High-order effects in action-variational approaches to lattice gauge theory

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A recently developed action-variational approach so far has been applied to various cases up to fourth order. To obtain more reliable information about the underlying mechanisms and to check if the accuracy of high-statistics Monte Carlo simulations can be reached computations up to the next even order turn out to be necessary. This was prevented up to now by the occurrence of huge combinatorial factors. In the present work we develop means to circumvent this obstacle. In addition, the case of finite temperatures is also considered. Our results allow us to establish the general features of the approach in detail and to predict the behavior of still higher orders. With respect to practical applications it turns out that the sixth order gives worse results than the fourth order, or, more generally, that there is no longer an improvement beyond the fourth order. This behavior appears to be related to the asymptotic nature of the expansion and to the conversion into powers of $1/\beta$ needed. Ultimately it reflects limitations in the possibilities of compensating the action by the trial action.

I. INTRODUCTION

Action-variational approaches to lattice gauge theory are an analytical alternative to Monte Carlo simulations. They work particularly well in the weak-coupling region and thus are of interest for circumventing the critical slowing down of simulations. Since these approaches started with mean-field methods [1,2] there have been a number of developments. Recently the accumulation-point approach has been introduced [3–5] which turns out to allow accurate higher-order calculations. It has been applied [3–5] to the gauge groups U(1), SU(2), and SU(3) and the inclusion of fermions has been studied [6] in the case of U(1).

Results with the accumulation-point approach so far have been obtained up to the fourth order (on the weak-coupling side). At this order one reaches the accuracy of simulations of moderate statistics. Certain systematic features allow some improvement of the accuracy. The important question which arises at this point is if at still higher order one can really compete with the accuracy of high-statistics simulations. A further question is if the systematic features can be established in a more general and precise way. Because at present there are no analytical or rigorous tools to deal with this question one has to rely on numerical investigations also for this purpose.

The computational effort when going to the next order increases considerably for two reasons. One is the magnitude of the combinatorial factors related to the huge number of terms which occur at higher order in the cumulant expansion of the correlation function. The other one is the large number of combinations then arising in the evaluation of SU(N) traces. This means that to be able to get beyond the fourth order new methods have to be developed within these two respects.

In addition to the applications considered so far [3–6] it is desirable to study the case of finite temperatures, too. Since the accumulation-point method appears well suited for weak coupling it offers an interesting alternative to perturbative calculations of thermodynamic quantities which suffer from infrared problems [7–9].

In the present paper the accumulation-point approach is extended to the sixth order. For this purpose methods are developed which can handle the huge numbers of terms in the expansion and of combinations in the trace evaluations. Calculations for SU(2) are carried out which show the numerical limits of the method. The higher orders obtained allow to work out the general features of the individual orders and to discuss some important theoretical aspects of the method. Furthermore, the results at finite temperature are used to discuss the situation also in this case.

In Sec. II the basis and the general details of the approach are pointed out. In Sec. III the methods of calculation and the improvements allowing to reach higher orders are explained. In Sec. IV the numerical results, their implications, and the theoretical aspects involved are discussed. Section V is devoted to the case of finite temperatures. In Sec. VI some main conclusions are collected.

II. BASIC FEATURES OF APPROACH

Correlation functions $\langle \cdots \rangle$ with respect to the action S can be expressed by correlation functions $\langle \cdots \rangle_0$ with respect to a trial action S_0 by the identity

$$\langle X \rangle = \frac{\langle e^{S-S_0} X \rangle_0}{\langle e^{S-S_0} \rangle_0} . \tag{2.1}$$

After expanding the exponentials, division in (2.1) leads to the cumulant expansion of correlation functions

$$\langle X \rangle = \sum_{\nu=0}^{\infty} \frac{1}{\nu!} \langle (S-S_0)^\nu X \rangle_0^c , \tag{2.2}$$

where $\langle \cdots \rangle_0^c$ are connected functions which have the general form

$$\langle X_1 X_2 \cdots X_n \rangle^c = \sum_{\text{partitions}} (-1)^{k-1}(k-1)! \underbrace{\langle X_1 \cdots X_r \rangle \cdots \langle X_s \cdots X_n \rangle}_{k \text{ factors}} . \tag{2.3}$$

Clearly neither (2.1) nor (2.2) depends on S_0. The series (2.2) is a formal one which is to be given sense by a suitable choice of S_0. The finite approximations of (2.2) (with summation only up to some finite order) then do depend on the particular choice of S_0 and it is crucial for the approach to choose an optimal S_0.

It turns out that there are two useful choices depending on the coupling in S. At strong coupling this is $S_0 \equiv 0$ by which (2.2) becomes a particular form of strong-coupling expansion for which it is easy to reach relatively high orders [4]. At weak coupling this is a trial action which is a sum of one-link terms and the parameter of which is fixed in the region of the mean-field estimate as is to be discussed in more detail later. In the crossover region the expansion breaks down. At the weak-coupling side this breakdown occurs at the coupling value of a possible phase transition [4]. In the present paper the investigation concentrates on the weak-coupling region.

The choice of the trial action to be a sum of one-link terms leads to factorization of $\langle \cdots \rangle_0$ in one-link contributions which can be evaluated. In the present paper we illustrate the details for the gauge group SU(2) with action

$$S = \frac{\beta}{2} \sum_p \mathrm{tr} U_p \tag{2.4}$$

and trial action

$$S_0 = \sum_l \mathrm{tr}(\tilde{J} U_l + J U_l^\dagger) , \tag{2.5}$$

where p runs over plaquettes and l over links. Completely analogous expressions and conditions as discussed here arise for the other gauge groups [3,5].

The trial action actually depends only on one parameter α because one can put $J = \tilde{J} = (\alpha/2)\mathbb{1}$ without restricting generality [4] for SU(2) and gets analogous relations for other groups [5] by requiring the same basic properties for S_0 as for S. The α dependence of the one-link contributions for SU(2) is expressed by the functions

$$V_r(\alpha) = I_{1+r}(2\alpha)/I_1(2\alpha) , \tag{2.6}$$

where the I_r are modified Bessel functions.

For the evaluation of (2.2) a crucial property is that the mathematical description by connected functions implies that only terms of S and S_0 geometrically connected to X (also via other terms from S) can contribute. This is the basis of our computations which enumerate the possible sets of configurations each of which can be characterized by a set of integers.

In this context a simple picture of the mean-field estimate arises which is illustrated in Fig. 1 and refers to an approximation of the contribution from $S - S_0$ attached to some link (from X or from another term of S). The factor related to the attached link is the same for the plaquette from S and for the link from S_0. For S there are $2(d-1)$ directions of plaquettes and a factor $V_1^3(\alpha)$ for the three free links of an attached plaquette. Thus the compensation of terms illustrated in Fig. 1 requires

$$\frac{\beta}{2} 2(d-1) V_1^3(\alpha) = \alpha , \tag{2.7}$$

which is the mean-field estimate for fixing the parameter α [applying to all orders in (2.2) and all terms in (2.3)]. Clearly there must be deviations from this estimate because plaquettes can be attached with more than one link, more than two objects can meet at a link and there are forbidden directions for plaquettes to avoid double counting.

From our investigations up to the fourth order, with prescriptions essentially requiring fastest convergence of the expansion, we find optimal α values in the vicinity of the mean-field estimate, however, with a definite and systematic deviation from it. We describe this by a quantity Δ, which for SU(2) is defined by

$$\Delta = \frac{\alpha}{V_1^3} \frac{2}{\beta} - 2(d-1) . \tag{2.8}$$

Our observation is that Δ is largely independent of gauge group, dimension d, and coupling β. The value of Δ depends on the geometry of X in (2.2), for example, being about two in the case of a plaquette, smaller for larger planar loops [3–5], and larger for twisted loops [6].

In view of the substantial deviations from the mean-field estimate which occur in part of the contributions, the universal character of Δ is remarkable. It appears to result from some "collective" phenomenon. There is, however, presently no way to get hold of such features analytically. Similarly, because of the nonpositive-definite nature of the cumulant expansion the usual rigorous methods fail. Therefore, sufficiently high orders are needed in the computations to be able to extract systematic features from the numerical results.

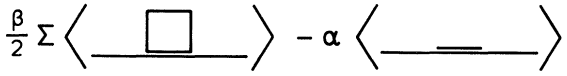

FIG. 1. Illustration of mean-field estimate.

III. METHODS OF CALCULATION

For the evaluation it is observed that (2.2) with (2.3) gets the form

$$\langle X \rangle = \sum_{\nu=0}^{\infty} \sum_{\mu=0}^{\nu} \frac{1}{(\nu-\mu)!} \frac{1}{\mu!} (\beta/2)^{\nu-\mu} (-\alpha)^\mu F_{\nu-\mu,\mu} , \tag{3.1}$$

where the $F_{\rho\mu}$ are weighted sums of monomials of the $V_r(\alpha)$ in (2.6), which means that one has

$$F_{\rho\mu} = \sum_j C_{\rho\mu j} V_1^{E_{\rho\mu j 1}} \cdots V_m^{E_{\rho\mu j m}} \tag{3.2}$$

where j numbers different configurations.

This form allows us to divide the calculations into two major parts. The first one of these is computationally very expensive. It concerns finding the weights and the exponents of the monomials which are integer constants determined by the possible geometric configurations of plaquettes (from S) and links (from S_0). The second part needs only modest computational effort. It consists of evaluating (3.1) up to some finite order using the integer constants from the first part and thus introduces the β and α dependences.

To get beyond the fourth order we have subdivided the mentioned computationally expensive part in several steps and have developed more effective methods within these steps. In this way the evaluation in terms of monomial exponents of about 10^{10} configurations occurring in the sixth order (which is not possible directly) has been reduced to that of less than 2×10^4 configurations. In addition the speed of the individual evaluations has been considerably increased.

The first step consists of attaching plaquettes (from S^ν) to X and finding the weights of the equivalence classes which occur. The crucial point here is that one can make use of the fact that each plaquette position is specified by an unique number in the algorithm. Therefore individual classes can be characterized by the plaquette numbers of one of its members. In this way one can avoid immediate evaluation in terms of monomial exponents which would be prohibitive at higher order.

The second step consists in attaching links (from S_0^μ) to the plaquette configurations (using one member of each equivalence class only) and finding the weights of the equivalence classes in this case, again using characterization by the corresponding numbers in the algorithm.

In the third step, collecting appropriate contributions from the first and second steps as needed according to (2.2) with (2.3) for a particular $F_{\rho\mu}$ in (3.1), one finds the weights and exponents of the monomials in (3.2) from the numbers specifying the configurations in the algorithm and the weights of the particular equivalence classes (needing only one member of each class which makes the procedure work at higher order).

The third step in the non-Abelian case also includes the trace evaluations. For this purpose, instead of relying on the usual generating of functions from the one-link integral, we here exploit the fact that the one-link correlation functions are related to direct tensor products and thus get the form [10]

$$\langle U_{ij}\cdots U_{km}\rangle_{0L}=\sum_r (Y_r)_j^{i\cdots k}{}_m V_r\ , \tag{3.3}$$

where the Y_r are the operators corresponding to the possible Young patterns and the V_r coefficients of the character expansion of $\exp[(\alpha/2)\mathrm{tr}(U+U^\dagger)]$ which for SU(2) are given by (2.6).

If factors $U^\dagger$ appear in the one-link correlation functions for SU(N) the relation

$$U_{ji}^\dagger=\frac{1}{(N-1)!}\epsilon^{ii_1\cdots i_{N-1}}_{jj_1\cdots j_{N-1}}U_{i_1j_1}\cdots U_{i_{N-1}j_{N-1}} \tag{3.4}$$

can be inserted, which for SU(2) is simply $U_{ji}^\dagger=\epsilon_{js}^{ir}U_{rs}$.

On the basis of (3.3) systematic and effective trace evaluations become possible also at high orders. In practice this is achieved by replacing the matrix multiplications by fast integer algorithms which involve the numbering of links in the occurring loops and which incorporate the general rules which hold for the Y_r. In particular, the properties of the Y_r of being projectors and orthogonal to each other lead to a major speedup. Furthermore, a number of rules derived from representation properties of the permutation group have been implemented to handle the joining of one-link correlation functions with different numbers of U matrices (and thus related to permutation groups of different order).

IV. RESULTS AND THEIR IMPLICATIONS

To investigate systematic features of the approach computations up to the sixth order have been done for the case of SU(2), $d=4$, and with X representing a plaquette. Figure 2 shows the typical behavior of the nth-order approximations W_n to (2.2) as functions of α compared with the Monte Carlo result [11]. This behavior is found throughout the weak-coupling region (with the oscillations at small α increasing in magnitude with β) as has been checked up to $\beta=14$. The arrows in Fig. 2 indicate the α value corresponding to the mean-field estimate where $\Delta=0$ and the α value corresponding to the characteristic deviation $\Delta=2$ found in our former investigations [4,5], respectively. It is obvious that in the vicinity of $\Delta=2$ optimal convergence occurs while the choices of α values in other regions do not make sense.

The typical accumulation in the vicinity of $\Delta=2$ is shown in more detail in Fig. 3, now considering the W_n as functions of Δ as defined by (2.8). Because of its universal character Δ is a more appropriate variable for studying finer details.

From Figs. 2 and 3 it is apparent that the conventional mean-field method, which amounts to using the first-order approximation W_1 at $\Delta=0$, suffers from three drawbacks: (1) the first order is not sufficient to come reasonably close to the actual value; (2) odd orders are worse in general; (3) $\Delta=0$ is not optimal.

From Fig. 3 it is seen that the series of even orders of

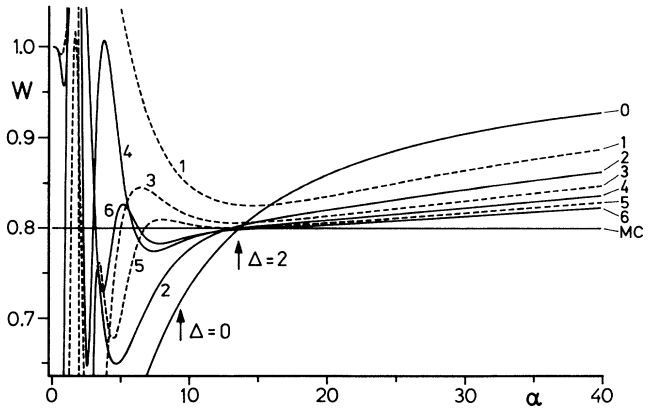

FIG. 2. Typical behavior of W_0 to W_6 as functions of α and Monte Carlo value (shown at $\beta=4$).

the W_n shows faster convergence in the region of interest. This phenomenon has been found [3,4] already up to the fourth order to appear independently of gauge group and dimension for all Wilson loops above some β, which for the plaquette is close to the crossover region. Thus, in the present investigation it appears over the whole range considered.

The origin of the indicated behavior of even orders can be inferred from Fig. 4 which shows the dependences on Δ of the contributions

$$u_\nu = \frac{1}{\nu!}\langle (S-S_0)^\nu X\rangle_0^c \tag{4.1}$$

to (2.2) for $\nu>0$ (in which case they do depend on $S-S_0$). It is seen that in the region of interest only the u_ν with odd ν change sign and thus are essentially responsible for the accumulation structure. In addition, it becomes obvious that u_1 and u_2, u_3 and u_4, u_5 and u_6 below the zeros largely compensate each other, respectively. Thus it is advantageous to consider the combinations u_1+u_2, u_3+u_4, u_5+u_6 which are much smaller there and which also change sign. This shows how the even-order phenomenon arises.

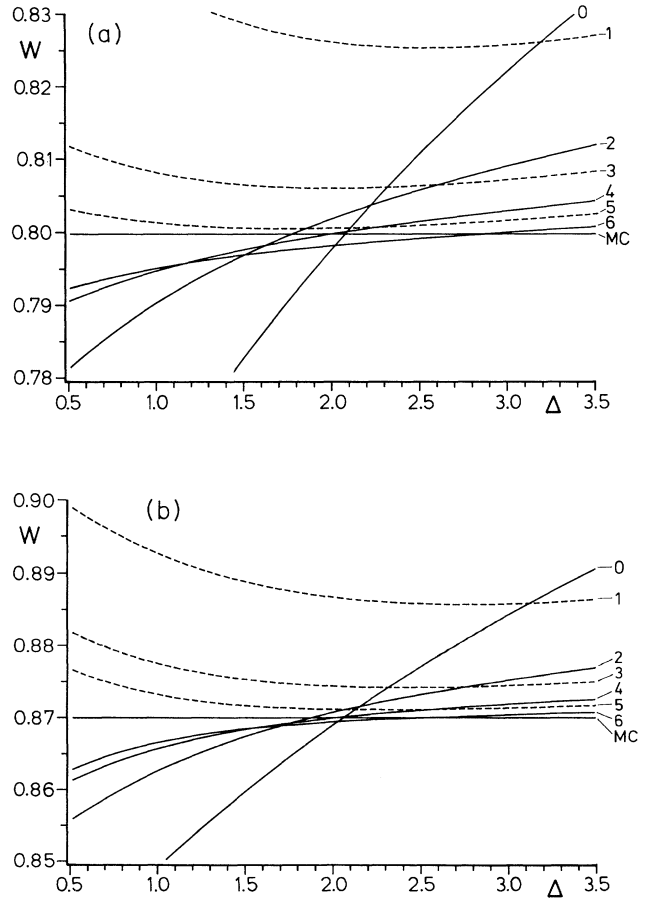

FIG. 3. Typical behavior of W_0 to W_6 as functions of Δ and Monte Carlo value in the vicinity of the mean-field estimate, shown at (a) $\beta=4$ and (b) $\beta=6$.

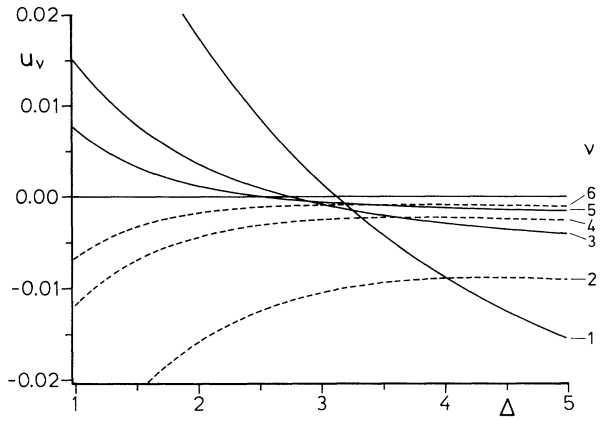

FIG. 4. Dependences of the contributions u_ν on Δ (shown for $\beta=6$).

The mean-field estimate (2.7) resulted from a simple picture of the compensation of S by S_0 relying on the vanishing of an idealized correlation function containing the difference $S-S_0$. Figures 2–4 illustrate the more sophisticated rules which are found in reality. As already pointed out, the vanishing does not occur at $\Delta=0$ but near $\Delta=2$. A further difficulty from the mean-field view is that the zeros of the contributions depending on $S-S_0$ change their position slightly from order to order (which stems from the complicated entering of $S-S_0$ as well as from the overall S_0 dependence of any correlation function $\langle\cdots\rangle_0$). Thus, one is lead to consider the more general criterion of the fastest convergence of subsequent orders (or even orders).

We now turn to the question of how exploiting finer details of the accumulation structure to obtain optimal accuracy when fixing α. Up to the fourth order a set of rules has been established [3–5] which applied to all of the considered gauge groups, dimensions, and Wilson loop sizes and by which the accuracy of Monte Carlo simulations of moderate statistics was reached. After rules based on the vanishing of the $S-S_0$ dependent contributions (related to intersections of W_n with W_0) refined rules emphasizing the fastest convergence of subsequent orders and accounting for the even-order phenomenon have been developed (related to intersections or closest approaches between $W_{2\nu}$ and $W_{2\nu-2}$ or W_n and W_{n-1}, respectively). For the plaquette average to be considered here, particularly high accuracy has been reached [4] by taking W_4 at the α value where $W_2-W_4=W_4-W_0$.

To get further insight it was necessary to obtain results up to the next even order, i.e., up to the sixth order, which has been achieved in the present work. The general features of the accumulation structure become transparent from these results. However, from the comparison with the Monte Carlo value in Fig. 3 the disappointing fact is apparent that the sixth order no longer leads to an improvement. Figures 3(a) and 3(b) show that at lower as well as at higher β the fourth order is better than the sixth order (with generally better results at larger β).

Inspection of Figs. 3 and 4 with respect to this (at first sight surprising) observation reveals the underlying

(monotonic) trend of consecutive orders according to which one has to expect still worse results for the eighth and higher orders. This holds independently of the particular prescription for fixing α (i.e., equally well for using intersections of $W_{2\nu}$ with $W_{2\nu-2}$, intersections of $W_{2\nu}$ with W_0, or anything similar that can be reasonably justified). Also involving odd orders somehow offers no way out because seventh and higher orders are to be expected well below the fifth order. Thus, from the practical point of view one arrives at the conclusion that the method fails to compete with high-statistics Monte Carlo simulations.

From the theoretical point of view the question arises why the expansion fails above a certain order. One immediately notes that such a behavior is typically found for asymptotic expansions [12] when increasing the order for fixed expansion parameter. In fact, providing a weak-coupling approximation the expansion considered here is expected to be asymptotic. Because of its construction it is, however, hard to get hold of its remainder and to investigate details of this rigorously. As compared with usual expansions there is an additional severe difficulty in the present case. The orders are primarily not specified in terms of powers of a parameter but in terms of powers of a difference of functions $S-S_0$. Therefore, in the evaluation somehow a conversion from orders of $S-S_0$ into orders of $1/\beta$ has to take place such that one arrives at a weak-coupling approximation. For this purpose it is obviously important to choose α appropriately depending on β.

From the discussions in Secs. II and IV it follows that our $\alpha(\beta)$ derived from requirements of optimal convergence is an approximate solution of

$$\frac{\beta}{2}[(2d-1)+\Delta]=\frac{\alpha}{V_1^3(\alpha)} . \tag{4.2}$$

Using the asymptotic expansion of modified Bessel functions it is seen that for large α the right-hand side of (4.2) can be replaced by $\alpha+\frac{9}{4}+99/(32\alpha)$. Cancellations of powers of β in (3.1) become thus possible, though only in an approximate way and with increasing difficulty at higher order. There are, however, further cancellations in (3.1) due to the asymptotic form $V_r(\alpha)=1-r(r+2)/(4\alpha)+O(1/\alpha^2)$ and because of the properties of (2.3). These are such that the constant parts of the monomials of $V_r(\alpha)$ in (3.2) drop out and one remains with powers of $1/\alpha$ which by (4.2) turn into powers of $1/\beta$. This saves the situation as far as the β dependence is concerned and is the reason why one gets a weak-coupling approximation.

The analytical details of the conversion into powers of $1/\beta$ are obviously complicated and may emphasize the effect that the approximation no longer improves above some order. From a more general point of view the limitations for compensating plaquette actions by link actions appear to show up.

V. THE CASE OF FINITE TEMPERATURES

In the case of finite temperatures calculations have again been done for SU(2) in the weak-coupling region and for $d=4$, now with periodicity and extension N_τ in the time direction and still infinite extensions in the three spatial directions.

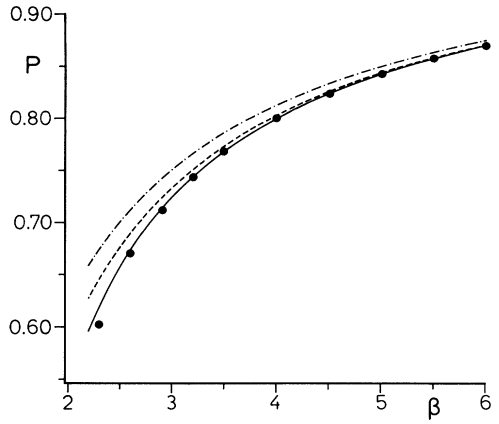

FIG. 5. Typical result for $P_{\rm sym}$ as a function of β compared with Monte Carlo values (dots) and with perturbative $O(1/\beta)$ (dash-dotted line) and $O(1/\beta^2)$ (dashed line) results.

To investigate the general situation space-space and space-time plaquette averages have been calculated up to the sixth order for $N_\tau=4$. The behavior of the individual orders turns out to be the same as that discussed in Sec. IV for the plaquette on the symmetric lattice. Comparison with Monte Carlo data [13] again shows that the sixth order no longer leads to an improvement as compared to the fourth order.

In perturbative calculations of thermodynamic quantities at higher order summations of an infinite set of diagrams are used to cure infrared divergences which, however, ultimately does not lead to satisfactory results [7]. On the lattice one is confronted with zero modes already at low order [14]. Therefore, the present weak-coupling approach is of interest as an alternative to these perturbative calculations.

To check the respective possibilities the internal energy of the gluon gas has been considered which, with appropriate coefficients [15] c_σ and c_τ, can be obtained [16] from

$$\epsilon=3\beta(P_\sigma-P_\tau)+c_\sigma(P_{\rm sym}-P_\sigma)+c_\tau(P_{\rm sym}-P_\tau) , \tag{5.1}$$

where P_σ and P_τ are the average plaquettes in space-space and space-time directions and $P_{\rm sym}$ the one on the symmetric lattice. According to the rules about accuracies found our computations (up to the sixth order) have been evaluated in the fourth order (using the $W_2-W_4=W_4-W_0$ prescription discussed in Ref. [4]) for P_σ and P_τ at $N_\tau=3,4,5$ and for $P_{\rm sym}$.

Figure 5 shows typical results for $P_{\rm sym}$ compared with Monte Carlo values [11] and with $O(1/\beta)$ and $O(1/\beta^2)$ results from lattice perturbation theory [14]. The corresponding figures for P_σ and P_τ have the same appearance (because the small differences are not visible at the scale of the figures). It is seen that our results for the average plaquettes are better than those from perturbation theory. However, inserting the perturbative results for the plaquettes into (5.1) leads to reasonable results for ϵ,

which apparently is due to cancellations of common deviations within the differences in (5.1). For our plaquette results cancellations of this type do not occur and thus the insertion into (5.1) does not lead to useful results for ϵ at the given accuracy.

VI. CONCLUSIONS

To get more insight in the underlying mechanisms of the accumulation-point approach and to decide if the approach is able to compete with high-statistics Monte Carlo simulations it was necessary to reach the sixth order by overcoming huge combinatorial factors. This has been achieved by two means. First, instead of treating all configurations contributing to the set of connected functions these configurations have been reduced to equivalence classes in several steps (getting from numbers of about 10^{10} to ones lower than 2×10^4). Second, instead of using the one-link integral as a generating function the tools of representation theory have been used evaluating tensor products (gaining up to a factor 3×10^9 for some contributions).

The results have allowed us to establish the general features of the individual orders. Details as the even-order phenomenon have been clarified. It has become possible to identify the general trend which then allows us to predict the behavior of still higher orders. This is important because it cannot be done by analytical and rigorous tools so far.

With respect to practical applications it has turned out that the sixth order gives worse results than the fourth order, or, more generally, that there is no longer an improvement beyond the fourth order. This behavior appears to be related to the asymptotic nature of the expansion and to the conversion into powers of $1/\beta$ needed. Ultimately it reflects limitations in the possibilities of compensating the action by the trial action.

The origin of the weak-coupling nature of the expansion is revealed. It has been found to follow from the properties of connected functions combined with the asymptotic behavior of the modified Bessel functions involved.

The extension of the approach to the case of finite temperatures has shown that there the same features occur as on the symmetric lattice. Comparing the calculations of thermodynamic quantities by the present approach and by perturbation theory it is seen that though higher accuracies are reached for average plaquettes the accuracy is not sufficient for energy densities.

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