PHYSICAL REVIEW
LETTERS

VOLUME 68 | 15 JUNE 1992 | NUMBER 24

Real-Space Quantum Renormalization Groups

S. R. White and R. M. Noack
Department of Physics, University of California, Irvine, California 92717
(Received 20 January 1992; revised manuscript received 27 April 1992)

Although originally thought to show great promise in solving quantum many-body problems on a lattice, numerical real-space renormalization-group techniques have had little success for such problems. We explore the nature of the difficulties involved by studying the application of the method to the simple tight-binding model in one dimension. The standard approach fails dramatically for this model. We show that the key to successfully applying the renormalization-group technique lies in applying a variety of boundary conditions to a block in order to simulate the effect of neighboring blocks.

PACS numbers: 05.30.Fk, 05.70.Fh, 71.10.+x

Shortly after Wilson's dramatic success in solving the Kondo problem with a numerical renormalization-group (RG) method [1], there was considerable excitement about the possibility of applying the same type of approach in a real-space form to a variety of difficult quantum lattice problems. These real-space RG techniques quickly developed a bad reputation, however, after several different applications of the methods gave poor results. For example, Lee [2] applied a real-space RG technique to the problem of Anderson localization on a two-dimensional square lattice. The major conclusion of this study, that there was a critical parameter that separated scaling towards extended or localized states, later was shown by Lee and Fisher [3] to be incorrect. RG studies of other systems, such as the one-dimensional (1D) Hubbard model [4], also gave poor results, and today the technique is little used. It has not been very well understood why the method fails.

In this Letter [5] we examine real-space RG methods for an extremely simple model, a 1D tight-binding lattice. The importance of understanding real-space RG in the context of this model was pointed out by Wilson several years ago in an informal, unpublished talk. The standard RG approach fails spectacularly in this model, and it is quite easy to see why. Here, in addition to showing why it fails, we provide several closely related variations of the standard approach which perform extremely well. Although the calculations reported here are for this very simple model, we believe the problem is generic and the general type of solution we give can be applied to virtually any quantum lattice model.

We consider a 1D chain of sites i with the single-particle Hamiltonian matrix

$$H_{ij}=\begin{cases}2, & i=j,\\ -1, & |i-j|=1,\\ 0, & \text{otherwise}.\end{cases} \tag{1}$$

This problem is equivalent in the continuum limit to a 1D particle in a box.

The standard real-space RG approach consists of considering a group of sites to be a "block," and diagonalizing that block to find a set of eigenstates. One then truncates the set of eigenstates, keeping only the lowest m states (ordered by energy), and uses those states to construct an approximate Hamiltonian for a new, larger block composed of two of the old blocks. At each iteration s we can write the Hamiltonian of the infinite chain as a block tridiagonal matrix in terms of diagonal blocks H^s and off-diagonal blocks T^s,

$$H=\begin{pmatrix} H^s & T^s & 0 & 0 & \cdots \\ T^{s\dagger} & H^s & T^s & 0 & \cdots \\ 0 & T^{s\dagger} & H^s & T^s & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}. \tag{2}$$

Initially, the block size is 1 and H^1 and T^1 are 1×1 matrices equal to 2 and -1, respectively. We start iteration s by forming the Hamiltonian matrix for a block composed of two blocks from the previous iteration

$$\bar{H}^s = \begin{pmatrix} H^{s-1} & T^{s-1} \\ (T^{s-1})^\dagger & H^{s-1} \end{pmatrix} \quad (3)$$

and

$$\bar{T}^s = \begin{pmatrix} 0 & 0 \\ T^{s-1} & 0 \end{pmatrix}. \quad (4)$$

We diagonalize $\bar{H}^s$ and take the lowest m eigenvalues E_l^s and eigenstates V_l^s, $l=1,\ldots,m$, discarding the rest. We then perform a change of basis to the eigenstates via

$$H_{ll'}^s = \sum_{i,j} V_{li}^s \bar{H}_{ij}^s V_{l'j}^s \quad (5)$$

and

$$T_{ll'}^s = \sum_{i,j} V_{li}^s \bar{T}_{ij}^s V_{l'j}^s . \quad (6)$$

Note that Eq. (5) puts H^s into diagonal form. We then proceed to the next iteration, starting with Eqs. (3) and (4). The idea is that the higher-energy states which are discarded at the current iteration are unimportant in making up the low-energy states at a later iteration. The accuracy can be increased by keeping more states, i.e., increasing m.

It is easy to see in this simple example, however, that this procedure is quite *poor* in describing large-scale, low-energy behavior. The Hamiltonian in this example is just a finite-difference discretization of the kinetic energy of a 1D particle, and in the limit of large block size, the eigenstates are just particle-in-a-box eigenstates. The boundary condition of ignoring the connections T to neighboring blocks corresponds to setting the wave function to 0 at the sites just outside the block. Figure 1 illustrates the difficulty. Any state made only of low-lying states from the previous iteration must have a "kink" in the middle. In order to accurately represent states in the larger block, one must make use of nearly all the states in the smaller block: Any truncation leads to large errors.

Wilson suggested one possible way to cure this problem. He suggested integrating out the higher-energy states via a unitary transformation, taking into account the interactions with other blocks perturbatively rather than ignoring them. (This approach is closely related to degenerate perturbation theory.) Ingersent and White [6] recently tried a variety of ways of implementing this, but were unable to find a satisfactory approach. We now believe that the set of low-lying states kept in the standard approach is too incomplete for the perturbative unitary transformation to help.

The key to fixing this simple example lies in the treatment of boundary conditions (BCs). However, simply choosing an alternative set of BCs is not adequate. The standard approach uses BCs in which the eigenstates vanish (in the large block limit) at the edges of a block. We call this type of BCs "fixed." Because fixed BCs must be used on the inside edges whenever two blocks are to be joined, fixed BCs are the most natural kind to use. However, the RG procedure can be modified to use other kinds of BCs. The alternative BCs would be used in forming the matrix that is diagonalized in order to determine the eigenfunctions V to be kept, but fixed BCs must still be used on the inner edges in forming larger blocks. Although H^s in Eq. (5) is no longer diagonal, the procedure is still well defined in the sense that it is exact when all states are kept at each iteration.

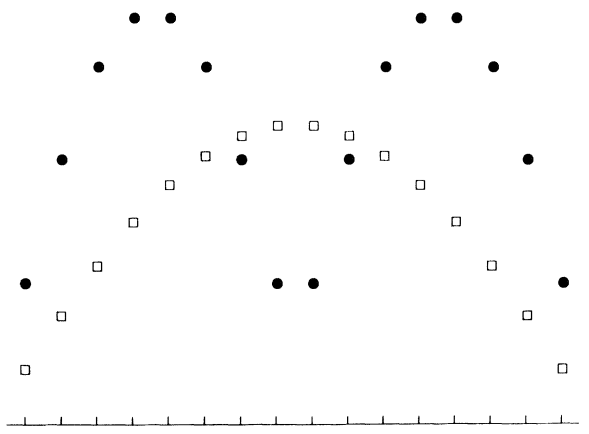

FIG. 1. Lowest eigenstates of two 8-site blocks (solid circles) and a 16-site block (open squares) for the one-dimensional tight-binding model with fixed boundary conditions.

One finds, however, that applying the RG procedure with BCs other than fixed does not eliminate the difficulties. For example, using periodic BCs results in the low-lying eigenstates being identical at the two edges, which prevents the accurate representation of anything but the ground state (which for periodic BCs is a constant function) on larger blocks. "Free" boundary conditions (obtained by changing H_{ii} from 2 to 1 on the edges) result in the slope of the eigenstate vanishing at the edges, and again excited states on larger blocks cannot be represented.

In order to obtain a working approach, we must *combine* eigenstates obtained from different boundary conditions. The block must be diagonalized several times, with different boundary conditions each time. We then extract a few low-lying eigenstates from each diagonalization, orthogonalize them, and keep this set of states for the next iteration. To be more specific, the following "fixed-free" procedure solves the simple problem almost exactly for fixed boundary conditions, in the sense that a finite number of the lowest energies of large blocks is obtained almost exactly even after many iterations, keeping only a few states at each iteration. This method uses the four possible combinations of free and fixed BCs at the two edges of each block. We keep track of four H matrices at each iteration, $\bar{H}_{b,b'}^s$, where b represents the left edge and takes on the values free or fixed, and b' similarly represents the right edge. For example, for an initial two-site block one would have

$$H^1_{\text{free,fixed}} = \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}. \quad (7)$$

We diagonalize $\bar{H}^s_{\text{free,fixed}}$ and extract the lowest $m/4$ eigenstates. Similarly, we extract the lowest $m/4$ eigenstates for $\bar{H}^s_{\text{free,free}}$, $\bar{H}^s_{\text{fixed,free}}$, and $\bar{H}^s_{\text{fixed,fixed}}$. This set of m states is not orthogonal, so we next orthonormalize them. This set of states forms the new basis, taking the place of the V^s_l, $l=1,\ldots,m$. (The orthogonal complement to these states are the states that are discarded.) We next perform a change of basis on the matrices $\bar{T}^s$ and $\bar{H}^s_{b,b'}$, as in Eq. (6). Finally, for the next iteration, we replace Eq. (3) by

$$\bar{H}^s_{b,b'} = \begin{pmatrix} H^{s-1}_{b,\text{fixed}} & T^{s-1} \\ (T^{s-1})^\dagger & H^{s-1}_{\text{fixed},b'} \end{pmatrix}. \quad (8)$$

Note the use of fixed BCs for the inner edges when joining two blocks together.

Table I compares the results of this procedure with the standard one. The eigenvalues of $\bar{H}^s_{\text{fixed,fixed}}$ are shown for the new procedure. A total of eight states ($m=8$) were kept for both procedures. Whereas the results from the standard procedure bear little relationship to the exact results, we find that the new procedure yields energies for the first four states even after ten (or more) iterations accurate to nine digits with 64-bit precision.

The lesson to be learned from this example is that the influence of the surrounding blocks not taken into account in the current iteration is to effectively apply a variety of boundary conditions to the current block. Hence, any approach using one set of boundary conditions on a block generates a set of states which is in some sense "incomplete," and it is very difficult to correct this incompleteness by keeping many states or by applying perturbative corrections.

Higher-energy states can also be found using the fixed-free method. In particular, if we are interested in states near a particular energy, we keep the m states at each iteration that is closest to that energy. Table II compares results for states at the center of the band using the fixed-free method with exact results and keeping fixed BCs only. We keep sixteen states at each iteration. The fixed-free results are accurate to nine digits, while the fixed BC results are quite inaccurate. This shows the general principle of keeping states from a variety of boundary conditions is also important for higher-energy states for which the wave function is rapidly varying in space.

The fact that the fixed-free method performs so well is not an accident specific to this problem or this choice of BCs. Accurate results are also obtained using the combination of periodic and antiperiodic BCs. For periodic or antiperiodic BCs, the matrix elements at the corners of the blocked Hamiltonian matrix are affected by the boundary conditions. In order to perform the real-space blocking transformation, one has to keep track of two additional off-diagonal matrices, T^s_{P} and T^s_{AP}, for periodic and antiperiodic BCs, in addition to T^s. One diagonalizes the blocked Hamiltonian

$$\bar{H}^s_b = \begin{pmatrix} H^{s-1} & T^{s-1}_b \\ (T^{s-1}_b)^\dagger & H^{s-1} \end{pmatrix} \quad (9)$$

for both periodic ($b=\text{P}$) and antiperiodic ($b=\text{AP}$) boundary conditions, keeps $m/2$ states from each BC, and orthonormalizes the resulting states. This set of states is then used to transform $\bar{H}^s$ and $\bar{T}^s$, formed using Eqs. (3) and (4), to the new basis.

The new off-diagonal matrices can be formed from the T^{s-1} using

$$\bar{T}^s_b = \begin{pmatrix} 0 & \pm(T^{s-1})^\dagger \\ T^{s-1} & 0 \end{pmatrix} \quad (10)$$

and then transformed to the new basis as in Eq. (6). Here the positive sign is for periodic BCs and the negative sign for antiperiodic BCs. Table III compares the energies of the lowest four eigenstates using this method for periodic BCs with the exact results and with renormalization-group results for which only periodic boundary conditions are kept. The results are calculated after ten iterations of the renormalization group, keeping eight states at each iteration.

A third approach to varying the BCs involves putting extra blocks around the block of interest. One diagonalizes a larger system containing p blocks (a "superblock"), where $p>2$, but with only *one* type of BC (typically periodic). Two of these blocks will form a larger block for the next iteration. The idea is that the surrounding blocks apply a variety of BCs to the block of interest. We

TABLE I. Lowest energies after ten blocking transformations for the noninteracting single particle on a 1D chain with fixed boundary conditions.

	Exact	Standard	Fixed free
E_0	2.3508×10^{-6}	1.9207×10^{-2}	2.3508×10^{-6}
E_1	9.4032×10^{-6}	1.9209×10^{-2}	9.4032×10^{-6}
E_2	2.1157×10^{-5}	1.9214×10^{-2}	2.1157×10^{-5}
E_3	3.7613×10^{-5}	1.9217×10^{-2}	3.7613×10^{-5}

TABLE II. Energies in the center of the band after ten blocking transformations for the noninteracting single particle on a 1D chain with fixed boundary conditions. Energies are measured relative to the band center.

	Exact	Standard	Fixed free
ΔE_{1023}	-4.5997×10^{-3}	-5.7054×10^{-3}	-4.5997×10^{-3}
ΔE_{1024}	-1.5332×10^{-3}	-4.0785×10^{-3}	-1.5332×10^{-3}
ΔE_{1025}	1.5332×10^{-3}	4.0785×10^{-3}	1.5332×10^{-3}
ΔE_{1026}	4.5997×10^{-3}	5.7054×10^{-3}	4.5997×10^{-3}

TABLE III. Lowest energies after ten blocking transformations for the noninteracting single particle on a 1D chain with periodic boundary conditions.

	Exact	Periodic only	Periodic antiperiodic
E_0	0.0	0.0	0.0
E_1	9.4124×10^{-6}	2.1281×10^{-3}	9.4161×10^{-6}
E_2	3.7649×10^{-5}	5.3888×10^{-3}	3.7659×10^{-5}
E_3	8.4711×10^{-5}	9.1936×10^{-3}	8.4732×10^{-5}

extract m states from the diagonalization of the superblock, then project out the portion of each wave function corresponding to the two spatial blocks of interest. The system size doubles at each iteration. For $p=2$, this procedure is equivalent to the conventional procedure for periodic BCs (results for which are given in Table III, column 2). As in the other methods, these projected states must be orthogonalized before they can be used to transform the Hamiltonian matrices.

The results for the superblock procedure are summarized in Table IV for various values of p, after ten iterations, keeping eight states at each iteration. The results are reasonably accurate even for $p=3$, and become more accurate for larger p. The $p=20$ results are accurate to ten decimal places, suggesting that this procedure becomes exact in the large-p limit.

In devising a procedure such as the three we have described here, it is important to make sure that the variation of the boundary conditions is sufficiently broad. For example, if one uses the superblock method with antiperiodic BCs, one finds that the ground state is not accurately obtained, but that excited states are. This is because the states kept are missing any very-low-momentum component. However, if one adds one extra state, the zero-momentum state $V_i=$const, to the list of states kept at each iteration, the method becomes even more accurate than the periodic BC superblock method.

The next challenge is to discover how to apply the general ideas discussed here to more difficult models, such as the localization model studied by Lee [2], or interacting models, such as the 1D Hubbard model. We believe the most promising method of the three we have described here is the superblock method, since one does not have to choose what BCs to apply—in a sense, the system does it for us. For interacting problems in particular, there may be many-body states of the system where one particle has a node in its wave function at the edge of a block and another particle has an antinode at the same edge. For this case, any combination of single-particle BCs, like fixed and free, would probably not work. Of course, for interacting problems, the superblock method is very difficult for large p. One can envision hybrids of the superblock method with other variations of the BCs, such as the periodic-antiperiodic method, in order to keep the number of extra blocks to a minimum.

TABLE IV. Average relative errors in the lowest three excited-state energies after ten blocking transformations for periodic boundary conditions using the superblock method with p blocks.

p	Average error (%)
3	5
4	0.08
5	0.002
6	0.0005
20	10^{-8}

We would like to thank K. Ingersent for a number of helpful discussions and collaboration. We would also like to thank S. Coppersmith and D. R. Hamann for helpful comments and suggestions. This work was supported by the Office of Naval Research under Grant No. N00014-91-J-1143 and in part by the University of California through an allocation of computer time on the UC Irvine Convex.

[1] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[2] P. A. Lee, Phys. Rev. Lett. **42**, 1492 (1979).
[3] P. A. Lee and D. S. Fisher, Phys. Rev. Lett. **47**, 882 (1981).
[4] J. W. Bray and S. T. Chui, Phys. Rev. B **19**, 4876 (1979); S. T. Chui and J. W. Bray, Phys. Rev. B **18**, 2426 (1978); J. E. Hirsch, Phys. Rev. B **22**, 5259 (1980); C. Dasgupta and P. Pfeuty, J. Phys. C **14**, 717 (1981).
[5] Parts of this work have appeared in S. R. White, in Proceedings of the International Meeting on Computational Physics for Condensed Matter Phenomena, Osaka, October, 1991 (to be published).
[6] K. Ingersent and S. R. White (unpublished).