Use of the recursion method in the study of disordered systems

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Applied to the determination of the density of states of disordered systems, the recursion method permits the local Green's function to be written as a continued fraction. We examine the effect that truncating this fraction has upon the local Green's function and present a means of reducing this effect. Further, a self-consistent approach for obtaining the local Green's function is developed. This approach is shown to be suitable for the study of disordered systems.

I GENERAL CONSIDERATIONS

The mathematical problems involved in the study of disordered systems are complicated ones primarily in that the matrix describing the physics of the disordered system is infinite and irreducible. One approach is a numerical one which usually starts with truncating the system matrix to a finite but large size and then applying direct methods such as Dean's method of negative mode counting to determine the distribution of eigenvalues.[1] However, computational difficulties prevent the studies of really large systems so that the approach to infinite systems can never be fully explored.

On the other hand, if the Green's-function approach is used, one needs to determine the diagonal elements of the resolvent operator to obtain the eigenvalues. For this purpose, the recursion method developed by Haydock, Heine, and Kelly[2] is very useful because the matrices for disordered systems are usually sparse matrices in the representation of local basis vectors.

It should be noted that for a finite system, there is really no appreciable advantage to using the recursion method rather than direct methods since the transformed (tridiagonal) matrix is still an $N \times N$ matrix. However, for an infinite system, the local Green's function can be expressed as a continued fraction in the transformed (tridiagonal) representation.

The coefficients in the continued fraction at a given level depend only on the properties of the particles enclosed within a sphere of observation defined by the shell r (see Fig. 1). As the continued fraction is developed, the situation is equivalent to an enlargement of the "sphere of observation". At any given step of the development, the number of particles included in the sphere of observation is always larger than the number of steps needed to reach the boundary of the sphere. Since it is known that the eigenmodes for disordered systems may be either fairly localized or fairly extended, it may happen that at a certain step further enlargement of the sphere of observation will not add any new feature to the results. In this situation the corresponding local Green's function has exhibited a trend toward convergence. It is this particular characteristic of the recursion method which makes it well suited for the study of disordered systems.

In this work we examine use of the recursion method in the study of disordered systems. Emphasis will be placed on the effect of truncation of the continued fraction on the properties of the system, a possible way to reduce that effect, and a proposal of a method which provides a self-consistent scheme to study all aspects of disordered systems.

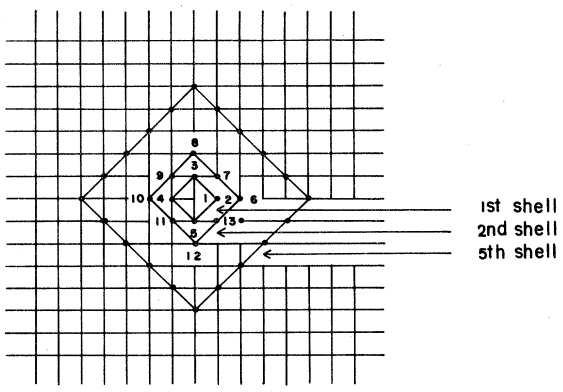

FIG. 1. Two-dimensional square lattice in the recursion representation.

II. THE EFFECT OF TRUNCATION OF THE LOCAL GREEN'S FUNCTION ON THE DISTRIBUTION OF THE EIGENVALUES

One of the advantages in using the recursion method is that the number of particles within a given shell, N, is always larger than the shell number. For localized states, convergence of the local Green's function can be expected to occur for a reasonably small shell number, r. One way to proceed with the calculation then is to truncate the continued fraction at that shell. Indeed, it is expected that such a procedure will be sufficient to obtain all the information desired about those states (but only for those states). However, some states can be quite extended and for those convergence of the local Green's function will not occur unless r becomes large enough to include all important correlations. Computing time and the progress of errors in the computer calculation makes the truncation scheme a very unattractive scheme to follow in those situations.

But, there is another factor to be considered when the continued fraction is truncated. This is the effect of truncation on the eigenvalues obtained. In order to study this effect, we shall use a concrete example of the dynamics of a two-dimensional square lattice.

Consider a two-dimensional periodic square lattice with nearest-neighbor interactions. The matrix equation describing the dynamics of the system may be written

$$MU=\lambda U\ . \tag{1}$$

In the system of reduced units of $\gamma/m=1$ (γ is the force constant and m is the mass), the smallest nontrivial matrix is

$$M=\begin{bmatrix} A & -1 & -1 & -1 & -1 \\ -1 & A & 0 & 0 & 0 \\ -1 & 0 & A & 0 & 0 \\ -1 & 0 & 0 & A & 0 \\ -1 & 0 & 0 & 0 & A \end{bmatrix}, \tag{2}$$

where $A=4$. The solution to the eigenvalue problem defined by Eq. (2) gives the following normal modes: $\omega^2=4$ (threefold degenerate), $\omega^2=2$, and $\omega^2=6$. If one plots the histogram of the eigenvalue distribution (Fig. 2), one sees that it agrees very well with the known frequency spectrum[3] of the two-dimensional square lattice considering the fact that only five particles are included in the consideration.

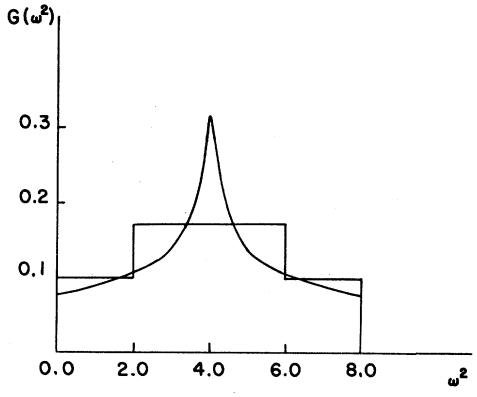

FIG. 2. Frequency spectrum of a periodic two-dimensional square lattice: Histogram represents a "five-particle" system; the solid curve represents the exact calculation.

Next we proceed to apply the recursion method to the matrix given by (2). In the new representation the matrix is tridiagonal with diagonal elements a_k and off-diagonal elements b_k. The local Green's function for the system $R_{00}(\omega^2)$ may now be written as a continued fraction:

$$R_{00}(\omega^2)=\cfrac{1}{(a_0-\omega^2)-\cfrac{b_1}{(a_1-\omega^2)-\cfrac{b_2}{\ddots}}}\ . \tag{3}$$

For the periodic two-dimensional square lattice as shown in Fig. 1, it can be shown that all the $a_k=A$. The coefficients b_k are given in Table I.

By examining Fig. 1 and Table I, it appears that up to the first shell all the information about the first five particles is included in the consideration. One might then expect to be able to obtain all the information about the eigenvalue problem of the

TABLE I. Coefficient b_r for a periodic square lattice.

r	b_r
1	4.000
2	5.000
3	3.800
4	4.305
5	3.873
6	4.169
7	3.908
8	4.114
9	3.929
10	4.085

five-particle system [Eq. (2)] by truncating the local Green's function, R_{00}, at the first shell. However, in doing so, one finds that the poles of R_{00} occur at $\omega^2=2$ and $\omega^2=6$, and apparently the degenerate mode at $\omega^2=4$ is not recovered. One might think that only two roots are found because truncation at the first level actually corresponds to considering a 2×2 matrix and that the complete picture for a five-particle system would be obtained by going to the fourth level before truncating. (The fourth level would yield a 5×5 transformed matrix.)

However, if the local Green's function is truncated at $r=4$, one finds that the poles of $R_{00}^{(4)}$ occur at $\omega^2=0.4$, 1.96, 4, 6.05, and 7.6. The frequency spectrum of the five-particle system is distorted; the two modes at $\omega^2=2$ and $\omega^2=6$ are shifted somewhat, the degeneracy at $\omega^2=4$ is removed, and two new modes appear at $\omega^2=0.4$ and $\omega^2=7.6$. A histogram constructed from these data shows no resemblence to the frequency spectrum of the two-dimensional square lattice. The reason for these changes is that there are actually 41 particles included in the sphere of observation when the continued fraction is truncated at the fourth shell ($r=4$). The mixing of the information about the particles in the three outer shells with the five particles in the inner shell apparently is responsible for the changes. Thus, it is important to note that *in the transformed representation simple truncation at any given step can result in a distorted picture of the system* except for those states where the trend of convergence of the local Green's function is established. *Simple truncation in the transformed tridiagonal representation is quite different from the truncation in the original representation.* Hence, extreme care must be exercised when using the truncation scheme in the recursion method, especially for those states which are not very localized. Some other scheme is needed if one is interested in obtaining a complete and accurate picture of the disordered system.

III. THE CONVERGENCE OF THE LOCAL GREEN'S FUNCTION

We have showed that if one is interested in the total picture of a disordered system (rather than just the limited region of very localized states), simple truncation of the continued fraction used for the local Green's function can often present a distorted picture of the system. Before attempting to devise a scheme to remedy the situation, we first examine how the truncated local Green's function behaves as r increases in different frequency regions.

We first consider the dynamics of a two-dimensional randomly and isotopically disordered binary system with 10% light impurities ($M_L/M_H=\frac{1}{3}$). The impurity configuration is randomly generated and is shown in Fig. 3. The coefficients a_r, b_r and the truncated local Green's function $R_{00}^{(r)}$ are calculated for different frequency regions. Some of the results are shown in Tables II and III. It is interesting to note that from $\omega^2=0$ to $\omega^2=7.5$, $R_{00}^{(r)}$ has not shown any trend of convergence for r up to $r=30$. However, at $\omega^2=7.85$ and beyond, the local Green's function has definitely demonstrated convergence. This indicates that there is no need to be beyond the 30th shell to determine the properties of these modes. The normal modes beyond $\omega^2=7.85$ are localized modes with localization lengths equal to or shorter than the length defining the 30th shell. We have also calculated the local Green's function at $\omega^2=13.5$ which is in the neighborhood of a prominent impurity mode[4] (outside the main band defined by $0<\omega^2<8$). It can be seen that this mode is indeed very localized (with localization restricted within the first shell).

The results of these calculations clearly indicate that for localized modes simple truncation at the level of convergence can determine the properties of these modes because the local Green's function has reached convergence. However, for the major part of the spectrum, the likelihood of $R_{00}^{(r)}$ reaching convergence for small r is remote. For these

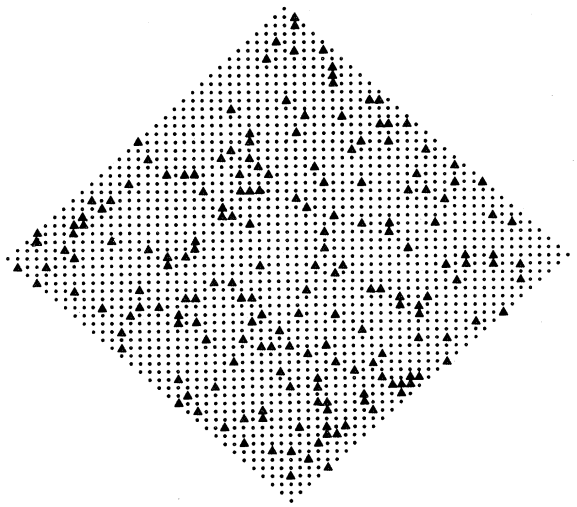

FIG. 3. Randomly generated two-dimensional binary system. The triangles represent the impurity atoms at 10% concentration.

TABLE II. Coefficients $(a_r-\omega^2)$ and the truncated local Green's function $R_{00}^{(r)}$ for the random configuration shown in Fig. 3 at $\omega^2=5.0$.

r	$a_r-\omega^2$	b_r	$R_{00}^{(r)}$
1	−1.000	4.000	0.333
2	−1.000	5.000	−0.500
3	−1.000	3.800	2.294
4	−0.674	4.305	−0.326
5	−0.136	4.853	3.426
6	−0.410	5.812	−0.244
7	−0.554	4.713	−3.235
8	−0.761	4.522	−0.0824
9	−0.289	4.650	−1.767
10	−0.0221	5.565	−0.0782
11	−0.330	5.654	−1.187
12	−0.623	4.568	0.0882
13	−0.717	4.290	−0.665
14	−0.549	4.230	0.310
15	0.0003	5.493	−0.665
16	−0.132	5.935	0.378
17	−0.173	5.198	−0.603
18	0.0375	5.754	0.360
19	−0.198	5.964	−0.543
20	−0.293	4.910	0.571

modes simple truncation will not work (see Sec. II). How can one then proceed to analyze the properties of these modes?

To look for clues to solve this problem, we consider a situation where all the modes are extended (so that the local Green's function will not converge for finite r). The periodic two-dimensional lattice is just such a case.

The local Green's function may be considered as the limit of the truncated continued fraction as the level of truncation approaches infinity. Ordinarily, when dealing with finite systems such as resulting from the truncation of the continued fraction, the poles of the truncated local Green's function determine the eigenvalues of the truncated system. In general, the eigenvalue spectrum for a finite system consists of a series of discrete poles. As the level of truncation increases, the density of the discrete poles also increases, leading eventually to a continuous spectrum as the level of truncation approaches infinity. Thus, following Wongtawatnugool and Wu,[5] we write

$$R_{00}(\omega^2)=\lim_{\eta\to 0\, r\to\infty} R_{00}^{(r)}(\omega^2+i\eta) \tag{4}$$

[where $R_{00}(\omega^2)$ is the local Green's function for the infinite system] or

$$|R_{00}^{(r)}(\omega^2+i\eta)-R_{00}^{(r')}(\omega^2+i\eta)|<\epsilon \quad \text{for } r>M \text{ and } r'>M\ . \tag{5}$$

For extended modes, M may approach infinity as ϵ and η approach zero. However, if instead of simply truncating the continued fraction one replaces the remainder of the continued fraction after a given level by a parameter Σ, one obtains (with $a_i'=a_i-\omega^2$),

$$R_{00}^{(r)}(\Sigma)=\cfrac{1}{a_0'-\cfrac{b_1}{a_1'-\ddots\cfrac{b_r}{a_r'-\Sigma}}}\ . \tag{6}$$

If the parameter Σ can be chosen to reflect the effect of the remainder of the continued fraction on the local Green's function, it may then be expected that $R_{00}^{(r)}(\Sigma)$ will approach the limit $R_{00}(\omega^2)$. This should also mean that

$$R_{00}^{(r)}(\Sigma)=R_{00}^{(r+1)}(\Sigma)\ . \tag{7}$$

In fact, Eq. (7) can be used as the self-consistent equation to determine Σ.

For a system with a fixed configuration, Eq. (7) indicates that

$$\Sigma=\frac{b_{r+1}}{a_{r+1}'-\Sigma} \tag{8}$$

or that the coefficients a_k and b_k must have reached convergence at $k=r+1$.

If one examines Table IV one finds that for the two-dimensional square lattice $a_i=A$ and the coefficients b_k have converged to within 1% at $k=15$. Chen and Wu computed the frequency spectrum of the two-dimensional periodic lattice[6] for $r=14$, using Eq. (8), and obtained excellent agreement with the known results. Thus for a periodic system with extended states, even though the truncated local Green's function does not show any trend of convergence at or in the neighborhood of $r=14$, Eq. (7) with $r=14$ nevertheless leads to excellent results. This certainly suggests that the concept leading to Eq. (7) is a valid one and as the situation requires, it should be modified to deal with disordered systems.

The discussion presented above indicates how the local Green's function behaves under different situations. *For the more localized states, the local Green's function is expected to converge at a reasonably small value of r* (see Table III). On the other hand, *for the extended states, it is the convergence of the coefficients a_r and b_r at reasonably small values of r which provides an efficient way of determining the local Green's function even though the local Green's function itself is not expected to converge until $r\to\infty$* (see Table IV). Since Eq. (7) is

TABLE III. Truncated local Green's function $R_{00}^{(r)}(\omega^2)$.

	ω^2					
r	7.0	7.5	7.8	7.85	7.9	13.5
1	−0.600	−0.424	−0.364	−0.356	−0.348	−0.110
2		−0.637	−0.457	−0.438	−0.422	−0.110
3	0.0316	−1.427	−0.551	−0.513	−0.482	−0.111
4	−0.325	0.219	−0.767	−0.647	−0.571	−0.111
5	0.507	−0.743	−0.470	−0.448	−0.428	−0.111
6	−0.174	16.270	−0.605	−0.550	−0.509	−0.111
7	−0.351	0.454	−0.680	−0.596	−0.538	−0.111
8	−0.880	−0.018	−0.763	−0.637	−0.561	−0.111
9	−0.151	−0.987	−0.166	1.813	−0.829	−0.111
10	−0.577	0.112	−0.725	−0.619	−0.551	−0.111
11	1.111	−0.141	−0.799	−0.651	−0.567	−0.111
12	−0.076	−0.319	−0.871	−0.674	−0.577	−0.111
13	−0.387	−1.928	−1.580	−0.761	−0.603	−0.111
14	0.112	−0.227	−0.831	−0.662	−0.572	−0.111
15	−0.218	−0.415	−0.898	−0.681	−0.579	−0.111
16	−0.443	−0.767	−0.971	−0.697	−0.585	−0.111
17	−0.162	−0.356	−0.878	−0.676	−0.578	−0.111
18	−0.335	−0.531	−0.924	−0.687	−0.582	−0.111
19	−0.642	−0.761	−0.953	−0.693	−0.583	−0.111
20	−0.254	−0.425	−0.896	−0.680	−0.579	−0.111
21	−0.471	−0.634	−0.939	−0.690	−0.582	−0.111
22	0.298	−1.064	−0.960	−0.694	−0.584	−0.111
23	−0.346	−0.515	−0.918	−0.686	−0.581	−0.111
24	10.200	−0.834	−0.952	−0.692	−0.583	−0.111
25	−0.154	−2.079	−0.963	−0.694	−0.584	−0.111
26	−0.328	−0.269	−1.004	−0.699	−0.585	−0.111
27	0.412	−0.946	−0.955	−0.693	−0.583	−0.111
28	−0.254	3.293	−0.967	−0.695	−0.584	−0.111
29	−0.379	−0.248	−0.984	−0.697	−0.584	−0.111

TABLE IV. Coefficients (a_r, b_r) and $R_{00}^{(r)}$ for the periodic square lattice at $\omega^2 = 0.5$.

r	$a_r - \omega^2$	b_r	$R_{00}^{(r)}$
1	3.500	4.000	0.424
2	3.500	5.000	0.637
3	3.500	3.800	1.427
4	3.500	4.305	−0.571
5	3.500	3.873	0.0805
6	3.500	4.169	0.274
7	3.500	3.908	0.411
8	3.500	4.114	0.595
9	3.500	3.929	1.151
10	3.500	4.085	−1.032
11	3.500	3.943	0.0269
12	3.500	4.067	0.245
13	3.500	3.952	0.384
14	3.500	4.055	0.549
15	3.500	3.959	0.944
16	3.500	4.047	−2.693
17	3.500	3.964	−0.0500
18	3.500	4.040	0.212
19	3.500	3.968	0.356
20	3.500	4.036	0.508

consistent with both aspects of the behavior of the local Green's function, its applicability to disordered systems where both localized states and extended states may exist is therefore expected.

However, because all possible configurations consistent with the distribution of disorder are present in an infinite disordered system, the quantity of interest is the ensemble average of the local Green's function, $\langle R_{00}^{(r)}(\Sigma)\rangle$. The self-consistent equation for the determination of the parameter Σ then becomes

$$\langle R_{00}^{(r)}(\Sigma)\rangle = \langle R_{00}^{(r+1)}(\Sigma)\rangle \ . \tag{9}$$

The direct procedure to determine Σ using Eq. (9) may now be set up as follows. For a given shell r consisting N_r particles, the ensemble average of $R_{00}^{(r)}(\Sigma)$ is computed over all possible configurations of the N_r particles,[7] i.e.,

$$\langle R_{00}^{(r)}(\Sigma)\rangle = \sum_c P_c \cfrac{1}{a_0'^c - \cfrac{b_1^c}{a_1'^c - \ddots - \cfrac{b_r^c}{a_r'^c - \Sigma}}} \ ,$$

where a_k^c and b_k^c are the coefficients of the continued fraction at kth shell for a given configuration c and P_c is the probability of occurence of that configuration. Similarly $R_{00}^{(r+1)}(\Sigma)$ can be set up in the same way. When these quantities are substituted into Eq. (9), we obtain

$$\sum_c P_c \cfrac{1}{a_0'^c - \cfrac{b_r^c}{a_1'^c - \ddots \cfrac{b_r^c}{a_r'^c - \Sigma}}} = \sum_c P_c \cfrac{1}{a_0'^c - \cfrac{b_1^c}{a_1'^c - \ddots \cfrac{b_{r+1}^c}{a_{r+1}'^c - \Sigma}}} . \tag{10}$$

The solution to Eq. (10) determines Σ from which other quantities of interest such as the frequency spectrum, can be calculated.

The actual computation of Σ starts with an arbitrarily chosen r and Eq. (10) is then solved. Next the same procedure is repeated for $r+1$. If either Σ_r and Σ_{r+1}, or the quantities calculated based on Σ_r and Σ_{r+1}, exhibit the trend of convergence, one may conclude the Σ_r has reached its limit, Σ. The degree of difficulty of computation of Σ thus depends on r. For the two-dimensional binary system under consideration, the number of particles enclosed within the rth shell is $N_r = 1 + 2r(r+1)$. For example for $r=2$, $N_{r+1}=25$. This means that in the summation at the right-hand side of Eq. (10), 2^{25} configurations need to be considered. Apparently the direct application of Eq. (10) will quickly become inefficient as r exceeds the first few shells.

On the other hand, consideration of the structural aspect of the two- and three-dimensional systems shows it is necessary to go beyond the first few shells in order to recover the features associated with those properties. For example, it can be seen from Fig. 1 that each of the four sites 2, 3, 4, and 5 in the first shell can be reached from site 1 in the zeroth shell in only one way. However, there are two types of "lattice sites" in the second shell, namely, the sites 6, 8, 10, and 12 which can be reached from the sites in the preceding shell one way only and the sites 7, 9, 11, and 13 which can be reached from the sites in the preceding shell two ways. As the shell number increases, the number of sites which are equivalent to the first type of site remains fixed at four while the number of sites of the second kind will increase. Eventually, the properties of the local Green's function will be determined mainly by the properties associated with sites of the second kind. In the calculation of the frequency spectrum of periodic lattices,[8] it was shown that for the extended states the coefficient b_r converged to within a few percent of its limiting value at about the tenth shell (see also Table IV). This indicates that a reliable calculation of the local Green's function must include at least the first ten shells. A direct calculation of Σ in the spirit of Eq. (10) using $r=10$ would involve 2^{221} configurations; an almost impossible task to carry out.

Another way to use Eq. (9) is to proceed as follows. Instead of averaging over all possible configurations corresponding to a cluster defined by a small shell number r (say $r=10$), the ensemble average of the local Green's function may be taken over a limited number of randomly generated configurations of a cluster defined by a reasonably large r (so that a sufficiently large number of particles is included within the rth shell), i.e.,

$$R_{00}^{(r)}(\Sigma) = \frac{1}{N_c} \Sigma P_c \cfrac{1}{a_0'^c - \cfrac{b_1^c}{a_1'^c - \ddots \cfrac{b_r^c}{a_r'^c - \Sigma}}} , \tag{11}$$

where N_c is the number of randomly generated configurations.

To demonstrate the feasibility of this approach, the coefficients (a_r, b_r) for a randomly generated configuration are shown in Table V. It is seen that the values of successive a_r and b_r do not exhibit any correlation. In fact, these values seem to fluctuate randomly. Furthermore, the local maxima and minima of a_r and b_r fluctuate within a range. From the results shown in Table VI, it can also be seen that the values of a_r and b_r for different configurations all exhibit the same behavior. In particular, their values all fluctuate within the same range. This then indicates that the ensemble averaging over a limited number of configurations may indeed give a realistic description of the disorder of the system as long as a sufficiently large number of shells (a sufficiently large r) is included in the consideration. In this spirit, the self-consistent equation for the determination of the parameter Σ using Eqs. (9) and (11) will be mean-

TABLE V. a_r and b_r for a randomly generated configuration.

r	a_r	b_r	r	a_r	b_r
1	4.000	6.000	27	10.625	23.724
2	8.000	25.000	28	8.053	14.115
3	7.360	8.310	29	7.705	13.303
4	6.424	20.208	30	5.984	6.187
5	11.379	19.471	31	5.800	17.466
6	6.861	19.348	32	9.345	11.750
7	10.397	17.668	33	5.852	19.919
8	6.630	10.487	34	13.615	24.815
9	7.345	17.567	35	6.361	13.121
10	8.259	13.205	36	10.239	25.010
11	7.702	24.276	37	7.703	11.062
12	11.871	30.965	38	7.661	20.429
13	8.338	9.685	39	8.852	17.574
14	6.480	17.602	40	8.466	14.511
15	9.602	16.992	41	6.429	9.679
16	6.513	10.578	42	8.045	28.598
17	8.829	23.002	43	10.518	16.558
18	7.327	7.872	44	7.530	18.040
19	6.785	25.661	45	9.274	18.236
20	10.852	12.198	46	7.254	10.932
21	5.166	8.591	47	7.452	23.442
22	8.021	20.612	48	10.500	17.066
23	7.923	9.018	49	6.615	9.563
24	5.110	8.440	50	6.622	16.038
25	7.976	19.327			
26	8.157	20.255			

ingful.

Since the numerical studies of the two-dimensional lattice indicate that a system of a few thousand particles usually yields reasonable and meaningful results,[4] it may be sufficient to use r in the neighborhood of $r=50$ (corresponding to a system of 5101 particles) for Eq. (11). Figure 4 shows the results of our calculation of the frequency spectrum of the system described earlier using Eq. (11). In this calculation, r was chosen to be 30 and 100 randomly generated configurations were used. In the figure, the histogram obtained by Payton and Visscher[4] by direct numerical calculation for a system of 900 particles is also shown. The agreement between the general features of the two spectra is indeed excellent. Some of the peaky fluctuation in the spectrum may be attributed to the limited number of configurations used or to the fact that not enough shells had been included. These factors have to be considered in light of the efficiency of the calculation. Thus, an attempt should be made to obtain an optimal combination of the size (r) and the number of configurations for achieving the best result with the most efficient effort. Work along this line is currently in progress.

VI. SUMMARY

The recursion method is certainly useful for the study of disordered systems,[8–11] in particular if one is interested in developing an approximate method for *an infinite system.* It transforms the matrix describing the physics of the system into a tridiagonal form and provides a scheme to incorporate the properties of the local environment into the transformed matrix. When the local Green's function is written in the form of a continued fraction, each pair of consecutive coefficients (a_k,b_k) contains information about all the N_r particles included within that shell. However, a simple truncation of the local Green's function at any given step will only present a distorted picture of the system except for those localized states for which the local Green's function has already converged at the level of truncation. The logical way to approach this problem is to carry the detailed description of the system to an appropriate level and then replace the remainder by an effective parameter reflecting the effect of the rest of the system. But, because of the transformation involved in the calculation of a_k and b_k, a critical factor determining the feasi-

TABLE VI. a_r and b_r for some randomly generated configurations.

	a_r				b_r			
r	Config. 1	Config. 2	Config. 3	Config. 4	Config. 1	Config. 2	Config. 3	Config. 4
15	6.944	7.475	9.624	9.976	22.987	23.377	18.037	22.176
16	5.935	9.958	7.752	10.578	6.762	15.623	19.160	20.562
17	9.514	6.178	9.140	7.728	16.400	21.202	17.325	26.528
18	6.886	5.461	6.956	5.710	15.996	7.143	17.192	8.227
19	9.791	6.897	10.064	8.878	16.452	10.459	14.329	12.380
20	7.754	6.947	9.007	7.541	21.595	10.180	27.498	19.316
21	6.081	11.121	8.690	9.318	10.873	22.807	18.001	14.729
22	5.403	7.952	9.217	9.793	8.137	20.383	18.108	26.624
23	7.661	8.980	10.465	7.621	8.594	19.264	29.186	19.516
24	8.079	6.231	9.936	7.097	21.190	14.457	21.165	10.375
25	5.174	6.456	7.375	8.758	8.144	8.456	24.445	20.162
26	9.362	7.549	6.130	5.986	10.152	12.940	7.414	10.533
27	9.518	9.126	11.127	10.307	31.410	17.231	20.524	16.028
28	8.660	8.526	8.599	6.536	15.303	19.132	21.159	19.053
29	9.993	9.816	9.885	9.542	23.685	23.119	25.846	11.681
30	9.490	7.582	5.340	7.999	25.188	15.969	12.548	26.693
31	6.778	11.764	5.871	6.628	15.297	24.703	6.199	9.561
32	10.232	6.000	10.263	10.132	16.502	20.362	17.716	16.385
33	7.069	6.006	6.206	9.783	20.043	5.996	16.449	31.437
34	12.216	9.113	8.281	7.363	17.006	17.318	9.770	14.495
35	7.330	5.508	9.569	10.291	31.332	12.719	25.954	21.090
36	7.679	6.592	7.886	7.813	8.317	6.794	15.216	18.673
37	10.445	9.735	11.604	10.248	30.115	19.614	25.417	19.528
38	9.002	8.556	8.821	10.923	15.356	19.803	26.452	29.594
39	8.749	10.661	10.589	9.519	28.210	22.606	21.318	26.931
40	5.369	9.218	7.326	9.317	8.969	26.145	22.824	21.217

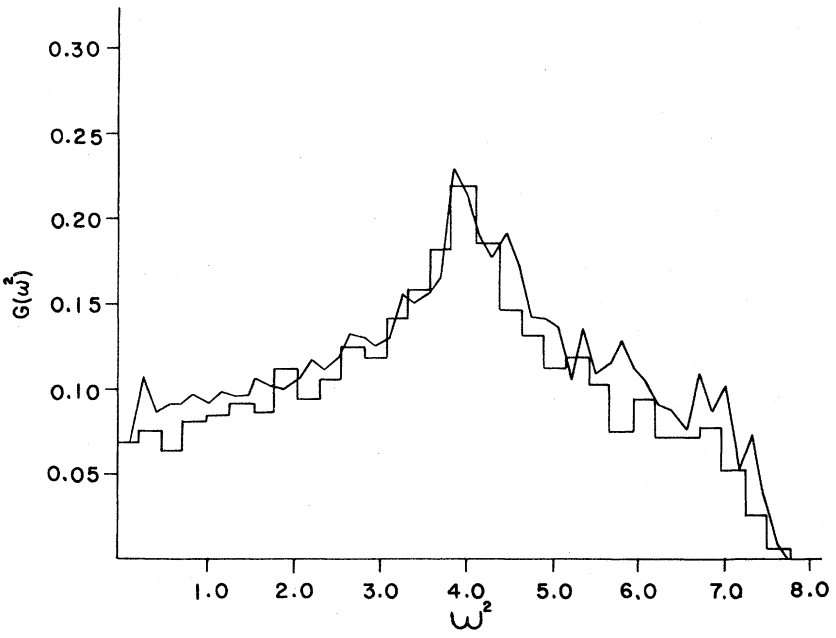

FIG. 4. Main band of a disordered square lattice. ($C_L=0.15$ and $M_L/M_H=\frac{1}{3}$.)

bility of any approach is the computation time. For example, Sinai, Wu, and Chen[12] recently used an effective-medium approach to get around the time-consuming problem of taking the average over all possible configurations of a large system. For the two-dimensional square lattice, they obtained good agreement with the numerical calculation by averaging over all configurations corresponding to particles only in the first two shells (corresponding to $r=1$). The tradeoff is the inclusion of an effective medium which has to be determined self-consistently. The self-consistent scheme requires the calculation of the coefficients a_k and b_k for each iteration. Hence, the computing time for complicated systems may become excessive. On the other hand, in the present scheme, the coefficients a_k and b_k for all the configurations need to be calculated only once. They can be stored away and recalled for repeated use. This feature alone will make this approach most attractive for treating more complicated, realistic systems.

In addition to the determination of the eigenvalue spectrum, the other important problem is the calculation of the eigenvectors. In the transformed tridiagonal representation, only the local Green's function can be directly linked to the amplitude of the eigenvector at the local site.[8] Recently Tong and co-workers[13,14] carried out a series of calculations to map out spatially the amplitudes of the eigenvector by calculating the local Green's function at each spatial point. In their approach, since the recursion method has to be used at every local site, the calculation becomes quite involved. Also, the calculation is carried out basically in the spirit of truncation of the continued fraction at finite step with allowance given to the boundary farther away from the region of calculation. Still, their scheme will probably only work well in the region of localized states. For the important problem of studying the transition from the region of localized states to the region of extended states near the band tail, their scheme may need to be modified along the lines as discussed in Sec. III.

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[1]P. Dean, Rev. Mod. Phys. 44, 127 (1972).
[2]R. Haydock, V. Heine, and J. J. Kelly, J. Phys. C 5, 2845 (1972).
[3]E. W. Montroll, *Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Problems* (University of California Press, Berkeley, California, 1956), Vol. III, p. 209.
[4]D. N. Payton III and W. M. Visscher, Phys. Rev. 154, 802 (1967).
[5]C. Wongtawatnugool and S. Y. Wu (unpublished).
[6]Y. C. Chen and S. Y. Wu, Bull. Am. Phys. Soc. 23, 236 (1978).
[7]S. Y. Wu, J. Math. Phys. (N.Y.) 15, 947 (1974); S. Y. Wu and M. Chao, Phys. Status Solidi B 68, 349 (1975); S. Y. Wu, S. P. Bowen, and K. S. Dy, CRC Crit. Rev. Solid State Phys. 10, 43 (1980).
[8]Y. C. Chen, S. Y. Wu, and J. J. Sinai, Phys. Status Solidi B 104, 441 (1981).
[9]J. Stein and U. Krey, Solid State Commun. 27, 797 (1978).
[10]J. Stein and U. Krey, Solid State Commun. 27, 1405 (1978).
[11]F. Yonezawa, J. Non-Cryst. Solids 35-36, 29 (1980).
[12]J. J. Sinai, S. Y. Wu, and Y. C. Chen, Phys. Status Solidi B 107, 367 (1981).
[13]B. Hede and B. Y. Tong, Solid State Comm. 25, 269 (1978).
[14]B. Y. Tong, M. M. Pant, and B. Hede, J. Phys. C 13, 1221 (1980); M. M. Pant and B. Y. Tong, J. Phys. C 13, 1237 (1980).