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Approximate Solutions for Large Transfer Matrix Problems

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A new approach is proposed for the determination of the dominant eigenvalues and their corresponding eigenvectors for one-spin transfer matrices. The matrices describe properties of spin systems on semi-infinite lattices. The method gives approximate solution for lattices of widths larger than previously tractable. © 1989 Academic Press, Inc.

The classic transfer matrix formalism has been most useful in yielding numerical results for lattice models that are not exactly soluble [1–4]. The standard procedure is to apply phenomenological renormalization to solutions of lattices which are infinite in one direction but finite in the other directions, e.g., in two dimensions, a strip of width n. From the determination of the leading eigenvalues $(\lambda_1 > \lambda_2 \geqslant \cdots)$ of the transfer matrix, one derives the free energy per lattice site F_n and the correlation lenghth ξ_n, where

$$F_n = -\ln(\lambda_1) \tag{1}$$

$$\xi_n^{-1} = \ln(\lambda_1/\lambda_2). \tag{2}$$

Then the application of finite size scaling yields the critical exponents and phase structure of the truly infinite system ($n \to \infty$ limit). More particulary, we have shown [5–6] how the critical properties of spin lattice systems may be calculated in terms of the duo-diagonal, sparse matrices of the type introduced by Kramers and Wannier [7-8]. The formulation is quite general [9], including two-, three-, and higher dimensional lattices as well as allowing nearest, next-nearest, and more distant neighbor interactions.

The difficulty in implementing the method is not its formulation but rather lies in the practical problems of large-scale computation. In the present work, we describe these problems and propose a new approach to their resolution. Although further work is needed, the basic principles appear to be sound.

The matrices we are interested in are extremely sparse: they have exactly two nonzero elements in every row and column. Their size is $2^n \times 2^n$, where n is as large

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as allowed by practical restrictions of computation such as storage space in memory and CPU time (closely related to money). The nonzero matrix elements are distributed in a pattern, characteristic of the nature of the interaction: (a) nearest neighbor, next-nearest neighbor, etc.; (b) dimensionality of the lattice. For example, the 2-dimensional Ising system gives rise to a transfer matrix of the form ($n = 3$)

$$M = \begin{bmatrix} a_1 & 0 & 0 & 0 & a_2 & 0 & 0 & 0 \\ a_3 & 0 & 0 & 0 & a_4 & 0 & 0 & 0 \\ 0 & a_1 & 0 & 0 & 0 & a_2 & 0 & 0 \\ 0 & a_3 & 0 & 0 & 0 & a_4 & 0 & 0 \\ 0 & 0 & a_3 & 0 & 0 & 0 & a_4 & 0 \\ 0 & 0 & a_5 & 0 & 0 & 0 & a_6 & 0 \\ 0 & 0 & 0 & a_3 & 0 & 0 & 0 & a_4 \\ 0 & 0 & 0 & a_5 & 0 & 0 & 0 & a_1 \end{bmatrix}. \tag{3}$$

The precise pattern is not essential for starting the mathematical problem, which is to find the largest eigenvalue(s) and the associated eigenvector(s) of the transfer matrix. The maximal eigenvalue λ_1 is simply the partition function per unit spin, and the knowledge of λ_1, allows one to determine the energy per spin, specific heat, etc. Knowledge of the associated eigenvector may be used to determine the magnetization, susceptibility, etc. The second largest eigenvalue then fixes the correlation length. All this is well known; we are concerned here with demonstrating the usefulness of a method for handling the very large matrices that arise in such problems.

The (sparse) transfer matrices have simple properties that are independent of the particular spin lattice model they describe. These are

(1) Duo-diagonal (described above).

(2) A few numbers appear in a repetitive pattern. For example, for the 2-dimensional nearest neighbor interaction model with a magnetic field H, six (not all independent) numbers suffice for fixed H and temperature T.

(3) The maximal eigenvalue is real, positive, and isolated; the other eigenvalues are complex, in general, since the matrix is not symmetric (although it is real).

It is conventional to use the classic "power" method of iteratively determining the maximal eigenvalue and its eigenvector. Because of the points (1) and (2) above, there is no need to store the matrix as a whole, and in fact there is no need to use ordinary matrix multiplication. A simple algorithm is sufficient for obtaining the $(n+1)$th iterate for the eigenvector from the nth. Because of point (3) above, the procedure converges to the desired result; the speed of convergence (the number of iterations) is determined by the nearness of the next largest eigenvalue since the error is of order $(\lambda_2/\lambda_1)^p$ for p iterations. Since $\lambda_2 \to \lambda_1$ as a phase boundary is

approached, the method is poorest there. Nevertheless, even there, $|\lambda_2| < \lambda_1$ for a finite lattice, so the procedure converges, just slowly (and the larger the lattice, the slower).

The limitation we encountered, however, was due to the length of the vectors being multiplied (and so that of the eigenvectors sought) rather than to the size of the matrix itself. The vector dimension of 2^n for $n \gtrsim 12$ led to a rapidly growing number of arithmetic operations and was, furthermore, limited by the CYBER bound of $2^{16} - 1$ on vector dimension. This latter constraint may be avoided (awkwardly) but the former comes into play in any event. Now, it is true that the maximal eigenvectors are rather sparse, in general. That is to say, only a small number of elements are "large" so long as the temperature and magnetic field are chosen such that the system is in an ordered phase. In our calculations we never made use of this information. For physical reasons, we are only interested in the dominant eigenvalues and the largest elements (and their positions) in the corresponding eigenvectors. By using the standard power method, we were multiplying and adding—most of the time—very small, uninteresting elements of the vectors. How can this be avoided?

The idea is to modify the power method as follows:

(1) Choose an arbitrary, sparse initial vector. For example, choose n_e elements of the vector u_1 to have value 1, and the remaining elements zero. Clearly, only n_e reals (the elements of u_1) and n_e integers (the indices corresponding to the nonzero elements of u_1) need to be stored at this step.

(2) Multiply u_1 by the (sparse) matrix M: $w_2 \equiv Mu_1$. Because of the simple structure of M—namely, because it has only two nonzero elements in every column —this will generate only $2 \times n_e$ nonzero elements in the vector w_2. That is, at this step, we are storing $2 \times n_e$ integers and $2 \times n_e$ reals.

(3) Sort the elements of the vector w_2 by magnetude, keeping track of the indices (that is, tag the elements). Employ an appropriate criterion to choose half of the elements to form the new iterate (u_2) for the approximate eigenvector; the vector u_2 will have n_e elements, with n_e indices.

(4) Repeat steps (1), then (3) in an analogous fashion for the transpose of the matrix, M^{T}, and its eigenvector v with maximal eigenvalue (also λ_1, of course).

(5) Compute the Rayleigh quotient at the ith iteration

$$R_i = \frac{(v_i, Mu_i)}{(v_i, u_i)} \tag{4}$$

and test for convergence. If the convergence criterion is satisfied, stop; R_i is the computed value of λ_1 and u_i, v_i are right and left eigenvectors of M. If the convergence criterion is not satisfied, return to step (2) and proceed analogously, using u_i, v_i as the new starting vectors.

(6) Using the resulting eigenvectors, compute the energy, spin configuration probabilities, etc. as usual.

There are two ambiguous points above: (a) the convergence criterion, referred to in (5), and (b) the selection criterion, referred to in (3). We have used the convergence criterion of requiring that the partition function (the logarithm of the eigenvalue), computed in three successive iterations, not vary by more than 10^{-12}. This is somewhat arbitrary; a much stronger constraint would be meaningless in view of the ever present round-off errors, while a weaker one might give spurious results that depended on choice of starting vectors (step (1) above). Clearly, there is some flexibility here. The choice of a selection criterion is not so straightforward and deserves some discussion.

The most obvious selection criterion is to choose the elements of the vector $w_2 = Mu_1$ of largest magnitude to form the next iterate, u_2. We have found that this gives reasonable results, but biases the physics in an undesirable way. That is, the spin configuration probabilities computed with this criterion guiding the algorithm are far from translation invariant. The problem arises essentially because of end effects of the finite lattice.

We give a specific example to illustrate this point. Suppose we are computing the approximate eigenvectors u, v for an Ising lattice of width 12 and we are using only $n_e = 2^5$ elements; suppose further that we choose $H = 0$ and $T \ll T_c$, so we are deep in the ferromagnetic phase. Then the most probable spin configurations are all aligned (2 such) and one spin flipped (24 such). The elements of the exact eigenvectors u, v with indices corresponding to the one-flip configurations are almost all equal—but not all. The ones corresponding to the configurations with an end spin flipped are quite different from the ones corresponding to an interior spin flipped (perhaps an order of magnitude larger or smaller). So the "largest magnitude" selection criterion does not pick up these elements in both approximate eigenvectors u and v. Thus, the spin configuration probabilities are found to be essentially equal for *almost* all the one-flip states but some configurations are simply missed, since the probabilities are simply the products of the corresponding elements of u and v (appropriately normalized).

As a consequence, we have used a somewhat more sophisticated convergence criterion. What we do is as follows. First multiply the right eigenvector approximation u_1 by M to get w_2, as described above. Then multiply the left eigenvector approximation v_1 by M^{T} to get the analogue of w_2, which we call x_2. Use the simple (largest magnitude) criterion to extract the next iterate v_2. The extraction of the next iterate u_2 from w_2 is done in two steps. First search for nonzero elements of w_2 which have indices that match those in the new vector v_2. If this fills all n_e available positions in u_2, we are done with this step; otherwise, choose the elements in w_2 of largest magnitude that have not already been chosen to complete the new vector u_2. In this way, all spin configurations that are physically related will be represented—if n_e is large enough to accomodate them, of cource. If n_e is less than the maximum (2^n), naturally this cannot always be true. However, the missing spin configurations are those with the smallest probabilities.

To illustrate these points, we display in Table I the results of computation of the maximal eigenvector for the simple 2-dimensional Ising lattice with a strip width of

TABLE I

The Maximal Eigenvector for the Isotropic Square 2-Dimensional Ising Lattice for $N = 8$

Index	Exact (n_e=256)	n_e=128	n_e=64	n_e=32
1	1.000 000 000 000	1.000 000 000 000	1.000 000 000 000	1.000 000 000 000
17	0.018 321 787 227	0.018 321 787 227	0.018 321 781 034	0.018 321 776 904
9	0.018 321 787 227	0.018 321 787 227	0.018 321 783 098	0.018 321 778 967
5	0.018 321 787 227	0.018 321 787 227	0.018 321 785 161	0.018 321 781 030
33	0.018 321 787 227	0.018 321 787 227	0.018 321 778 971	0.018 321 774 841
65	0.018 321 787 227	0.018 321 787 227	0.018 321 776 907	0.018 321 772 777
3	0.018 321 787 226	0.018 321 787 226	0.018 321 787 223	0.018 321 783 093
2	0.018 321 785 164	0.018 321 785 164	0.018 321 785 160	0.018 321 785 157
97	0.000 335 800 502	0.000 335 800 502	0.000 335 800 310	0.000 335 574 974
49	0.000 335 800 501	0.000 335 800 501	0.000 335 800 348	0.000 335 575 012
25	0.000 335 800 501	0.000 335 800 501	0.000 335 800 386	0.000 335 575 050
13	0.000 335 800 500	0.000 335 800 500	0.000 335 800 423	0.000 335 575 087
7	0.000 335 800 499	0.000 335 800 499	0.000 335 800 461	0.000 335 575 125
4	0.000 335 800 423	0.000 335 800 423	0.000 335 800 423	0.000 335 575 163
81	0.000 335 687 928	0.000 335 687 928		
41	0.000 335 687 923	0.000 335 687 928	0.000 335 575 164	
21	0.000 335 687 923	0.000 335 687 927	0.000 335 575 201	
11	0.000 335 687 923	0.000 335 687 926	0.000 335 575 239	
73	0.000 335 687 890	0.000 335 687 890		
37	0.000 335 687 889	0.000 335 687 889		
69	0.000 335 687 889	0.000 335 687 889		
19	0.000 335 687 889	0.000 335 687 889		
35	0.000 335 687 889	0.000 335 687 889		
67	0.000 335 687 889	0.000 335 687 889		
128	0.000 335 687 888	0.000 335 687 888	0.000 335 687 737	0.000 335 687 509
6	0.000 335 687 888	0.000 335 687 888	0.000 335 575 277	
10	0.000 335 687 850	0.000 335 687 850		
66	0.000 335 687 850	0.000 335 687 850		
18	0.000 335 687 850	0.000 335 687 850		
34	0.000 335 687 850	0.000 335 687 850		
127	0.000 012 298 777	0.000 012 298 778	0.000 012 298 768	
113	0.000 006 156 782	0.000 006 156 782	0.000 006 154 562	
57	0.000 006 156 744	0.000 006 156 744	0.000 006 154 562	
29	0.000 006 156 706	0.000 006 156 706	0.000 006 154 562	
15	0.000 006 156 668	0.000 006 156 668	0.000 006 154 564	
8	0.000 006 152 628	0.000 006 152 628		
105	0.000 006 152 618	0.000 006 152 618		
89	0.000 006 152 618	0.000 006 152 618		
53	0.000 006 152 580	0.000 006 152 580		
45	0.000 006 152 580	0.000 006 152 580		

Note. The approximate eigenvector computed with n_e elements is shown for $n_e = 32$, 64, and 128 (as well as the exact result $n_e = 256$). Only the largest elements in the exact result and the corresponding elements in the approximations are given. The temperature $T = 0.5$ and the magnetic field $H = 0$.

$n = 8$. The eigenvector dimension is $2^8 = 256$; however, for $T = 0.5$ the system is deep in the ferromagnetic region of the phase diagram, so only a very few spin configurations are important. This implies that only a few eigenvector elements are significant, so we give in Table I only the largest of these. In the first two columns are the index and corresponding element of the exact eigenvector; in subsequent columns are the corresponding elements of the approximate eigenvector computed using the indicated number (n_e) of elements. Since (taking $H = 0$) the vector is symmetric, $u(i) = u(2^n - i + 1)$, only values of $i \leqslant 128$ are presented. It is clear from Table I that for such a low temperature only a very few elements of the eigenvector are significant. Recall that physical quantities—matrix elements—are in general

much less sensitive to variations in parameters than are eigenfunctions; uncertainties in eigenfunctions are propagated only in higher order in the matrix elements. We will briefly discuss this below. For the moment, we would simply note that an examination of Table I shows that as n_e is increased the exact eigenvector is approached in a regular fashion; that the most significant elements are found even for a value of n_e which is only 1/8 the dimension of the eigenvector.

One does not expect this extremely simple situation to persist as a phase boundary is approached that leads to a rapid increase in the number of configurations that must be considered. For the Ising model, the boundary of the ferromagnetic phase is such a place; how does our approximation behave in this case? In Table II we present the results of calculation for the same system as in Table I except that here we have set the temperature $T=2.0$, close to the transition temperature $T_c=2.269...$. Again, in Table II the same quantities are given as in Table I; however, as expected, the method is no longer so powerful. It is no longer true that only a few eigenvector elements are dominant (whatever precisely one means by that word). Nevertheless, it is apparent that the approximate eigenvectors are cap-

TABLE II

Same as Given Table I, except the Temperature $T=2.0$, near the Phase Boundary

Index	Exact (n_e=256)	n_e=128	n_e=64	n_e=32
1	1.000 000	1.000 000	1.000 000	1.000 000
65	0.451 134	0.433 336	0.383 327	0.367 540
33	0.449 530	0.434 114	0.392 138	0.375 006
17	0.448 434	0.436 940	0.401 152	0.382 624
9	0.447 381	0.439 787	0.410 373	0.392 396
5	0.445 944	0.439 765	0.419 806	0.398 326
3	0.442 795	0.437 124	0.429 456	0.406 418
2	0.431 183	0.427 302	0.420 693	0.414 673
97	0.243 794	0.210 867	0.188 939	0.135 210
49	0.240 702	0.211 797	0.193 282	0.137 957
25	0.238 193	0.217 372	0.197 725	0.140 759
13	0.235 370	0.222 939	0.202 270	0.143 619
7	0.230 644	0.220 457	0.206 919	0.146 537
4	0.217 484	0.209 069	0.200 804	0.149 513
81	0.216 332	0.185 267		
41	0.213 826	0.179 124		
21	0.211 455	0.195 071		
73	0.209 351	0.174 658		
11	0.208 026	0.199 440	0.150 968	
37	0.206 795	0.179 216		
69	0.206 632	0.170 685		
128	0.204 517	0.192 140	0.169 849	0.150 096
67	0.204 350	0.174 481		
19	0.203 627	0.183 984		
35	0.203 105	0.175 151		
6	0.199 485	0.193 406	0.154 438	
66	0.198 191	0.183 894		
34	0.196 335	0.179 123		
10	0.196 191	0.188 118	0.150 968	
18	0.185 765	0.179 721		
127	0.176 362	0.157 170	0.137 695	
113	0.161 746	0.127 168	0.101 011	
57	0.156 205	0.130 447	0.103 333	
29	0.150 972	0.133 873	0.105 708	

TABLE III

Spin Configuration Probabilities for the Same System as That of Tables I and II

Configuration	Exact (n_e=256)	n_e=32
++++++++	0.499 999 549	0.499 999 549
-+++++++	5.632×10^{-8}	5.631×10^{-8}
++++++-	5.632×10^{-8}	5.632×10^{-8}
+-++++++	5.631×10^{-8}	5.631×10^{-8}
++-+++++	5.631×10^{-8}	5.631×10^{-8}
+++-++++	5.631×10^{-8}	5.631×10^{-8}
++++-+++	5.631×10^{-8}	5.631×10^{-8}
+++++-++	5.631×10^{-8}	5.631×10^{-8}
++++++-+	5.631×10^{-8}	5.631×10^{-8}

Note. Only the most probable configurations are given. The temperature $T=0.5$ and the magnetic field $H=0$.

TABLE IV

Spin Configuration Probabilities for the Same System as That of Tables I and II

Configuration	Exact (n_e=256)	n_e=128	n_e=64	n_e=32
++++++++	0.368 045	0.383 144	0.401 939	0.423 867
-+++++++	0.011 940	0.011 472	0.010 566	0.008 596
++++++-	0.011 940	0.011 552	0.010 566	0.009 582
+++-++++	0.009 993	0.009 945	0.008 955	0.008 538
++++-+++	0.009 993	0.009 940	0.008 955	0.008 518
++-+++++	0.009 985	0.009 877	0.008 955	0.008 557
+++++-++	0.009 985	0.009 871	0.008 955	0.008 499
+-++++++	0.009 950	0.009 764	0.008 955	0.008 577
++++++-+	0.009 950	0.009 813	0.008 955	0.008 479
--++++++	0.003 539	0.002 965	0.002 642	
++++++--	0.003 539	0.002 970	0.002 127	0.001 125
+++--+++	0.002 826	0.002 435	0.002 127	0.001 132
++--++++	0.002 822	0.002 435	0.002 127	0.001 135
++++--++	0.002 822	0.002 429	0.002 127	0.001 130
+--+++++	0.002 801	0.002 347	0.002 127	0.001 138
+++++--+	0.002 801	0.002 397	0.002 127	0.001 127

Note. Only the most probable configurations are given. The temperature $T=2.0$ and the magnetic field $H=0$.

turing the essential characteristics of the system even at this elevated temperature. Let us be more precise about this and discuss the calculation of physical quantities.

At low temperatures, when the system is essentially always in a single configuration, the method gives precise results with n_e quite small. This was seen in Table I and is reflected as well in Table III, which gives the probabilities for the most likely spin configurations. There we only display results for the exact solution and for the crudest ($n_e = 32$) approximation, since even in this latter case the results are essentially exact. On the other hand, at a higher temperature ($T = 2.0$), the situation is more complex, as seen in Table IV. It is clear that in order to extract physically meaningful results, some method of extrapolation is required. Of course, for the exact eigenfunctions and eigenvalues, since the very lattice itself, being finite, is necessarily an approximation to the problem of interest. Consequently, an extrapolation scheme is needed which takes approximate solutions to approximating lattice systems to obtain results for the infinite lattice system. This is a separate issue and will be taken up at a later time.

In a low-temperature phase, i.e., far below the critical point, the correlation length will be only a few lattice spacings and so will be small compared to the system size. One might therefore expect a conventional finite-lattice approximation to be adequate and see no need for the scheme developed here. Indeed, one may question whether our approach applied to a system of size larger than n_e is any better than the exact (numerical) eigensolution of the transfer matrix for a lattice of $\ln_2 (n_e)$ sites. We turn now to an examination of this question.

In Table V we present the results of calculation of the free energy per lattice site, F_n, for the Ising model at temperature $T = \frac{1}{2}T_c \approx 1.135$ and for a variety of lattice sizes (n) as well as dimensions of approximating vectors (n_e). The exact solution for each finite lattice lies on the diagonal $n_e = 2^n$ and is underlined; the conventional approach would be to compute some physical quantity (the free energy, energy, magnetization,...) as a function of n for $n_e = 2^n$ and extrapolate appropriately to infinite n. The present scheme is more complex in that extrapolation is done in the 2-dimensional parameter space (n_e, n). The most obvious generalization of the

TABLE V

Values of the Partition Function for the Same System as in Preceding Tables, with Temperature $T = \frac{1}{2}T_c$ and Various Choices for the Lattice width (n) and the Number of Approximating Elements (n_e)

n_e \ n=	7	8	9	10	11	12	16	20
2^5	1.763 663 851	1.763 659 772	1.763 658 903	1.763 631 520	1.763 630 723	1.763 629 928	1.763 602 135	1.763 628 334
2^6	1.763 667 724	1.763 664 205	1.763 663 817	1.763 662 151	1.763 660 417	1.763 659 565	1.763 653 033	1.763 623 648
2^7	1.763 669 740	1.763 668 488	1.763 668 141	1.763 666 436	1.763 664 756	1.763 663 893	1.763 658 797	1.763 653 692
2^8	--	1.763 668 685	1.763 668 446	1.763 668 299	1.763 668 103	1.763 667 933	1.763 664 460	1.763 658 676
2^9	--		1.763 668 471	1.763 668 418	1.763 668 389	1.763 668 375	1.763 667 784	1.763 667 405
2^{10}	--			1.763 668 428	1.763 668 416	1.763 668 399	1.763 668 340	1.763 668 020
2^{11}					1.763 668 416	1.763 668 415		
						1.763 668 416		

standard method would be to extrapolate along a line of fixed ratio $n_e/2^n$. It appears from the table that such an extrapolation procedure might be possible, but would not be as smooth for smaller ratios than for a ratio of unity (corresponding to exact solution for each strip with n). What is the origin of the irregular behavior? We argue here that it arises from the treatment of subdominant spin configurations: their neglect or inclusion for various n_e.

The dominant spin configurations for $T=\frac{1}{2}T_c$ is of cource totally aligned, since we are in the ferromagnetic region of the phase diagram. The subdominant configurations are modifications of this one in which there is one kink–antikink pair, two such pairs, etc. For example, with $n=8$, the dominant configuration is $[+++++++++]$; the next most important configurations are $[++++++++-]$ and its related partners (see Tables III and IV for temperatures $T=0.5$, 2.0). It is a simple exercise to count the number of such configurations for any given n; results are presented in Table VI. Now, an examination of Table V reveals sudden jumps in the approximate free energy for fixed n around certain values of n_e. For example, for $n=8$ there is a jump when n_e is increased from 2^6 to 2^7. Refering to Table VI, we see that for $n=8$ one requires at least $n_e=74$ to account for two kink–antikink pairs, so we may attribute the improvement in the calculation of F_n to the inclusion of these configurations. A similar jump for $n=9$, 10 occurs for the same n_e values and has the same explanation. This argument is confirmed by examining $n=11$: the jump now occurs when n_e is increased from 2^7 to 2^8, and the minimum value of n_e needed to account for two kink–antikink pairs for $n=11$ is 134. Similarly, for $n=20$, the jump occurs for n_e increasing from 2^8 to 2^9, while the minimum n_e needed for $n=20$ is 380. Table VI indicates that the number of these configurations grows much more slowly than does the total number of configurations. For example, there are about seven times more configurations with up to three kink–antikink pairs for $n=20$ than for $n=10$, but over 1000 times more total congigurations.

The lessons to be learned from this exercise are that the method is useful for situations in which only a few spin configurations are important; that the precision will worsen in a manner which can be well understood by enumeration of subdomi-

TABLE VI

Number of Spin Configurations with *at most* n_k Kink–Antikink Pairs, for Various Choices of the Lattice Width n

n_k \ n	7	8	9	10	11	12	16	20
2	58	74	92	112	134	158	274	380
3	128	186	260	352	464	598	1120	2280
4		256	512	772	1124	1588	3640	9690
5				1024	2048	3172	8736	31008
6						4096	16016	77520

nant configurations; finally, that the most probable configurations are relatively easy to extract even for large n, but the neglect of the contribution of large numbers of low-probability configurations will lead to controlled errors in estimation of physical quantities.

The effect of projecting out only certain vector components varies with the physical quantity being computed. For example, if spin configuration probabilities are being computed, then there is not much loss of precision. However, if the partition function (maximal eigenvalue) is desired, then one computes the Rayleigh quotient, R_i, of Eq. (4); this requires one further multiplication, and thus one further projection. The ratio must be computed by first determining the intersection of the sets of indices for the vectors v_i, u_i, and Mu_i and then computing the ratio R_i by restricting the inner products to this common index set. Clearly, this does not make use of all the information known of the eigenvectors, but it is a conservative method of physical quantities (such as energy per site, correlations) which require additional multiplications will lead to yet more deterioration in precision. To illustrate the point, consider the application of the method for temperature $T = 0.99T_c$, $n = 12$, and $n_e = 1024$, i.e., only 1/4 the dimension of the exact solution eigenvector. We find that when convergence occurs there are 1000 matching indices in vectors u_i and v_i, but only 882 matching indices of these vectors and these of Mu_i; thus only 882 elements are used in computing R_i, which means 142 elements are computed but not used there. The dominant configurations are spins all aligned, one spin flipped, two neighboring spins flipped, and three spins in a row flipped. In Table VII we give some results which allow comparison of the method with exact diagonaliza-

TABLE VII

Comparison of Results for $n_e = 1024$ with Those for Exact Diogonalization ($n_e = 4096$), for $n = 12$ and Temperatures near the Critical Temperature T_c

$T = 0.95T_c$, $n = 12$	$n_e = 1024$	$n_e = 4096$
Free energy	0.963 595	0.966 177
Energy	1.672	1.570
All spins aligned	0.547	0.486
1 spin flip	0.247	0.235
2 spins in row flipped	0.076	0.079
3 spins in row flipped	0.023	0.031
$T = 0.99T_c$, $n = 12$	$n_e = 1024$	$n_e = 4096$
Free energy	0.933 318	0.937 874
Energy	1.617	1.446
All spins aligned	0.467	0.375
1 spin flipped	0.255	0.226
2 spins in row flipped	0.090	0.090
3 spins in row flipped	0.040	0.049

tion, for a particulary poor choice of temperatures $T=0.95T_c$, $0.99T_c$. We see that even very near T_c roughly 1% of all spin configurations make up 80% or so of the configuration probabilities. The partition function is determined to better than a percent while the energy is only good to 10%, as expected. The spin configuration probabilities are qualitatively correct (the most important are identified), while the projection of large components of the eigenvectors skews the probabilities towards the dominant ones: the purely aligned and one flip configurations are overestimated, the three spins in a row flipped are underestimated.

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