# Optimization of order parameters in lattice SU(2)gauge theory using the linear delta expansion

M.Sci. final year project

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to my parents

#### Abstract

The linear  $\delta$  expansion is applied to the calculation of order parameters in lattice SU(2) pure gauge theory and all the diagrams up to order four are tabulated. The principle of minimal sensitivity is applied to fix the variational parameters. The results are satisfactory for zero temperature, but at finite temperature there are indications that the method fails to produce a valid expansion in the region where a second order phase transition is expected.

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# 1 Introduction

The success of the eightfold way of Gell-Mann and Ne'eman [1], the large cross sections and their angular dependence in deep inelastic lepton-hadron scattering, together with the celebrated explanation of the charmonium and upsilon spectra in terms of excitations of bound quark states, all support a model of quarks interacting via some gauge field as the fundamental theory of the strong interaction. However, an isolated quark has never been observed in experiments and this motivates the postulation of an exact confinement. In other words, the gauge field mediating the strong force must be self interacting which is possible if it is non-Abelian.

The clearest evidence of confinement in non-Abelian gauge theories is provided by Wilson's formulation of gauge fields on a Euclidean lattice [15]. The lattice is particularly suited for non-perturbative calculations which are essential in the strong coupling limit. In fact, in this limit non-Abelian gauge theories on the lattice turn out to be confining, but it cannot be immediately deduced that this property survives in the continuum limit as a deconfining phase transition may be encountered.

A lot of recent work has been devoted to showing that confinement survives in the continuum. One way of approaching this problem is to consider various order parameters which could monitor the phase structure of the system. Both Monte Carlo simulations and semi-analytical methods have been applied in the evaluation of the order parameters with considerable success.

In this project we calculate two order parameters for pure SU(2) lattice gauge theory, the plaquette energy and the Polyakov line, using a variational-perturbative method, the linear  $\delta$  expansion. Our initial aim was to go up to the fourth order for the plaquette energy and up to the third order for Polyakov line, but the development of a new technique for the evaluation of the diagrams involved in these expansions has enabled us to calculate the fourth order of the Polyakov line as well.

# 2 Theory

### 2.1 Gauge theories

#### 2.1.1 Continuum and lattice gauge fields

A gauge field is most naturally introduced by requiring that the global invariance of a Lagrange density  $\mathcal{L}$  under a gauge group  $\mathcal{G}$  is promoted to a local one. Here we concentrate on SU(N) gauge fields on the Euclidean four dimensional space.

Consider N complex scalar fields  $\phi^i(x)$ , i = 1, ..., N which form the components of a complex SU(N)-vector field  $\phi(x)$ . Then the (Euclidean) free Lagrange density

$$\mathcal{L} = \frac{1}{2} \partial_{\mu} \phi^T(x) \partial^{\mu} \phi(x) + \frac{1}{2} m^2 \phi^T(x) \phi(x)$$
(1)

is invariant under the global SU(N) transformation

$$\phi(x) \to \phi'(x) = V\phi(x), \tag{2}$$

where  $V \in SU(N)$  is independent of x. However, if V depends on x the invariance is lost due to the derivatives in the kinetic term. To extend the invariance of the Lagrange



Figure 1: An elementary plaquette on a hypercubic lattice

density to local SU(N) transformations we introduce the covariant derivative

$$D_{\mu} := \partial_{\mu} + igA_{\mu}(x) \tag{3}$$

and demand that

$$D_{\mu}\phi(x) \to D'_{\mu}\phi'(x) = V(x)D_{\mu}\phi(x) \tag{4}$$

or in operator form

$$D'_{\mu} = V(x)D_{\mu}V^{\dagger}(x). \tag{5}$$

The transformation law for the SO(4)-vector field  $A_{\mu}(x)$  (Lorentz vector in Minkowski space) is then found to be

$$A_{\mu}(x) \to A'_{\mu}(x) = V(x)A_{\mu}(x)V^{\dagger}(x) - \frac{i}{g}V(x)\partial_{\mu}V^{\dagger}(x).$$
(6)

So, if we replace  $\partial_{\mu}$  with the covariant derivative  $D_{\mu}$  in Equation 1 the Lagrange density will be invariant under local SU(N) transformations of the fields when accompanied by the gauge transformation 6.

To give a standing on its own to the gauge field  $A_{\mu}(x)$  we need to introduce a gauge invariant kinetic term for it. To this end we define the gauge invariant SO(4)-tensor

$$F_{\mu\nu} := -\frac{i}{g} [D_{\mu}, D_{\nu}] = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu} + ig[A_{\mu}, A_{\nu}]$$
(7)

which transforms covariantly under SU(N):

$$F'_{\mu\nu}(x) = V(x)F_{\mu\nu}(x)V^{\dagger}(x).$$
(8)

A free Lagrange density for the gauge field can then be defined as

$$\mathcal{L}_{YM} = \frac{1}{2} \operatorname{Tr}(F_{\mu\nu} F^{\mu\nu}) \tag{9}$$

which is the Yang-Mills Lagrange density in Euclidean space. Here the Euclidean metric tensor  $\delta^{\mu\nu}$  ( $\delta = diag(1, 1, 1, 1)$ ) has been used to raise the indices.

We now proceed to introduce gauge fields on the Euclidean lattice. A free Lagrange density for the SU(N)-vector field  $\phi(x)$  on the lattice can be defined as

$$\mathcal{L} = \frac{a^4}{2} \sum_{x} \left( \Delta_{\mu} \phi^T(x) \Delta^{\mu} \phi(x) + m^2 \phi^T(x) \phi(x) \right)$$
(10)

where a is the lattice spacing and  $\Delta_{\mu}$  is a forward difference in the direction  $\mu(=1, 2, 3, 4)$ indicated by the unit vector  $\hat{\mu}$  (See Figure 1)

$$\Delta_{\mu}\phi(x) := \frac{1}{a} \left( \phi(x + a\hat{\mu}) - \phi(x) \right).$$
(11)

In the continuum limit this reduces to  $\partial_{\mu}$  as it should.

The Lagrange density 10 is clearly invariant under the global SU(N) transformation in 2 but not under a local one. As in the continuum we introduce the covariant derivative which now takes the form

$$D_{\mu}\phi(x) := \frac{1}{a} \left( U^{\dagger}(x,\mu)\phi(x+a\hat{\mu}) - \phi(x) \right).$$
(12)

Here I have used the notation of [3] which I find most illuminating and displays the geometrical significance of the gauge fields in terms of parallel transport. So,  $U(x, \mu) \equiv U(x + a\hat{\mu}, x) \in SU(N)$  is the parallel transporter from the point x to  $x + a\hat{\mu}$  and can be expressed as

$$U(x,\mu) = e^{-iagA_{\mu}(x)} \tag{13}$$

where the gauge field  $A_{\mu}(x) \in su(N)$ , the algebra of SU(N). Then, expanding in a one gets

$$D_{\mu}\phi(x) = \frac{1}{a} \left( \phi(x + a\hat{\mu}) - \phi(x) + iagA_{\mu}(x)\phi(x) + \mathcal{O}(a^2) \right)$$
(14)

which correctly reduces to 3 in the continuum limit.

Demanding that  $D_{\mu}$  transforms covariantly (Equation 5) under local SU(N) transformations leads to the transformation law of the parallel transporters

$$U'(x,\mu) = V(x+a\hat{\mu})U(x,\mu)V^{\dagger}(x).$$
(15)

Before we introduce a free Lagrange density for the gauge field let me define the antisymmetric tensor

$$F_{\mu\nu} = -\frac{i}{g} [D_{\mu}, D_{\nu}]$$
(16)

by analogy to the continuum case. Applying  $F_{\mu\nu}$  on  $\phi(x)$  and expanding in *a* we find, after some algebra, the reassuring result

$$F_{\mu\nu}(x) = \Delta_{\mu}A_{\nu}(x) - \Delta_{\nu}A_{\mu}(x) + ig[A_{\mu}(x), A_{\nu}(x)] + \mathcal{O}(a).$$
(17)

The action that has been proposed by Wilson [15] for the pure lattice gauge theory is defined in terms of the parallel transporters:

$$S[U] = \sum_{p} S_p(U_p) \tag{18}$$

with

$$S_p(U) = \beta \left( 1 - \frac{1}{N} \operatorname{Re}(\operatorname{Tr} U) \right)$$
(19)

and

$$U_p \equiv U(x, x + a\hat{\nu})U(x + a\hat{\nu}, x + a\hat{\mu} + a\hat{\nu})U(x + a\hat{\mu} + a\hat{\nu}, x + a\hat{\mu})U(x + a\hat{\mu}, x)$$
(20)

is a parallel transporter around an elementary plaquette (Figure 1), called a *plaquette* variable. The sum over all plaquettes p stands for

$$\sum_{p} \equiv \sum_{x} \sum_{1 \le \mu < \nu \le 4} = \frac{1}{2} \sum_{x} \sum_{\mu,\nu} .$$
 (21)

It should be noted that this action is invariant under the gauge transformation 15.

A lattice gauge theory is of direct physical significance only if it is related to the continuum theory, which should be recovered in the appropriate limit of the lattice theory. It is instructive then to confirm that this is the case. Firstly,

$$U_{p}(x) = U(x, x + a\hat{\nu})U(x + a\hat{\nu}, x + a\hat{\mu} + a\hat{\nu})U(x + a\hat{\mu} + a\hat{\nu}, x + a\hat{\mu})U(x + a\hat{\mu}, x)$$
  
$$= e^{iagA_{\nu}(x)}e^{iagA_{\mu}(x+a\hat{\nu})}e^{-iagA_{\nu}(x+a\hat{\mu})}e^{-iagA_{\mu}(x)}$$
  
$$= e^{iagA_{\nu}(x)}e^{iag(A_{\mu}(x)+a\Delta_{\nu}A_{\mu}(x))}e^{-iag(A_{\nu}(x)+a\Delta_{\mu}A_{\nu}(x))}e^{-iagA_{\mu}(x)}$$
(22)

which upon using the Campbell-Baker-Hausdorff formula

$$e^{A}e^{B} = e^{A+B+(1/2)[A,B]+\dots}$$
(23)

reduces to

$$U_p(x) = e^{-ia^2 g F_{\mu\nu}(x) + \mathcal{O}(a^3)}.$$
(24)

Therefore,

$$S_{p} = \beta \left( 1 - \frac{1}{2N} \operatorname{Tr}(U_{p} + U_{p}^{\dagger}) \right)$$
$$= \frac{\beta g^{2}}{2N} a^{4} \operatorname{Tr}(F_{\mu\nu}F_{\mu\nu}) + \mathcal{O}(a^{5})$$
(25)

giving

$$S[U] = \frac{\beta g^2}{2N} a^4 \sum_x \frac{1}{2} \sum_{\mu,\nu} \operatorname{Tr}(F_{\mu\nu}F_{\mu\nu}) + \mathcal{O}(a^5)$$
  

$$\rightarrow \frac{\beta g^2}{2N} \int d^4x \frac{1}{2} \operatorname{Tr}(F_{\mu\nu}F^{\mu\nu})$$
(26)

as  $a \to 0$ . So we recover the Yang-Mills action (Equation 9) provided we identify

$$\beta = \frac{2N}{g^2}.$$
(27)

Now we have confirmed the physical relevance of the lattice theory, we can go on to define the appropriate path integral and the corresponding generating function.

#### 2.1.2 Functional integral

By analogy to the continuum theory, the expectation value of an observable  $\mathcal{O}$  is defined to be

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_{l} dU_{l} \mathcal{O} e^{-S[U]}, \qquad (28)$$

where

$$Z = \int \prod_{l} dU_{l} e^{-S[U]}$$
<sup>(29)</sup>

is the partition function and  $U_l$  are the parallel transporters from one lattice site to its nearest neighbours, each pair of nearest neighbours (or link) being labeled by l. The integration measure  $dU_l$  on the link l is the Haar measure of the gauge group (SU(N)) in this case).

As we are mainly interested in SU(2) here, we consider this gauge group as an example. A parametrization of SU(2) which will be useful in our later considerations is

$$U = e^{i\varphi\vec{n}\cdot\vec{\sigma}/2}$$
  
=  $\mathbf{1}\cos(\varphi/2) + i\vec{n}\cdot\vec{\sigma}\sin(\varphi/2), \qquad 0 \le \varphi < 2\pi,$  (30)

where

$$\vec{n} = \vec{i}\cos\phi\sin\theta + \vec{j}\sin\phi\sin\theta + \vec{k}\cos\theta, \quad 0 \le \phi < 2\pi, \\ 0 \le \theta < \pi$$
(31)

and  $\sigma^i$  are the Pauli matrices. In this parametrization the Haar measure is

$$dU = \frac{1}{4\pi^2} d\phi d\theta \sin\theta d\varphi \sin^2(\varphi/2).$$
(32)

#### 2.1.3 Finite physical temperature

It turns out that Euclidean quantum field theory on a lattice is mathematically equivalent to a system of classical statistical mechanics in four dimensions. In particular it is analogous to the generalised Ising model for spins. However, this is just a formal mathematical correspondence and should not be confused with a quantum system at finite physical temperature. To introduce a finite physical temperature for a quantum system let me review how the path integral in quantum mechanics is related to quantum statistical mechanics.

In quantum statistical mechanics the partition function for a system at finite temperature T is

$$Z = \operatorname{Tr}\left(e^{-\beta H}\right), \qquad \beta = \frac{1}{k_B T}$$
(33)

where H is the Hamiltonian of the system and  $k_B$  is Boltzmann's constant. This  $\beta$  is not the same as that of the previous section, which was introduced in view of the mathematical analogy between statistical mechanics and Euclidean lattice field theory mentioned above. The thermal expectation value of an observable  $\mathcal{O}$  is then given by

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \operatorname{Tr} \left( \mathcal{O} e^{-\beta H} \right).$$
 (34)

Now, the Euclidean (i.e.  $t \to -i\tau$ ) path integral for an one dimensional quantum system described by a Hamiltonial H(q, p) is

$$F(q', -i\tau; q, 0) := \langle q' \mid e^{-\tau H} \mid q \rangle = \int \mathcal{D}[q] e^{-S_E[q]}, \tag{35}$$

where

$$S_E[q] = \int_0^\tau d\tau' \left(\frac{1}{2}m\left(\frac{dq}{d\tau'}\right)^2 + V(q)\right),\tag{36}$$

is the Euclidean action with the boundary conditions q(0) = q,  $q(\tau) = q'$ . Therefore, we can make the formal identification

$$Z = \int dq \langle q \mid e^{-\beta H} \mid q \rangle \equiv \int_{periodic \ paths} \mathcal{D}[q] e^{-S_E[q]}, \tag{37}$$

provided  $\beta = \tau$  and the path integration is over all periodic paths with period  $\beta$ .

The extension to Euclidean field theory is now straightforward. The action integral takes the form

$$S = \int_0^\beta dx^4 \int d^3x \mathcal{L},\tag{38}$$

where  $\mathcal{L}$  is the Lagrange density and the fields are periodic in  $x^4$  with period  $\beta$ . On the lattice the integration is replaced by a summation over all lattice sites and  $\beta = Na$  is the length of the lattice in the time direction. All spatial directions have infinite length.

#### 2.1.4 Phase transitions and order parameters

The mathematical correspondence between Euclidean lattice field theory and statistical mechanics allows us to use powerful techniques from solid state physics to obtain results about field theory. In particular, we are interested in suitable order parameters that can distinguish between different phases of the system. In the Ising model such an order parameter is the magnetization, which vanishes identically at the high temperature rotationally symmetric phase of the spin system and takes on a non-zero value at low temperature where the rotational symmetry is broken.

In non-Abelian lattice gauge theories we need to distinguish between the confined phase, where the energy of a quark-antiquark pair grows with their spatial separation, and the deconfinement phase, where a quark and an antiquark can exist separately. It can be shown that in the strong coupling limit (i.e.  $g \to \infty$ ) gauge theories on a lattice are confining ([2], chapter 10). Now, since physical results can only be obtained in the continuum limit we naturally ask the question whether confinement survives in the continuum. Asymptotic freedom, the vanishing of the coupling constant at short distances in non-Abelian gauge theories, and renormalization, however, require that as the lattice constant approaches zero the coupling constant must tend to zero as well ([2] chapter 12). Therefore, in taking the continuum limit we are forced into the weak coupling regime. Along the way a deconfining phase transition may be encountered implying that the lattice and continuum formulations of gauge fields are not continuously connected. If this is the case, a deconfinement phase in the continuum may be possible.

In lattice gauge theory the order parameter corresponding to the magnetization in the Ising model is the expectation value of a single parallel transporter between two nearest neighbours,  $\langle U(x,\mu)\rangle$ . However, this local quantity, and in fact any local quantity, cannot be used as an order parameter since it vanishes identically for all values of the coupling constant. This is guaranteed by Elitzur's theorem [4] and is a consequence of the gauge dependence of local quantities. Therefore, any order parameter in pure lattice gauge theory must be non-local. The simplest such quantity is the *plaquette energy* 

$$E_p := \left\langle \frac{1}{N} \operatorname{ReTr}(U_p) - 1 \right\rangle = \frac{2}{N_l(d-1)} \frac{\partial \ln Z}{\partial \beta}, \tag{39}$$

where d is the dimension of the lattice (4 in our case) and  $N_l (= d \times \text{number of sites})$  is the number of links in the system. The number of plaquettes is then  $N_p = N_l (d-1)/2$ . Although this is not as good an order parameter as the magnetization of the Ising model, it can exhibit the phase structure of the system with phase transitions appearing as jumps (for first order phase transitions) in its value as a function of the coupling constant ([2] chapter 9). Other, more complicated order parameters can be constructed as discussed in [2].

At finite physical temperature the time direction of the lattice is distinct from the spatial directions since it has a finite length. Therefore, the plaquette energy is not well defined as plaquettes containing temporal links will have a different contribution from those that contain only spatial links. The appropriate order parameter (again non-local) is then the *Polyakov line* 

$$L_{\mathbf{x}} := \frac{1}{N_{\tau}} \operatorname{Tr} \left( \prod_{x^4=1}^{N_{\tau}} U(\mathbf{x}, x^4; \hat{4}) \right), \tag{40}$$

where  $N_{\tau}$  is the number of links along the time direction and  $\hat{4}$  is a unit vector in the same direction. In the confined phase the expectation value of L vanishes whereas in the deconfinement phase it is non-zero ([3] chapter 5), which means that L is a suitable order parameter.

Next we turn to the question of how to evaluate these order parameters for the SU(2) pure gauge theory on the lattice. However, most of our methodology is applicable to SU(N) after minor modifications.

### 2.2 The linear delta expansion

#### 2.2.1 The Toy Model

The linear  $\delta$  expansion (LDE) is a variational-perturbative technique that provides a systematic approximation method. Before we apply it to the problem of solving lattice gauge theories let me demonstrate the main ideas involved by evaluating the integral

$$I = \int_{-\infty}^{+\infty} dx e^{-gx^4 - \mu^2 x^2}, \qquad g > 0, \tag{41}$$

which corresponds to the path integral for zero dimensions scalar field theory.

For simplicity we set  $\mu = 0$ , but the case  $\mu \neq 0$  can be treated in a similar way after completing the square. The integral then can be evaluated exactly:

$$I = \int_{-\infty}^{+\infty} dx e^{-gx^4} = \frac{\Gamma(1/4)}{2g^{1/4}}.$$
(42)

Now we let

$$I(\delta;\lambda) = \int_{-\infty}^{+\infty} dx e^{-\lambda x^2 + \delta(\lambda x^2 - gx^4)}$$
(43)

so that  $I = I(1; \lambda)$ .  $\lambda$  is introduced here as a variational parameter which we will try to optimize. An expansion of  $I(\delta; \lambda)$  in powers of  $\delta$  gives

$$I(\delta;\lambda) = \sqrt{\frac{\pi}{\lambda}} \left\{ 1 + \frac{\delta}{2} \left( 1 - \frac{3g}{2\lambda^2} \right) \right\} + \mathcal{O}(\delta^2).$$
(44)

This expression depends on the parameter  $\lambda$  which must be chosen so that the truncated expansion 44 approximates the exact result 42 as closely as possible. The criterion we

adopt to optimize  $\lambda$  is the Principle of Minimal Sensitivity (PMS), which states that since I must be independent of the parameter  $\lambda$ , the closest approximation to the true value of I we can get by truncating the expansion at order  $\delta^N$  is  $I_N(1;\lambda_N)$ , where  $\lambda_N$  is the solution of the equation

$$\frac{\partial I_N(1;\lambda)}{\partial \lambda} = 0. \tag{45}$$

This guarantees that, at least locally, I does not depend on the variational parameter  $\lambda$ . So, in the above example, by truncating the expansion at order  $\delta$  and finding the stationary point with respect to  $\lambda$ , we get

$$\lambda_1 = \sqrt{\frac{5g}{2}},\tag{46}$$

which gives

$$I \approx I_1(1; \lambda_1) = \frac{6}{5} \left(\frac{2\pi^2}{5g}\right)^{1/4}.$$
(47)

It is important to note that even at first order we get the correct dependence on g, which cannot be obtained by perturbation methods. In this particular example it can be proved rigorously that the sequence  $I_N(1; \lambda_N)$  tends to I as  $N \to \infty$  and the proof can be found in [16].

#### **2.2.2** Lattice SU(2) gauge theory

Now we will apply the linear  $\delta$  expansion to SU(2) lattice gauge theory. The dynamics of the pure gauge field is determined by Wilson's action 18. However, the additive constant is physically unimportant as it does not affect any expectation value. We shall, therefore, use the action

$$S = \frac{\beta}{2} \sum_{p} \text{Tr} U_p, \qquad (48)$$

where we have used the fact that the trace of any SU(2) element, at least in the fundamental representation, is real and have absorbed the minus sign into the action.

This action leads to a non-solvable theory and we have to rely on some approximation method. The linear  $\delta$  expansion begins by introducing the trial action

$$S_0 = J \sum_l \text{Tr} U_l.$$
(49)

Here,  $U_l$  are parallel transporters on single links and J is the variational parameter. The summation is now over all links in the system. The reason for choosing this trial action, despite its gauge dependence, is that it leads to a solvable theory which can be used as the zero order approximation in our expansion. Other choices are possible, however.

Before we proceed further with the LDE, it is worth checking that  $S_0$  gives a solvable theory by evaluating the corresponding partition function  $Z_0$ . We have,

$$Z_{0} = \int \prod_{l} dU_{l} e^{S_{0}} = \int \prod_{l} \left( dU_{l} e^{J \operatorname{Tr} U_{l}} \right) = \left( \int dU_{l} e^{J \operatorname{Tr} U_{l}} \right)^{N_{l}}, \qquad (50)$$

where  $N_l$  is the total number of links in the system. Then consider

$$f(J) := \int dU e^{J \operatorname{Tr} U}.$$
(51)

If we use the parametrization of SU(2) given in Equation 30 this can be written as:

$$f(J) = \int_0^{2\pi} \frac{d\varphi}{\pi} \sin^2(\varphi/2) e^{2J\cos(\varphi/2)}.$$
(52)

Now, the exponential of the cosine can be expanded in terms of the modified Bessel functions of integer order  $I_n(z)$ :

$$e^{z\cos\theta} = I_0(z) + 2\sum_{k=1}^{\infty} I_k(z)\cos(k\theta).$$
(53)

Finally, expressing the cosines in this expansion in terms of the characters of the (2j+1)dimensional irreducible representations of SU(2)

$$\chi^{j}(\varphi) = \frac{\sin\left((j+1/2)\varphi\right)}{\sin(\varphi/2)},\tag{54}$$

and using their orthogonality with respect to the inner product

$$(\chi,\xi) := \int_0^{2\pi} \frac{d\varphi}{\pi} \sin^2(\varphi/2) \chi^*(\varphi) \xi(\varphi), \tag{55}$$

we obtain

$$f(J) = I_0(2J) - I_2(2J) = \frac{I_1(2J)}{J},$$
(56)

by the properties of the modified Bessel functions. Therefore, we have found a closed form expression for the partition function  $Z_0$ :

$$Z_0 = \left(\frac{I_1(2J)}{J}\right)^{N_l}.$$
(57)

However, the quantity we are really interested in is Z, the partition function of the Wilson action, and not  $Z_0$ . So we introduce the action

$$S_{\delta} = S_0 + \delta(S - S_0), \tag{58}$$

which reduces to S for  $\delta = 1$ . Then,

$$Z := \int \prod_{l} dU_{l} e^{S_{\delta}} = \int \prod_{l} dU_{l} e^{(1-\delta)S_{0}} e^{\delta S}$$
(59)

is the desired partition function if  $\delta = 1$ . For mathematical convenience we absorb  $(1 - \delta)$  into  $S_0$  by defining  $J(\delta) := (1 - \delta)J$ . This redefinition of  $S_0$  does not affect our earlier results for  $Z_0$ , but we should keep it in mind and take into account the  $\delta$  dependence of J in the end. Implementing this we get:

$$Z = \int \prod_{l} dU_{l} e^{S_{0}} e^{\delta S} =$$

$$Z_{0} \left\langle e^{\delta S} \right\rangle_{0} =$$

$$Z_{0} \sum_{n=0}^{\infty} \frac{\delta^{n}}{n!} \langle S^{n} \rangle_{0}.$$
(60)

Here,  $\langle \cdot \rangle_0$  denotes the expectation value with respect to  $Z_0$ . Having found an expression for the partition function of the system we can go on and evaluate the order parameters we are interested in.

Let us first consider the plaquette energy. It is expressed in terms of the free energy  $W = -\ln(Z)$  as

$$E_p = -\frac{2}{N_l(d-1)} \frac{\partial W}{\partial \beta}.$$
(61)

So, it suffices to calculate W:

$$W = -\ln Z = -\ln Z_0 - \ln \left( \sum_{n=0}^{\infty} \frac{\delta^n}{n!} \langle S^n \rangle_0 \right) = W_0 - \sum_{n=1}^{\infty} \frac{\delta^n}{n!} \langle S^n \rangle_c,$$
(62)

where the connected averages  $\langle \cdot \rangle_c$  are defined by

$$\left\langle \prod_{j=1}^{N} X_{j}^{n_{j}} \right\rangle_{c} := \left( \prod_{j=1}^{N} \frac{n_{j}!}{2\pi i} \oint_{C_{j}} \frac{dz_{j}}{z_{j}^{n_{j}+1}} \right) \ln \left\langle e^{\sum_{k=1}^{N} z_{k} X_{k}} \right\rangle_{0}.$$
(63)

 $X_j$  are arbitrary statistical variables and the contour  $C_j$  is the unit circle on the complex  $z_j$ -plane. We can then write  $\langle S^n \rangle_c$  in the form

$$\langle S^n \rangle_c = (\beta/2)^n \sum_{i=1}^{\xi(n)} \alpha_{n,i} \langle D_{n,i} \rangle_c, \tag{64}$$

where  $D_{n,i}$  are  $\xi(n)$  inequivalent diagrams with multiplicities  $\alpha_{n,i}$ . These diagrams can be evaluated directly and they are listed in Appendix C.1 together with their multiplicities. In the next section we will deal exclusively with the methods for evaluating these diagrams.

The evaluation of the Polyakov line is not a very different task. We start with the action 48

$$S = \frac{\beta}{2} \left( \sum_{p_{\sigma}} \operatorname{Tr} U_{p_{\sigma}} + \sum_{p_{\tau}} \operatorname{Tr} U_{p_{\tau}} \right), \tag{65}$$

where  $p_{\tau}$  indicates plaquettes that contain temporal links and  $p_{\sigma}$  plaquettes that contain only spatial links. The fields are periodic in the time direction with period  $N_{\tau}a$ . The trial action we now use is

$$S_0 = J \sum_{\sigma} \text{Tr} U_{\sigma} + K \sum_{\tau} \text{Tr} U_{\tau}.$$
 (66)

We have introduced two variational parameters because we need to distinguish between temporal and spatial links. Then, a similar argument as for zero temperature, gives

$$Z_0 = [f(J)]^{N_s} [f(K)]^{N_t}, (67)$$

with f(z) defined as previously.  $N_s$  and  $N_t$  are the total numbers of spatial and temporal links respectively. The  $\delta$  expansion then proceeds by introducing  $S_{\delta}$  as before, but now, instead of evaluating the partition function we would like to calculate the expectation value of the Polyakov line. To this end, a generating function:

$$Z(\lambda) := \int \prod_{l} dU_{l} e^{S_{\delta} + \lambda \mathcal{O}}$$
(68)

can be introduced to evaluate

$$\langle \mathcal{O} \rangle = \frac{\int \prod_l dU_l \mathcal{O} e^{S_\delta}}{\int \prod_l dU_l e^{S_\delta}}.$$
(69)

A straightforward calculation, written out explicitly in [9], gives:

$$\langle \mathcal{O} \rangle = \langle \mathcal{O} \rangle_0 + \sum_{n=1}^{\infty} \frac{\delta^n}{n!} \langle \mathcal{O} S^n \rangle_c,$$
 (70)

where we have again redefined  $S_0$  by introducing  $J(\delta)$  and  $K(\delta)$  as before. The Polyakov line is now easily evaluated as

$$\langle L \rangle = \langle L \rangle_0 + \sum_{n=1}^{\infty} \frac{\delta^n}{n!} \langle LS^n \rangle_c.$$
(71)

With  $N_{\tau} = 2$ , as we assume from now on,  $\langle LS^n \rangle_c$  take the form:

$$\langle LS^n \rangle_c = \frac{1}{2} (\beta/2)^n \sum_{i=1}^{\xi(n)} \alpha_{n,i} \langle L_{n,i} \rangle_c.$$
(72)

The inequivalent diagrams  $L_{n,i}$ , together with their multiplicities, are listed in Appendix C.2. We will now develop the methodology for evaluating these inequivalent diagrams.

# 3 Method of calculation

Equation 63 allows us to relate connected averages to non-connected expectation values. We shall, therefore, consider the evaluation of non-connected averages first.

Let U be an element of SU(2) in the fundamental representation, i.e. a  $2 \times 2$  unitary matrix with unit determinant. Then, using the parametrization 30 of SU(2) we find:

$$\int dU U_j^i e^{J \operatorname{Tr} U} = \frac{1}{2} \delta_j^i \int dU \operatorname{Tr}(U) e^{J \operatorname{Tr} U} = \frac{1}{2} \frac{dZ_0}{dJ} \delta_j^i = \frac{1}{2f} \frac{df}{dJ} \delta_j^i =: \omega_1 \delta_j^i.$$
(73)

This result is more general than it may seem. In fact, the expectation value of any product of SU(2) matrix elements is a linear combination of products of Kronecker deltas. This motivates the digression into the representation theory of the symmetric groups that follows.

### 3.1 Projection operators and evaluation of non-connected averages

We will start by presenting some powerful results from the theory of finite groups that will allow us to evaluate expectation values in a very elegant and general way. Consider a finite group  $\mathcal{G}$  of order |G| and define the vector space  $\mathcal{V}_G$ , over the field of complex numbers C, by

$$\mathcal{V}_G := \left\{ \sum_{i=1}^{|G|} \alpha_i g_i | \alpha_i \in C, g_i \in \mathcal{G} \right\}.$$
(74)

Vector addition and scalar multiplication are defined in the usual way:

Given  $u, v \in \mathcal{V}_G$ ,

$$u + v = \sum_{i=1}^{|G|} \alpha_i g_i + \sum_{i=1}^{|G|} \beta_i g_i := \sum_{i=1}^{|G|} (\alpha_i + \beta_i) g_i$$
(75)

and

$$\lambda u = \lambda \left( \sum_{i=1}^{|G|} \alpha_i g_i \right) := \sum_{i=1}^{|G|} (\lambda \alpha_i) g_i, \qquad \forall \lambda \in C.$$
(76)

Then, if we define the product between two elements of  $\mathcal{V}_G$  by

$$uv = \left(\sum_{i=1}^{|G|} \alpha_i g_i\right) \left(\sum_{j=1}^{|G|} \beta_j g_j\right) := \sum_{i=1}^{|G|} \sum_{j=1}^{|G|} \alpha_i \beta_j (g_i g_j), \quad \forall u, v \in \mathcal{V}_G,$$
(77)

 $\mathcal{V}_G$  is a linear algebra over the field of complex numbers. The following theorem concerns the structure constants of this algebra.

**Theorem 1** Let  $c_i = \sum_{g \in K_i} g$ ,  $i = 1, 2, ..., \kappa$ , be the element of  $\mathcal{V}_G$  corresponding to the sum of the elements of the conjugacy class  $K_i \subset \mathcal{G}$ . By the closure of the algebra under multiplication, there exist complex numbers  $\xi_{ijl}$  such that

$$c_i c_j = \sum_{l=1}^{\kappa} \xi_{ijl} c_l.$$
(78)

Then, the structure constants  $\xi_{ijl}$  are given by

$$\xi_{ijl} = \frac{k_i k_j}{|G|} \sum_{\mu=1}^{\kappa} \frac{1}{\dim(\mathcal{V}_{\mu})} \chi^{\mu}(K_i) \chi^{\mu}(K_j) \chi^{\mu*}(K_l),$$
(79)

where  $k_i = |K_i|$  and  $\chi^{\mu}$  denotes the character of the irreducible representation of  $\mathcal{G}$  on the vector space  $\mathcal{V}_{\mu}$ .

The proof of this theorem is given in Appendix A.1.

We now construct projection operators corresponding to the irreducible representations of the group  $\mathcal{G}$ . In [17] it is proved that if  $U : \mathcal{G} \to \operatorname{Perm}(\mathcal{V})$  is a representation of  $\mathcal{G}$  on  $\mathcal{V}$  and  $D_{\mu} : \mathcal{G} \to GL(dim(\mathcal{V}_{\mu}), C)$  is an irreducible matrix representation of  $\mathcal{G}$ , then the operator

$$P_{\mu} := \frac{\dim(\mathcal{V}_{\mu})}{|G|} \sum_{g \in \mathcal{G}} \chi^{\mu}(g^{-1}) U(g), \qquad (80)$$

is a projection operator on  $\mathcal{V}$  in the sense that

$$P_{\mu}P_{\nu} = \delta_{\mu\nu}P_{\mu}, \qquad \sum_{\mu=1}^{\kappa} P_{\mu} = \mathbf{1}.$$
 (81)

$$S_{1}: Y_{\Box} = E, \qquad E = (1)$$

$$S_{2}: Y_{\Box\Box} = \frac{1}{2}(E + B) \\Y_{\Box} = \frac{1}{2}(E - B), \qquad E = (1^{2}), B = (2)$$

$$S_{3}: Y_{\Box\Box} = \frac{1}{6}(E + B + C) \\Y_{\Box} = \frac{1}{3}(2E - C) \\Y_{\Box} = \frac{1}{6}(E - B + C), \qquad E = (1^{3}), B = 3(2, 1), C = 2(3)$$

$$S_{4}: Y_{\Box\Box\Box} = \frac{1}{24}(E + D + B + C + F) \\Y_{\Box\Box} = \frac{1}{8}(3E + D - B - F) \\Y_{\Box} = \frac{1}{8}(3E - D - B + F)$$

Table 1: The projection operators for the symmetric group  $S_n$ ,  $1 \leq n \leq 4$ , in Young Tableaux notation. The structure of the conjugacy classes in terms of the partitions of nis also shown.

In particular, if  $D_{\mu}$  is unitary (for a finite group this is guaranteed by Maschke's theorem provided the representation is carried on an inner product space),

$$P_{\mu} = \frac{\dim(\mathcal{V}_{\mu})}{|G|} \sum_{g \in \mathcal{G}} \chi^{\mu*}(g) U(g) =$$
  
$$\frac{\dim(\mathcal{V}_{\mu})}{|G|} \sum_{i=1}^{\kappa} \chi^{\mu*}(K_i) \sum_{g \in K_i} U(g) =$$
  
$$\frac{\dim(\mathcal{V}_{\mu})}{|G|} \sum_{i=1}^{\kappa} \chi^{\mu*}(K_i) \tilde{U}(c_i), \qquad (82)$$

where  $\tilde{U}: \mathcal{V}_G \to \operatorname{Perm}(\mathcal{V})$  is the representation of the algebra  $\mathcal{V}_G$  induced by the representation of  $\mathcal{G}$  on  $\mathcal{V}$ . So, for the symmetric group  $S_n$  the projection operators take the form:

$$Y^{(\mu)} = \frac{\dim(\mathcal{V}_{\mu})}{|G|} \sum_{i=1}^{\kappa} \chi^{\mu}(K_i) \tilde{U}(c_i),$$
(83)

since the characters are real. These can be constructed immediately from the character table. The projection operators for the symmetric groups of order 1, 2, 3 and 4 are listed in Table 1.

As mentioned before, the expectation value of a product of n SU(2) matrix elements can be written as a linear combination of Kronecker deltas. In fact, in a more compact fashion, it can be written as a linear combination of the projection operators of  $S_n$  acting on (say) the lower indices of n Kronecker deltas. A further simplification is possible if the possible index values are less than n. This is guaranteed by the following lemma.

$$S_{1}: Y_{\Box} = E$$

$$S_{2}: Y_{\Box} = \frac{1}{2}(E + B)$$

$$Y_{\Box} = \frac{1}{2}(E - B)$$

$$S_{3}: Y_{\Box} = \frac{1}{3}(E + C)$$

$$Y_{\Box} = \frac{1}{3}(2E - C)$$

$$Y_{\Box} = 0, \qquad B = E + C$$

$$S_{4}: Y_{\Box} = \frac{1}{12}(E + B + C)$$

$$Y_{\Box} = \frac{1}{4}(3E - B)$$

$$Y_{\Box} = 0$$

$$Y_{\Box} = \frac{1}{12}(2E + 2B - C)$$

$$Y_{\Box} = 0, \qquad D = 2E + C/2, \ F = B + C/2 - E$$

Table 2: The reduced projection operators for  $S_n$ ,  $1 \le n \le 4$ . The relation of the odd conjugacy classes to the even ones can be determined by expressing the former as a linear combination of the latter and then deducing the coefficients by requiring that the structure of the algebra is maintained.

**Lemma 1** An odd permutation acting on N indices, at least two of which are equal, is equivalent to an even permutation acting on these N indices.

proof:

The odd permutation can be followed by an interchange of the two equal indices. The resulting permutation is even. QED

The consequence of this lemma is that not all the conjugacy classes of  $S_n$ , n > 2, are independent. The ones that consist of odd permutations can be reexpressed in terms of the rest. The union of the remaining even conjugacy classes is the alternating group  $A_n$ , a normal subgroup of  $S_n$ . The reduced projection operators are shown in Table 2.

Now we are in a position to evaluate the expectation values of products of up to four SU(2) matrix elements. First, we write the expectation value as a general linear combination of the non-vanishing projection operators of the corresponding symmetric group and then, by summing over various indices, we determine the coefficients. The results of this procedure are summarized in Table 3. The expectation values given there are sufficient to calculate the diagrams up to order four for the plaquette energy and order three for the Polyakov line.

### **3.2** Evaluation of connected averages

Now we turn to the evaluation of the connected averages, which, in fact, are the ones that appear in the  $\delta$  expansion. We will begin by the conventional construction of these averages from the non-connected expectation values and then, I will present a powerful

$$\begin{split} \langle U_a^i \rangle_0 &= (\omega_1 \mathbf{Y}_{\Box})_a^i \\ \langle U_a^i U_b^j \rangle_0 &= (\Omega \mathbf{Y}_{\Box\!\Box} + \mathbf{Y}_{\Box\!\Box})_{ab}^{ij}, \qquad \qquad \Omega = (\omega_2 - 1)/3 \\ \langle U_a^i U_b^j U_c^k \rangle_0 &= (\Lambda \mathbf{Y}_{\Box\!\Box} + \omega_1 \mathbf{Y}_{\Box\!\Box})_{abc}^{ijk}, \qquad \qquad \Lambda = (\omega_3 - 4\omega_1)/4 \\ \langle U_a^i U_b^j U_c^k U_d^l \rangle_0 &= (M \mathbf{Y}_{\Box\!\Box\!\Box} + \Omega \mathbf{Y}_{\Box\!\Box\!\Box} + \mathbf{Y}_{\Box\!\Box})_{abcd}^{ijkl}, \qquad M = (\omega_4 - 3\omega_2 + 1)/5 \end{split}$$

Table 3: The expectation values of products of SU(2) matrix elements in terms of projection operators. Here,  $\omega_1 = (1/2f)df/dJ$  and  $\omega_n = (1/f)d^nf/dJ^n$ , for  $n \ge 2$ .

method which allows one to calculate the connected averages of the vast majority of diagrams efficiently with no reference to non-connected averages. As far as I know, this method is used here for the first time, although special cases of it have appeared in some PhD theses(e.g. [10]).

To express the connected averages in terms of the non-connected ones we use Equation 63. For one, two, three and four statistical variables it gives:

$$\langle U \rangle_{c} = \langle U \rangle_{0}$$

$$\langle UV \rangle_{c} = \langle UV \rangle_{0} - \langle U \rangle_{0} \langle V \rangle_{0}$$

$$\langle UVW \rangle_{c} = \langle UVW \rangle_{0} - \langle UV \rangle_{0} \langle W \rangle_{0} - \langle UW \rangle_{0} \langle V \rangle_{0} - \langle VW \rangle_{0} \langle U \rangle_{0} + 2 \langle U \rangle_{0} \langle V \rangle_{0} \langle W \rangle_{0}$$

$$\langle UVWX \rangle_{c} = \langle UVWX \rangle_{0} - \langle U \rangle_{0} \langle VWX \rangle_{0} - \langle V \rangle_{0} \langle UWX \rangle_{0} - \langle W \rangle_{0} \langle UVX \rangle_{0} - \langle X \rangle_{0} \langle UVW \rangle_{0} - \langle UV \rangle_{0} \langle WX \rangle_{0} - \langle UW \rangle_{0} \langle VX \rangle_{0} - \langle UX \rangle_{0} \langle VW \rangle_{0} + 2 \langle U \rangle_{0} \langle V \rangle_{0} \langle WX \rangle_{0} + 2 \langle U \rangle_{0} \langle V \rangle_{0} \langle VX \rangle_{0} + 2 \langle U \rangle_{0} \langle X \rangle_{0} \langle UW \rangle_{0} + 2 \langle W \rangle_{0} \langle X \rangle_{0} \langle UV \rangle_{0} - 6 \langle U \rangle_{0} \langle W \rangle_{0} \langle X \rangle_{0}$$

$$(84)$$

Here, the statistical variables are identified with the trace of different plaquette variables and the non-connected averages are obtained as in the previous section. These expressions are sufficient for the diagrams up to order four for the plaquette energy and up to order three for the Polyakov line.

The above procedure is easily carried out for low order diagrams, but it quickly becomes too cumbersome as we go to higher orders. Eventually, we will have to perform the calculation with the help of a computer. Though, the following theorem sets the basis for an efficient, systematic evaluation of connected averages which can take us a few orders further in the  $\delta$  expansion.

**Theorem 2** Given a set of N statistical variables  $\{X_{\ell,i}\}_{i=1,2,...,N}$ , defined on the link  $\ell$ , the connected averages of these variables satisfy:

$$\frac{d}{dJ} \left\langle \prod_{i=1}^{N} X_{\ell,i}^{n_i} \right\rangle_c = \left\langle \operatorname{Tr} U_\ell \prod_{i=1}^{N} X_{\ell,i}^{n_i} \right\rangle_c,$$
(85)

The proof is given in Appendix A.2. The implications of this theorem are not immediately obvious, but they are indeed far going. In effect, it means that if a diagram can be formed from a lower order diagram by attaching a single plaquette or the Polyakov line to *one* of its links, then the connected average of the new diagram can be obtained from that of the lower order diagram. One simply needs to differentiate with respect to J the *part* of the connected average of the lower order diagram which corresponds to the link where the new plaquette was attached. An example would be helpful:

Suppose we want to calculate 
$$\left\langle \boxed{2} \right\rangle_{c}^{}$$
. Given that  $\left\langle \boxed{2} \right\rangle_{c}^{} = 3\Omega^{4} + 1 - 4\omega_{1}^{8},$  (86)

we conclude that

$$\left\langle \boxed{2} \right\rangle_{c} = \omega_{1}^{3} (3\Omega^{3}\Omega' - 8\omega_{1}^{7}\omega_{1}'), \qquad (87)$$

where the prime denotes differentiation with respect to J. Note that we have differentiated only one factor of  $\Omega$  and two factors of  $\omega_1$  since only those factors correspond to the link where we have attached the third plaquette. The  $\omega_1^3$  outside the parentheses corresponds to the free links of the new plaquette.

Therefore, to evaluate all diagrams of a certain order, the following procedure should be followed: First we identify the diagrams that cannot be obtained by attaching plaquettes to lower order diagrams. Generally, these are a small minority of all the diagrams. We evaluate the connected averages of these 'irreducible' diagrams using their non-connected expectation values as described in the beginning of this section. Then, the connected average of the rest of the diagrams is obtained from that of the corresponding lower order diagrams as in the above example.

### 3.3 Evaluation of diagrams with FORM

As the evaluation of the diagrams eventually becomes too lengthy for any analytical method, it is instructive to consider possible computer algorithms for doing this calculation. No such algorithms were developed as part of this project, but existing codes, by H.F.Jones, were employed to check the analytical calculations. These algorithms were written for the programming language FORM of J.A.M.Vermaseren (1989).

Both connected and non-connected averages can be calculated for each diagram. First, the diagram is defined in terms of its link structure and then external routines for the evaluation of connected and non-connected averages are invoked to complete the calculation.

A sample of these codes is shown in Appendix B.1. Their disadvantage is that each diagram must be defined manually by explicitly adjusting the appropriate parameters and the calculation is performed for one diagram at a time. Moreover, different order diagrams need different external routines to do the calculation. An improved version of these algorithms would probably be along the lines of W.Kerler's codes [7], where the classification and enumeration of the diagrams is also part of the computer calculation. This not only allows the evaluation of the averages to be more efficient, but also provides an effective way for the calculation of the multiplicities at the same time.

### **3.4** Calculation of the multiplicities

Finally, before I discuss the results of our calculations, I will briefly describe how the multiplicities of the inequivalent diagrams on a *d*-dimensional hypercubic lattice can be calculated.

Each lattice site has 2d nearest neighbours, two in each of the d orthogonal directions of the lattice. Now attaching a plaquette to this site would occupy two of these directions. Then, the desired diagram is built by attaching extra plaquettes to this initial plaquette and counting the number of ways this can be done without changing the link structure. As an example, the multiplicity of  $\langle 2 \\ 2 \\ \rangle_c$  is  $\frac{3!}{1!2!}4[2(d-1)-1]$ . The combinatorial factor appears because it is immaterial which of the plaquettes is the single one. Then, 4 is the number of links where the single plaquette can be attached to the other two, and the expression in the parentheses is the number of possible directions it can have relative to them.

Some care must be taken when calculating the multiplicity of diagrams containing the Polyakov line. In this case the lattice is periodic in the fourth direction, which must not be counted with the spatial directions. Also, this periodicity implies that the two extreme plaquettes of a diagram extending along the entire period of the lattice in the fourth direction will share a link.

A Fortran routine to enumerate the possible link structures and evaluate their multiplicities has been developed by H.F.Jones. However, I have not used this code in this project.

### 4 Results and discussion

Now that we have learnt how to evaluate the terms of the  $\delta$  expansions for the plaquette energy and the Polyakov line (Equations 62 and 72) we consider the results of such a calculation. However, a couple of technical comments are in order here. Firstly, we should remember that the averages that appear in these expansions are functions of  $J(\delta) =$  $(1 - \delta)J$  and  $K(\delta) = (1 - \delta)K$  and so, to obtain the full expansion in powers of  $\delta$  each average must be expanded first. This will introduce derivatives of the averages which can be calculated recursively using the identities:

$$\omega_1' = (\omega_2 - 4\omega_1^2)/2 \tag{88}$$

$$\omega_n' = \omega_{n+1} - 2\omega_1 \omega_n. \tag{89}$$

Although these follow from the properties of the modified Bessel functions if  $\omega_n$  is defined as previously, they can be proved purely from the action integral if  $\omega_n$  is defined geometrically through the expectation value of the trace of n plaquettes stack one on top of the other. Then it is seen that they are generally true for SU(N).

Secondly, the 'order' of the expansion is counted by the corresponding power of  $\delta$ . However, in order to agree with the counting of orders in [5], I have adopted the convention that for the plaquette energy order n is the expansion up to the coefficient of  $\delta^{n+1}$  inclusive.



Figure 2: Plots of the plaquette energy as a function of  $r = J/3\beta$  for  $\beta = 3.2$ . MC stands for Monte Carlo data, taken from Ref. [12]

### 4.1 Optimization of the plaquette energy

Figure 2 shows the first three orders (after order 0) of the plaquette energy as functions of the variational parameter. The Monte Carlo value shown is from Ref. [12].

The Principle of Minimal Sensitivity dictates that at each order, and for each value of  $\beta$ , the optimum value of the variational parameter should correspond to a stationary point of the plaquette energy. If more than one stationary points exist, the broader one should be chosen. This optimization procedure was done using the C++ routines, listed in Appendix B.2. The algorithms for the modified Bessel functions were taken from the Numerical Recipes library. However, some of them were impossible to adjust to achieve the required accuracy and so, slower algorithms, based on a power series expansion, were devised. For the location of the stationary points I used the interval bisection method as given in [14].

Once the optimum curve  $J(\beta)$  is found, it is inserted into the plaquette energy, which is now considered as a function of  $\beta$  only. The results for the first three orders are shown in Figure 3.

A few things should be observed. Firstly, not all orders have PMS points. Here, orders 1 and 3 have but order 2 does not. So instead of order 2 the Padé approximant P(1,1) is plotted. The existence of PMS points for even or odd orders only is a quite general phenomenon. It also appears in the  $\delta$  expansion for zero dimensions field theory [16], and it has been observed by Kerler [7], who also provides a qualitative explanation.

Another feature is that, at least for the orders shown, as we go to higher orders the optimized plaquette energy tends to the Monte Carlo result. This is encouraging but it is accompanied by a gradual increase in the value of  $\beta_{min}$ , the point where the broad minimum ceases to exist. In other words, higher order approximations are valid in a smaller part of the weak coupling region. This is clearly a disadvantage of our method since the expansion fails to give adequate information for the transition region between



Figure 3: Plot of the optimized plaquette energy as a function of  $\beta/2$ . Since the second order does not have any PMS points, the Padé approximant P(1, 1) is shown instead. The Monte Carlo data are taken from Refs. [11] and [23].

strong and weak coupling and, therefore, little can be deduced about the existence or the nature of a deconfining phase transition in this region. This unfortunate phenomenon has also been observed by J.O.Akeyo and H.F.Jones [5] who attempted to extend the expansion beyond  $\beta_{min}$  by adopting a 'weak PMS'. In the absence of stationary points of the plaquette energy, they looked at stationary points of its slope. This enabled them to extend the  $\delta$  expansion down to  $\beta/2 = 1.23$  for order 3. However, such a criterion is not well justified and their conclusion that there is no signal of the breakdown of the expansion as higher orders are reached is rather misleading. Indeed the increase of  $\beta_{min}$  with order seems to be a universal feature of the  $\delta$  expansion for lattice gauge theories. As we will see below it also appears in the Polyakov line expansion and in that case it is much more disastrous.

The failure of the expansion in the transition region is not unique to the  $\delta$  expansion with the PMS criterion though. Kerler [6] has used the same expansion for the plaquette energy but with a different criterion for fixing the variational parameter. Instead of the PMS he uses the 'accumulation' points of successive orders of the expansion. For example, such an accumulation occurs just after 1.0 in Figure 2. Kerler observed that as the transition region is approached from either the weak or the strong coupling side, the accumulation suddenly disappears. This change in the accumulation point systematics occurs at  $\beta/2 = 0.76$  for the strong coupling side and at  $\beta/2 = 1.0$  for the weak coupling side. Therefore, at least for the first order of the  $\delta$  expansion, the disappearance of the PMS point (at  $\beta/2 = 1.07$ ) almost coincides with the change in the accumulation point systematics. The failure of the expansion in the transition region is taken by Kerler as an indication for the location of a phase transition, but not for its existence or its nature.

Finally, Zheng, Tan and Wang [8] use a third criterion for optimizing the variational

parameter at each order. They use the convexity inequality:

$$W \le W_{eff,1}(\beta, J),\tag{90}$$

where  $W_{eff,1}(\beta, J)$  is the first order approximation to the free energy, together with the variational principle

$$\frac{\delta}{\delta J} W_{eff,1}(\beta, J) = 0.$$
(91)

From the variational principle they obtain a double-valued curve  $J(\beta)$  and they choose the appropriate branch by employing the convexity inequality. With this approach there seems to be no problem in extrapolating the expansion into the transition region and the criterion for the existence of a (first-order) phase transition is taken to be the matching or the mismatching of the strong and weak coupling branches of the expansion. Zheng et al. found that the first order expansions fail to join smoothly indicating a first-order transition at  $\beta/2 = 1.41$ . The second order, however, produces a smooth curve over the whole range of couplings, thus removing the unwanted phase transition. The interesting result is that the next order shows a discontinuity again in the transition region, although the fit of the expansion to the Monte Carlo data in the strong and the weak coupling regions is improved. This situation is analogous to the behaviour of the  $\delta$  expansion as we go to higher orders. Namely, the fit to the Monte Carlo data is improved in the weak coupling region, but the validity of the expansion is restricted to a smaller region. To overcome this difficulty Zheng et al. used gauge fixing, thus improving slightly their results. However, this approach is not better justified than the weak PMS adopted by Akeyo and Jones.

### 4.2 Optimization of the Polyakov line

The trial action for the Polyakov line has two variational parameters both of which must be optimized. As a first attempt we follow Tan and Zheng [9] and set J = K. This follows from the convexity inequality and the variational principles

$$\frac{\delta}{\delta J}W_{eff,1} = 0, \qquad \frac{\delta}{\delta K}W_{eff,1} = 0.$$
(92)

However, we could adopt a more sophisticated approach by using our PMS criterion for the Polyakov line in the J-K plane. Since this introduces some computational difficulties, we only consider the case J = K here.

Figure 4 shows plots of the Polyakov line for  $\beta = 2.5$  as a function of the variational parameter. Only order 2 exhibits a PMS point for  $\beta \ge 2.4$ . H.F.Jones has done the calculation for order 4 and it seems that a PMS point exists for larger values of  $\beta$ . So, as for the plaquette energy, not all orders exhibit a PMS point and higher order approximants are valid for a smaller range of couplings. The optimized second order is plotted in Figure 5. Monte Carlo results and the first three orders of the cumulant expansion of Tan and Zheng [9], based on the free energy variational principle, are also shown. It should be emphasized that here Tan and Zheng have used gauge fixing for all orders. The fourth order of the  $\delta$  expansion is not shown since it has not been optimized yet. Based on the results for the plaquette energy we expect that it will give a better approximation to the Monte Carlo data in the weak coupling region.



Figure 4: Plots of the Polyakov line as a function of J = K for  $\beta = 2.5$ .



Figure 5: Plot of the optimized Polyakov line as a function of  $\beta$ . The first three orders of the cumulant expansion of Tan and Zheng [9] are also shown together with Monte Carlo points from Ref. [13]

The disadvantage of the  $\delta$  expansion is that it cannot be extrapolated well into the transition region which is the region of major interest. The gauge fixed cumulant expansion, however, does extend into the transition region and it seems to approach the Monte Carlo results as the order increases. In fact,  $\langle L \rangle = 0$  in the strong coupling region up to  $\beta_c \approx 1.6$ , where  $\langle L \rangle$  takes on a non-zero value in a continuous way. This is the qualitative behaviour of a second order phase transition, which according to Tan and Zheng may exist near  $\beta_c$ . The Monte Carlo data support this possibility.

## 5 Conclusions

The plaquette energy and the Polyakov line have been calculated up to the fourth order for SU(2) pure gauge theory on the lattice using the linear  $\delta$  expansion. The calculation of the fourth order of the Polyakov line was beyond our initial expectations, but the development of a new method for the evaluation of connected averages has made it possible. In the near future we intend to complete the optimization of the Polyakov line and compare the results with the calculation of H.F.Jones.

Our results so far suggest that the linear  $\delta$  expansion is a competent semi-analytical approach to zero temperature lattice gauge theories. However, there are strong indications that at finite temperature the method fails to produce an expansion valid in the range of couplings where a deconfining second-order phase transition is expected. The results could be improved by using a different trial action, preferably gauge invariant, or, in the case of the Polyakov line, by applying the PMS criterion in the J - K plane instead of setting J = K on an ad hoc basis.

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# Appendix

# A Proofs of important results

## A.1 Proof of theorem 1

Consider an irreducible representation of the finite group  $\mathcal{G}$  on the vector space  $\mathcal{V}_{\mu}$ 

$$T^{(\mu)}: \mathcal{G} \to \operatorname{Perm}(\mathcal{V}_{\mu}).$$
 (93)

Also, define the map

$$\tilde{T}^{(\mu)}: \mathcal{V}_G \to \operatorname{Perm}(\mathcal{V}_{\mu}),$$
(94)

$$\tilde{T}^{(\mu)}(u) = \tilde{T}^{(\mu)}\left(\sum_{i=1}^{|G|} \alpha_i g_i\right) := \sum_{i=1}^{|G|} \alpha_i T^{(\mu)}(g_i), \qquad \forall u \in \mathcal{V}_G.$$
(95)

This is a representation of the algebra  $\mathcal{V}_G$  on  $\mathcal{V}_\mu$  with the property

$$\tilde{T}^{(\mu)}(c_i)T^{(\mu)}(g) = T^{(\mu)}(g)\tilde{T}^{(\mu)}(c_i), \qquad \forall g \in \mathcal{G}.$$
(96)

Therefore, by Shur's First Lemma,

$$\tilde{T}^{(\mu)}(c_i) = \lambda_i^{\mu} \mathbf{1},\tag{97}$$

where  $\lambda_i^{\mu}$  is a complex number. By taking the trace on both sides we find:

$$\lambda_i^{\mu} = \frac{k_i \chi^{\mu}(K_i)}{\dim(\mathcal{V}_{\mu})},\tag{98}$$

which is called the *Dirac Character*.

Then,

$$c_i c_j = \sum_{l=1}^{\kappa} \xi_{ijl} c_l \Rightarrow$$

$$\tilde{T}^{(\mu)}(c_i c_j) = \sum_{l=1}^{\kappa} \xi_{ijl} \tilde{T}^{(\mu)}(c_l) \Rightarrow$$

$$\tilde{T}^{(\mu)}(c_i) \tilde{T}^{(\mu)}(c_j) = \sum_{l=1}^{\kappa} \xi_{ijl} \tilde{T}^{(\mu)}(c_l) \Rightarrow$$

$$\lambda_i^{\mu} \lambda_j^{\mu} = \sum_{l=1}^{\kappa} \xi_{ijl} \lambda_l^{\mu},$$
(99)

which, uppon using the orthogonality relation

$$\sum_{\mu=1}^{\kappa} k_i \chi^{\mu}(K_i) \chi^{\mu*}(K_j) = |G| \delta_{ij}, \qquad (100)$$

gives

$$\xi_{ijl} = \frac{k_i k_j}{|G|} \sum_{\mu=1}^{\kappa} \frac{1}{\dim(\mathcal{V}_{\mu})} \chi^{\mu}(K_i) \chi^{\mu}(K_j) \chi^{\mu*}(K_l).$$
(101)

This completes the proof.

### A.2 Proof of theorem 2

Firstly, we easily find

$$\frac{\partial}{\partial J} \left\langle e^{\sum_{i=1}^{N} z_i X_{\ell,i}} \right\rangle_0 = \left\langle \operatorname{Tr} U_\ell e^{\sum_{i=1}^{N} z_i X_{\ell,i}} \right\rangle_0 - \left\langle \operatorname{Tr} U_\ell \right\rangle_0 \left\langle e^{\sum_{i=1}^{N} z_i X_{\ell,i}} \right\rangle_0.$$
(102)

Then, using Equation 63, we get

$$\frac{d}{dJ} \left\langle \prod_{i=1}^{N} X_{\ell,i}^{n_i} \right\rangle_c = \left( \prod_{j=1}^{N} \frac{n_j!}{2\pi i} \oint_{C_j} \frac{dz_j}{z_j^{n_j+1}} \right) \left\langle \operatorname{Tr} U_\ell e^{\sum_{i=1}^{N} z_i X_{\ell,i}} \right\rangle_0 / \left\langle e^{\sum_{i=1}^{N} z_i X_{\ell,i}} \right\rangle_0 = \left( \prod_{j=1}^{N} \frac{n_j!}{2\pi i} \oint_{C_j} \frac{dz_j}{z_j^{n_j+1}} \right) \left( \frac{\partial}{\partial z} \ln \left\langle e^{z \operatorname{Tr} U_\ell} e^{\sum_{i=1}^{N} z_i X_{\ell,i}} \right\rangle_0 \right)_{z=0} = \left\langle \operatorname{Tr} U_\ell \prod_{i=1}^{N} X_{\ell,i}^{n_i} \right\rangle_c.$$
(103)

This completes the proof.

# **B** Routines used in the calculation

### **B.1** Samples of FORM routines

\*program c3 \*26/11/93

```
f Z,D,[d/dy],[d/dz];
s [1/Z],j,k,l,w1,V3;
g fig3c=Z(1,0,0)*D;
multiply left [d/dy]*[d/dz];
repeat;
id [d/dy]*Z(j?,k?,l?)=Z(j,k+1,l)+Z(j,k,l)*[d/dy];
id [d/dy]*D=-Z(0,1,0)*D^2+D*[d/dy];
id [d/dz]*Z(j?,k?,l?)=Z(j,k,l+1)+Z(j,k,l)*[d/dz];
id [d/dz]*D=-Z(0,0,1)*D^2+D*[d/dz];
endrepeat;
id [d/dy]=0;
id [d/dz]=0;
id D = [1/Z];
bracket [1/Z];
id [1/Z]=1;
id Z(1,0,0)=[A](w1,V3);
id Z(0,1,0)=[B](w1,V3);
id Z(0,0,1)=[C](w1,V3);
id Z(1,1,0)=[AB](w1,V3);
id Z(1,0,1)=[AC](w1,V3);
id Z(0,1,1)=[BC](w1,V3);
```

```
*program fig3c
*26/11/93
Nwrite statistics;
d 2;
i a,b,c,d,e,f;
G y3(a,b,c,d)=(d_(a,c)*d_(b,d)+d_(a,d)*d_(b,c))/2;
G y1(a,b,c,d)=(d_(a,c)*d_(b,d)-d_(a,d)*d_(b,c))/2;
G y4(a,b,c,d,e,f)=(d_(a,d)*d_(b,e)*d_(c,f)+
d_(a,e)*d_(b,f)*d_(c,d)+d_(a,f)*d_(b,d)*d_(c,e))/3;
G y2(a,b,c,d,e,f)=d_(a,d)*d_(b,e)*d_(c,f)-y4(a,b,c,d,e,f);
.store
.global
d 2;
i a,b,c,d,e,f,g,h,i,j,k;
s w1,V1,V2,V3,V4,n;
сU
#do i=1,4
   A'i', B'i',C'i'
#enddo
;
set AA:
#do i=1,4
A'i'
#enddo
;
set BB:
#do i=1,4
B'i'
#enddo
;
set CC:
#do i=1,4
C'i'
#enddo
;
i
#do i=1,4
```

id Z(1,1,1)=[ABC](w1,V3);

```
a'i', b'i', c'i'
#enddo
;
set first:
#do i=1,4
a'i', b'i', c'i'
#enddo
;
set last:
#do i=2,4
a'i', b'i',c'i'
#enddo
a1, b1, c1;
set Dag:
#do i=3,4
A'i', B'i', C'i'
#enddo
;
G[A](w1,V3) =
#do i=1,4
 * A'i'(a'i',a'i')
#enddo
;
G [B] (w1,V3) =
#do i=1,4
* B'i'(b'i',b'i')
#enddo
;
G[C](w1,V3) =
#do i=1,4
 * C'i'(c'i',c'i')
#enddo
;
G [AB](w1,V3) = [A] * [B];
G [AC](w1,V3) = [A]*[C];
G [BC](w1,V3) = [B]*[C];
G [ABC](w1,V3) = [A] * [B] * [C];
id U?(i?,j?first[n])=U(i,last[n],0);
id U?Dag[n](i?,j?,0)=U(i,j,1);
```

#procedure subs3

```
#do i=1,4
 if (count(A'i',1)=1);
 id A'i'(a?,b?,j?)=w1*d_(a,b);
endif;
 if (count(B'i',1)=1);
 id B'i'(a?,b?,j?)=w1*d_(a,b);
endif;
 if (count(C'i',1)=1);
 id C'i'(a?,b?,j?)=w1*d_(a,b);
endif;
#enddo
repeat;
id U?(a?,b?,i?)*U?(c?,d?,i?)*U?(e?,f?,i?)
= V4*y4(a,c,e,b,d,f)+V2*y2(a,c,e,b,d,f);
id U?(a?,b?,i?)*U?(c?,d?,i?)\
= V3*y3(a,c,b,d)+y1(a,c,b,d);
id U?(a?,b?,i?)*U?(c?,d?,j?)\
= ((V3+1)*y3(a,c,b,d)+(3*V3-1)*y1(a,c,b,d))/2;
endrepeat;
#endprocedure
```

```
*program fig3p1c
*26/11/93
#include fig3c
nwrite statistics;
```

-----Fig. 3.1-----\* \* \* \_\_\_\_\_ 1 \* 3 \* \* \* \* id U?BB[n](i?,j?,k?)=AA[n](i,j,k); id U?CC[n](i?,j?,k?)=AA[n](i,j,k); \*-----\_\_\_\_\_ #call subs3 .store \*NB!!! #-#include c3 nwrite statistics; b w1;

```
s V2;
id V2=w1;
p;
.e
```

### B.2 C++ routines

```
//SU(2) - PMS for the Plaquette Enegry - John Papadimitriou 13/01/2000
//(last updated 5/5/00)
#include <iostream.h>
#include <math.h>
#include <fstream.h>
#include <stdlib.h>
#include "factor.h"
#include "bessi0.h"
#include "bessi1.h"
#include "bessi.h"
//Function prototypes:
double root(double x1, double x2, double f1, double f2, int &depth,
double y, double dx);
double find_root(double x1, double x2,int &depth, double y, double dx);
double f(double,double);
double f_derivative(double, double, double);
int main(void)
{
const double dx=0.1, dy=0.1;
int i:
ofstream file("su2opt1.dat");
char opt;
cout<<"Enter 'p' to plot the function or 'm' to minimize it: ";</pre>
cin>>opt;
switch(opt)
{
case 'p': {
for(i=1;i<=300;i++) {</pre>
cout<<i*dx/9.6<<'\t'<<f(i*dx,1.6)<<endl;
file<<i*dx/9.6<<'\t'<<f(i*dx,1.6)<<endl;
}
}break;
```

```
case 'm': {
double x=0, y;
int j;
for(i=0;i<30;i++){</pre>
y=(i+15)*dy;
//Initial approximation for x-----
for(j=80; j<=600; j++)</pre>
{
if(fabs(f_derivative(j*dx, y, dx))<=0.02)</pre>
{x=j*dx;
break;
}
}
//-----
int depth=0;
if (x==0){
x=find_root(3, 50, depth, y, dx);
}
else {
x=find_root(x-1.0, x+18.0, depth, y, dx);
}
//output of optimum contour
cout<<x<<'\t'<<'y<<endl;</pre>
file<<y<<'\t'<<'\t'<<x<<endl;
//cout<<y<<'\t'<<f(x,y)<<endl;</pre>
//file<<y<<'\t'<<f(x,y)<<endl;</pre>
}
}break;
default:{cout<<"No file written"<<endl;}</pre>
}
return 0;
}
//function to be studied
double f(double x,double y)
{
double Ep;
int const d=4;int const R0=2*d-3;int const R1=2*d-4;
int const R2=2*d-5;int const R=4*R0;
//Omegas
double w1=bessi(2,2*x)/bessi1(2*x);
double w^{2=4-6*w^{1/x}};
double V3=bessi(3,2*x)/bessi1(2*x);
```

```
double V4=bessi(4,2*x)/bessi1(2*x);
double w3=4*(V4+w1);
double V5=bessi(5,2*x)/bessi1(2*x);
double w4=5*V5+3*w2-1;
//Derivatives of wn
double dw1=0.5*(w2-4*w1*w1);
double ddw1=0.5*(w3-6*w1*w2+16*w1*w1*w1);
double dddw1=0.5*(w4-8*w1*w3-3*w2*w2+48*w1*w1*w2-96*pow(w1,4));
double dw2=w3-2*w1*w2;
double ddw2=w4-2*w1*w3-2*dw1*w2-2*w1*dw2;
   double dw3=w4-2*w3*w1;
//Connected diagrams by new method
double fig1p1=2*pow(w1,4);
double fig2p1c=1+3*pow(V3,4)-4*pow(w1,8);;
double fig2p2c=2*pow(w1,6)*dw1;
double fig3p1c=4*pow(V4,4)-18*pow(w1*V3,4)-2*pow(w1,4)+16*pow(w1,12);
double fig3p2c=pow(w1,3)*(pow(V3,3)*dw2-8*pow(w1,7)*dw1);
double fig3p3c=2*pow(w1,9)*ddw1;
double fig3p4c=pow(w1,6)*(3*pow(V3,3)+4.5*V3*V3+0.5-6*w2*pow(w1,4)+
16*pow(w1,6));
double fig3p5c=2*pow(w1,8)*dw1*dw1;;
double fig4p1c=5*pow(V5,4)+9*pow(V3,4)+2-8*pow(w1,4)*(4*pow(V4,4)-
18*pow(w1,4)*pow(V3,4)-2*pow(w1,4))-3*pow((1+3*pow(V3,4)),2)-
96*pow(w1,16);
double fig4p2c=pow(w1,3)*(pow(V4,3)*(dw3-4*dw1)-18*pow(w1,3)*pow(V3,3)*
(dw1*V3+w1*dw2/3.)-2*pow(w1,3)*dw1+48*pow(w1,11)*dw1);
double fig4p3c=pow(V3,6)*(5*V5+w2)+6*pow(V3,4)+1-8*pow(w1,7)*
(pow(V3,3)*dw2-8*pow(w1,7)*dw1)-pow(1+3*pow(V3,4),2)-
2*pow(w1,12)*(w2*w2-16*pow(w1,4));
double fig4p4c=pow(w1,6)*(pow(V3,3)*ddw2-8*pow(w1,6)*(dw1*dw1+w1*ddw1));
double fig4p5c=2*pow(w1,12)*dddw1;
double fig4p6c=pow(w1,4)*(V3*V3*(4*V3*(2*V4+w1)*(2*V4+w1)/3.+(1-V3)*
(2*V4*V4+w1*w1))+w1*w1*w2-12*pow(w1,6)*pow(V3,3)-2*pow(w1,6)*
(3*(3*V3*V3-8*pow(w1,4)*dw1)+1)-4*pow(w1*V3,3)*dw2-
8*pow(w1,8)*dw1*dw1-w1*w1*w2*(1+3*pow(V3,4))+32*pow(w1,12));
double fig4p7c=pow(w1,6)*(V3*V3*dw2*dw2/3.-16*pow(w1,6)*dw1*dw1);
double fig4p8c=pow(w1,5)*dw1*(pow(V3,3)*dw2-8*pow(w1,7)*dw1);
double fig4p9c=pow(w1,9)*(V3*(V3+1)*dw2-2*pow(w1,4)*dw2-16*pow(w1,3)*
dw1*dw1);
double fig4p10c=2*pow(w1,11)*ddw1*dw1;
double fig4p11c=pow(w1,6)*(3*pow(V3,3)*(V3+1)*(V3+1)+(3*V3*V3+1)*
(3*V3*V3+1)/4.-12*pow(w1,4)*pow(V3,3)-2*pow(w1,4)*
(2*(3*V3*V3-8*pow(w1,4)*dw1)+3*V3*V3-8*pow(w1,4)*dw1+1)-
8*pow(w1,6)*w2*dw1-4*pow(w1,8)*w2+32*pow(w1,10));
double fig4p12c=pow(w1,8)*dw1*(3*pow(V3,3)+4.5*V3*V3+0.5-6*w2*pow(w1,4)+
```
```
16*pow(w1,6));
double fig4p13c=pow(w1,8)*((21*pow(V3,4)+24*pow(V3,3)+18*V3*V3+1)/4.-
24*pow(w1,4)*dw1*dw1-32*pow(w1,6)*dw1-16*pow(w1,8));
double fig4p14c=2*pow(w1,10)*pow(dw1,3);
double fig4p15c=2*pow(w1,10)*pow(dw1,3);
//Derivatives of connected diagrams
double Dfig1p1=8*pow(w1,3)*(0.5*w2-2*w1*w1);
double DDfig1p1=4*(w3*pow(w1,3)+1.5*w2*w2*w1*w1-18*w2*pow(w1,4)+40*pow(w1,6)
);
double DDDfig1p1=4*(pow(w1,3)*(w4-2*w1*w3)+3*w1*w1*(w2-6*w1*w1)*(w3-2*w1*w2)+
(3*w3*w1*w1+3*w2*w2*w1-72*w2*pow(w1,3)+240*pow(w1,5))*(0.5*w2-2*w1*w1));
double Dfig2p1c=4*pow(V3,3)*(w3-2*w1*w2)-16*pow(w1,7)*(w2-4*w1*w1);
double Dfig2p2c=pow(w1,5)*((3*w2-16*w1*w1)*(w2-4*w1*w1)+w1*(w3-2*w1*w2));
double DDfig2p1c=4*(pow(V3,3)*(w4-2*w1*w3)+(V3*V3*(w3-2*w1*w2)-2*w1*pow(V3,3))
-4*pow(w1,7))*(w3-2*w1*w2)+(144*pow(w1,8)-28*pow(w1,6)*w2-2*w2*pow(V3,3))*
(0.5*w2-2*w1*w1));
double DDfig2p2c=pow(w1,4)*((6*w3*w1+15*w2*w2-210*w2*w1*w1+576*pow(w1,4))*
(0.5*w2-2*w1*w1)+w1*(6*w2-30*w1*w1)*(w3-2*w1*w2)+w1*w1*(w4-2*w1*w3));
double Dfig3p1c=4*pow(V4,3)*(w4-2*w1*w3)-24*pow(w1,4)*pow(V3,3)*(w3-2*w1*w2)+
(192*pow(w1,11)-8*pow(w1,3)-72*pow(w1,3)*pow(V3,4)-16*pow(V4,3))*
(0.5*w2-2*w1*w1);
double Dfig3p2c=pow(w1*V3,3)*(w4-2*w1*w3)+(pow(w1,3)*V3*V3*(w3-2*w1)-
8*pow(V3,3)*pow(w1,4)-4*pow(w1,10))*(w3-2*w2*w1)+(0.5*w2-2*w1*w1)*
(3*w1*w1*pow(V3,3)*(w3-2*w1)-2*pow(w1*V3,3)-24*pow(V3,4)*pow(w1,3)-
40*pow(w1,9)*w2+192*pow(w1,11));
double Dfig3p3c=pow(w1,9)*(w4-2*w1*w3)-6*pow(w1,10)*(w3-2*w1*w2)+
pow(w1,8)*(9*w3-60*w1*w2+192*w1*w1)*(0.5*w2-2*w1*w1);
double Dfig3p4c=(6*pow(w1,5)*(V3*V3*(w2+3.5)+0.5)-60*w2*pow(w1,9)+
192*pow(w1,11))*(0.5*w2-2*w1*w1)+(3*pow(w1,6)*V3*(V3+1)-6*pow(w1,10))*
(w3-2*w1*w2);
double Dfig3p5c=pow(w1,7)*(w2-4*w1*w1)*(w1*(w3-2*w1*w2)+2*(w2*w2-10*w1*w1*w2+
24*pow(w1,4)));
//Expansion coefficients
double a0=0.5*fig1p1;
double a1=0.5*y*(fig2p1c+R*fig2p2c)-0.5*x*Dfig1p1;
double a2=0.25*(y*y*(fig3p1c+3.*R*fig3p2c+R*R1*fig3p3c+8.*R1*fig3p4c+
3.*(3.*R*R0-8.*R1)*fig3p5c)-2.*x*y*(Dfig2p1c+R*Dfig2p2c)+
x*x*DDfig1p1);
double a3=(y*y*y*(fig4p1c+4.*R*fig4p2c+3.*R*fig4p3c+6.*R*R1*fig4p4c+
R*R1*R2*fig4p5c
+48.*R1*fig4p6c+6.*(3.*R*R0-8.*R1)*fig4p7c+12.*(3.*R*R0-8.*R1)*fig4p8c+
96.*R1*R1*fig4p9c+48.*R1*(R0*R0+4.*R1+2.*R2*R2)*fig4p10c+48.*R1*fig4p11c+
192.*R1*R1*fig4p12c+12.*(2.*R0+R1+2.*R1*R2)*fig4p13c
+96.*(R0*R0*R0-2.*R1*R1-R1)*fig4p14c
+48.*(9.*R0*R0+14.*R0*R0+19.*R0-7.)*fig4p15c)
```

```
34
```

```
-3.*x*y*y*(Dfig3p1c+3.*R*Dfig3p2c+R*R1*Dfig3p3c+8.*R1*Dfig3p4c+
3.*(3.*R*R0-8.*R1)*Dfig3p5c)+3.*x*x*y*(DDfig2p1c+R*DDfig2p2c)-
x*x*x*DDDfig1p1)/12.0;
//Plaquette Energy to order delta<sup>3</sup>
Ep=a0+a1;
//Pade Approximant P(1,1)
double P11=a0+a1*a1/(a1-a2);
return Ep;
}
//first derivative of f(x,y) with respect to x
double f_derivative(double x, double y, double dx)
ſ
return (f(x+dx,y)-f(x-dx,y))/(2.0*dx);
}
double root(double x1, double x2, double f1, double f2, int &depth,
double y, double dx)
//Finds a root of f_derivative(x, y, dx)=0 using bisection for fixed y and dx
//Assumes that x2>=x1 and f1*f2<0.0 (D.M. CAPPER, Introduction to C++
//for scientists, engineers and mathematicians)
{
const int max_depth=50;
const double x_limit=1e-5;
double estimated_root;
double x_mid=0.5*(x1+x2);
if (x2-x1 \le x_{\min}) {
//cout<<"Root found at recursion depth="<<depth<<"\n";</pre>
estimated_root=x_mid;
}
else if (++depth>max_depth){
cout<<"WARNING: maximum limit of "<<max_depth<<</pre>
" bisections reached"<<"\n";</pre>
estimated_root=x_mid;
}
else {
double f_mid=f_derivative(x_mid, y, dx);
if (f_mid==0.0) {
//Zero at x_mid.
estimated_root=x_mid;
}
else if (f_derivative(x1, y, dx)*f_mid<0.0) {</pre>
//Zero in first segment.
```

```
estimated_root=root(x1, x_mid, f1, f_mid, depth, y, dx);
}
else {
//Zero in second segment
estimated_root=root(x_mid, x2, f_mid, f2, depth, y, dx);
}
}
   return estimated_root;
}
double find_root(double x1, double x2,int &depth, double y, double dx)
{
double f1=f_derivative(x1, y, dx);
double f2=f_derivative(x2, y, dx);
if (f1*f2>0.0) {
cout<<"Error in find_root(): "<<"end-points have same sign\n";</pre>
//exit(EXIT_FAILURE);
return 100;
}
if (x2-x1>0.0)
return root(x1, x2, f1, f2, depth, y, dx);
else
return root(x2, x1, f2, f1, depth, y, dx);
}
```

```
//Pkovline - PMS for the Polyakov Line - John Papadimitriou 11/02/2000
#include <iostream.h>
#include <math.h>
#include <fstream.h>
#include <stdlib.h>
#include "factor.h"
#include "bessi0.h"
#include "bessi1.h"
#include "bessi.h"
//Function prototypes:
double root(double x1, double x2, double f1, double f2, int &depth,
double y, double dx);
double find_root(double x1, double x2,int &depth, double y, double dx);
double f(double,double,double);
double f_derivative(double, double, double);
int main(void)
{
const double dx=0.1, dy=0.1;
int i;
ofstream file("pkov3.dat");
char opt;
cout<<"Enter 'p' to plot the function or 'm' to minimize it: ";</pre>
cin>>opt;
switch(opt)
{
case 'p': {
for(i=1;i<=100;i++) {</pre>
cout<<i*dx<<'\t'<<f(i*dx,i*dy,2.5)<<endl;
file<<i*dx<<'\t'<<f(i*dx,i*dy,2.5)<<endl;
}
}break;
case 'm': {
double x=0, y;
int j;
for(i=0;i<30;i++){</pre>
y=(i+15)*dy;
//Initial approximation for x-----
for(j=80; j<=600; j++)</pre>
{
if(fabs(f_derivative(j*dx, y, dx))<=0.02)</pre>
{x=j*dx;
```

```
break;
}
}
//-----
            -----
int depth=0;
if (x==0){
x=find_root(3, 50, depth, y, dx);
}
else {
x=find_root(x-1.0, x+18.0, depth, y, dx);
}
//output of optimum contour
//cout<<x<<'\t'<<y<endl;</pre>
//file<<y<<'\t'<<'x<<endl;</pre>
cout<<y<<'\t'<<f(x,y,z)<<endl;
file<<y<<'\t'<<f(x,y,z)<<endl;
}
}break;
default:{cout<<"No file written"<<endl;}</pre>
}
return 0;
}
//function to be studied
double f(double x,double y, double z)
{
int const D=4; int const r=2*(D-1); int const R0=r-1; int const R1=r-2;
   int const R2=r-3;
double L;
//Definition of variables
double w1=bessi(2,2*x)/bessi1(2*x);
double w^{2=4-6*w^{1/x}};
double V3=bessi(3,2*x)/bessi1(2*x);
double V4=bessi(4,2*x)/bessi1(2*x);
double w3=4*(V4+w1);
double V5=bessi(5,2*x)/bessi1(2*x);
double w4=5*V5+3*w2-1;
double x1=bessi(2,2*y)/bessi1(2*y);
double x^{2=4-6*x^{1/y}};
double V3K=bessi(3,2*y)/bessi1(2*y);
double V4K=bessi(4,2*y)/bessi1(2*y);
double x3=4*(V4K+x1);
```

```
double V5K=bessi(5,2*y)/bessi1(2*y);
double x4=5*V5K+3*x2-1;
//Derivatives of x1 and w1
double dw1=0.5*(w2-4*w1*w1);
double ddw1=0.5*(w3-6*w1*w2+16*w1*w1*w1);
double dddw1=0.5*(w4-8*w1*w3-3*w2*w2+48*w1*w1*w2-96*pow(w1,4));
double dw2=w3-2*w1*w2;
//-----
double dx1=0.5*(x2-4*x1*x1);
double ddx1=0.5*(x3-6*x1*x2+16*x1*x1*x1);
double dddx1=0.5*(x4-8*x1*x3-3*x2*x2+48*x1*x1*x2-96*pow(x1,4));
double dx2=x3-2*x1*x2;
double ddx2=x4-2*x1*x3-2*dx1*x2-2*x1*dx2;
//-----
//Non-connected diargams
//A. Diagrams including line
double L0p1=2*x1*x1;
double L1p1=w1*w1*x1*x1*x2;
double L2p1=0.5*pow(w1,4)*x1*x1*w2*x2;
double L2p2=x1*(2*x1+(x3-2*x1)*V3K*V3*V3);
double L2p3=pow(w1,4)*pow(x1,3)*x3;
double L2p4=0.5*pow(w1,4)*x1*x1*x2*x2;
double L2p5=L2p4;
double L2p6=0.5*x1*x1*(V3*V3*x2*x2+(1-V3*V3)*(1+3*V3K*V3K));
double L3p1=0.5*w1*x1*x1*x2*(2*w1+(w3-2*w1)*V3*V3*V3);
double L3p2=0.25*pow(w1,6)*x1*x1*w2*w2*x2;
double L3p3=L3p2;
double L3p4=0.5*pow(w1,7)*x1*x1*x2*w3;
double L3p5=pow(w1,3)*x1*(4*w1*x1+(w3-2*w1)*(x3-2*x1)*V3*V3K/3.0);
double L3p6=0.5*pow(w1,6)*pow(x1,3)*w2*x3;
double L3p7=pow(w1,4)*pow(x1,3)*((1+V3)*V3*x3+(1-V3)*(1-V3)*x1);
double L3p8=0.5*pow(w1,4)*x1*x1*x2*((1+V3)*V3*x2+0.5*(1-V3)*(1-V3));
double L3p9=0.25*pow(w1,4)*pow(x1,4)*w2*w2*x2;
double L3p10=0.25*pow(w1,6)*x1*x1*w2*x2*x2;
double L3p11=L3p10;
double L3p12=0.25*pow(w1,4)*x1*x1*(w2*x2*(2*V3*V3K+V3+V3K)+
(1-V3)*(1-V3K)*(1+3*V3*V3K));
double L3p13=L3p10;
double L3p14=pow(w1,3)*x1*x1*((w3-2*w1)*(x2*x2-1-3*V3K*V3K)*V3/6.0+
w1*(1+3*V3K*V3K));
```

```
double L3p15=x1*(2*w1*w1*x1*x2+(x4-2*x2)*(0.25*w3-w1)*(0.25*w3-w1)*
(0.25 \times x3 - x1));
double L3p16=w1*w1*x1*x1*(x2+(x4-x2)*V3*V3*V3K);
double L3p17=w1*w1*x1*x1*(4*x1*x1+(x3-2*x1)*(x3-2*x1)*V3*V3/3.);
double L3p18=0.5*w1*w1*x1*x2*(2*x1+(x3-2*x1)*V3*V3*V3K);
double L3p19=0.5*pow(w1,6)*pow(x1,3)*x2*x3;
double L3p20=pow(w1,6)*pow(x1,4)*x4;
double L3p21=L3p19;
double L3p22=0.5*w1*w1*x1*x2*(2*x1+(x3-2*x1)*V3*V3*V3K);
double L3p23=0.25*pow(w1,6)*x1*x1*x2*x2*x2;
double L3p24=L3p19;
double L3p25=L3p23;
double L3p26=x1*((x3-2*x1)*V3K*(V3K+1)*(w1*w1+2*(0.25*w3-w1)*(0.25*w3-w1))/3.0+
w1*w1*x1*(1+4*V3K-V3K*V3K)+0.5*V3K*(V3K-1)*((2*w1*w1+(0.25*w3-w1)*(0.25*w3-w1))*
(x3+4*x1)/3.0-4*w1*w1*x1));
double L3p27=0.5*w1*w1*x1*x1*(x2*x3*V3*V3+(1-V3*V3)*(2*x1+(x3-2*x1)*V3K));
double L3p28=0.25*w1*w1*x1*x1*x2*(x2*x2*V3*V3+(1-V3*V3)*(1+3*V3K*V3K));
double L3p29=0.25*w1*w1*pow(x1,4)*x2*x2*(1+3*V3*V3);
```

```
//B. Diagrams not including line
```

```
double D1p1=2*pow(w1,4);
double D1p2=2*w1*w1*x1*x1;
double D2p1=1+3*pow(V3,4);
double D2p2=1+3*V3*V3*V3K*V3K;
double D2p3=pow(w1,6)*w2;
double D2p4=pow(w1,4)*x1*x1*x2;
double D2p5=pow(w1,4)*x1*x1*w2;
double D2p6=pow(x1,4)*(1+3*V3*V3);
double D3p1=x1*x1*w1*((w3-2*w1)*pow(V3,3)+2*w1);
double D3p2=0.5*x1*x1*pow(w1,6)*w2*w2;
double D3p3=D3p2;
double D3p4=x1*x1*pow(w1,7)*w3;
double D3p5=w1*w1*w1*((w3-2*w1)*V3*V3K*V3K+2*w1);
double D3p6=0.5*x1*x1*pow(w1,6)*x2*w2;
double D3p7=x1*x1*pow(w1,4)*(3*V3*V3K*(V3+1)+1.5*V3*V3+0.5);
double D3p8=0.5*pow(x1,4)*pow(w1,4)*w2*w2;
double D3p9=pow(x1,4)*w1*w1*w1*((w3-2*w1)*V3+2*w1);
double D3p10=4*((0.25*w3-w1)*(0.25*w3-w1)*(0.25*x3-x1)*(0.25*x3-x1)+w1*w1*x1*x1);
double D3p11=x1*w1*w1*((x3-2*x1)*V3*V3*V3K+2*x1);
double D3p12=x1*x1*x1*pow(w1,6)*x3;
double D3p13=0.5*x1*x1*pow(w1,6)*x2*x2;
double D3p14=2*x1*x1*(2*V3K*V3K*(0.25*w3-w1)*(0.25*w3-w1)+(V3K*V3K+1)*w1*w1);
double D3p15=0.5*pow(x1,4)*w1*w1*x2*(3*V3*V3+1);
```

```
//Connected diagrams
double L0p1c=2*x1*x1;
double L1p1c=2*x1*x1*w1*w1*dx1;
double L2p1c=2*x1*x1*pow(w1,4)*dx1*dw1;
double L2p2c=L2p2-L0p1*D2p2-2*L1p1*D1p2+2*L0p1*D1p2*D1p2;
double L2p3c=2*x1*x1*pow(w1,4)*ddx1;
double L2p4c=2*x1*x1*pow(w1,4)*dx1*dx1;
double L2p5c=L2p4c;
double L2p6c=L2p6-L0p1*D2p6-2*L1p1*D1p2+2*L0p1*D1p2*D1p2;
double L3p1c=L3p1-L0p1*D3p1-2*L2p1*D1p1+L0p1*D1p2*D2p1-L1p1*D2p1+2*L0p1*D1p1*D2p5+
2*L1p1*D1p1*D1p1-2*L0p1*D1p2*D1p1*D1p1;
double L3p2c=2*x1*x1*pow(w1,6)*dx1*dw1*dw1;
double L3p3c=2*x1*x1*pow(w1,6)*dx1*dw1*dw1;
double L3p4c=2*x1*x1*pow(w1,7)*dx1*ddw1;
double L3p5c=L3p5-L0p1*D3p5-L2p2*D1p1-2*L2p1*D1p2-2*L1p1*D2p5+4*L1p1*D1p2*D1p1+
L0p1*D1p1*D2p2+4*L0p1*D2p5*D1p2-4*L0p1*D1p2*D1p2*D1p1;
double L3p6c=2*x1*x1*x1*pow(w1,6)*ddx1*dw1;
double L3p7c=L3p7-L0p1*D3p7-2*L2p1*D1p2-L2p3*D1p1-2*L1p1*D2p5+4*L1p1*D1p2*D1p1+
L0p1*D2p4*D1p1+4*L0p1*D2p5*D1p2-4*L0p1*D1p1*D1p2*D1p2;
double L3p8c=L3p8-L0p1*D3p7-L2p1*D1p2-L2p4*D1p1+2*L0p1*D2p5*D1p2+2*L1p1*D1p1*D1p2+
L0p1*D2p4*D1p1-2*L0p1*D1p2*D1p2*D1p1-L1p1*D2p5;
double L3p9c=2*pow(x1,4)*pow(w1,4)*dx1*dw1*dw1;
double L3p10c=2*x1*x1*pow(w1,6)*dx1*dx1*dw1;
double L3p11c=2*x1*x1*pow(w1,6)*dx1*dx1*dw1;
double L3p12c=L3p12-L0p1*D3p8-2*L2p1*D1p2-L2p5*D1p1-2*L1p1*D2p5+4*L1p1*D1p2*D1p1+
4*L0p1*D1p2*D2p5-3*L0p1*D1p2*D1p2*D1p1;
double L3p13c=2*x1*x1*pow(w1,6)*dx1*dx1*dw1;
double L3p14c=L3p14-L0p1*D3p9-L2p6*D1p1-2*L2p1*D1p2-2*L1p1*D2p5+L0p1*D2p6*D1p1+
4*L1p1*D1p2*D1p1+4*L0p1*D2p5*D1p2-4*L0p1*D1p2*D1p2*D1p1;
double L3p15c=L3p15-L0p1*D3p10-3*L2p2*D1p2-3*L1p1*D2p2+6*L1p1*D1p2*D1p2+
6*L0p1*D2p2*D1p2-6*L0p1*D1p2*D1p2*D1p2;
double L3p16c=L3p16-L0p1*D3p11-L2p2*D1p2-2*L2p3*D1p2-L1p1*D2p2-2*L1p1*D2p4+
6*L1p1*D1p2*D1p2+4*L0p1*D2p4*D1p2+2*L0p1*D2p2*D1p2-6*L0p1*D1p2*D1p2*D1p2;
double L3p17c=L3p17-L0p1*D3p11-L2p2*D1p2-2*L2p4*D1p2-2*L1p1*D2p4+L0p1*D2p2*D1p2+
4*L1p1*D1p2*D1p2+4*L0p1*D2p4*D1p2-4*L0p1*D1p2*D1p2*D1p2;
double L3p18c=L3p18-L0p1*D3p11-2*L2p4*D1p2+L0p1*D2p2*D1p2-L1p1*D2p2+
2*L0p1*D2p4*D1p2+2*L1p1*D1p2*D1p2-2*L0p1*D1p2*D1p2*D1p2;
double L3p19c=2*x1*x1*x1*pow(w1,6)*dx1*ddx1;
double L3p20c=2*pow(x1,4)*pow(w1,6)*dddx1;
double L3p21c=2*x1*x1*x1*pow(w1,6)*ddx1*dx1;
double L3p22c=L3p22-L2p2*D1p2-2*L2p5*D1p2+L0p1*D2p2*D1p2+4*L1p1*D1p2*D1p2-
L1p1*D2p2-2*L0p1*D1p2*D1p2*D1p2;
double L3p23c=2*x1*x1*pow(w1,6)*dx1*dx1*dx1;
```

```
double L3p24c=2*x1*x1*x1*pow(w1,6)*ddx1*dx1;
double L3p25c=2*x1*x1*pow(w1,6)*dx1*dx1*dx1;
double L3p26c=L3p26-L0p1*D3p14-L2p2*D1p2-2*L2p6*D1p2-2*L1p1*D2p6-L1p1*D2p2+
6*L1p1*D1p2*D1p2+4*L0p1*D2p6*D1p2+2*L0p1*D2p2*D1p2-6*L0p1*D1p2*D1p2*D1p2;
double L3p27c=L3p27-L0p1*D3p15-L2p6*D1p2-L2p3*D1p2-L2p5*D1p2-L1p1*D2p6-L1p1*D2p4+
5*L1p1*D1p2*D1p2+2*L0p1*D2p6*D1p2+2*L0p1*D2p4*D1p2-4*L0p1*D1p2*D1p2*D1p2;
double L3p28c=L3p28-L0p1*D3p15-L2p6*D1p2-L2p4*D1p2+2*L1p1*D1p2*D1p2*D1p2;
double L3p28c=L3p28-L0p1*D3p15-L2p6*D1p2-L2p4*D1p2+2*L1p1*D1p2*D1p2-L1p1*D2p4+
L0p1*D2p6*D1p2+2*L0p1*D2p4*D1p2-2*L0p1*D1p2*D1p2;
double L3p29c=L3p29-L0p1*D3p15-L2p4*D1p2+L1p1*D1p2*D1p2;
L0p1*D2p6*D1p2+L3p29-L0p1*D3p15-L2p4*D1p2+L1p1*D1p2*D1p2+L0p1*D2p6*D1p2+
L0p1*D2p4*D1p2-L1p1*D2p6-L0p1*D1p2*D1p2;
```

```
//Derivatives of the connected diagrams
double d1KL0p1c=4*x1*dx1;
double d2KLOp1c=4*(dx1*dx1+x1*ddx1);
double d3KL0p1c=4*(3*dx1*ddx1+x1*dddx1);
//-----
double d1JL1p1c=4*w1*dw1*x1*x1*dx1;
double d1KL1p1c=2*w1*w1*x1*(2*dx1*dx1+x1*ddx1);
double d2JL1p1c=4*x1*x1*dx1*(dw1*dw1+w1*ddw1);
double d2KL1p1c=2*w1*w1*(2*dx1*dx1*dx1+6*x1*dx1*dx1+x1*x1*dddx1);
double d1Jd1KL1p1c=4*w1*dw1*x1*(2*dx1*dx1+x1*ddx1);
//-----
                                                            _____
double d1JL2p1c=2*x1*x1*dx1*(pow(w1,4)*ddw1+4*w1*w1*w1*dw1*dw1);
double d1KL2p1c=2*pow(w1,4)*dw1*(x1*x1*ddx1+2*x1*dx1*dx1);
double d1JL2p2c=2*V3*dw2*V3K*x1*dx2/3.0-32*w1*w1*w1*dw1*pow(x1,4)*dx1;
double d1KL2p2c=V3*V3*(x1*dx2*dx2/3.0+V3K*dx1*dx2+V3K*x1*ddx2)-8*pow(w1,4)
*x1*x1*x1*(4*dx1*dx1+x1*ddx1);
double d1JL2p3c=8*w1*w1*w1*dw1*x1*x1*x1*ddx1;
double d1KL2p3c=2*pow(w1,4)*(3*x1*x1*dx1*ddx1+x1*x1*x1*ddx1);
double d1JL2p4c=8*w1*w1*w1*dw1*x1*x1*dx1*dx1;
double d1KL2p4c=2*pow(w1,4)*(2*x1*dx1*dx1*dx1+2*x1*x1*dx1*dx1);
double d1JL2p5c=d1JL2p4c;
double d1KL2p5c=d1KL2p4c;
double d1JL2p6c=x1*x1*(2*V3*dw2*(V3K*V3K+V3K-2*pow(x1,4))-
32*w1*w1*w1*dw1*x1*x1*dx1);
double d1KL2p6c=2*x1*dx1*(3*V3*V3*(V3K*V3K+V3K-2*pow(x1,4))
+0.5*(1+3*V3K*V3K-4*pow(x1,4))-8*pow(w1,4)*x1*x1*dx1)+
x1*x1*(V3*V3*((2*V3K+1)*dx2-24*x1*x1*x1*dx1)+V3K*dx2-
8*x1*x1*x1*dx1-8*pow(w1,4)*x1*(x1*ddx1+2*dx1*dx1));
//Expansion coefficients
double L0=0.5*L0p1c;
double L1=0.5*(-y*d1KL0p1c+0.5*z*2*r*L1p1c);
double L2=0.25*(y*y*d2KL0p1c-z*2*r*(x*d1JL1p1c+
y*d1KL1p1c)+0.25*z*z*(8*r*R1*L2p1c+2*r*L2p2c+
2*r*R0*L2p3c+4*r*R0*L2p4c+2*r*R0*L2p5c+2*r*L2p6c));
```

```
double L3=(-y*y*y*d3KL0p1c+1.5*z*2*r*(x*x*d2JL1p1c+2*x*y*d1Jd1KL1p1c+
y*y*d2KL1p1c)-0.75*z*z*(8*r*R1*(x*d1JL2p1c+y*d1KL2p1c)+
2*r*(x*d1JL2p2c+y*d1KL2p2c)+2*r*R0*(x*d1JL2p3c+y*d1KL2p3c)+
4*r*R0*(x*d1JL2p4c+y*d1KL2p4c)+2*r*R0*(x*d1JL2p5c+y*d1KL2p5c)+
2*r*(x*d1JL2p6c+y*d1KL2p6c))+0.125*z*z*z*(12*r*R1*L3p1c+
12*r*R1*R1*L3p2c+72*r*R1*R2*L3p3c+12*r*R1*R2*L3p4c+
12*r*R1*L3p5c+24*r*R1*R1*L3p6c+12*r*R1*L3p7c+24*r*R1*L3p8c+
72*r*R1*L3p9c+24*r*R1*R1*L3p10c+24*r*R1*R1*L3p11c+
12*r*R1*L3p12c+24*r*R1*R1*L3p13c+12*r*R1*L3p14c+2*r*L3p15c+
6*r*R0*L3p16c+6*r*R0*L3p17c+6*r*R0*L3p18c+6*r*R0*R1*L3p19c+
2*r*R0*R1*L3p20c+6*r*R0*R1*L3p21c+6*r*R0*L3p22c+
12*r*R0*R0*L3p23c+12*r*R0*R0*L3p24c+12*r*R0*R0*L3p25c+
6*r*L3p26c+12*r*R0*L3p27c+12*r*R0*L3p28c+12*r*R0*L3p29c))/12.0;
L=L0+L1+L2+L3;
return L;
}
//first derivative of f(x,y) with respect to x
double f_derivative(double x, double y, double dx)
{
return (f(x+dx,y,x)-f(x-dx,y,x))/(2.0*dx);
}
double root(double x1, double x2, double f1, double f2, int &depth,
double y, double dx)
//Finds a root of f_derivative(x,y,dx)=0 using bisection for fixed y and dx
//Assumes that x_2 = x_1 and f_1 + f_2 < 0.0 (D.M. cAPPER, Introduction to c++
//for scientists, engineers and mathematicians)
{
const int max_depth=50;
const double x_limit=1e-5;
double estimated_root;
double x_mid=0.5*(x1+x2);
if (x2-x1 \le x_{\min}) {
//cout<<"Root found at recursion depth="<<depth<<"\n";</pre>
estimated_root=x_mid;
}
else if (++depth>max_depth){
cout<<"WARNING: maximum limit of "<<max_depth<<</pre>
" bisections reached"<<"\n";</pre>
estimated_root=x_mid;
}
else {
double f_mid=f_derivative(x_mid, y, dx);
if (f_mid==0.0) {
//Zero at x_mid.
estimated_root=x_mid;
```

```
}
else if (f_derivative(x1, y, dx)*f_mid<0.0) {</pre>
//Zero in first segment.
estimated_root=root(x1, x_mid, f1, f_mid, depth, y, dx);
}
else {
//Zero in second segment
estimated_root=root(x_mid, x2, f_mid, f2, depth, y, dx);
}
}
   return estimated_root;
}
double find_root(double x1, double x2,int &depth, double y, double dx)
{
double f1=f_derivative(x1, y, dx);
double f2=f_derivative(x2, y, dx);
if (f1*f2>0.0) {
cout<<"Error in find_root(): "<<"end-points have same sign\n";</pre>
//exit(EXIT_FAILURE);
return 100;
}
if (x2-x1>0.0)
return root(x1, x2, f1, f2, depth, y, dx);
else
return root(x2, x1, f2, f1, depth, y, dx);
}
//Factorial function
//John Papadimitriou (12/12/1999)
#include <math.h>
double factorial(int);
//factorial function
double factorial(int n)
{
int i;
double f=0;
for(i=1;i<=n;i++)</pre>
{
```

```
f+=log(i);
}
return exp(f);
}
```

```
//Returns Modified Bessel function of order zero
//John Papadimitriou 19/01/2000
#include <math.h>
double bessi0(double x)
{
double ans=0;
int n;
int const N=90;
for(n=0;n<=N;n++)
{
ans += pow(0.5*x,2*n)/pow(factorial(n),2);
}
return ans;
}
//Returns Modified Bessel function of order one
//John Papadimitriou 19/01/2000
#include <math.h>
double bessi1(double x)
{
double ans=0;
int n;
int const N=90;
for(n=0;n<=N;n++)
{
ans += pow(0.5*x,2*n)/(factorial(n)*factorial(n+1));
}
```

```
return 0.5*x*ans;
}
```

```
#include <math.h>
#include <iostream.h>
#define ACC 100.0
#define BIGNO 1.0e10
#define BIGNI 1.0e-10
double bessi(int n, double x)
{
double bessi0(double x);
int j;
double bi,bim,bip,tox,ans;
if (n < 2) cout<<"Index n less than 2 in bessi";
if (x == 0.0)
return 0.0;
else {
tox=2.0/fabs(x);
bip=ans=0.0;
bi=1.0;
for (j=2*(n+(int) sqrt(ACC*n));j>0;j--) {
bim=bip+j*tox*bi;
bip=bi;
bi=bim;
if (fabs(bi) > BIGNO) {
ans *= BIGNI;
bi *= BIGNI;
bip *= BIGNI;
}
if (j == n) ans=bip;
}
ans *= bessi0(x)/bi;
return x < 0.0 && (n & 1) ? -ans : ans;
}
}
#undef ACC
#undef BIGNO
#undef BIGNI
/* (C) Copr. 1986-92 Numerical Recipes Software s>%-OL12w-'<;w#!. */
```

## C List of inequivalent diagrams

## C.1 Inequivalent diagrams for the plaquette energy

n	i	$D_{n,i}$	$lpha_{n,i}$	$\left\langle D_{n,i} \right\rangle_c$
1	1		1	$2\omega_1^4$
2	1	2	1	$3\Omega^4 + 1 - 4\omega_1^8$
	2		R	$2\omega_1^6\omega_1'$
3	1	3	1	$4\Lambda^4 - 18\omega_1^4\Omega^4 - 2\omega_1^4 + 16\omega_1^{12}$
	2	2	3R	$\omega_1^3(3\Omega^3\Omega'-8\omega_1^7\omega_1')$
	3		$RR_1$	$2\omega_1^9\omega_1''$
	4		$8R_1$	$\omega_1^6(3\Omega^3 + \frac{9}{2}\Omega^2 + \frac{1}{2} - 6\omega_1^4\omega_2 + 16\omega_1^6)$
	5		$3(3RR_0 - 8R_1)$	$2\omega_1^8\omega_1'^2$
4	1	4	1	$5M^4 + 9\Omega^4 + 2 - 8\omega_1^4 (4\Lambda^4 - 18\omega_1^4 \Omega^4 - 2\omega_1^4) - 3(1 + 3\Omega^4)^2 - 96\omega_1^{16}$
	2	3	4R	$ \omega_1^3 (\Lambda^3 (\omega_3' - 4\omega_1') - 18\omega_1^3 \Omega^3 (\omega_1' \Omega + \omega_1 \Omega') -2\omega_1^3 \omega_1' + 48\omega_1^{11} \omega_1') $
	3	2 2	3R	$ \begin{aligned} &\Omega^6(5M+\omega_2)+6\Omega^4+1-\\ &8\omega_1^7(\Omega^3\omega_2'-8\omega_1^7\omega_1')-(1+3\Omega^4)^2-\\ &2\omega_1^{12}(\omega_2^2-16\omega_1^4) \end{aligned} $
	4		$6RR_1$	$\omega_1^6(\Omega^3 \omega_2'' - 8\omega_1^6(\omega_1'^2 + \omega_1 \omega_1''))$
	5		$RR_1R_2$	$2\omega_1^{12}\omega_1^{\prime\prime\prime}$
	6	2	$48R_{1}$	$\begin{split} &\omega_1^4 (\Omega^2 (4\Omega (2\Lambda + \omega_1)^2/3 + \\ &(1 - \Omega)(2\Lambda^2 + \omega_1^2)) + \omega_1^2 \omega_2 - \\ &12\omega_1^6 \Omega^3 - 2\omega_1^6 (3(3\Omega^2 - 8\omega_1^4 \omega_1') + 1) - \\ &4\omega_1^3 \Omega^3 \omega_2' - 8\omega_1^8 \omega_1'^2 - \\ &\omega_1^2 \omega_2 (1 + 3\Omega^4) + 32\omega_1^{12}) \end{split}$



$$R_n = 2d - 3 - n, R = 4R_0.$$
  

$$\Omega = (\omega_2 - 1)/3, \Lambda = (\omega_3 - 4\omega_1)/4, M = (\omega_4 - 3\omega_2 + 1)/5.$$









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 $r = 2(d-1), R_n = r - 1 - n$ 

 $\xi_i, \Xi, \overline{\Lambda} \text{ and } \overline{M} \text{ are the counterparts of } \omega_i, \Omega, \Lambda \text{ and } M \text{ respectively, for } K.$