} \right\} = 1 + ig \varphi^a \frac{\tau^a}{2} + \ldots \]  \hspace{1cm} (17)

Hence at leading order one can take

\[ U \simeq 1 , \quad \partial_i U \simeq ig \partial_i \varphi^a \frac{\tau^a}{2}. \]  \hspace{1cm} (18)

Thus, the gauge transformations (2) reduce to

\[ A_i^a \rightarrow A_i^a - \partial_i \varphi^a \]  \hspace{1cm} (19)

and the Hamiltonian (13) reduces to

\[ \mathcal{H} = \frac{1}{2} \left[ E_i^a + (\epsilon_{ijk} \partial_j A_{k}^a)^2 \right]. \]  \hspace{1cm} (20)

These last two equations describe the theory \( U(1)^{N^2-1} \): in the leading order
of \( \sigma \)-model perturbation theory, the \( SU(N) \) Yang–Mills theory reduces to
the \( U(1)^{N^2-1} \) free theory. Moreover, the density matrix eq. (1) becomes
Gaussian again, because the gauge transformations are linear:

\[ \rho[A, A'] = \int D\varphi \exp \left\{ -\frac{1}{2} \left[ AG^{-1}A + (A' - \partial \varphi)G^{-1}(A' - \partial \varphi) \right. \right. \]
\[ \left. \left. - 2AH(A' - \partial \varphi) \right] \right\}. \]  \hspace{1cm} (21)
The theory of $N^2 - 1$ $U(1)$ free fields in $3 + 1$ dimensions is completely tractable; the variational analysis for the $U(1)$ theory (with Gaussian ansatz (21)) was discussed in [12]. The free energy in momentum space in terms of the arbitrary kernels $G^{-1}$ and $H$ is

$$F = \frac{N^2 - 1}{2} \int \frac{d^3 p}{(2\pi)^3} \left[ G^{-1}(1 + GH) + p^2 G(1 - GH)^{-1} \right.$$

$$\left. - 4T \left( \ln \left[ \frac{GH}{\xi} \right] - \ln \left[ \frac{\eta}{GH} \right] \cdot \frac{\eta}{\xi} \right) \right], \quad (22)$$

where $\eta = 1 - (1 - (GH)^2)^{1/2}$ and $\xi = (1 - (GH)^2)^{1/2} - (1 - GH)$. The kernels which minimize the free energy are

$$G^{-1} = p \left( \frac{1 + e^{-\frac{2\pi}{p}}}{1 - e^{-\frac{2\pi}{p}}} \right), \quad H = 2p \left( \frac{e^{-\frac{p}{4\pi}}}{1 - e^{-\frac{2\pi}{p}}} \right) \quad (23)$$

and the minimal value of the free energy at temperature $T$ is

$$F = -\frac{\pi^2 N^2 T^4}{45}. \quad (24)$$

So we see that the free energy of $SU(N)$ is minimised with $M = M_c$ in the disordered phase of the $\sigma$-model for temperatures from zero up to a temperature $T_c$ where

$$F = -\frac{N^2 M_c^4}{30 \pi^2} = -\frac{\pi^2 N^2 T_c^4}{45}, \quad (25)$$

which in turn implies

$$T_c = \left( \frac{3}{2} \right)^{1/4} \frac{M_c}{\pi} \simeq 470 \text{MeV}. \quad (26)$$

Although the actual value of the transition temperature is considerably larger than the lattice estimate it makes more sense to look at dimensionless quantities. In particular, if we identify $2M_c$ with the mass of the lightest glueball [11] (see also the discussion in [1]), we find

$$\frac{T_c}{2M_c} = \frac{1}{2\pi} \left( \frac{3}{2} \right)^{1/4} \simeq 0.18. \quad (27)$$

This is in excellent agreement with the lattice estimate for $SU(3)$ pure gauge theory [8].
4. Conclusions

In 3+1 dimensional gluodynamics, this variational method gives results which on the qualitative level at least, conform with our intuition about the structure of the ground state. We find a first order phase transition which corresponds to the Polyakov loop acquiring a non-zero average. Although we have not calculated the string tension directly, the behavior of the Polyakov loop is very much indicative that this is indeed the deconfining phase transition. The value of the critical temperature (in units of glueball mass) we find is in good agreement with lattice results. We also found that in the low temperature phase the entropy remains zero all the way up to the transition temperature. This is a rather striking result, which has not been built into our variational ansatz, but rather emerged as the result of the dynamical calculation.

An important lesson we learned is that the projection of the Gaussian trial state onto the gauge invariant Hilbert subspace dictates most, if not all, of the important aspects of the non-perturbative physics. It was absolutely essential to perform the projection non-perturbatively, fully taking into account the contribution of the overlap between gauge rotated Gaussians into the variational energy prior to minimization. We have seen that from the point of view of the effective $\sigma$-model the energy is minimized in the disordered phase. In other words, the low momentum fluctuations of the field $U$ are large, unlike in the perturbative regime, where $U$ is close to a unit matrix. From the point of view of the trial wave functional, this means that the off-diagonal contributions, coming from the Gaussian WF gauge rotated by a slowly varying gauge transformation, are large. It is these “off diagonal” contributions to the energy that lowered the energy of the best trial state below the perturbative value. In the low temperature phase the vanishing of the entropy was also a direct consequence of the effective $\sigma$-model being in the disordered phase, and thus of the non-perturbative nature of the gauge projection.

This variational method appears to be a good candidate for a useful calculational scheme for strongly interacting gauge theories. However, many outstanding questions remain. Is the best variational state confining? How do we calculate the interaction potential between external sources? How do we understand better the relation between the variational parameter and the glueball masses? Can we extend the Ansatz to include (massless) fermions?

Personally, I believe that these results are genuine and that there is
enough scope for further development of the approach which warrants continuing active investigations.

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