PHYSICAL REVIEW
LETTERS

VOLUME 73 | 3 OCTOBER 1994 | NUMBER 14

Contractor Renormalization Group Method: A New Computational Technique for Lattice Systems

Colin J. Morningstar
Department of Physics & Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, Scotland

Marvin Weinstein
Stanford Linear Accelerator Center, Stanford University, Stanford, California 94309
(Received 23 May 1994)

The contractor renormalization group (CORE) method, a new approach to solving Hamiltonian lattice systems, is introduced. The method combines contraction and variational techniques with the real-space renormalization group approach. It applies to lattice systems of infinite extent and is ideal for studying phase structure and critical phenomena. The CORE approximation is systematically improvable and can treat systems with dynamical fermions. The method is tested using the (1+1)-dimensional Ising model.

PACS numbers: 02.70.Rw, 05.50.+q, 11.15.Ha

Many problems in particle and condensed matter physics cannot be studied with conventional perturbation theory. Aside from Monte Carlo simulations, few tools allow one to deal with general Hamiltonian systems and fewer tools deal directly with their infinite-volume behavior. This paper introduces a new tool, the contractor renormalization group (CORE) approximation, which can handle this class of problems. The CORE approach is a simple, systematic procedure for improving any Hamiltonian real-space renormalization group calculation. Its virtues are the following: it is a variational procedure which is systematically improvable to any desired degree of accuracy; it applies to lattice systems of infinite extent, allowing direct study of phase structure and critical phenomena; it provides tools for error estimation; it requires modest computer resources by modern standards; it is complementary to Monte Carlo methods; systems with dynamical fermions can be treated.

We start with a brief description of the CORE approximation, then illustrate and test the method in two different applications to the (1+1)-dimensional Ising model.

Baisc ideas.—Choosing a good trial state is crucial to the success of any variational calculation, especially one involving a large number of degrees of freedom. The Hamiltonian real-space renormalization group (RSRG) method [1] is an algorithm for constructing a class of trial states appropriate for lattice systems. In this approach, one partitions the lattice into blocks containing a few sites and diagonalizes the Hamiltonian associated with each block. One then *thins* the Hilbert space by discarding all states except those which are tensor products of some chosen subset of low-lying block eigenstates, and an effective Hamiltonian which describes the mixing of the retained states is computed. This truncation process is iterated until the effective Hamiltonian evolves into a fixed form which can be easily diagonalized.

Unfortunately, simple RSRG truncation procedures tend to severely underestimate the effects of block-to-block couplings and this hinders the accurate description of long-wavelength modes on the full lattice. Past approaches to overcoming this problem have concentrated on using larger blocks, increasing the number of states retained per block, or introducing more sophisticated truncation schemes [2,3]. The t expansion has also been used [4]. The CORE approximation is a new approach to this problem which emphasizes simplicity, versatility, and insensitivity to the precise details of the truncation scheme. This insensitivity, or robustness, frees one from the need to develop clever truncation algorithms or to retain many states per block. This

0031-9007/94/73(14)/1873(5)$06.00

feature of CORE, combined with its simplicity, greatly enhances its usefulness for higher dimensional systems. CORE also allows the use of manifestly gauge-invariant RSRG schemes when studying lattice gauge theories; such simple schemes cannot be exploited in the naive multistate approach since gauge-noninvariant states are necessary for coupling neighboring blocks after the first truncation step. Furthermore, the CORE method does not suffer from the series reconstruction difficulties which plague the t expansion.

The basic idea of the CORE approach is to use contraction techniques to steer the RSRG iteration. In the limit $t \to \infty$, the operator e^{-tH} *contracts* any trial state $|\Phi_{\rm var}\rangle$ onto the lowest eigenstate of H with which it has a nonvanishing overlap. Therefore, the expectation value

$$\mathcal{E}(t) = \frac{\langle \Phi_{\rm var}|e^{-tH}He^{-tH}|\Phi_{\rm var}\rangle}{\langle \Phi_{\rm var}|e^{-2tH}|\Phi_{\rm var}\rangle} \quad (1)$$

tends to the corresponding eigenvalue ϵ_0 of H as t becomes large. In general, $\mathcal{E}(t)$ cannot be computed exactly. Reliably approximating $\mathcal{E}(t)$ is an integral part of the steering process in the CORE method.

An important step in building a CORE approximation to $\mathcal{E}(t)$ is to construct an easily *computable* operator $T(t)$ which closely approximates e^{-tH} for t in some range $0 < t < t_{\rm max}$. To find such an operator [5], first divide H into two (or more) parts, i.e., $H = H_1 + H_2$, where the individual parts H_1 and H_2 are chosen such that e^{-tH_1} and e^{-tH_2} can be computed exactly. Next, rewrite e^{-tH} as a symmetric product

$$e^{-tH} = e^{-tH_1/2}\, e^{-tH_2/2}\, e^{C_3(t)}\, e^{-tH_2/2}\, e^{-tH_1/2}, \quad (2)$$

where $C_3(t)$ is a sum of terms all of which begin in order t^3 or higher. The simplest $T(t)$ is obtained by replacing $e^{C_3(t)}$ by the identity operator. One way to construct a better approximation is to retain low-order terms in $C_3(t)$ and rewrite the exponential of these operators as a symmetric product of explicitly computable terms. Another is to use the operators $T_p(t) = [T(t/p)]^p$. In any case, it is very important to ensure the approximate contractor satisfies all the symmetries of H.

Given a contractor $T(t)$, ϵ_0 can then be bounded from above by computing

$$\mathcal{E}_T(t) = \frac{\langle \Phi_{\rm var}|T(t)\,H\,T(t)|\Phi_{\rm var}\rangle}{\langle \Phi_{\rm var}|T(t)^2|\Phi_{\rm var}\rangle}. \quad (3)$$

A best estimate for ϵ_0 is obtained by minimizing $\mathcal{E}_T(t)$ with respect to t and any parameters in $|\Phi_{\rm var}\rangle$. For a trial state $|\Phi_{\rm var}\rangle = \sum_{j=1}^{n} \alpha_j|\phi_j\rangle$, where $\{|\phi_j\rangle\}$ is some set of orthonormal states, one can show that minimizing $\mathcal{E}_T(t)$ with respect to the α_j parameters is equivalent to solving the generalized eigenvalue problem

$$\det\left(\llbracket T(t)HT(t)\rrbracket - \lambda\llbracket T(t)^2\rrbracket\right) = 0, \quad (4)$$

where $\llbracket\cdots\rrbracket$ denotes truncation to the subspace spanned by the $|\phi_j\rangle$ states. In particular, for an operator O, $\llbracket O\rrbracket = POP^\dagger$ where P is the projection operator $P = \sum_{j=1}^{n}|\phi_j\rangle\langle\phi_j|$. Thus, finding the best trial state $|\Phi_{\rm var}\rangle$ is equivalent to diagonalizing the *effective Hamiltonian*

$$H_{\rm eff}(t) = \llbracket T(t)^2\rrbracket^{-1/2}\llbracket T(t)\,H\,T(t)\rrbracket\llbracket T(t)^2\rrbracket^{-1/2}. \quad (5)$$

Developing *this* operator in the RSRG iteration instead of $\llbracket H\rrbracket$ is a key innovation of the CORE approach.

The effective Hamiltonian defined by Eq. (5) cannot be exactly computed. Another novel feature of the CORE approach is the use of the finite *cluster* method to evaluate $H_{\rm eff}(t)$. In this method, $H_{\rm eff}(t)$ (or any other *extensive* quantity) is calculated as a sum of finite-volume contributions (see Ref. [6]). The finite cluster method, which will be described later when applying CORE to the Ising model, is simple to implement, provides numerous computational checks, and does little or no harm to the variational bound in $\mathcal{E}_T(t)$.

The final ingredient in the CORE approximation is the selection of a best value for t in each RSRG step. This can be done in a number of ways. One can extract the coefficient of the identity operator in $H_{\rm eff}$ and vary t to minimize this quantity. Better yet, one can evaluate $H_{\rm eff}$ in a simple product state to produce a mean-field estimate of the ground state energy and minimize this with respect to t.

In summary, the CORE method generates a sequence of effective Hamiltonians $H_{\rm eff}^{(n)}(t_n^*)$ by successive thinning of degrees of freedom using the recursion relation

$$H_{\rm eff}^{(n+1)}(t) = R_n(t)\llbracket T^{(n)}(t)H_{\rm eff}^{(n)}(t_n^*)T^{(n)}(t)\rrbracket R_n(t), \quad (6)$$

where $R_n(t) = \llbracket T^{(n)}(t)^2\rrbracket^{-1/2}$ and the contractor $T^{(n)}(t)$ is constructed to approximate $\exp[-tH_{\rm eff}^{(n)}(t_n^*)]$. Equation (6) is evaluated using the finite cluster method and a best $t = t_{n+1}^*$ must be chosen. As the recursion proceeds, the effective Hamiltonian evolves eventually into a simple form which can be trivially diagonalized, yielding estimates of the ground state energy and the energies of some low-lying excited states.

The expectation value of an extensive operator O can also be evaluated in the CORE method. One develops O using the same RSRG transformations as for H, producing a sequence of effective operators $O_{\rm eff}^{(n)}(t_n^*)$. The matrix element of $O_{\rm eff}$ is then evaluated once $H_{\rm eff}$ has evolved to the point where its ground state can be easily determined.

Note that from a programming point of view, CORE calculations involve mainly matrix multiplications; diagonalizations and inversions of only very small matrices are

required. Often the matrices will be sparse and one can exploit efficient algorithms for multiplying them.

The (1+1)-dimensional Ising model.—We illustrate and test the CORE approximation in two different applications to the (1+1)-dimensional Ising model. The Hamiltonian in this model is given by

$$H_{\text{Ising}} = -\sum_j [c_\lambda \sigma_z(j) + s_\lambda \sigma_x(j)\sigma_x(j+1)], \quad (7)$$

where j labels the sites in the infinitely long chain, $c_\lambda = \cos(\lambda\pi/2)$, and $s_\lambda = \sin(\lambda\pi/2)$, for $0 \le \lambda \le 1$. This model exhibits a second-order phase transition at $\lambda = 1/2$. For $\lambda < 1/2$, the ground state is unique and the order parameter $\langle \sigma_x(j)\rangle = 0$, for some site j. When $\lambda > 1/2$, the ground state is twofold degenerate and the order parameter takes values $\langle \sigma_x(j)\rangle = \pm[1 - \cot^2(\lambda\pi/2)]^{1/8}$.

The CORE approximation is best applied in the following sequence of steps: (1) choose an RSRG algorithm by specifying how to partition the lattice into blocks and which states to retain on each block; (2) specify the truncation order in the cluster expansion of H_{eff}; (3) deduce the general form of H_{eff} based on the choices made in steps (1) and (2); (4) construct a contractor $T(t)$ which closely approximates $\exp(-tH_{\text{eff}})$ and is easily computable; (5) choose a method of determining the optimal value of t in each RSRG step; (6) iteratively compute H_{eff} using Eq. (6) with initial condition $H_{\text{eff}}^{(0)} = H$, where H is the Hamiltonian of interest, until H_{eff} can be easily diagonalized.

In our first application, we partition the lattice into two-site blocks and truncate the Hilbert space to the lowest two eigenstates in each block. Since our intention here is to carry out only the *simplest* of calculations, we choose to truncate the cluster expansion of $H_{\text{eff}}(t)$ after three-block clusters. The general form of $H_{\text{eff}}(t)$ may then be deduced by considering how it is computed in the finite cluster method.

Evaluation of $H_{\text{eff}}(t)$ by the finite cluster method is accomplished in the following sequence of steps. First, compute $H_{\text{eff}}(t)$ using Eq. (5) on a sublattice which contains only a single block. This yields

$$h_{\text{eff}}^{(1)}(t) = H_{\text{eff}}^{(1)}(t) = c_u^{(1)}(t)u + c_z^{(1)}(t)\sigma_z, \quad (8)$$

where u is a 2×2 identity matrix. Next, calculate $H_{\text{eff}}(t)$ for a theory defined on a sublattice made up of two adjacent blocks. This Hamiltonian takes the form

$$H_{\text{eff}}^{(2)}(t) = c_u^{(2)}(t)u^L u^R + c_z^{(2)}(t)(\sigma_z^L u^R + u^L \sigma_z^R) + c_{zz}^{(2)}(t)\sigma_z^L \sigma_z^R + c_{xx}^{(2)}(t)\sigma_x^L \sigma_x^R + c_{yy}^{(2)}(t)\sigma_y^L \sigma_y^R, \quad (9)$$

where L and R refer to the left and right blocks, respectively, in the cluster. Remove from the two-block calculation those contributions which arise from terms already included in the single-block calculation:

$$h_{\text{eff}}^{(2)}(t) = H_{\text{eff}}^{(2)}(t) - u^L \otimes h_{\text{eff}}^{(1R)}(t) - h_{\text{eff}}^{(1L)}(t) \otimes u^R. \quad (10)$$

Repeat this procedure for sublattices containing successively more connected blocks, then sum the contributions $h_{\text{eff}}^{(m)}(t)$ from these sublattices with weights given by the number of ways each sublattice can be embedded in the full lattice. The stage at which one cuts off this cluster expansion determines the maximum range of the interactions which will appear in H_{eff}. For our choices, the effective Hamiltonian in this model takes the general form

$$H_{\text{eff}}(t) = -\sum_{\alpha,j} c_\alpha(t) O_\alpha(j), \quad (11)$$

$$O_\alpha(j) = \sigma_{\alpha_0}(j)\sigma_{\alpha_1}(j+1)\cdots\sigma_{\alpha_r}(j+r), \quad (12)$$

where $c_\alpha(t)$ are the couplings, α labels the different types of operators, and j is a site label. There are only two one-site operators: $\alpha^{(1)} = \{u, z\}$, where u denotes the identity operator. In other words, the only one-site operators are $O_u(j) = \sigma_u(j) = 1$ and $O_z(j) = \sigma_z(j)$. There are three two-site operators: $\alpha^{(2)} = \{xx, yy, zz\}$. The three-site operators are $\alpha^{(3)} = \{xzx, xux, xxz, zxx, yzy, yuy, yyz, zyy, zuz, zzz\}$.

Our first contractor is built using the approximation $\exp[-tH_{\text{eff}}(t^*)] \approx S^\dagger(t)S(t)$, where the operator $S(t) = \prod_\alpha\{\prod_j \exp[tc_\alpha(t^*)O_\alpha(j)/2]\}$. The operators in the α product are ordered according to their site range, increasing in size from right to left. This operator can be simplified using $\exp[yO_\alpha(j)] = \cosh^N y[1 + \tanh y O_\alpha(j)]$, where N is the (infinite) number of sites in the lattice. Discarding the unimportant $\cosh^N y$ factors, one obtains a contractor given by $T_1(t) = S_1^\dagger(t)S_1(t)$, where $S_1(t) = \prod_\alpha\{\prod_j[1 + \tanh(c_\alpha t/2)O_\alpha(j)]\}$.

Last, t is chosen in each RSRG step to minimize the expectation value of $H_{\text{eff}}(t)$ evaluated in the mean-field state given by $|\psi_{\text{mf}}\rangle = \prod_j(\cos\theta|\uparrow_j\rangle + e^{i\phi}\sin\theta|\downarrow_j\rangle)$, where $\sigma_z(j)|\uparrow_j\rangle = |\uparrow_j\rangle$ and $\sigma_z(j)|\downarrow_j\rangle = -|\downarrow_j\rangle$. The matrix element $\langle\psi_{\text{mf}}|H_{\text{eff}}(t)|\psi_{\text{mf}}\rangle$ is minimized with respect to t, θ, and ϕ, simultaneously.

For our second application of the CORE method, the lattice is divided into blocks containing three sites and the Hilbert space is again truncated to the lowest two eigenstates in each block. The cluster expansion is taken only to three-block clusters, so H_{eff} takes the general form shown in Eqs. (11) and (12). We use an approximate contractor given by $T_2(t) = S_2^\dagger(t)S_2(t)$ with $S_2(t) = \exp(-tV/2)\exp(-tH_b/2)$, where H_b contains all intrablock interactions and V contains all interblock operators (those which cross block boundaries). Note that $\exp(-tH_b/2) = \prod_p \exp[-tH_b(p)/2]$ and $\exp(-tV/2) = \prod_p \exp[-tV(p)/2]$, where $H_b(p)$ contains all operators which solely act on block p and $V(p)$ contains only

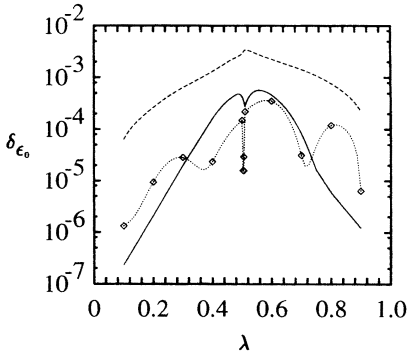

FIG. 1. Fractional error δ_{ϵ_0} in the ground-state energy density estimates against λ. Results using T_1^2 (dashed curve), T_1^{16} (solid), and T_2^{12} (diamonds with dotted curve, to guide the eye) are shown.

interactions between block p and $p+1$. The operators $H_b(p)$ and $V(p)$ can be exponentiated numerically with no difficulty. We fix t by minimizing the expectation value of H_{eff} in the mean-field state $|\psi_{\text{mf}}\rangle$ as described previously.

Selected estimates E_0 of the ground-state energy density from both variants of the CORE approach described above are compared to the exact [7] energy density ϵ_0 in Fig. 1. Calculations were done using $T_1^n(t/n)$ and $T_2^n(t/n)$ for various values of n. The fractional errors δ_{ϵ_0} shown in this figure are defined by $\delta_{\epsilon_0} = |(E_0 - \epsilon_0)/\epsilon_0|$. Selected mass gap estimates Δ are compared to the exactly known gap in Fig. 2. Figure 3 illustrates the amounts by which the T_2^{12} CORE estimates of the magnetization $\mathcal{M} = |\langle\sigma_x(j)\rangle|$, for some site j, differ from the exact values. The accuracy of the results is striking, especially considering that only the first three terms in the cluster expansion were included in the calculations. The CORE method reproduces the correct location of the critical point with remarkable precision. The critical exponent ζ was extracted from a straight-line fit of our T_2^{12} results for $\ln \mathcal{M}$ by the form $\ln \mathcal{M} = \zeta \ln(1 - \Lambda_c^2/\Lambda^2)$, where $\Lambda = \tan(\lambda\pi/2)$, $\Lambda_c = \tan(\lambda_c\pi/2)$, and λ_c is our computed value for the critical point. For $\lambda_c = 0.5053$ and fitting in the range $0.51 \leq \lambda \leq 1.0$, we obtain $\zeta = 0.12437$, to be compared to the exact value of 0.125. The CORE procedure produces better results for a given effort than multistate RSRG methods previously used [3]. The results also compare very favorably to previous t-expansion calculations [4]. Using larger blocks or including more terms in the cluster expansion should further improve these results.

In conclusion, given its simple theoretical foundations, the relative ease of implementation, and our success in applying it to the $(1+1)$-dimensional Ising model, we believe that the CORE approximation will prove to be a powerful tool for analyzing intrinsically nonperturbative systems. One particularly exciting feature of this method is that it can be applied to systems containing dynamical fermions, systems which resist treatment by present stochastic means. In general, we feel that the possibility of eliminating the quenched approximation in lattice quantum chromodynamics, better studying spontaneous symmetry breaking and other nonperturbative phenomena in relativistic field theories, and probing the low-energy physics of the Hubbard and t-J models warrants further work with the CORE approximation.

This work was supported by the U.S. DOE, Contract No. DE-AC03-76SF00515, NSERC of Canada, and the UK SERC, Grant No. GR/J 21347.

[1] The Hamiltonian RSRG procedure was introduced in S. Drell, M. Weinstein, and S. Yankielowicz, Phys. Rev. D **16**, 1769 (1977), and was motivated by the work of Kadanoff and Wilson [for reviews, see K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975), and L.P. Kadanoff, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic Press, London, 1974), Vol. 5a, p. 1]. For applications to spin systems and lattice gauge theories, see R. Jullien, J. Fields, and S. Doniach, Phys. Rev. Lett. **38**, 1500 (1977); S.D. Drell,

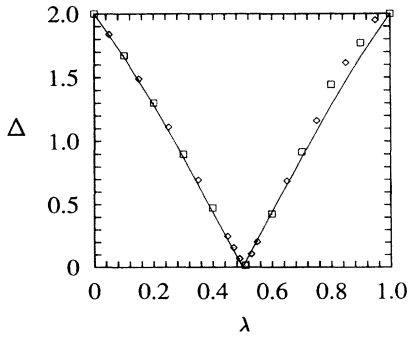

FIG. 2. Mass gap estimates Δ against λ. The diamonds and squares indicate CORE estimates obtained using T_1^{16} and T_2^{12}, respectively. The exact mass gap appears as a solid curve.

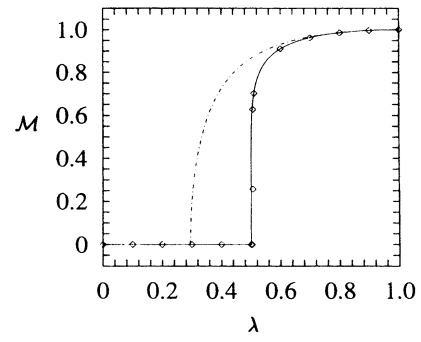

FIG. 3. Magnetization $\mathcal{M}$ against λ. The diamonds indicate CORE estimates obtained using T_2^{12}, the solid curve shows the exact magnetization, and the dot-dashed curve shows the estimates from mean-field theory.

B. Svetitsky, and M. Weinstein, Phys. Rev. D **17**, 523 (1978); S. D. Drell and M. Weinstein, *ibid.* **17**, 3203 (1978); D. Horn and S. Yankielowicz, Nucl. Phys. **B161**, 533 (1979); D. Horn, M. Karliner, and S. Yankielowicz, *ibid.* **B170**, 467 (1980); D. Horn and M. Weinstein, Phys. Rev. D **25**, 3331 (1982).

[2] R. Jullien, J. N. Fields, and S. Doniach, Phys. Rev. B **16**, 4889 (1977); K. Uzelac, P. Pfeuty, and R. Jullien, Phys. Rev. Lett. **43**, 805 (1979); J. Rabin, Phys. Rev. B **21**, 2027 (1980); J. B. Bronzan and R. L. Sugar, Phys. Rev. D **21**, 1564 (1980); S. Ben-Menahem, *ibid.* **26**, 455 (1982); J. Abad, J. G. Esteve, and A. F. Pacheco, *ibid.* **32**, 2729 (1985); G. Lana, *ibid.* **38**, 1954 (1988); S. R. White and R. M. Noack, Phys. Rev. Lett. **68**, 3487 (1992); S. R. White, *ibid.* **69**, 2863 (1992); S. R. White, Phys. Rev. B **48**, 10 345 (1993).

[3] R. Jullien, P. Pfeuty, J. N. Fields, and S. Doniach, Phys. Rev. B **18**, 3568 (1978); A. Pacheco, Phys. Rev. D **19**, 3173 (1979); M. Aelion and M. Weinstein, Report No. SLAC-PUB-2460, 1980 (unpublished); H. R. Quinn and M. Weinstein, Phys. Rev. D **25**, 1661 (1982).

[4] D. Horn, W. G. J. Langeveld, H. R. Quinn, and M. Weinstein, Phys. Rev. D **38**, 3238 (1988); C. Stubbins, *ibid.* **44**, 488 (1991).

[5] Marvin Weinstein, Phys. Rev. D **47**, 5499 (1993).

[6] Colin J. Morningstar, Phys. Rev. D **46**, 824 (1992), and references cited therein; see also C. Domb, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic Press, London, 1974), Vol. 3, p. 1.

[7] P. Pfeuty, Ann. Phys. (N.Y.) **57**, 79 (1970).