Variational Calculations in the Gluon Sector of the Lattice QCD

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Abstract. The partition function of d dimensional systems is estimated with the help of a variational Ansatz in terms of quasi-(d–1)-dimensional systems. The internal energy and the string tension derived in this framework agree reasonably with the Monte Carlo data.

1. Introduction

MC simulations [1] in the pure gluonic sector present high-quality tests of the theoretical ideas on non-Abelian gauge theories. The standard approach consists of calculating strong coupling series up to quite high order, manipulating them to improve their convergence and confront with the data [2]. Also the few first terms of the weak coupling expansions for some quantities are known. None of them can account for the data in the full range of variation of the coupling constant.

The variational calculus might complement the above perturbative methods. This has been recognized recently [3] in the Hamiltonian formulation and applied to the Ising gauge model. The present paper is devoted to the application of the variational method in the Euclidean version of the theory, which is directly comparable to the Monte Carlo results. The variational problem will be solved without any perturbative tool what is different from the attitude adopted in [3].

The method which is based on the transfer matrix is known in statistical physics for some time [4–6]. For the selfcontainness of our paper we introduce it through the example of the 2 dimensional Heisenberg spin model in Sect. 2. Several Monte Carlo studies have been performed on this model recently [7–9] because it is expected to share some properties of the 4-dimensional gauge models. The simplest variational Ansatz reproduces the internal energy of the system with 3% accuracy. Also the maximum of the specific heat is described correctly. The method is applied to the 3 dimensional $G=SU(2)$ gauge model (Wilson’s formulation), in Sect. 3. The expectation value of the plaquette action is reproduced with 9% maximal error in the $\beta=\frac{4}{g^2a} \in (0,8)$ range. Also Wilson’s correlation function is calculated and a good numerical agreement is achieved, although the weak coupling asymptotics of the calculated string tension is shown to be different from that found in the Monte Carlo simulation [10]. In Sect. 4 we discuss in detail the improvements of the present approach and point out the interest of a possible marriage of the variational approach with the Monte Carlo methods.

2. The $O(3)$ Spin Model in two Dimensions

The partition function is defined as

$$Z = \int \prod_n d\Omega_{\mathbf{s}_n} \exp \left\{ K \sum_{\langle\mathbf{n},\mathbf{m}\rangle} \mathbf{s}_n \cdot \mathbf{s}_m \right\},$$

(2.1)

where $\mathbf{s}_n$ is a 3-vector of unit length defined at the $n$-th site of the configurational plane. $d\Omega_{\mathbf{s}_n}$ is the spherical angular element around the direction of $\mathbf{s}_n$. $K$ is the coupling (scaled by the temperature) between two nearest neighbour vectors $\mathbf{n}$ and $\mathbf{m}$. $Z$ can be calculated as the $N_1$-th power of the largest eigenvalue of the transfer matrix defined by

$$\prod_{i=1}^{N_2} d\Omega_{\mathbf{s}_i} \exp \left\{ K \sum_{l=1}^{N_2} \mathbf{s}_l \cdot \left( \mathbf{s}_{l+1} + \mathbf{s}'(l+1) \right) \right\} \cdot \Psi_0(\mathbf{s}_l) = \lambda_0 \Psi_0(\mathbf{s}_l),$$

(2.2)

where $\mathbf{s}_i$ denotes the “spins” in the $l$-th row and $\mathbf{s}'$ those of the $(l+1)$-th ($l \leq N_2$ and periodic boundary conditions are subsumed). The free energy and internal
energy densities of the system are given by

\[ N_1N_2 \mathcal{F} = -\ln \lambda_0^{N_1}, \quad \mathcal{F}_b = 2 \frac{d \mathcal{F}}{dK}. \]  

The simplest Ansatz for the nodeless, translationally invariant groundstate is offered by

\[ \psi_0 = \exp \left\{ x \sum_i s_i s_{i+1} \right\}, \]  

which is invariant also under global $O(3)$ rotations. Therefore (2.4) might describe the disordered phase, which is the whole temperature range in the present case. One has

\[ \lambda_0 \geq \lambda_a \]

where \( \lambda_a \) is given by

\[ \int \prod_i d\Omega_{s_i} d\Omega_{s_{i+1}} \exp \left\{ K \sum_i s_i s_{i+1} + \tilde{K} \sum_i (s_i s_{i+1} + s_{i+1} s_{i+2}) \right\} \]

\[ \times \int \prod_i d\Omega_{s_i} \exp \left\{ 2x \sum_i s_i s_{i+1} \right\}, \]  

where \( \tilde{K} = \frac{K}{2} + x \).

The most important remark is that both the numerator and denominator of (2.5) can be interpreted as the partition function of some spin system. The numerator corresponds to the $O(3)$ symmetric system of two parallel lines with anisotropic couplings. The denominator is a 1-dimensional Heisenberg-chain of coupling $2x$. One readily writes down the corresponding transfer matrix eigenvalue equations. Using the well-known expansion:

\[ e^{Ks_{i}s_{i+1}} = 4\pi \sum_{l,m} J_{l+1/2}^{(2)}(K) Y_l^n(s_i) Y_l^m(s_{i+1}) \]  

(\( J_{l+1/2}^{(2)}(K) \) denotes the spherical Bessel functions of imaginary argument), one can calculate the denomi-

\[ \lim_{N_2 \to 0} \prod_{i=1}^{N_2} d\Omega_{s_i} \exp \left\{ 2x \sum_i s_i s_{i+1} \right\} = J_{1/2}(2x)^{N_2}. \]  

Next we turn to the transfer-matrix of the numerator system. In order to maximize \( \lambda_a \) we ask for the highest eigenvalue (\( \equiv \lambda_0^{(0)} \)). The corresponding eigenfunction \( \Phi_0(s_0, s) \) will depend only on the scalar product \( s_0 s \). By subsequent use of (2.6) one can show that the eigenvalue equation written down originally as an integral equation of four variables reduces to that of a single variable:

\[ \lambda_0^{(0)} \Phi_0(\cos \Theta_{1,2}) = \int_{-1}^1 d\cos \Theta_{1,2} \Phi_{1,2} \cos \Theta_{1,2} \Phi_{2,1} \]

\[ \Phi_0(\cos \Theta_{1,2}) \]  

where \( \Theta_{1,2} \) and \( \Theta_{2,1} \) are the angles between two neighbouring pairs in the infinite parallel sequence. The kernel K is given by

\[ K(x, y) = 8 \pi^2 \sum_{l} J_{l+1/2}^{(2)}(k) P_l(x) P_l(y) e^{K/2(l+1)}(2l+1), \]  

\[ J_{l+1/2}(x) = (-1)^l x^l \frac{d^l}{dx^l} \frac{1}{x} \]  

One can solve (2.9) on a computer with an accuracy appropriate for the comparison with the Monte Carlo data. The free energy density is given by minimalizing \( -\ln \lambda_a \), that is

\[ \mathcal{F}_a = \min_{a} \left( -\ln \lambda_0^{(0)}(K, x) + \ln J_{1/2}(2x) \right). \]  

We have truncated the l-sum in (2.9) at \( l_{\max}(K) \), increasing with \( K (5 \leq l_{\max}(K) \leq 10) \). The integration in (2.8) was done by Gauss's quadrature of increasing order with \( K \). It turned out however that an 8-point quadrature gives the first five digits of \( \lambda_0^{(0)} \) correctly in the range \( K \in (0, 3) \). We have compared our results for the internal energy to the figures published in [7-9] (Fig. 1). The deviation is less than 1% outside the region \( K \in (1, 3, 2) \). In this interval we could compare the variational internal energy with the numbers published by Berg and Lüscher [9] and we found the maximal error between \( K = 1.5-1.6 \) to be 3% (Table 1). This is the region where the strong coupling regime changes rapidly into the weak coupling behaviour. The behaviour of the variational parameter \( \alpha = \alpha(K) \) is very characteristic (Fig. 2). It starts close to \( K = 0 \) with a linear variation \( \alpha = \frac{1}{2} K \). An easy calculation shows that our Ansatz reproduces the right high-temperature asymptotics of \( Z \) with this \( K \)-dependence. Then from about \( K = 0.5 \) it turns into a transient regime approaching very slowly the \( \alpha = K \) straight line. This transition enables the Ansatz to interpolate between