7 Lattice methods

Analytic calculations of observables in the non-Abelian lattice gauge theories are available only in the strong-coupling regime $g^2 \to \infty$, while one needs $g^2 \to 0$ for the continuum limit. When g^2 is decreased, the lattice systems can undergo phase transitions as often happens in statistical mechanics.

To look for phase transitions, the mean-field method was first applied to lattice gauge theories [Wil74, BDI74]. It turned out to be useful for studying the first-order phase transitions which very often happen in lattice gauge systems but do not affect the continuum limit.

The second-order phase transitions are better described by the lattice renormalization group method. The approximate Migdal–Kadanoff recursion relations [Mig75, Kad76] were the first implementation of the renormalization group transformation on a lattice, which indicated the absence of a second-order phase transition in the non-Abelian lattice gauge theories and, therefore, quark confinement.

A very powerful method for practical nonperturbative calculations of observables in lattice gauge theories is the numerical Monte Carlo method. This method simulates statistical processes in a lattice gauge system and for this reason is often called a numerical simulation. The idea of applying it to lattice gauge theories is due to Wilson [Wil77], while the practical implementation was done by Creutz, Jacobs and Rebbi [CJR79] for Abelian gauge groups and by Creutz [Cre79, Cre80] for the SU(2) and SU(3) groups.

In this chapter we briefly describe the mean-field method, the lattice renormalization group method and the Monte Carlo method. A few results from Monte Carlo simulations will also be discussed.

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Fig. 7.1. Typical β -dependence of the plaquette average for a first-order phase transition which occurs at $\beta = \beta_*$.

7.1 Phase transitions

As was pointed out in Sect. 6.7, analytic calculations of the string tension are available only in the strong-coupling regime $g^2 \to \infty$, while one needs $g^2 \to 0$ for the continuum limit. A question arises as to what happens with lattice systems when g^2 is decreased. In particular, does an actual picture of the dependence of the string tension on g^2 look like that shown in Fig. 6.10?

We know from statistical mechanics that lattice systems can undergo phase transitions with a change of parameters, say the temperature, which completely alters the macroscopic properties. The simplest example is that of the first-order phase transition which occurs in a teapot.

First-order phase transitions very often happen in lattice gauge theories. They are usually seen as a discontinuity in the β - (or $1/g^2$ -) dependence of the plaquette average (6.65) as is depicted in Fig. 7.1. The form of $W(\partial p)$ at small β is given to the leading order of the strong-coupling expansion by Eq. (6.72), while that at large β is prescribed by the lattice perturbation theory^{*} to be

$$W(\partial p) = 1 - \frac{d_G}{\beta d} + \mathcal{O}(\beta^{-2}), \qquad (7.1)$$

where d_G is the dimensionality of the gauge group G ($d_G = N^2 - 1$ for SU(N), $d_G = N^2$ for U(N)) and d is the dimensionality of the lattice as before.

This behavior of the plaquette average is quite analogous to the dependence of the internal energy per unit volume (called the specific energy) in statistical systems. In order to see the analogy between the specific en-

^{*} It is often called, for obvious reasons, the weak-coupling expansion.

ergy and $(1 - W(\partial p))$, let us remember that β is analogous to the inverse temperature and rewrite Eq. (6.65) as

$$W(\partial p) = 1 + \frac{1}{N_p} \frac{\partial}{\partial \beta} \ln Z(\beta), \qquad (7.2)$$

where the partition function is given by Eq. (6.31) and the number of plaquettes N_p is analogous to the volume of a statistical system.

Problem 7.1 Derive Eq. (7.1) for the SU(N) gauge group.

Solution The partition function (6.31) can be calculated at large β (weak coupling) using the saddle-point method. The saddle-point configurations are given by solutions of the classical equation (6.24). The appropriate solution reads as

$$U^{\rm sp}_{\mu}(x) = Z_{\mu} \,, \tag{7.3}$$

where Z_{μ} is an element of the Z(N) group, the center of SU(N),

$$Z_{\mu} = \mathbb{I} \cdot e^{2\pi i n_{\mu}/N}, \qquad n_{\mu} = 1, \dots, N.$$
 (7.4)

It is evident that this is a solution because elements of the center commute so that Z_{μ} and $Z_{-\mu}$ cancel each other in $U_{\mu,\nu}(x) \equiv U(\partial p)$.

In order to take into account fluctuations around the saddle-point solution (7.3), let us expand

$$U_{\mu}(x) = U_{\mu}^{\rm sp}(x) e^{i t^{a} \epsilon_{\mu}^{a}(x)}, \qquad (7.5)$$

where the order of multiplication is not essential since Z_{μ} commute with the generators t^a . The expansion of tr $U(\partial p)$ to the quadratic order in ϵ^a is given by

$$\frac{1}{N} \operatorname{tr} U_{\mu,\nu}(x) = 1 - \frac{1}{2N} \mathcal{E}^2_{\mu,\nu}(x) , \qquad (7.6)$$

where

$$\mathcal{E}^{a}_{\mu,\nu}(x) = \epsilon^{a}_{\mu}(x) + \epsilon^{a}_{\nu}(x+a\hat{\mu}) - \epsilon^{a}_{\mu}(x+a\hat{\nu}) - \epsilon^{a}_{\nu}(x).$$
(7.7)

Owing to the local gauge invariance, we can always choose, say, $\epsilon_d(x) = 0$ so that there are only $N_l - N_s$ independent ϵ_s .

Substituting into Eq. (6.31) and expanding the Haar measure, we obtain

$$Z(\beta) \propto \prod_{\nu=1}^{d} \sum_{n_{\nu}=1}^{N} \prod_{a,x,\mu < d} \int_{-\infty}^{+\infty} \mathrm{d}\epsilon_{\mu}^{a}(x) \,\mathrm{e}^{-\beta \mathcal{E}_{\mu,\nu}^{2}(x)/2N}.$$
 (7.8)

The sum over n_{ν} , which arises from the degenerate saddle points, is just an irrelevant constant.

We see from Eq. (7.8) that only

$$\epsilon^a_\mu(x) \sim \frac{1}{\sqrt{\beta}}$$
 (7.9)

are essential which justifies the expansion in ϵ . Rescaling the integration variables in Eq. (7.8), we therefore find

$$Z(\beta) \propto \beta^{-(N_l - N_s) d_G/2}.$$
(7.10)

Substituting into Eq. (7.2) and remembering that $(N_l - N_s)/N_p = 2/d$ (see Eq. (6.5)), we obtain Eq. (7.1).

Problem 7.2 Repeat the derivation of the previous Problem for the adjoint action (6.29).

Solution The only difference with respect to the Wilson action (6.16) is that the saddle-point solution (7.3) is now modified as

$$U^{\rm sp}_{\mu}(x) = Z_{\mu}(x), \qquad (7.11)$$

i.e. may take on different values at different links. It is evident that this is a minimum of the action (6.29).

The only modification of Eq. (7.8) is

$$\prod_{\nu=1}^{d} \sum_{n_{\nu}=1}^{N} \implies \prod_{x} \prod_{\nu=1}^{d} \sum_{n_{\nu}(x)=1}^{N}, \qquad (7.12)$$

which only changes an irrelevant overall constant. Therefore, Eq. (7.1) remains unchanged providing the plaquette average is also taken in the adjoint representation. This supports the expectation that the continuum limits for both actions coincide.

The first-order phase transitions of the type given in Fig. 7.1 are usually harmless and are not associated with deconfinement. They are related with dynamics of some lattice degrees of freedom (say, with large fluctuations of the link variable $U_{\mu}(x)$ which occur independently at adjacent links) which do not affect the continuum limit and are called *lattice artifacts*. Moreover, these lattice degrees of freedom become frozen for $\beta > \beta_*$, which is necessary for the continuum limit to exist.

Another possibility for a lattice system is to undergo a second-order phase transition in analogy with spin systems. In this case $W(\partial p)$ is continuous but the derivative $\partial W(\partial p)/\partial \beta$ becomes infinite at the critical point $\beta = \beta_*$ as depicted in Fig. 7.2. Given Eq. (7.2), this derivative is to be considered as an analog of the specific heat of statistical systems. Its behavior at small and large β is governed by Eqs. (6.72) and (7.1), respectively.

Differentiating Eq. (6.65) with respect to β , the derivative $\partial W(\partial p)/\partial \beta$ can be expressed via the sum of the connected correlators:

$$\frac{\partial W(\partial p)}{\partial \beta} = \frac{1}{2} \sum_{\text{orient } p'} \left\langle \frac{1}{N} \operatorname{tr} U(\partial p) \frac{1}{N} \operatorname{tr} U(\partial p') \right\rangle_{\text{conn}}.$$
 (7.13)

This formula also shows that $\partial W(\partial p)/\partial \beta$ is positive definite, since the



Fig. 7.2. Typical β -dependence of $\partial W(\partial p)/\partial \beta$ for a second-order phase transition which occurs at $\beta = \beta_*$.

RHS can be rewritten using translational invariance as

$$\frac{1}{2} \sum_{\text{orient } p'} \left\langle \frac{1}{N} \operatorname{tr} U(\partial p) \frac{1}{N} \operatorname{tr} U(\partial p') \right\rangle_{\text{conn}} \\
= \frac{1}{4N_p} \left\langle \left[\sum_{\text{orient } p} \frac{1}{N} \operatorname{tr} U(\partial p) \right]^2 \right\rangle - \frac{1}{4N_p} \left[\left\langle \sum_{\text{orient } p} \frac{1}{N} \operatorname{tr} U(\partial p) \right\rangle \right]^2 \ge 0, \\$$
(7.14)

where the equality is possible only for a Gaussian averaging, i.e. for a free theory. This repeats the standard proof of the positivity of specific heat in statistical mechanics.

Since each term of the sum in Eq. (7.13) is finite (remember that the trace of a unitary matrix takes on values between -N and N), the only possibility for the RHS to diverge is for the sum over plaquettes p' to diverge. This is possible only when long-range (in the units of the lattice spacing) correlations are essential or, in other words, the correlation length is infinite. Thus, once again we have reproduced the argument that the continuum limit of lattice theories is reached at the points of second-order phase transitions.

Such a second-order phase transition seems to occur in compact QED (i.e. the U(1) lattice gauge theory with fermions) at $e_*^2 \sim 1$. It is associated there with deconfinement of electrons. Electrons are confined for $e^2 > e_*^2$, similarly to quarks in lattice QCD, and are liberated for $e^2 < e_*^2$. The interaction potential looks like that of Fig. 6.9b for $e^2 < e_*^2$ and like that of Fig. 6.9a in the confinement region $e^2 > e_*^2$.* In order to reach the continuum limit with deconfined electrons, the bare charge

^{*} The latter statement is not quite correct for reasons which are discussed in Sect. 9.5.

 e^2 should be chosen to be slightly below the critical value. Then the renormalized physical charge can be made as small as the experimental value ($\alpha \approx 1/137$) according to the renormalization group arguments which are presented in the Remarks in Sect. 6.7.

The nature of the phase transition in a four-dimensional compact U(1) lattice gauge theory without fermions was investigated using numerical methods. While the very first paper [LN80] indicated that the phase transition is of second order, some more advanced later investigations noted [EJN85] that it may be weakly first order. Anyway, we need fermions which usually weaken a phase transition that happens in a pure lattice gauge theory.

There are no indications that a second-order phase transition occurs in non-Abelian pure lattice gauge theories at intermediate values of β . This supports very strongly the behavior of the string tension being of the type depicted in Fig. 6.10. The second-order phase transition occurs in four dimensions at $\beta = \infty$ (or $g^2 = 0$) according to the general arguments of Sect. 6.7, which is necessary for the continuum limit to exist.

Remark on confinement in $4 + \epsilon$ dimensions

In $4+\epsilon$ dimensions ($\epsilon > 0$), a second-order deconfining phase transition always occurs in non-Abelian pure lattice gauge theories at some finite value of $\beta < \infty$ (or $g^2 > 0$). The case of $\epsilon \ll 1$ can be considered to be analogous to the ϵ -expansion in statistical mechanics [WK74]. An ultraviolet-stable fixed point exists at $g_*^2 \sim \epsilon$ since the theory is asymptotically free in d = 4. This phase transition is associated with deconfinement quite analogously to compact QED in d = 4. The deconfining phase is realized when the bare coupling $g < g_*$, while the confining phase is realized when $g > g_*$.

7.2 Mean-field method

The idea of applying the mean-field method, which is widely used in statistical systems, to study phase transitions in the lattice gauge theories was proposed by Wilson [Wil74] and first implemented for Abelian theories by Balian, Drouffe and Itzykson [BDI74]. A mean field usually works well when there are many neighboring degrees of freedom, interacting with a given one.

In the simplest version of the mean-field method, the link variable $U_{\mu}(x)$ is replaced by the mean-field value $m \cdot \mathbb{I}$ everywhere but at a given link (see Fig. 7.3) at which the self-consistency condition

$$\left\langle \left[U_{\mu}(x)\right]^{ij}\right\rangle_{0} = m\,\delta^{ij}$$
(7.15)

is imposed.



Fig. 7.3. Graphical representation of the self-consistency condition (7.17). The link variables are replaced by $m \cdot \mathbb{I}$ at all links except for a given one denoted by the bold line.

The average on the LHS of Eq. (7.15) is calculated with the action which is obtained from (6.16) by the substitution of $m \cdot \mathbb{I}$ for all the link variables (or their Hermitian conjugates) except at the given link. Since the given link enters 2(d-1) plaquettes, the average on the LHS of Eq. (7.15) is to be calculated with the action

$$S_0[U] = 2(d-1)m^3 \operatorname{Re} \operatorname{tr} U_{\mu}(x) + \operatorname{const}.$$
 (7.16)

Therefore, the self-consistency condition (7.15) can be written using the substitution of the mean-field ansatz into the lattice partition function (6.31) as

$$\frac{\int dU e^{\bar{\beta}N \operatorname{Re} \operatorname{tr} U} \frac{1}{N} \operatorname{tr} U}{\int dU e^{\bar{\beta}N \operatorname{Re} \operatorname{tr} U}} = m$$
(7.17)

with

$$\bar{\beta} = 2(d-1)m^3\frac{\beta}{N^2}.$$
 (7.18)

The meaning of Eq. (7.17) is very simple: the average of the normalized trace of the link variable at the given link should coincide with m, which is substituted for all other links of the lattice.

In order to verify whether the self-consistency condition (7.17) admits nontrivial solutions, one should first calculate the group integral on the LHS and then solve the self-consistency equation for m versus β . Typical behavior of the solution is depicted in Fig. 7.4. For all values of β , there exists a trivial solution m = 0 that is associated with no mean field. At



Fig. 7.4. Typical behavior of the mean-field solutions of the self-consistency equation (7.17). The only solution with m = 0 exists for $\beta < \beta_*$. Two more solutions appear for $\beta > \beta_*$. The solution depicted by the dashed line is unstable. The actual value of m versus β is depicted by the bold lines. A first-order phase transition is associated with $\beta = \beta_*$.

some value β_* , two more solutions of the self-consistency equation appear. The upper one is associated with positive specific heat, while the lower one corresponds to negative specific heat. This can be seen by noting that

$$W(\partial p) = m^4 \tag{7.19}$$

in the mean-field approximation which follows from the substitution of the link variables in the definition (6.65) by the mean-field values. This nontrivial solution is preferred for $\beta > \beta_*$, since the partition function for it is larger (or the free energy is smaller) than for the m = 0 solution. The value of β_* is often associated with the point of a first-order phase transition.

The mean-field method in such a simple form was first applied to non-Abelian lattice gauge theories in [GL81, CGL81]. For the cases when a first-order phase transition occurs (say, for the SU(N) groups with N > 3or for the SO(3) group), agreement with numerically calculated positions of the phase transitions is remarkable.

Problem 7.3 Calculate β_* for the $SU(\infty)$ lattice gauge theory, when the group integral on the LHS of Eq. (7.17) equals $\bar{\beta}/2$ for $\bar{\beta} \leq 1$ (a strong-coupling phase) and $1 - 1/2\bar{\beta}$ for $\bar{\beta} \geq 1$ (a weak-coupling phase).

Solution For the strong-coupling phase, the self-consistency equation

$$(d-1)m^3\frac{\beta}{N^2} = m (7.20)$$

has the only solution m = 0. The other solutions are unacceptable owing to the stability criterion.

The nontrivial solutions of the self-consistency equation appear in the weakcoupling phase when $dm/d\beta = \infty$ or $d\beta/dm = 0$. Differentiating, we obtain then in d = 4

$$\frac{\partial \beta^{-1} N^2}{\partial m} = 12 \left(3m^2 - 4m^3 \right) , \qquad (7.21)$$

which yields

$$m_* = \frac{3}{4}, \qquad \frac{\beta_*}{N^2} = \frac{4^3}{3^4} \approx 0.79.$$
 (7.22)

It is still left to verify that the proper $\bar{\beta}$ is indeed associated with the weakcoupling phase. From Eq. (7.18), we find $\bar{\beta}_* = 2$ and this is the case.

How one can calculate the one-matrix integral on the LHS of Eq. (7.17) at large N is explained in Sect. 12.9.

7.3 Mean-field method (variational)

There are some puzzles with the simplest mean-field ansatz described above. First of all, the average value of the link variable $U_{\mu}(x)$ in a lattice gauge theory must vanish owing to the gauge invariance (remember that $U_{\mu}(x)$ changes under the gauge transformation according to Eq. (6.13), while the action and the measure are gauge invariant). This is in accordance with Elitzur's theorem [Eli75], which says that a local gauge symmetry cannot be broken spontaneously, so that any order parameter for phase transitions in lattice gauge theories must be gauge invariant.

A way out of this is to reformulate the mean-field method in lattice gauge theories as a variational method [BDI74] which is similar to that proposed by R. Peierls in the 1930s. It is based on Jensen's inequality^{*}

$$\langle e^F \rangle_0 \ge e^{\langle F \rangle_0}$$
 (7.23)

which arises from the convexity of the exponential function, where $\langle \cdots \rangle_0$ denotes averaging with respect to a trial action.

Let us choose the trial partition function

$$Z_0 = \int \prod_{x,\mu} \mathrm{d}U_{\mu}(x) \,\mathrm{e}^{\bar{\beta}N\sum_{x,\mu} \operatorname{Retr} U_{\mu}(x)}$$
(7.24)

as a product of one-link integrals. Adding and subtracting the trial action, we write down the following bound on the partition function (6.31):

$$Z \geq Z_0 \exp\left\langle \frac{\beta}{N} \sum_p \operatorname{Re} \operatorname{tr} U(\partial p) - \bar{\beta} N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} U_{\mu}(x) \right\rangle_0, \qquad (7.25)$$

* More detail can be found, for example, in the books [Fey72, Sak85].

where $\langle \cdots \rangle_0$ denotes averaging with respect to the same action as in Eq. (7.24).

Since the expression that is averaged in the exponent in Eq. (7.25) is linear in each of the link variables, it can be calculated via the one-matrix integral given by the LHS of Eq. (7.17). Therefore, we find

$$\left\langle \frac{\beta}{N} \sum_{p} \operatorname{Re} \operatorname{tr} U(\partial p) - \bar{\beta} N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} U_{\mu}(x) \right\rangle_{0} = \beta N_{p} m^{4} - \bar{\beta} N^{2} N_{l} m,$$
(7.26)

where Eq. (7.19) has been used.

The idea of the variational mean-field method is to fix $\bar{\beta}$ from the condition for the trial ansatz (7.24) to give the best approximation to Z in the given class. Calculating the derivative of the RHS of Eq. (7.25) with respect to $\bar{\beta}$ and taking into account the fact that m depends on $\bar{\beta}$ according to Eq. (7.17), we find the maximum at $\bar{\beta}$ given by Eq. (7.18), which reproduces the simplest version of the mean-field method described above.

To restore Elitzur's theorem, a more sophisticated trial ansatz [Dro81] can be considered:

$$Z_0 = \int \prod_{x,\mu} dU_{\mu}(x) e^{N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} B^{\dagger}_{\mu}(x) U_{\mu}(x)}, \qquad (7.27)$$

where we choose $B_{\mu}(x)$ to be an arbitrary complex $N \times N$ matrix. Now the best approximation is reached for

$$B_{\mu}(x) = \bar{\beta} \Omega(x) \Omega^{\dagger}(x + a\hat{\mu}), \qquad (7.28)$$

where $\bar{\beta}$ is given by exactly the same equation as before, while $\Omega(x) \in SU(N)$ but is arbitrary otherwise. Now $\langle U^{ij}_{\mu}(x) \rangle_0$ vanishes after summing over equivalent maxima which results in integrations over $d\Omega(x)$.

Problem 7.4 Perform the variational mean-field calculation with the ansatz (7.27).

Solution Let us denote

$$M_{\mu}^{ij}(x) = \frac{\int \prod_{x,\mu} dU_{\mu}(x) e^{N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} B_{\mu}^{\dagger}(x) U_{\mu}(x)} U_{\mu}^{ij}(x)}{\int \prod_{x,\mu} dU_{\mu}(x) e^{N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} B_{\mu}^{\dagger}(x) U_{\mu}(x)}}.$$
 (7.29)

Then the analog of Eq. (7.26) is

$$\left\langle \frac{\beta}{N} \sum_{p} \operatorname{Re} \operatorname{tr} U(\partial p) - N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} B^{\dagger}_{\mu}(x) U_{\mu}(x) \right\rangle_{0}$$
$$= \frac{\beta}{N} \sum_{p} \operatorname{Re} \operatorname{tr} M(\partial p) - N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} B^{\dagger}_{\mu}(x) M_{\mu}(x)$$
(7.30)

so that the inequality (7.25) takes the form

$$Z \geq Z_0 \exp\left[\frac{\beta}{N} \sum_{p} \operatorname{Re} \operatorname{tr} M(\partial p) - N \sum_{x,\mu} \operatorname{Re} \operatorname{tr} B^{\dagger}_{\mu}(x) M_{\mu}(x)\right].$$
(7.31)

 $B_{\mu}(x)$ can now be determined by maximizing with respect to $B_{\mu}(x)$ and taking into account Eq. (7.29).

It is easy to see that if $B_{\mu}(x) = \overline{\beta} \cdot \mathbb{I}$ is a solution as before, then (7.28) is also a solution. Therefore, we find

$$\left\langle U^{ij}_{\mu}(x) \right\rangle_{0} = m \int \mathrm{d}\Omega(x+a\hat{\mu}) \,\mathrm{d}\Omega(x) \,\Omega(x+a\hat{\mu}) \,\Omega^{\dagger}(x) = 0 \,, \qquad (7.32)$$

where the integration over Ω takes into account different equivalent maxima. Thus, all gauge-invariant quantities for the ansatz (7.27) are the same as for the ansatz (7.24), while gauge-noninvariant quantities now vanish in agreement with Elitzur's theorem.

Remark on the criterion for phase transition

Another puzzle with the simplest mean-field method is why the point of the first-order phase transition is chosen as explained in Fig. 7.4 but not when the free energy of both phases coincide (the standard Maxwell rule in statistical physics). Perhaps, the criterion of Fig. 7.4 should be chosen if a barrier between two phases is impenetrable, which happens at large N or if quantum fluctuations are not taken into account such as for the simplest mean field. The mean-field calculations of [FLZ82], which take into account fluctuations around the mean-field solution (7.28), agree for the Maxwell-rule criterion with numerical data. These results are reviewed in [DZ83].

7.4 Lattice renormalization group

While the mean-field method is useful for studying the first-order phase transitions, the second-order phase transitions in lattice statistical systems are better described by the renormalization group method (see, for example, the review by Wilson and Kogut [WK74]). The idea of applying a similar method to lattice gauge theories is due to Migdal [Mig75].

A simple renormalization group transformation in lattice gauge theories is associated with doubling of the lattice spacing a. Originally one has a lattice as depicted in Fig. 7.5a. The lattice renormalization group (r.g.) transformation consists in integrating over the link variables $U_{\mu}(x)$ on the links shown by the thin lines which results in a lattice with spacing 2a,

$$a \stackrel{\text{r.g.}}{\Longrightarrow} 2a$$
, (7.33)



Fig. 7.5. Lattice renormalization group transformation (7.33). The thin lines of the old lattice (a) represent links on which integration is performed. The new lattice (b) has a lattice spacing of 2a but the same spatial extent La.

which is depicted in Fig. 7.5b. The space size of the lattice is L before the transformation and becomes L/2 after the transformation,

$$L \stackrel{\text{r.g.}}{\Longrightarrow} \frac{L}{2},$$
 (7.34)

so that the lattice extent is $L \cdot a$ in both cases, which is expected to reduce the influence of finite-size effects on the transformation.

The Wilson action on the lattice of Fig. 7.5a becomes a more general one under the renormalization group transformation:

$$S[U] = \sum_{p} \beta \frac{1}{N} \operatorname{tr} U(\partial p)$$

$$\stackrel{\text{r.g.}}{\Longrightarrow} S'[U] = \sum_{p} \beta'_{1} \frac{1}{N} \operatorname{tr} U(\partial p) + \sum_{p_{2}} \beta'_{2} \frac{1}{N} \operatorname{tr} U(\partial p_{2})$$

$$+ \sum_{p_{3}} \beta'_{3} \frac{1}{N} \operatorname{tr} U(\partial p_{3}) + \cdots .$$
(7.35)

The new action S'[U] is not necessarily a single-plaquette action and can involve traces of the Wilson loops for boundaries of double plaquettes, triple plaquettes and so on.

The new action would be the same as the old one only at a fixed point. This usually happens after the renormalization group transformation is applied several times when the lattice theory does have a fixed point. The resulting action is then associated with an action of the continuum theory.

The great success of non-Abelian lattice gauge theories with the Wilson action in describing the continuum limit even at a relatively small spatial extent or, which is the same, at relatively large g^2 and a, is because it is not far away from the fixed-point action of the renormalization group. The proper numerical results will be presented in a moment (Fig. 7.6).

If both actions S[U] and S'[U] are the single-plaquette Wilson actions, then

$$\beta \stackrel{\text{r.g.}}{\Longrightarrow} \beta' = \beta - \Delta\beta \tag{7.36}$$

under the renormalization group transformation on the lattice.

Since the Gell-Mann–Low function $\mathcal{B}(g^2)$ in the continuum is known, $\Delta\beta$ versus β is determined by the equation

$$\int_{\beta-\Delta\beta}^{\beta} \frac{\mathrm{d}x}{x^2 \mathcal{B}(3/x)} = -\frac{\ln 2}{3}.$$
(7.37)

Here ln 2 on the RHS arises from Eq. (7.33) and the relation (6.32) between β and g^2 is used with N = 3.

For the pure SU(3) gauge theory, we obtain from Eq. (7.37)

$$\Delta\beta = 0.579 + \frac{0.204}{\beta} + \mathcal{O}(\beta^{-2})$$
(7.38)

at asymptotically large β .

One can integrate over the thin links in Fig. 7.5a either approximately or numerically. The following procedure for an approximate integration is known as the Migdal–Kadanoff recursion relations.

Let us expand the exponential of the old action in the characters

$$e^{-S[U]} = \sum_{r} f_r d_r \chi_r(U),$$
 (7.39)

where

$$d_r = \chi_r(\mathbb{I}) \tag{7.40}$$

is the dimension of a given representation r and f_r are the coefficients which depend on the form of S[U].

Migdal [Mig75] proposed to approximate the new action, which appears after

$$a \implies \rho a$$
, (7.41)

by the formula

$$e^{-S'[U']} = \left[\sum_{r} (f_r)^{\rho^2} d_r \chi_r(U')\right]^{\rho^{d-2}},$$
 (7.42)



Fig. 7.6. Monte Carlo data from Akemi *et al.* [Ake93] for $\Delta\beta$. The error bars represent statistical errors. The solid line represents the asymptote (7.38).

which is exact in d = 2 dimensions. Kadanoff [Kad76] modified slightly the recursion relation (7.42).

The study of the Migdal-Kadanoff recursion relations was historically the first argument that second-order phase transitions do not occur in the non-Abelian lattice gauge theory when g^2 is decreased. Moreover, these relations in d = 4 are the same as for spin systems (with the same symmetry group) in d = 2 where this phenomenon is known. A disadvantage of the method is that it is difficult to estimate its accuracy.

A final answer to the question of whether or not a second-order phase transition occurs in the non-Abelian lattice gauge theory was given by the numerical integration. This is known as the Wilson Monte Carlo renormalization group. Some typical results [Ake93] for $\Delta\beta$, which is defined by Eq. (7.36), versus β are depicted in Fig. 7.6. The solid line represents the asymptote (7.38). The agreement confirms that the continuum limit is reached already at these values of β , while the deviation of the Monte Carlo data from the asymptotic behavior for smaller values of β is owing to lattice nonperturbative effects.

7.5 Monte Carlo method

The idea of the Monte Carlo method is to calculate the partition function (6.31) and the averages (6.39) for arbitrary values of β numerically, using the fact that the multiplicity of the integral is large. For an $L \times L \times L \times L$ lattice in 4 dimensions, a typical multiplicity of the integral is as large as $4 \cdot (N^2 - 1) \cdot L^4$ (~ 10⁷ for L = 24). It is hopeless to calculate such an integral exactly. In contrast, the larger the multiplicity the better the Monte Carlo method works. As usual, the Monte Carlo method is applied not to sequential integrals over $U_{\mu}(x)$ at each link but rather to the multiple integral as a whole, which can be viewed as the sum over states of a statistical system.

A state is identified with a gauge field configuration which is described by the values of the link variables at all the links of the lattice:

$$C = \{ U^{ij}_{\mu}(x), \dots, \dots, \dots, \dots, \dots, \dots, \dots, \dots \}.$$
 (7.43)

There are as many positions in this row as the multiplicity of the integral.

Then the sequential integral can be represented as

$$\int \prod_{x,\mu} \mathrm{d}U_{\mu}(x) \cdots = \sum_{C} \cdots .$$
 (7.44)

The averages (6.39) can be rewritten as

$$\langle F(C) \rangle = \frac{\sum_{C} e^{-\beta S(C)} F(C)}{\sum_{C} e^{-\beta S(C)}},$$
(7.45)

where S(C) and F(C) are the values of S and F for the given configuration C.

The task of Monte Carlo calculations is not to sum over all possible configurations, the number of which is infinite, but rather to construct an ensemble, say, of n configurations

$$E = \{C_1, \dots, C_n\}$$
(7.46)

such that a given configuration C_k is encountered with the Boltzmann probability

$$P_{\text{Bol}}(C_k) = Z^{-1}(\beta) e^{-\beta S(C_k)}.$$
 (7.47)

Such a sample of configurations is called the *equilibrium ensemble*.

Given an equilibrium ensemble, the averages (7.45) take the form of the arithmetic mean

$$\langle F[U] \rangle = \frac{1}{n} \sum_{k=1}^{n} F(C_k)$$
 (7.48)

because each configuration "weights" already as much as is required. In particular, the Wilson loop average for a rectangular contour is given by

$$W(R \times \mathcal{T}) = \frac{1}{n} \sum_{k=1}^{n} \frac{1}{N} \operatorname{tr} U(R \times \mathcal{T}; C_k).$$
 (7.49)

If all configurations in the equilibrium ensemble are independent, then the RHS of Eq. (7.49) will approximate the exact value of $W(R \times \mathcal{T})$ with an accuracy of $\sim \sqrt{n}$.

The analogy between this method of calculating averages and statistical physics is obvious. The equilibrium ensemble simulates actual states of a statistical system, while the index k describes the time evolution.

A crucial point in the Monte Carlo method is to construct the equilibrium ensemble. It is not simple to do that because the Boltzmann probability is not known at the outset. A way around this problem is to establish a random process for which each new configuration in the sequence (7.46) is obtained from the previous one by a definite algorithm but stochastically. In other words, the random process is completely determined by the probability $P(C_{k-1} \to C_k)$ for a transition from a state C_{k-1} to a state C_k and does not depend on the history of the system, i.e.

$$P(C_{k-1} \to C_k) = P(C_{k-1}, C_k).$$
 (7.50)

Such a random process is known as the *Markov process*.

The transition probability P(C, C') should be chosen in such a way as to provide the Boltzmann distribution (7.47). This is ensured if P(C, C')satisfies the detailed balance condition

$$e^{-\beta S(C)} P(C, C') = e^{-\beta S(C')} P(C', C).$$
 (7.51)

Then

- (1) an equilibrium sequence of states will transform into another equilibrium sequence,
- (2) a nonequilibrium sequence will approach an equilibrium one when moving through the Markov chain.

Problem 7.5 Prove statements (1) and (2) listed in the previous paragraph using the detailed balance condition (7.51).

Solution Let a state C be encountered in ensembles E and E' with probability densities P(C) and P'(C), respectively. Then the distance between the two ensembles can be defined as

$$||E - E'|| = \sum_{C} |P(C) - P'(C)|.$$
 (7.52)

For a Markov process when Eq. (7.50) holds, we have

$$P'(C) = \sum_{C'} P(C, C') P(C')$$
(7.53)

if E' is obtained from E by a Monte Carlo algorithm. The transition probability

P(C, C') is nonnegative and obeys

$$\sum_{C} P(C, C') = \sum_{C'} P(C, C') = 1$$
(7.54)

since each new state is obtained from an old one and vice versa.

It is now easy to prove statement (1). Summing the detailed balance condition (7.51) over C', we obtain

$$P_{\rm Bol}(C) = \sum_{C'} P(C, C') P_{\rm Bol}(C'), \qquad (7.55)$$

i.e. the Boltzmann distribution is an eigenvector of P(C, C'). Comparing with Eq. (7.53), we see that the new distribution is again the Boltzmann one, which proves statement (1).

To prove statement (2), let us compare the distances from E and E' to some equilibrium ensemble E_{Bol} associated with the Boltzmann distribution (7.47). We have the inequality

$$\begin{aligned} \left\| E' - E_{Bol} \right\| &= \sum_{C} \left| P'(C) - P_{Bol}(C) \right| \\ &= \sum_{C} \left| \sum_{C'} P(C, C') \left[P(C') - P_{Bol}(C') \right] \right| \\ &\leq \sum_{CC'} P(C, C') \left| P(C') - P_{Bol}(C') \right| \\ &= \sum_{C'} \left| P(C') - P_{Bol}(C') \right| \\ &= \left\| E - E_{Bol} \right\|, \end{aligned}$$
(7.56)

where Eqs. (7.53), (7.55) and (7.54) are used. Thus, statement (2) is proven.

Specific Monte Carlo algorithms differ in the choice of the transition probability P(C, C'), while the detailed balance condition (7.51) is always satisfied. The two most popular algorithms, which act at one link, are as follows.

Heat bath algorithm

A new link variable $U'_{\mu}(x)$ is selected randomly from the group manifold with a probability given by the Boltzmann factor

$$P(U'_{\mu}(x)) \propto e^{-\beta S(C')}.$$
 (7.57)

Then this procedure is repeated for the next link and so on until the whole lattice is passed. This can be imagined as if a reservoir at temperature $1/\beta$ touches each link of the lattice in succession. It is clear from physical intuition that the system will be brought to thermodynamic equilibrium sooner or later.

Metropolis algorithm

This algorithm is used in statistical physics since the 1950s and consists of several steps.

- (1) A trial new link variable $U'_{\mu}(x)$ is selected (suppose randomly on the group manifold).
- (2) The difference between the action for this trial configuration and that for the old one is calculated:

$$\Delta S = S(C') - S(C). \qquad (7.58)$$

- (3) A random number $r \in [0, 1]$ is generated.
- (4) If

$$e^{-\beta\Delta S} > r, \qquad (7.59)$$

then $U'_{\mu}(x)$ is accepted. Otherwise, $U'_{\mu}(x)$ is rejected and the old value $U_{\mu}(x)$ is kept.

(5) All of this is repeated for the next links.

An advantage of the Metropolis algorithm is that it is usually more easy implemented in practical calculations.

A new configuration C', which is obtained by applying once either Monte Carlo algorithm to each link of the lattice (this procedure is often called the Monte Carlo sweep), will be strongly correlated with the old one, C. This is because the lattice action depends not only on the variable at the given link but also on those at the neighboring links which form plaquettes with the given one. In order for C' to become independent of C, this procedure should be repeated many times or special tricks should be used to reduce the correlations. Then this new configuration can be added to the equilibrium ensemble (7.46) as C_k .

More details concerning the Monte Carlo algorithms as well as their practical implementation in lattice gauge theories can be found in the review [CJR83] and the books [Cre83, MM94].

7.6 Some Monte Carlo results

The first Monte Carlo calculation in non-Abelian lattice gauge theories, which is relevant for the continuum limit, was performed by Creutz [Cre79] who evaluated the string tension for the SU(2) gauge group. His result is reproduced in Fig. 7.7 and looks very much like what is expected in Fig. 6.10 on p. 120. This calculation was the first demonstration that the continuum limit sets in for relatively large $g^2 \approx 0.91$



Fig. 7.7. Monte Carlo data from Creutz [Cre79] for the string tension in the SU(2) pure lattice gauge theory.

 $(\beta \approx 2.2)$ and that results for the continuum can therefore be extracted from relatively small lattices.

The restoration of rotational symmetry for these values of g^2 was demonstrated explicitly by Land and Rebbi [LR82]. They calculated equipotential surfaces for the interaction between static quarks. In the strong-coupling region $g^2 \to \infty$, they appear as in Fig. 7.8a since the interaction potential is given by

$$E(x, y, z) = K(|x| + |y| + |z|)$$
(7.60)

because the distance between the quarks is measured along the lattice. This is associated with the cubic symmetry on the lattice (i.e. rotations through an angle which is a multiple of $\pi/2$ around each axis and translations by a multiple of the lattice spacing along each axis) rather than with the Poincaré group. The rotational symmetry must be restored in the continuum limit.

The Monte Carlo data of Land and Rebbi [LR82] are shown in Figs. 7.8b and c. They demonstrate the restoration of rotational symmetry when passing from $\beta = 2$ (Fig. 7.8b) to $\beta = 2.25$ (Fig. 7.8c).

The early Monte Carlo calculations played a very important role in the development of the method. Their main result is that the Monte Carlo



Fig. 7.8. Behavior of equipotential lines at different values of β : (a) the strongcoupling limit $\beta = 0$; (b) $\beta = 2$; (c) $\beta = 2.25$. (b) and (c), taken from the paper by Lang and Rebbi [LR82], show how the rotational symmetry is restored as β is increased.

calculation of physical quantities in QCD is possible on relatively small lattices.

A dramatic improvement of the Monte Carlo technology in lattice gauge theories has taken place over the last 20 years. New calculations are performed on larger lattices and with better statistics. The best way to follow current developments of the subject is via plenary talks published in the proceedings of the annual Lattice Conference (currently [Lat00]).