Supercomputing the Effective Action

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We describe a new method for large-scale computer simulation of the effective action in lattice field theories. As a first application, the scalar ϕ^4 model with spontaneous symmetry breaking is studied, and the renormalization of physical parameters is calculated from the effective action. Mean-field scaling behavior with calculable logarithmic scaling corrections at the trivial Gaussian fixed point (vanishing renormalized coupling) is supported by our results. Applications to the electroweak theory are outlined and a bound on the Higgs-boson mass is estimated.

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We introduce a new method for large-scale computer simulation of the effective action from which one calculates the renormalization of masses, coupling constants, field operators, and composite operators for bare input parameters. The effective action when restricted to constant order parameters is reduced to the better known effective potential which is the focus of our first investigations. We find that our method is very useful in the numerical study of the Higgs-boson sector in electroweak models with spontaneous symmetry breaking.

For illustration, we investigate here the continuum limit of scalar lattice field theory with quartic self-interaction in four dimension. The Euclidean lattice action is given by

$$S=\frac{1}{2}\sum_i\left[\sum_{\hat{\mu}}(\phi_{i+\hat{\mu}}-\phi_i)^2+m_0^2\phi_i^2\right]+\lambda_0\sum_i\phi_i^4, \qquad (1)$$

where m_0^2 and λ_0 are bare-mass and coupling-constant parameters. The scalar field variables ϕ_i are defined on lattice sites labeled by i. The unit vector $\hat{\mu}$ points along the four positive lattice directions (the lattice spacing is set to unity in our calculations).

The effective potential $U_\Omega(\bar{\phi})$ has the definition[1]

$$\exp[-\Omega U_\Omega(\bar{\phi})]=\int D[\phi]\delta(\bar{\phi}-\Omega^{-1}\textstyle\sum_i\phi_i)e^{-S[\phi]}, \qquad (2)$$

where Ω designates the finite lattice volume and the integration is over scalar field variables ϕ_i on sites labeled by i. $U_\Omega(\bar{\phi})$ is related to $W_\Omega(J)$, the generator of Schwinger functions, by a Laplace transformation:

$$\int e^{\Omega[J\bar{\phi}-U_\Omega(\bar{\phi})]}d\bar{\phi}=e^{\Omega W_\Omega(J)}. \qquad (3)$$

In standard textbook definitions the effective potential $\Gamma_\Omega(\bar{\phi})$ is derived from $W_\Omega(J)$ by Legendre transformation.[2] $W_\Omega(J)$ and $\Gamma_\Omega(\bar{\phi})$ can always be calculated from $U_\Omega(\bar{\phi})$.

The known convexity of $\Gamma_\Omega(\bar{\phi})$ makes it impractical in computer simulations or analytic nonperturbative investigations of the broken-symmetry phase.[3] The effective potential $U_\Omega(\bar{\phi})$ which we will use is nonconvex in the broken-symmetry phase and has a direct physical interpretation. The probability density $P(\bar{\phi})$ to find the system in a state of "magnetization" $\bar{\phi}$ is given by

$$P(\bar{\phi})=e^{-\Omega U_\Omega(\bar{\phi})}\left(\int d\bar{\phi}e^{-\Omega U_\Omega(\bar{\phi})}\right)^{-1}, \qquad (4)$$

close in spirit to similar definitions in statistical mechanics. With this unique feature we can develop a direct and visual physical picture of spontaneous symmetry breaking and maintain at the same time other important theoretical properties of $\Gamma_\Omega(\bar{\phi})$. All observables of lattice field theories can be derived from $U_\Omega(\bar{\phi})$, or its natural generalization to the effective action $S_\Omega[\bar{\phi}]$ which will be introduced later. In the infinite volume limit $U(\bar{\phi})=\lim_{\Omega\to\infty}U_\Omega(\bar{\phi})$ becomes convex and the relation $U(\bar{\phi})=\Gamma(\bar{\phi})$ can be shown.[3]

From $U_\Omega(\bar{\phi})$ we extract the Euclidean Green's functions at zero momentum:

$$\frac{1}{\Omega^n}\sum_{i_1,\ldots,i_n}\langle\phi_{i_1}\cdots\phi_{i_n}\rangle=\frac{\int d\bar{\phi}\bar{\phi}^n e^{-\Omega U_\Omega(\bar{\phi})}}{\int d\bar{\phi}e^{-\Omega U_\Omega(\bar{\phi})}}. \qquad (5)$$

In saddle-point approximation it follows from Eq. (5) that

$$\lim_{\Omega\to\infty}\left.\frac{\partial^2U_\Omega(\bar{\phi})}{\partial\bar{\phi}^2}\right|_{\bar{\phi}=\bar{\phi}_{\min}}=\frac{m_R^2}{Z_\phi}, \qquad (6)$$

$$\lim_{\Omega\to\infty}\left.\frac{\partial^4U_\Omega(\bar{\phi})}{\partial\bar{\phi}^4}\right|_{\bar{\phi}=\bar{\phi}_{\min}}=24\frac{\lambda_R}{Z_\phi^2}, \qquad (7)$$

where Z_ϕ is the wave-function renormalization of the ϕ field, m_R^2 is the renormalized mass squared in lattice spacing units, and λ_R is the renormalized quartic coupling constant. In order to determine the renormalization constant Z_ϕ, we can use the relation

$$\partial\tilde{G}(p^2)^{-1}/\partial p^2|_{p^2=0}=Z_\phi^{-1},$$

where $\tilde{G}(p^2)$ is the two-point connected Green's function in momentum space.

For an independent determination of Z_ϕ we can generalize Eq. (2) and introduce the effective action

$S_{\rm eff}[\bar\phi(x)]$ which becomes a functional of the space-time-dependent order parameter $\bar\phi(x)$:

$$\exp(-\Omega S_{\rm eff}[\bar\phi])=\int D[\phi]\delta_f(\bar\phi-\phi)e^{-S[\phi]}. \quad (8)$$

In Eq. (8) the "functional δ-function" $\delta_f(\bar\phi-\phi)$ is a symbolic notation for integrating all field configurations orthogonal to $\bar\phi(x)$. In practice, Eq. (8) is implemented for selected $\bar\phi(x)$ configurations which correspond to fixed Fourier modes. In continuum notation we write[4]

$$S_{\rm eff}[\bar\phi]=\int d^4x[U(\bar\phi)+\tfrac{1}{2}Z_{\rm eff}^{-1}(\bar\phi)(\partial\bar\phi)^2+\cdots], \quad (9)$$

and $Z_\phi=Z_{\rm eff}(\bar\phi_{\rm min})$, by definition; $Z_{\rm eff}(\bar\phi)$ can be determined from our simulation technique as it will be outlined next.

It is easy to show from Eq. (2) that the identity

$$\partial U_\Omega(\bar\phi)/\partial\bar\phi=\langle V'(\phi)\rangle_{\bar\phi} \quad (10)$$

holds for the derivative of the effective potential. On the right side of Eq. (10) the expectation value of the derivative of the classical potential is calculated when all field configurations orthogonal to $\bar\phi$ are summed. Technically we work in Fourier space and the zero momentum Fourier mode is not integrated. To calculate $Z_{\rm eff}(\bar\phi)$, or other terms in the effective action, one has to keep other Fourier modes fixed in the functional integral.

We used two independent methods to generate the probability distribution of the field configurations for fixed $\bar\phi$. The first method is a complete implementation of the third-order Langevin algorithm in momentum space.[5] We also developed a second algorithm in momentum space which is based on the recently introduced unbiased hybrid Monte Carlo method.[6] We found the unbiased hybrid Monte Carlo algorithm to be superior to the third-order Langevin algorithm in efficiency. Our production runs of the O(4) model are now exclusively based on the hybrid Monte Carlo method. The speed of both algorithms is proportional to $\Omega\ln\Omega$ with helical boundary condition and fast Fourier transform. One microcanonical sweep in the ϕ^4 model takes about 5×10^{-3} s on a 8^4 lattice using fast Fourier transform. A typical run for a given value of $\bar\phi$ contains about 10^4 momentum refreshes with ten microcanonical steps between refreshes.

We first determine the critical line in the parameter space of bare coupling and bare mass squared at the crossover of the effective potential from a double-well function to single well. We can only present here results for the ϕ^4 model at one value of the bare coupling constant. Other results will be reported elsewhere.[7] At $\lambda_0=25$, which is strong coupling with respect to earlier computer simulations,[8,9] the critical point of the second-order phase transition for infinite lattice volume is found at $m_{0c}^2(\infty)=-24.55(5)$ from finite-size scaling analysis.[10]

We calculated the effective potential at seven different values of m_0^2 within a narrow range on both sides of the critical point. The two-point function in momentum space was also measured in unconstrained runs at every value of m_0^2 for an independent determination of m_R and Z_ϕ. The inverse of the two-point function in momentum space was fitted against the inverse of the free and massless propagator which is defined by $G_0^{-1}=4\sum_\mu\sin^2(p_\mu/2)$ on the finite lattice with discrete momentum components p_μ appropriate for helical boundary condition. The slope of the fit determines Z_ϕ and the intercept at zero momentum corresponds to m_R^2/Z_ϕ (Fig. 1 represents a typical fit).

From the analysis of the momentum space propagator and the effective potential we determined the renormal-

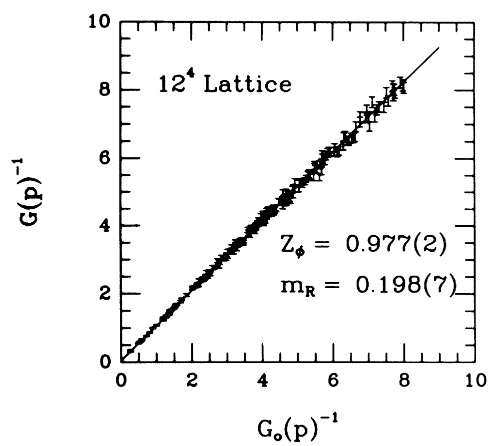

FIG. 1. The inverse of the momentum-space lattice propagator is plotted against the inverse of the massless free momentum-space lattice propagator of the finite lattice for $m_0^2=-24.6$. $1/Z_\phi$ is the slope and m_R is obtained from the intercept.

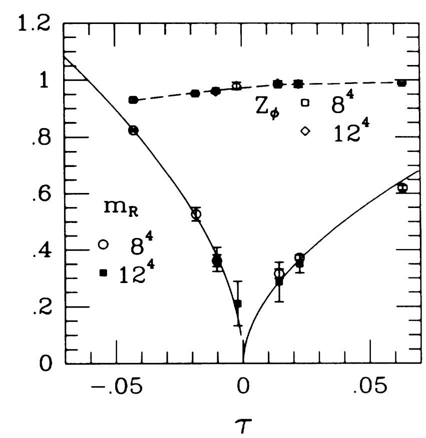

FIG. 2. The renormalized mass m_R and the wave-function renormalization constant Z_ϕ are plotted against $\tau=1-m_0^2/m_{0c}^2$. The solid line indicates the scaling law for $m_R\sim\sqrt{|\tau|}\,|\ln|\tau||^{-1/6}$. The dashed line for Z_ϕ is drawn to guide the eye.

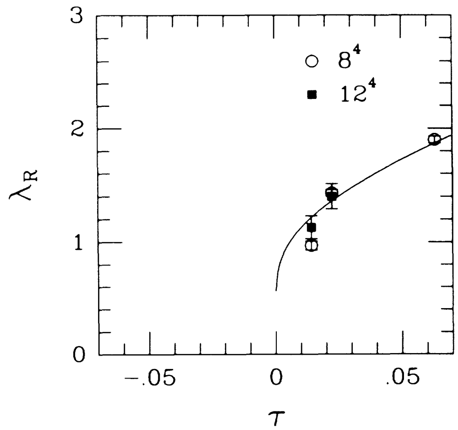

FIG. 3. The renormalized coupling constant λ_R is plotted as a function of τ. The solid line with the scaling behavior $\lambda_R \sim |\ln|\tau||^{-1}$ was calculated in one-loop perturbation theory at the Gaussian fixed point.

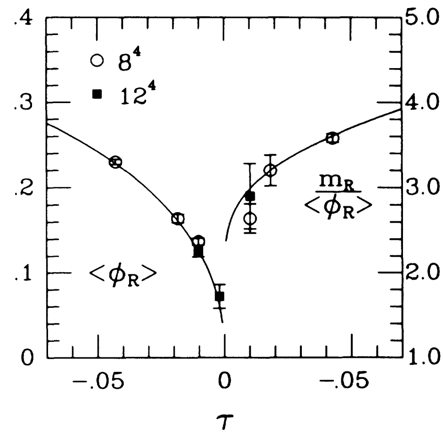

FIG. 4. The left curve is the scaling law of the vacuum expectation value of ϕ_R, $\langle\phi_R\rangle \sim \sqrt{|\tau|}\,|\ln|\tau||^{1/3}$, and the right curve corresponds to $m_R/\langle\phi_R\rangle \sim |\ln|\tau||^{-1/2}$ with the same scaling behavior as $\sqrt{\lambda_R}$. Both sides of the figure correspond to the broken phase.

ized coupling constant λ_R in the symmetric phase, the renormalized mass m_R and the wave-function renormalization constant Z_ϕ in both phases, and the vacuum expectation value of the renormalized field operator in the broken-symmetry phase. The renormalized mass and Z_ϕ are shown in Fig. 2 as functions of the bare-mass parameter for different lattice sizes. As depicted in Fig. 3, although the bare coupling is strong, λ_R is small and rapidly decreasing as we approach the critical line.

Assuming a Gaussian fixed point at $\lambda_R = 0$, the logarithmic corrections to mean-field critical behavior at the higher critical dimension $d = 4$ were calculated earlier.[11] Measuring the horizontal distance from the critical line by $\tau = 1 - m_0^2/m_{0c}^2$ in the phase diagram, one finds

$$\begin{aligned} \langle\phi_R\rangle &\approx |\tau|^{1/2}\,|\ln|\tau||^{3}, \\ m_R &\approx |\tau|^{1/2}\,|\ln|\tau||^{-1/6}, \\ \lambda_R &\approx |\ln|\tau||^{-1}. \end{aligned} \tag{11}$$

The logarithmic scaling corrections are consistent with the data points as shown in Figs. 2, 3, and 4 where the amplitudes are fitted.

The wave-function renormalization constant Z_ϕ in our calculation was found very close to one in the critical region.[9] This result is consistent with a recent effort to match the scaling behavior and high-temperature expansion.[12] We find Z_ϕ close to one also in the broken-symmetry phase where the high-temperature expansion is not applicable. Our own results on the high-temperature expansion which we used mainly for testing and orientation will be discussed elsewhere.[7]

The analysis we presented here was repeated for weaker and stronger bare couplings along the critical line. Our results demonstrate to a high degree of accuracy that in a whole range of the bare coupling constant the critical behavior of the theory is consistent with a Gaussian fixed point at $\lambda_R = 0$.

Although the Gaussian fixed point we found is trivial, inside the scaling region we have a reasonable effective theory with nonvanishing renormalized coupling λ_R. The ratio $m_R/\langle\phi_R\rangle$ according to Fig. 4 cannot grow very large before leaving the scaling region where explicit cutoff dependence begins to show in physical observables. Therefore, at fixed bare coupling a bound exists[13,14] on the Higgs-boson mass $m_R = M_H$ in units of $M_W^2 = g^2/4\langle\phi_R\rangle^2$ where $g^2 \approx 0.4$ is the SU(2) gauge coupling and M_W is the mass of the W boson. For $\lambda_0 = 25$ this bound is about $M_H/M_W \approx 12$ at $\tau = -0.061$ which corresponds to $M_H^{-1} = 1$ in lattice spacing units. The Higgs-boson bound would change to $M_H/M_W \approx 8.5$ at $\tau = -0.018$ with $M_H^{-1} = 5$. We do not expect significant changes in the upper bound in the $\lambda_0 \to \infty$ limit. We should also note that our estimate of the Higgs-boson bound in the one-component ϕ^4 model which does not exhibit Goldstone particles in the broken phase is not a very realistic one. A more realistic determination of the Higgs-boson bound in the O(4) model will be reported elsewhere.[15]

The generalization of our method to more complicated lattice field theories with spontaneous symmetry breaking is straightforward. We have already successfully applied our method to the O(4) approximation of the lattice SU(2) Higgs model.[15] The critical line in the bare parameter space is observed at the crossover points of the effective potential from convex to nonconvex shape. Although there is no conventional order parameter for spontaneous breaking of the continuous O(4) symmetry in a finite volume, with the effective potential we solved this difficulty and a clean signal is provided for the transition. The O(3) symmetry of the nonconvex effective potential in the broken phase accounts for the three Goldstone particles associated with spontaneous symmetry breaking. The renormalization of physical parameters has been determined accurately in the vicinity of the critical line. Work on the SU(2) Higgs model with nonvanishing gauge coupling is also in progress.

During the course of our work we learned about a computer simulation[16] of the traditional effective potential $\Gamma_\Omega(\bar{\phi})$ but our results on m_R, λ_R, $\langle \phi_R \rangle$, and Z_ϕ are quite different.

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[1]R. Fukuda and E. Kyriakopoulos, Nucl. Phys. **B85**, 354 (1975).

[2]U. M. Heller and N. Seiberg, Phys. Rev. D **27**, 2980 (1983).

[3]L. O'Raifeartaigh, A. Wipf, and H. Yoneyama, Nucl. Phys. **B271**, 653 (1986).

[4]C. Itzykson and J. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).

[5]H. S. Greensite and E. Helfand, Bell Syst. Tech. J. **60**, 1927 (1981).

[6]S. Daune, A. D. Kennedy, B. J. Pendleton, and D. Roweth, Florida State University Report No. FSU-SCRI 87-27, 1987 (to be published).

[7]J. Kuti, S. Meyer, and Y. Shen, to be published.

[8]B. Freedman, P. Smolensky, and D. Weingarten, Phys. Lett. **113B**, 481 (1982).

[9]I. T. Drummond, S. Duane, and R. R. Horgan, Nucl. Phys. **B280**, 25 (1987); I. A. Fox and I. G. Halliday, Phys. Lett. **159B**, 148 (1985).

[10]M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8.

[11]E. Brézin, J. C. LeGuillou, and J. Zinn-Justin, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1976), Vol. 6.

[12]M. Lüscher and P. Weisz, DESY Report No. DESY 87-017, 1987 (to be published).

[13]R. Dashen and H. Neuberger, Phys. Rev. Lett. **50**, 1897 (1983).

[14]P. Hasenfratz and J. Nager, Bern University Report No. BUTP-86/20, 1986 (to be published); W. Langguth and I. Montvay, DESY Report No. DESY 87-020, 1987 (to be published); A. Hasenfratz and T. Neuhaus, Florida State University Report No. FSU-SCRI 87-29, 1987 (to be published).

[15]J. Kuti, L. Lin, and Y. Shen, University of California, San Diego, Report No. UCSD/PTH 87-18, 1987 (to be published).

[16]K. Huang, E. Manousakis, and J. Polonyi, Phys. Rev. D **35**, 3187 (1987).