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CORE—A New Computational Technique for Lattice Systems*

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ABSTRACT

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 to any desired degree of accuracy. It is complementary to standard Monte Carlo methods and incorporating dynamical fermions presents no problems. The method is tested using the 1+1-dimensional Ising model.

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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. Its virtues are: it is systematically improvable to any desired degree of accuracy; it is a variational procedure which can produce an upper bound on the energy of the lowest eigenstate of the Hamiltonian in any sector of the theory defined by a distinguishable set of quantum numbers; it applies to lattice systems of infinite extent allowing one to directly study phase structure and critical phenomena; it provides tools for checking convergence and estimating the size of contributions which have not yet been computed; it requires modest computer resources by modern standards; it is complementary to standard Monte Carlo methods; incorporating dynamical fermions presents no new problems.

We start with a brief description of the method, then apply two variants of the CORE approximation to the 1+1-dimensional Ising model. Numerical results are presented for each calculation. A comparison of these calculations demonstrates the flexibility of the CORE approach. A thorough discussion of these results and convergence properties of the method is deferred to a later paper.

Description of the Method In the limit $t \to \infty$, the operator e^{-tH} *contracts* any trial state $|\Phi_{\text{var}}\rangle$ onto the lowest eigenstate of H with which it has a non-vanishing overlap. Therefore, the expectation value

$$\mathcal{E}(t) = \frac{\langle \Phi_{\text{var}} \, | e^{-tH} H e^{-tH} | \, \Phi_{\text{var}} \rangle}{\langle \Phi_{\text{var}} \mid e^{-2tH} \mid \Phi_{\text{var}} \rangle} \tag{1}$$

tends to the corresponding eigenvalue ϵ_0 of H as t becomes large. In general, $\mathcal{E}(t)$ cannot be computed exactly. Reliably approximating $\mathcal{E}(t)$ and other similar matrix elements is the primary goal of the CORE method.

The first step in building a CORE approximation to $\mathcal{E}(t)$ is to construct a computable operator $T(t)$ which closely approximates e^{-tH} for t in some range $0 < t < t_{max}$. To find

such an operator, 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, follow the approach of Ref. [1] and rewrite e^{-tH} as a symmetric product

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

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

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

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

$$\det\left(\llbracket T(t) H T(t) \rrbracket - \lambda \llbracket T(t)^2 \rrbracket\right) = 0, \tag{4}$$

where $\llbracket \ldots \rrbracket$ denotes truncation to the subspace spanned by the $|\phi_j\rangle$ states. In particular, for a given 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

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

This operator plays a key role in the CORE approach.

To simplify the computation of $H_{\rm eff}(t)$, one partitions the lattice into separate blocks and chooses a trial state which is a tensor product of identical block states. Truncating the

Hilbert space on a block-by-block basis allows the efficient evaluation of $H_{\text{eff}}(t)$ by the finite *cluster* method. In this method, $H_{\text{eff}}(t)$ (or any other *extensive* quantity) is calculated as a specific sum of finite-volume contributions. A general statement of the cluster method has been given in Ref. [2] and references cited therein; only a brief description can be presented here. Evaluation of $H_{\text{eff}}(t)$ by the finite cluster method is accomplished in the following sequence of steps. First, compute $H_{\text{eff}}(t)$ on a sub-lattice which contains only a single block. This yields all of the so-called range-one terms in the cluster expansion of the effective Hamiltonian. Next, calculate $H_{\text{eff}}(t)$ for a theory defined on a sub-lattice made up of two adjacent (*connected*) blocks. The range-two contributions to the cluster expansion are obtained by removing from the two-block calculation those contributions which arise from terms already included in the single-block calculation. Repeat this procedure for sub-lattices containing successively more connected blocks, then sum the connected contributions from these sub-lattices with weights given by the number of ways each sub-lattice 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}. The finite cluster method is simple to implement, provides numerous means of detecting computational errors, and does little or no harm to the variational bound in $\mathcal{E}_T(t)$.

The cluster expansion of $\mathcal{E}_T(t)$ converges rapidly, except near a critical point where the correlation length of the system becomes large. Near such a point, choosing a starting state having significant overlap with the exact ground state is crucial to improving the convergence of the cluster expansion. Fortunately, there exists an iterative procedure which allows simultaneous construction of a good trial state and the cluster-expansion computation of $\mathcal{E}_T(t)$ in that state. This procedure, which we refer to as a Hamiltonian real-space renormalization group (RG) method because of its similarity to the approach used in Ref. [3], treats the problem of infinite volume and vanishing mass gap quite successfully.

Our real-space renormalization group method develops H_{eff} by successive thinning of degrees of freedom. First, one specifies the RG algorithm by deciding how to partition the lattice into blocks of sites and which states on each block to eliminate. The Hilbert space is

then thinned by a truncation to the same chosen subset of states on each block and $H_{\text{eff}}(t)$ is calculated using the cluster expansion. The last step in this initial RG transformation is to select a best value for t. This can be done in a number of ways. For example, one can extract the coefficient of the identity operator in H_{eff} and vary t to minimize this quantity. Better yet, one can evaluate H_{eff} in a simple product state to produce a mean-field estimate of the ground state energy and minimize this with respect to t. Once a best $t = t_1^*$ is chosen and an effective Hamiltonian $H_{\text{eff}}^{(1)}(t_1^*)$ is obtained, the above procedure is repeated, constructing a new contractor $T^{(1)}(t)$ to approximate $\exp[-tH_{\text{eff}}^{(1)}(t_1^*)]$. Thus, the renormalization group procedure generates a sequence of effective Hamiltonians $H_{\text{eff}}^{(n)}(t_n^*)$, where

$$H_{\text{eff}}^{(n+1)}(t) = R_n(t)[\![T^{(n)}(t)H_{\text{eff}}^{(n)}(t_n^*)T^{(n)}(t)]\!]R_n(t), \tag{6}$$

and $R_n(t) = [\![T^{(n)}(t)^2]\!]^{-1/2}$. As the recursion proceeds, the effective Hamiltonian evolves eventually into a simple form which can be trivially diagonalized, yielding an estimate of the ground state energy.

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 being multiplied will be sparse and so one can exploit efficient algorithms for carrying out these computations, resulting in even greater economies of time and memory usage.

Excited States and Matrix Elements There are many ways of extracting the energies of excited states in a CORE calculation. If one retains r states per block in the RG algorithm, then about $r/2$ energy levels may be reliably obtained from the excited-state energies of the effective Hamiltonian $H_{\text{eff}}^{(n)}(t_n^*)$ for n sufficiently large. One can also construct an operator Ω such that $|\Phi_{\text{var}}\rangle$ and $\Omega\,|\Phi_{\text{var}}\rangle$ do not mix under H and $T(t)$ and $\Omega = \sum_b e^{i\boldsymbol{p}\cdot\boldsymbol{x}_b}\,\Omega(b)$, where b labels blocks, $\boldsymbol{p}$ is a momentum label, $\boldsymbol{x}_b$ is the position vector associated with block b, and the operator $\Omega(b)$ acts only on the single block b. Then the energy gap Δ_Ω associated with Ω is given by a ratio of extensive quantities $\Delta_\Omega = \langle M_\Omega(t)\rangle \;/\; \langle Z_\Omega(t)\rangle$, where

$$Z_\Omega(t) = [\![T(t)^2]\!]^{-1/2}[\![\Omega^\dagger T(t)^2\Omega]\!][\![T(t)^2]\!]^{-1/2}, \tag{7}$$

$$H_\Omega(t) = [\![T(t)^2]\!]^{-1/2}[\![\Omega^\dagger\, T(t)HT(t)\Omega]\!][\![T(t)^2]\!]^{-1/2}, \tag{8}$$

$$M_\Omega(t) = H_\Omega(t) - \frac{1}{2}\left\{Z_\Omega(t),\ H_{\text{eff}}(t)\right\}, \tag{9}$$

and $\langle \ldots \rangle$ denotes evaluation in the ground state of H_{eff}. Each of the operators $M_\Omega(t)$ and $Z_\Omega(t)$ has a cluster expansion and can be developed using the same sequence of RG transformations as for $H_{\text{eff}}^{(n)}(t_n^*)$.

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

The 1+1-Dimensional Ising Model The Ising model in $1+1$ dimensions is often used as a testing ground for new calculational methods. The Hamiltonian in this model is given by

$$H_{\text{Ising}} = -\sum_j \left[c_\lambda \sigma_z(j) + s_\lambda \sigma_x(j)\sigma_x(j+1)\right], \tag{10}$$

where j labels the sites in the infinite 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 of the system is unique and the order parameter $\langle \sigma_x(j) \rangle = 0$. When $\lambda > 1/2$, the system has a twofold-degenerate ground state corresponding to values of the order parameter given by $\langle \sigma_x(j) \rangle = \pm(1 - \cot^2(\lambda\pi/2))^{1/8}$.

In any application of the CORE method, one must choose a contraction operator $T(t)$, a renormalization group algorithm, a method of determining the optimal value of t in each RG step, and the truncation order to use in the cluster expansion of $H_{\text{eff}}(t)$. Symmetry, the choice of RG algorithm, and the truncation order used in the cluster expansion determine the general form of the effective Hamiltonian. Here, we test the CORE approximation in two different applications to the Ising model. In both applications, we chose an RG algorithm in which the Hilbert space is truncated to the lowest two eigenstates in each block. We also chose to truncate the cluster expansion of $H_{\text{eff}}(t)$ after two- and three-block clusters. For these choices, the effective Hamiltonian in this model takes the general form

$$H_{\text{eff}}(t) = -\sum_{\alpha} c_\alpha(t) V_\alpha, \tag{11}$$

$$V_\alpha = \sum_i O_\alpha(i), \tag{12}$$

$$O_\alpha(i) = \sigma_{\alpha_0}(i)\sigma_{\alpha_1}(i+1)\ldots\sigma_{\alpha_r}(i+r), \tag{13}$$

where $c_\alpha(t)$ are the couplings, α labels the different types of operators V_α, and i 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 $O_u(i) = \sigma_u(i) = 1$ and $O_z(i) = \sigma_z(i)$. There are three two-site operators: $\alpha^{(2)} = \{xx, yy, zz\}$. The three-site operators are $\alpha^{(3)} = \{xzx, xux, xxz, zxx, yzy, yuy, yyz, zyy, zuz, zzz\}$.

In our first application, we used a contraction operator given by $T_1(t) = S_1^\dagger(t)S_1(t)$, where $S_1(t) = \prod_\alpha U_\alpha(t)$ and $U_\alpha(t) = \prod_i [1 + \tanh(c_\alpha t/2)O_\alpha(i)]$. The operators in this product were ordered according to their site range, increasing in size from right to left. For the RG algorithm, two-site blocking was used and the Hilbert space was truncated to the lowest two eigenstates in each block. In each RG step, t was chosen to minimize the mean-field energy density of $H_{\text{eff}}(t)$. Calculations were done using $T_1^n(t/n)$ for various values of n and truncating the cluster expansion of $H_{\text{eff}}(t)$ after two- and three-block clusters.

For our second application of the CORE method, the lattice was divided into blocks containing three sites and the Hilbert space was again truncated to the lowest two eigenstates in each block. We used 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 intra-block interactions and V contains all inter-block 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 p labels the blocks. The operators $H_b(p)$ and $V(p)$ can be exponentiated numerically with no difficulty. We fixed t by minimizing the expectation value of H_{eff} in a mean-field state. Calculations were done using $T_2^n(t/n)$ for various values of n and stopping the cluster computation after two- and three-block clusters.

Selected estimates E_0 of the ground-state energy density from both variants of the CORE approach described above are compared to the exact energy density ϵ_0 in Fig. 1. 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 Δ_{exact} in Fig. 2. In this figure, the difference between the CORE estimates and the exact gap is denoted by $\delta_\Delta = \Delta - \Delta_{\text{exact}}$. Fig. 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 $\ln\mathcal{M}$ to 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. Using larger blocks or including more terms in the cluster expansion should significantly improve this result.

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 easily applied to systems containing dynamical fermions, systems which resist treatment by present stochastic means. Another is the fact that by a suitable choice of truncation algorithm, one can use the techniques introduced in this paper to generate *effective Hamiltonians* for the composite particles of a theory. For example, one could truncate the small-block problem in lattice QCD to the lowest-lying hadronic states and then develop the Hamiltonian computed in this subspace using the CORE approximation. The CORE approach should also be useful for investigating resonance phenomena. 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.

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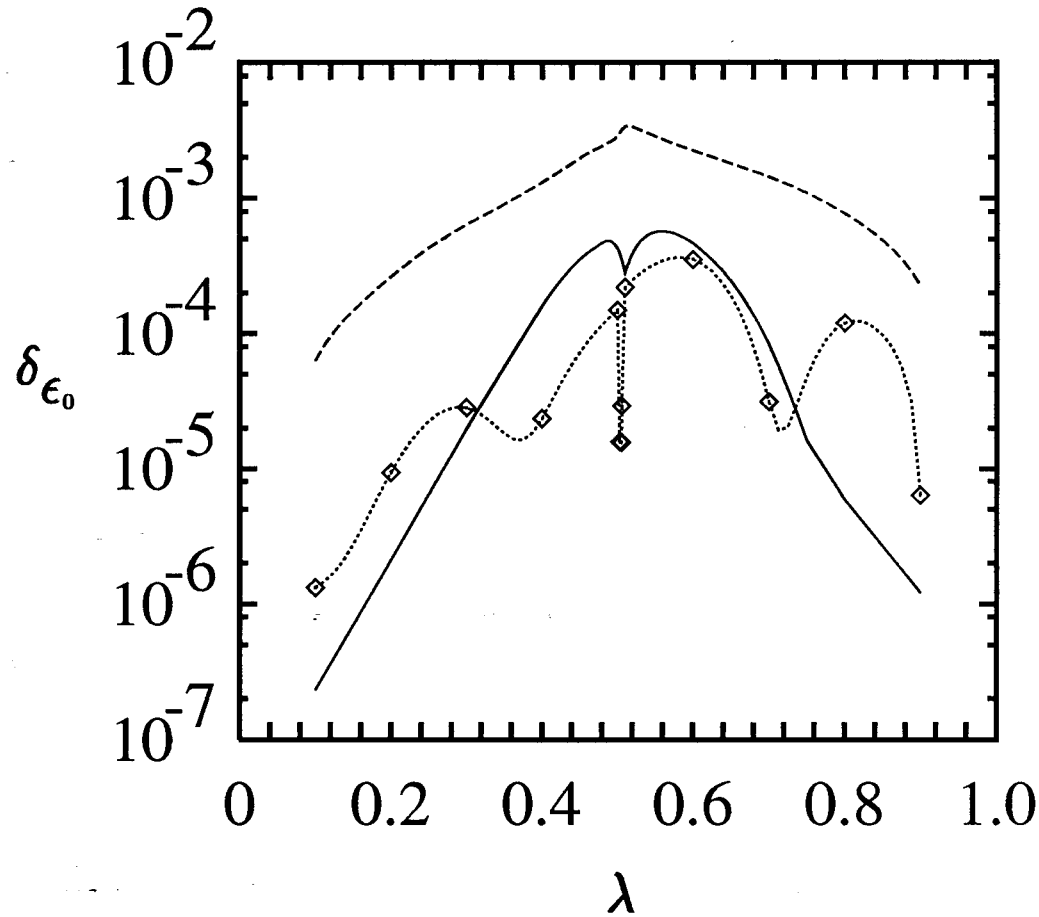

FIG. 1. Fractional error δ_{ϵ_0} in the ground-state energy density estimates against λ. Results using T_1^2 (dashed curve), T_1^{16} (solid), and T_2^{12} (dotted) are shown.

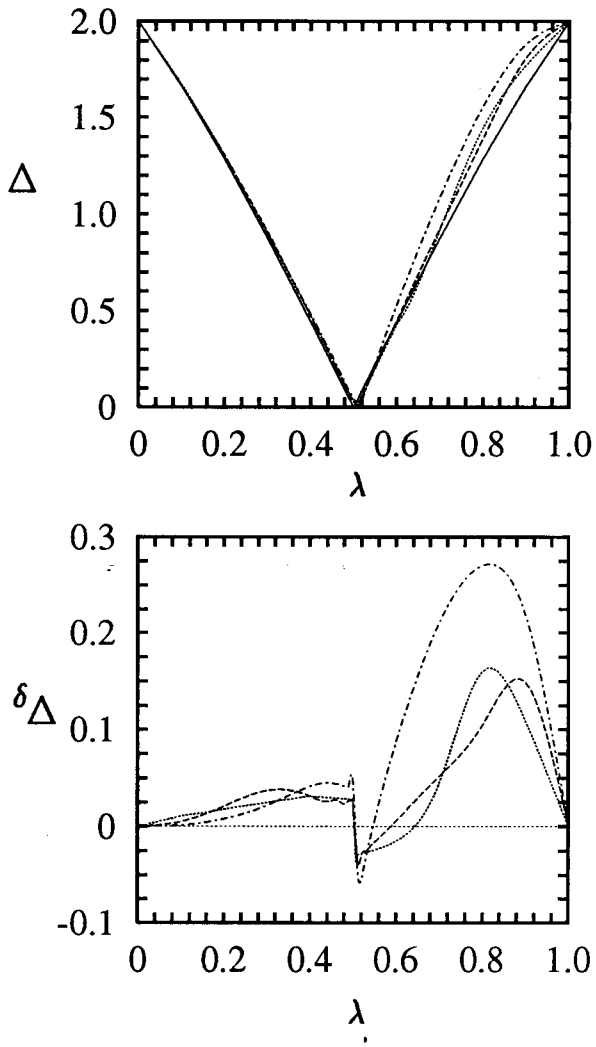

FIG. 2. (a) Mass gap estimates Δ against λ. (b) Differences δ_Δ between mass gap estimates and exact results against λ. Results using T_1^2 (dot-dashed curve), T_1^{16} (dashed), and T_2^{12} (dotted) are shown. The exact mass gap appears as a solid curve in (a).

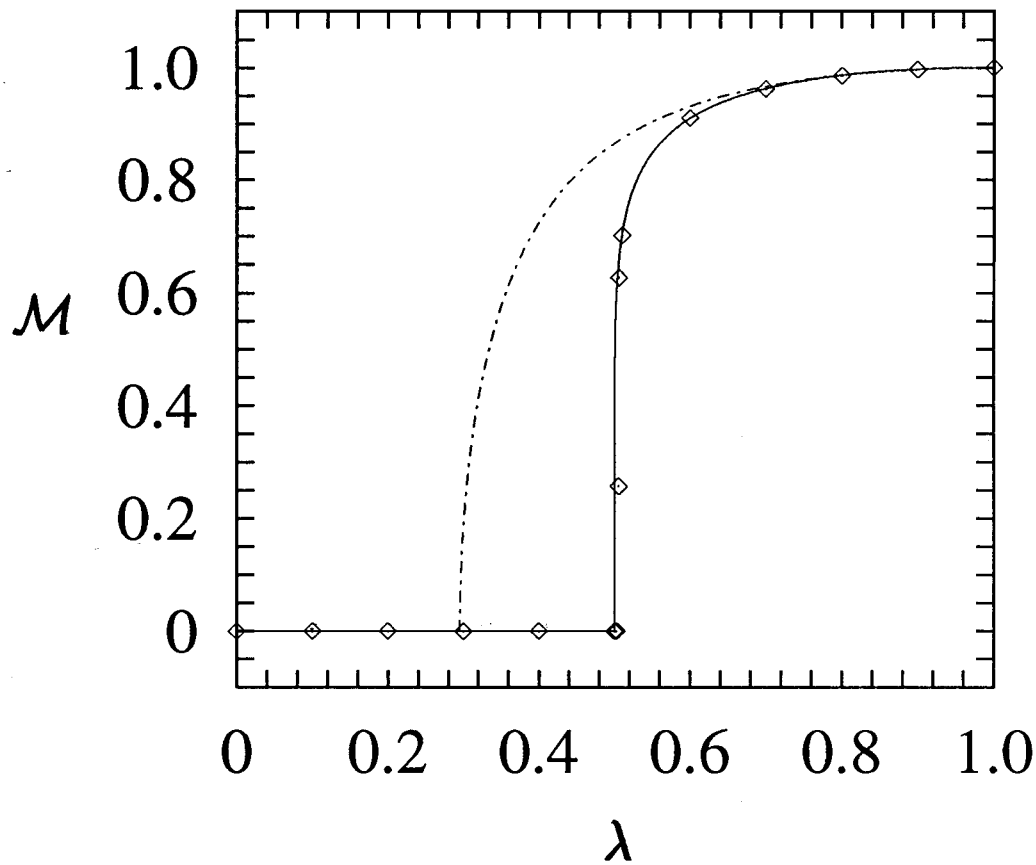

FIG. 3. Magnetization $\mathcal{M}$ against λ. The diamonds indicate CORE estimates obtained using T_2^{12}, the solid curve shows the exact magnetization, and the dot-dashed curve shows the estimates from mean-field theory.