Optimization in the extended variational approach to SU(2) gauge theory on the lattice

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The linear δ expansion is applied to SU(2) gauge theory on the lattice, with a trial action based on single links. In contrast with previous calculations using this action, we use the principle of minimal sensitivity to determine the arbitrary parameter J which occurs in the interpolating action. We obtain a good fit to the Monte Carlo data on the weak-coupling side of the transition region: this can be combined with results using a different trial action to cover the entire range of β. There is no sign that the procedure fails to converge.

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I. INTRODUCTION

Over the last few years, a promising new analytic approach to field theory has emerged and has been applied to a variety of problems (see, e.g., Ref. [1]). The method, the linear δ expansion, is nonperturbative in character; i.e., it is not an expansion in the coupling constant, although the Feynman diagrams encountered are not radically different from those of conventional perturbation theory. An important ingredient of the method, which makes it a generalization of the variational method, is the optimization of an arbitrary parameter λ appearing in the Lagrangian and/or action.

The essential idea is to construct an action S_δ which interpolates linearly between the action S of the theory one is trying to solve and the action S_0 of a soluble theory chosen to reflect as much of the physics of S as possible. That is,

$$S_\delta = \delta S + \lambda(1-\delta)S_0 = \lambda S_0 + \delta(S - \lambda S_0) , \quad (1)$$

with the property that $S_{\delta=0}=\lambda S_0$, while $S_{\delta=1}=S$, independent of λ. The vacuum-generating functional, or an appropriate Green's function, is then evaluated as a truncated expansion in δ, which is finally set equal to 1.

Because one can necessarily only calculate a finite number of terms, the truncated expansion will contain a residual λ dependence which would not be there in the infinite sum, and it is therefore necessary to have some criterion for choosing the optimum value of λ. The criterion which has been most widely adopted is the principle of minimal sensitivity (PMS). This chooses λ so as to minimize, at least locally, the dependence on λ of the result being calculated. Thus, if $R_K(\lambda)$ is the result truncated at order K, the criterion reads

$$\frac{\partial R_K}{\partial \lambda} = 0 . \quad (2)$$

The importance of this (or some similar) ingredient of the linear δ expansion (LDE) can hardly be overstressed. In the first place, it is here that nonperturbative dependence on the coupling constant g emerges, as it does in variational principles, of which the LDE can now be seen as a generalization. Second, it is the PMS criterion which produces a convergent sequence of approximants out of what would otherwise be an asymptotic or divergent series. This latter property certainly holds in practice in a large number of different situations, and it has recently been proved rigorously [2] in $d=0$ field theory, i.e., in the evaluation of $\int dx\, e^{-gx^4}$ by rewriting the exponential as $\exp[-\delta g x^4 - \lambda(1-\delta)x^2]$.

The linear δ expansion has much in common with other nonperturbative approaches to field theory. At $O(\delta)$ it can be variously identified, depending on the context, with the Gaussian approximation [3] or mean-field theory. The calculations of Killingbeck [4] on the anharmonic oscillator can now be recognized as an early application of the LDE which goes beyond first order, and the generalization of the Gaussian approximation, developed independently [5] by Okopińska and others, is again the linear δ expansion by another name.

In the context of lattice gauge theories, there have been several applications to the calculation of the average plaquette energy E_P, to be compared with the results of lattice Monte Carlo calculations. Depending on the choice of the trial action S_0, the expansion can be more appropriate to the strong-coupling ($\beta \ll 1$) or weak-coupling ($\beta \gg 1$) regime. In the strong-coupling regime, an approach based on choosing a maximal tree of plaquettes in four dimensions [6], following earlier work in three dimensions [7], has proved very successful in reproducing the whole of the strong-coupling side of the curve for SU(2). The results of an $O(\delta^4)$ calculation are shown in Fig. 1.

An attempt was made earlier [8] to calculate the weak-coupling side of the curve using a noncompact quadratic action S_0 which was the weak-coupling limit of S. Although at first sight this would appear to be the appropriate S_0 to use, difficulties with gauge invariance and the computational effort involved in evaluating the resulting lattice Gaussian integrals limit the practical utility of this particular choice of the action. In the event, it proved very difficult to go beyond $O(\delta)$; nonetheless, a hybrid "optimized $1/\beta$ expansion" turned out to give a reasonably good fit to the data.

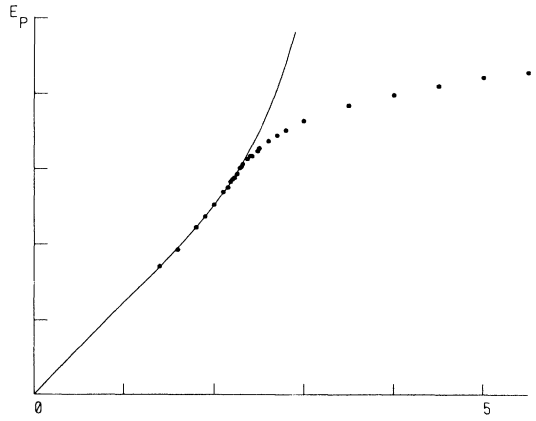

FIG. 1. Order-δ^3 linear δ expansion, based on the action of Ref. [6], for the plaquette energy E_P in the strong-coupling regime. Monte Carlo points from Refs. [13,14].

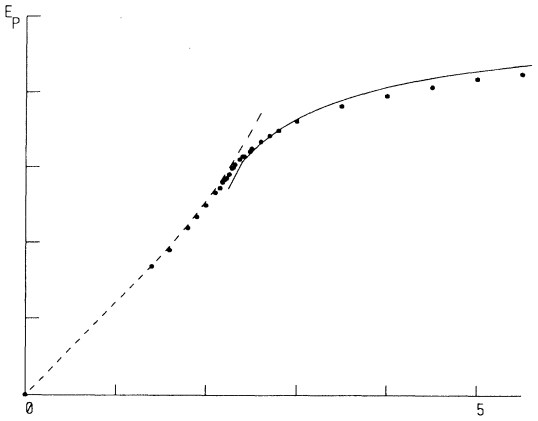

FIG. 2. Order-δ^3 "variational cumulant expansion" of Ref. [9], based on the action of Eq. (5) and the criterion $\partial F_1/\partial J=0$, for E_P in the weak-coupling regime. Also shown (dashed line) is the augmented $O(\beta^5)$ character of Ref. [13].

Independently, a related approach had been developed by Zheng, Tan, and Wang [9], termed the variational cumulant expansion. Although not formulated as such, it can now be seen as a variant of the linear δ expansion, with a trial action S_0 based on single links:

$$S_0=\sum_l \mathrm{tr}U_l \ , \tag{3}$$

with a multiplicative factor J taking the role of λ. The crucial difference from the LDE as now generally formulated lay in the criterion used for determining J. Influenced by the rigorous inequalities on the free energy F which occur at $O(\delta)$, they imposed the condition $\partial F_1/\partial J=0$, even though the actual quantity being calculated was the plaquette energy E_P to some higher order [up to $O(\delta^3)$]. This is clearly at variance with the spirit of the PMS: the resulting values do not satisfy $\partial E_P/\partial J=0$. The calculations were only moderately successful (see Fig. 2), and it was found necessary to impose a gauge-fixing condition, whereby all the timelike links were set equal to unity, to improve the agreement with experiment.

The shortcomings of the criterion $\partial F_1/\partial J=0$ were recognized by Kerler [10], who took the calculation to $O(\delta^4)$ and suggested a new criterion based on looking for "accumulation points," where the graphs for several different orders converged. While being somewhat *ad hoc,* this approach did give improved numerical results and encouraged an extension [11] of the calculations to $O(\delta^6)$. However, the conclusion of that paper was that going to higher orders failed to produce an improvement, and doubts were cast on the convergence of the procedure.

It is our experience in other contexts that the linear δ expansion, used in conjunction with the PMS criterion, does converge, and in zero dimensions it can be proved [2], by saddle-point methods, that the LDE produces a sequence converging to the exact answer with an error like $\exp(-cK)$ for large K. Thus it seemed worthwhile to reexamine the calculations of Refs. [9–11], using the same action, but the standard PMS criterion $\partial E_P/\partial J=0$ for determining J. This calculation is given in the next section, followed by our conclusions.

II. OPTIMIZATION FOR SU(2)

As explained in the Introduction, we are using the same bare action as in Refs. [9–11]. We consider pure SU(2) gauge theory on a hypercubic lattice with action

$$S=\beta\sum_P \mathrm{tr}U_P \ , \tag{4}$$

where U_P is the product of group elements U_l around the plaquette and $\beta=4/g^2$. We choose a trial action $S_0=J\sum_l \mathrm{tr}U_l$, as in Eq. (3). The variational parameter is J, taken to be the same on all links. The linear interpolating action is then of the form[1]

$$S_\delta=J\sum_L \mathrm{tr}U_l+\delta\left[\beta\sum_P \mathrm{tr}U_P-J\sum_l \mathrm{tr}U_l\right] . \tag{5}$$

The parameter δ, which was not included explicitly in those references, is the formal expansion parameter which generates the "variational cumulant expansion" [9] when the free energy, or connected vacuum-generating functional, is evaluated. That is,

$$\begin{aligned} Z=e^{-W}&=\int\prod_l dU_l e^{S_0}e^{\delta(S-S_0)} \\ &=Z_0\langle e^{\delta(S-S_0)}\rangle_0 \ , \end{aligned} \tag{6}$$

where the expectation value of a variable X with respect to S_0 is defined as

$$\langle X\rangle_0=\frac{1}{Z_0}\int\prod_l dU\, e^{S_0}X \tag{7}$$

[1]Here we are using the notation of Zheng, Tan, and Wang [9]. The β of Kerler [10] differs from this by a factor of 2: $\beta_K=2\beta_Z$.

and

$$Z_0=\int\prod_l dU_l e^{S_0}=[f(J)]^{N_l}\ , \tag{8}$$

where $f(J)=I_1(2J)/J$. Here N_l is the total number of links and $I_r(x)$ is the modified Bessel function of order r. Expanding the exponential in Eq. (6) gives

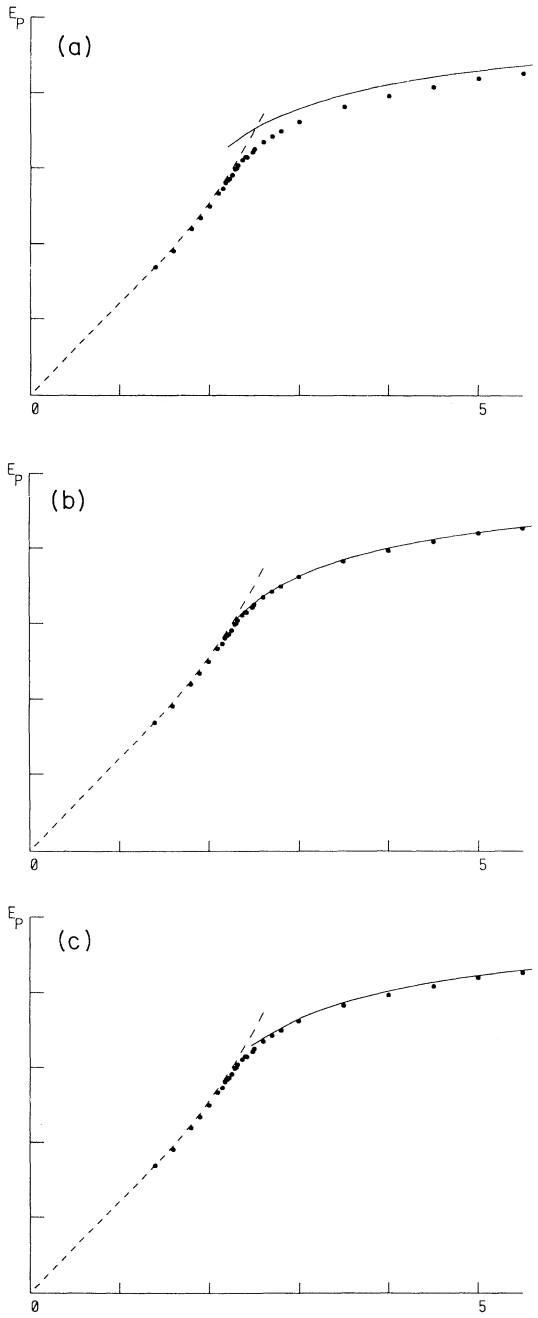

FIG. 3. Linear δ expansion, based on the action of Eq. (5) and the PMS criterion $\partial E_P/\partial J=0$, for E_P in the weak-coupling regime: (a) order δ, (b) the order-δ^2 Padé approximant $P(1,1)$, and (c) order δ^3.

$$W=W_0-\sum_{n=1}^{\infty}\frac{\partial^n}{n!}\langle(S-S_0)^n\rangle_C\ , \tag{9}$$

where the subscript C denotes the connected expectation value. This will, of course, be truncated as some finite order K, and δ then set to equal to 1. The plaquette energy E_P is obtained from W, the free energy of the system, by

$$E_P=-\frac{1}{N_l(d-1)}\frac{\partial W}{\partial\beta}\ . \tag{10}$$

Here $d=4$ is the number of space-time dimensions.

The general methodology for evaluating the expectation values has been described in Ref. [9]. The crux of the matter is that the exponential brings down powers of S whose expectation value has to be evaluated under the group integration $\int\prod_l dU_l e^{S_0}$. To $O(\delta^0)$ for E_P, one simply has to evaluate $\langle\mathrm{tr}U_P\rangle_0$. The invariance of S_0 under the group transformation $U_i=V^\dagger U_i V$ and the SU(2) identity $\int[dV]V^\dagger_{ik}V_{lj}=\frac{1}{2}\delta_{ij}\delta_{kl}$ readily give the result

$$\begin{aligned}\langle\mathrm{tr}U_1U_2\rangle_0&=\tfrac{1}{2}\langle\mathrm{tr}U_1\mathrm{tr}U_2\rangle_0\\&=\tfrac{1}{2}\langle\mathrm{tr}U_1\rangle_0\langle\mathrm{tr}U_2\rangle_0\ .\end{aligned} \tag{11}$$

Applying this twice, one finds that

$$\langle\mathrm{tr}U_P\rangle_0=\langle\mathrm{tr}U_1U_2U_3^\dagger U_4^\dagger\rangle_0=2\omega_1^4\ , \tag{12}$$

where

$$\langle\mathrm{tr}U_l\rangle_0=2\omega_1=(1/f)df/dJ\ .$$

In general,

$$\langle(\mathrm{tr}U)^n\rangle_0=\omega_n=(1/f)d^nf/dJ^n\ .$$

In first order an additional plaquette U_Q is brought down from the exponent. By connectedness, this must have at least one link in common with U_P, which means that it either has just one link in common or is identical to U_P. In the first case, each of the free links gives a factor ω_1, while the shared link gives a factor ω_2. The second case is more involved, but can be evaluated in a straightforward way using the relations in Ref. [9]. To evaluate expectations involving more than two connected plaquettes, we have another simplifying relation:

$$\langle\mathrm{tr}U_1U_2\mathrm{tr}U_1^\dagger U_3\rangle_0=\langle\Omega\,\mathrm{tr}U_2\mathrm{tr}U_3+\tfrac{1}{2}(1-\Omega)\mathrm{tr}U_2U_3\rangle_0\ , \tag{13}$$

where $\Omega=I_3(2J)/I_1(2J)$. Proceeding in this fashion, the expectation values associated with the different inequivalent diagrams have been evaluated and the number of diagrams of each type tabulated.[2]

[2]We believe, however, that there is a slight mistake in the number given in Ref. [9] for diagram 15, of $O(\delta^3)$. By breaking up the diagram into its constituent parts in the timelike gauge, and by comparison with Ref. [12], we believe that the number should be $48(9R_0^3-14R_0^2+19R_0-7)+36R_1$.

Up to this point, our calculation is identical to that of Refs. [9–11]. The difference between the various treatments hinges on the criterion used to fix the parameter J. As already mentioned, Zheng, Tan, and Wang [9] used the criterion $\partial F_1/\partial J=0$, even though the quantity being calculated was E_P to $O(\delta^3)$. Kerler worked with E_P itself, and devised a criterion of searching for accumulation points, where the results of various different orders converged. The approach of the present paper is simply to use the PMS criterion on E_P, namely $\partial E_P/\partial J=0$.

The first nontrivial dependence on J appears at $O(\delta)$. A broad minimum of E_P exists for large β, which persists down to $\beta\approx 1.07$. The calculated values are somewhat above the Monte Carlo points [13,14], as is shown in Fig. 3(a).

There are reasons for believing [2] that odd and even orders behave differently with respect to optimization. Indeed, we find that at $O(\delta^2)$ there is no corresponding minimum. However, if the Padé approximant $P(1,1)$ is formed, the results are surprisingly good, as shown in Fig. 3(b). The values at the minimum give good agreement with the data, and the minimum extends well down into the transition region, to $\beta\cong 1.23$.

Inclusion of the $O(\delta^2)$ terms gives a curve which agrees well with the data for larger β. As is to be expected, it shows a marked improvement on the $O(\delta)$ calculation, but a disappointing feature is that the broad minimum disappears well before the transition region, at $\beta\cong 1.47$. This feature corresponds to the change in the accumulation point systematics [10] as one goes from the "upper part" to the "lower part" of the weak-coupling region. It is possible to extend the graph downward, however, if one adopts a weaker form of the PMS criterion. In the absence of a solution to $\partial E_P/\partial J=0$, one can instead look for the values of J where the slope is least, i.e., a point of inflection: $\partial^2 E_P/\partial J^2=0$. Adopting this "weak PMS" allows one to extend the curve down to $\beta\cong 1.15$ in the $O(\delta^2)$ case and $\beta\cong 1.23$ in the $O(\delta^3)$ case, as shown in Fig. 3(c).

A variant of the chosen action is to use a gauge-fixing procedure, setting timelike links $U_l=1$. This procedure was found necessary in Ref. [9] in order to obtain results in reasonable agreement with experiment. We have repeated our calculations in this temporal gauge, but find that in our case the results are not thereby improved.

III. CONCLUSIONS

If one combines the results of Ref. [8] and the present paper (Figs. 1 and 3, respectively), it can be seen that the linear δ expansion provides a viable calculation method for the evaluation of the average plaquette energy. By judicious choice of the trial action S_0, the method can deal with both large and small coupling constants. The different contributions can be evaluated using the elegant techniques of group characters, and connectedness is easily implemented (in contrast with the strong-coupling expansion).

If the PMS criterion is used for determining the arbitrary parameter in the LDE, the results continue to improve as one goes to higher order, and we do not see any sign of the breakdown of the expansion. As is emphasized in Ref. [2], for *fixed* λ the LDE indeed gives a divergent alternating series, but when λ is optimized order by order, the result is a convergent sequence of approximants. It would be interesting to extend the calculation to $O(\delta^5)$: Figure 3 of Ref. [11] shows that in the upper part of the weak-coupling region the broad minimum for odd orders indeed converges rapidly to the Monte Carlo result.

Given the success of the technique as applied to the plaquette energy, one can be optimistic about its application to other quantities and features, such as the phase structure of the mixed SU(2)-SO(3) action, SU(2) at finite temperatures, string tension, mass gap, etc. Some of these topics have already been treated by Tan and Zheng [15], but always with a criterion based on the first-order free energy rather than the quantity being calculated. Work on these extensions of the method is currently in progress.

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