

## Real-space rescaling method for disordered systems

B. W. Southern, A. A. Kumar, and J. A. Ashraff

*Department of Physics, University of Manitoba, Winnipeg, Manitoba, Canada R3T 2N2*

(Received 14 March 1983)

An exact real-space rescaling approach for disordered tight-binding model Hamiltonians is presented. The method provides a direct way of obtaining the local Green's functions and the local density of states. The behavior of the eigenstates in a given region of energy can be determined from the behavior of the rescaling transformation under iteration. Localized-mode behavior is characterized by a fixed point of the transformation and the inverse localization length can be obtained directly from an analysis of the approach to this fixed point. The problem of a single impurity is studied in detail and our method is compared with the standard treatment of such problems.

### I. INTRODUCTION

In a recent paper<sup>1</sup> a real-space rescaling approach for the study of the spectral properties of tight-binding Hamiltonians was described. The method can be applied to a wide variety of problems: for example, electrons in pure and defect structures, magnetic systems with impurities, and in general, any excitation obeying a linear equation of motion. The approach provides a direct method of calculating the local Green's functions which contain all the detailed information about the dynamics of the system.

The basic idea of the method is to take a system of equations which describe  $N$  degrees of freedom and perform a transformation on the system which reduces the number of degrees of freedom to a fraction of  $N$  but leaves the equations invariant in form with modified (renormalized) parameters. The relationship between the renormalized parameters and the original set is used to define a scaling transformation on the equations of motion. This procedure can then be repeated indefinitely by simply iterating the transformation many times until there is only one degree of freedom left. In this limit, the local Green's functions are trivially obtained from the limiting values of the renormalized parameters. Also, the behavior of the transformation under iteration can be used to obtain detailed information about the nature of the eigenstates. The transformation exhibits certain fixed points, or special points, where the parameters do not change their values under iteration. The study of the accessibility of these various fixed points can be used to locate the different regions of energy in which the spectrum consists of extended states, localized states, or gaps.

In our previous paper<sup>1</sup> (hereafter referred to as SKLT) the method was applied to the study of the dynamical equations of a translationally invariant tight-binding system on a one-dimensional (1D) lattice with arbitrary range of interaction. We showed how to set up a general scaling transformation for the system and illustrated the method using the uniform chain with both first- and second-neighbor interactions as an example. A general procedure for calculating the local density of states (LDOS) at any given site was outlined.

In this paper we apply the rescaling method to systems which are not translationally invariant. In particular, we

consider a 1D disordered chain with both first- and second-neighbor interactions. The motivation for this study stems from the fact that most applications of the real-space methods have been restricted to systems with only nearest-neighbor (NN) interactions. Such a study, while being applicable to real systems, which in general possess interactions beyond nearest neighbors, is also important for the application of the scaling methods to higher dimensional lattices where the elimination procedure generates longer-ranged interactions. The expressions that we obtain are valid for an arbitrary number of impurities in the chain or any amount of randomness in the interactions between the lattice sites. To illustrate the approach, we consider in detail the problem of a 1D magnetic system with a single impurity. In contrast to the conventional treatments of this problem, our approach is a direct attack on the disordered system and does not require knowledge of the Green's functions of the pure system.

This paper is organized as follows. In Sec. II we describe how to set up the rescaling transformation for a 1D tight-binding Hamiltonian with arbitrary first- and second-neighbor interactions. A general rescaling transformation is obtained for the completely random case. In Sec. III we consider the conventional treatment of a single impurity in a ferromagnetic chain when the exchange interactions extend beyond nearest neighbors. We derive the equations which determine the energies of the localized modes associated with the impurity and discuss some limiting cases. In Sec. IV we examine the same problem using the expressions derived in Sec. II and demonstrate how the localized modes can be identified by studying the behavior of the scaling transformation under iteration. In addition, we discuss how information about the wave function of the localized modes can be extracted. Finally in Sec. V we summarize our results and discuss further possible applications of the method to systems with a finite concentration of impurities and also to higher dimensional lattices.

### II. RESCALING TRANSFORMATION

We consider the following tight-binding model Hamiltonian:

$$H = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{i,j} |i\rangle V_{ij} \langle j|, \quad (1)$$

where each state  $|i\rangle$  is an atomiclike orbital centered at site  $i$  and the sites form a regular 1D lattice. The parameters  $\varepsilon_i$  and  $V_{ij}$  represent the diagonal and off-diagonal matrix elements of the Hamiltonian in this basis. A Hamiltonian of this form is often the starting point for the investigation of the excitation spectrum of electronic, magnetic, and elastic degrees of freedom in both pure and disordered solids. The spectral properties are obtained by solving the following set of equations for the lattice Green's functions<sup>2</sup>  $G_{ij}$ :

$$(E - \varepsilon_i)G_{ij} = \delta_{ij} + \sum_k V_{ik}G_{kj}, \quad (2)$$

where

$$G_{ij}(E + i0^+) = \left\langle i \left| \frac{1}{E + i0^+ - H} \right| j \right\rangle$$

and  $\delta_{ij}$  is the Kronecker delta.

In SKLT we considered the case where (1) is translationally invariant and the  $V_{ij}$  were of arbitrary range. As discussed in that paper, when the range of interactions extends beyond nearest neighbors the inhomogeneous term in (2) is modified under the rescaling transformation. For this reason we must replace the Kronecker delta by a matrix  $Z_{ij}$  which is  $\delta_{ij}$  only at the initial stage. In the present case we limit the range of interactions to first and second neighbors only but allow each  $V_{ij}$  and  $\varepsilon_i$  to be arbitrary and hence Eq. (2) reduces to

$$(E - \varepsilon_i)G_{ij} = Z_{ij} + \sum_{n=\pm 1, \pm 2} V_{i,i+n}G_{i+n,j}. \quad (3)$$

If we now divide the sites into two groups which we simply label as "even" or "odd," then we can eliminate the odd sites from (3) and the equations for the even sites can be written in the form

$$(E - \varepsilon'_i)G_{ij} = Z'_{ij} + \sum_{n=\pm 2, \pm 4} V'_{i,i+n}G_{i+n,j}, \quad (4)$$

where the primes indicate that the parameters in the original set (3) have been renormalized. This elimination procedure actually generates two sets of equations which are completely decoupled from each other, and each involves only  $N/2$  sites. If we now rescale all distances in each set by a factor of 2 (the scaling factor), or equivalently redefine the lattice constant  $a' = a/2$ , then Eq. (4) has the same form as Eq. (3) and the procedure can be repeated again. This procedure is illustrated schematically in Fig. 1.

The renormalized parameters are given by

$$(E - \varepsilon'_i) = (E - \varepsilon_i) - \sum_{n=\pm 1, \pm 2} L(i,n)V_{i+n,i}, \quad (5a)$$

$$Z'_{ij} = Z_{ij} + \sum_{n=\pm 1, \pm 2} L(i,n)Z_{i+n,j}, \quad (5b)$$

$$V'_{i,i\pm 1} = V_{i,i\pm 2} - L(i,\pm 2)(E - \varepsilon_{i\pm 2}) + L(i,\pm 1)V_{i\pm 1,i\pm 2}, \quad (5c)$$

$$V'_{i,i\pm 2} = L(i,\pm 2)V_{i\pm 2,i\pm 4}, \quad (5d)$$

$$L(i,\pm 2) = -\frac{V_{i\pm 1,i\pm 3}}{V_{i\pm 2,i\pm 3}}L(i,\pm 1), \quad (5e)$$

$$L(i,\pm 1) = \frac{X_{i,i\pm 1}D_{\pm}^{(i)} + X_{i,i\mp 1}X_{i\mp 1,i\pm 1}}{D_{+}^{(i)}D_{-}^{(i)} - X_{i-1,i+1}X_{i+1,i-1}}, \quad (5f)$$

where

$$D_{\pm}^{(i)} = 1 + \frac{X_{i\pm 2,i\pm 1}X_{i\pm 1,i\pm 3}}{X_{i\pm 2,i\pm 3}} \quad (5g)$$

and

$$X_{i,j} = V_{i,j}/(E - \varepsilon_i). \quad (5h)$$

The above expressions were obtained by multiplying Eq. (3) for each neighbor  $n$  of the reference site  $i$  by  $L(i,n)$  and determining the  $L(i,n)$  subject to the condition that the odd sites are eliminated when we sum over the equations for site  $i$  and its neighbors.

In the uniform case these expressions reduce to those given in SKLT and can be used to calculate the various Green's functions for the uniform first- and second-neighbor problem. For a detailed discussion of the recursion relations and their fixed points in the uniform case, we refer the reader to SKLT.

The elimination procedure together with the rescaling of lengths defines the rescaling transformation and the renormalized parameters become the new effective interactions within each set. With these renormalized parameters the procedure can be repeated to generate twice as many additional sets of decoupled equations. Each  $G_{ij}$  thus belongs to a smaller and smaller set until finally each set contains only the  $G_{ij}$  of interest which is equal to the limiting value of the ratio  $Z_{ij}^{(\infty)}/(E - \varepsilon_i^{\infty})$ .

Our expressions are exact for any degree of disorder on the chain and can be easily implemented on any programmable device in order to obtain the Green's functions for any initial values of the parameters in (4). This point will be discussed further in Sec. IV where we will consider the problem of a ferromagnetic chain with defects. We treat a single impurity in a uniform host when the impurity has both first- and second-neighbor interactions with the host. In the next section, we outline the standard treatment of this problem and in Sec. IV we use the expressions obtained above to show how the scaling approach can be used to obtain the same results.

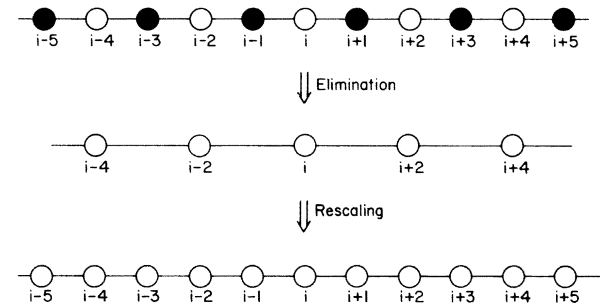


FIG. 1. Schematic illustration of the rescaling procedure. The first step consists of "eliminating" the odd sites (closed circles) leaving a chain with only even sites (open circles). The second step consists of rescaling all the lattice distances by a factor of  $\frac{1}{2}$  and relabeling the sites.

### III. SECOND-NEIGHBOR CHAIN WITH A SINGLE IMPURITY

In this section we work out the problem of a single impurity in a chain with extended range (beyond nearest neighbors) interactions. The basic purpose of this calculation is to allow a detailed comparison between the conventional treatment of this problem and the scaling approach developed in the preceding section. In order to fix our ideas, we discuss the case of the impurity spin in a ferromagnetic chain with first- and second-neighbor exchange interactions. However, the approach is not restricted to magnetic problems and, with proper identification of the parameters characterizing the impurity, the final expressions can be also applied to other types of defects. The analysis in this section follows the general procedure outlined by Wolfram and Callaway.<sup>3,4</sup> We omit the details of the calculation here and give only the essential features.

The system is defined by the Hamiltonian

$$H = -\frac{1}{2} \sum_{i,n=\pm 1,\pm 2} J_{|n|} \vec{S}_i \cdot \vec{S}_{i+n} - \sum_{n=\pm 1,\pm 2} (J'_{|n|} \vec{S}'_0 - J_{|n|} \vec{S}_0) \cdot \vec{S}_n, \quad (6)$$

where  $S(S')$  is the host (impurity) spin and  $J_1, J_2(J'_1, J'_2)$  are the host-host (impurity-host) first- and second-neighbor interactions, respectively. The impurity spin is located at the site labeled 0. This Hamiltonian can be expressed in a basis of single-spin deviation states<sup>3,4</sup> and takes the following tight-binding form:

$$H = H_0 + H_1,$$

where

$$H_0 = \text{const} + \sum_i |i\rangle \varepsilon \langle i| + \sum_{i,n=\pm 1,\pm 2} |i\rangle V_{|n|} \langle i+n| \quad (7)$$

with

$$\begin{aligned} \varepsilon &= -2V_1(1+A), \\ V_1 &= -2J_1S, \\ V_2 &= V_1A, \\ A &= J_2/J_1, \end{aligned} \quad (8)$$

and

$$H_1 = \sum_{n=0,\pm 1,\pm 2} |n\rangle \Delta \varepsilon_{|n|} \langle n| + \sum_{n=\pm 1,\pm 2} \Delta V_{|n|} (|0\rangle \langle n| + |n\rangle \langle 0|) \quad (9)$$

with

$$\begin{aligned} \Delta \varepsilon_0 &= 2V_1(\epsilon_1 + \epsilon_2), \\ \Delta \varepsilon_1 &= V_1\rho_1, \\ \Delta \varepsilon_2 &= V_1\rho_2, \\ \Delta V_1 &= V_1\gamma_1, \\ \Delta V_2 &= V_1\gamma_2, \end{aligned} \quad (10)$$

and

$$\begin{aligned} \rho_i &= -(J'_i S' - J_i S)/J_1 S, \\ \epsilon_i &= -(J'_i - J_i)/J_1, \\ \gamma_i &= \left[ J'_i \left[ \frac{S'}{S} \right]^{1/2} - J_i \right] / J_1 \quad (i=1,2). \end{aligned} \quad (11)$$

Our definitions of  $\rho_1$  and  $\epsilon_1$  are the negatives of those used by Wolfram and Callaway<sup>3,4</sup> whereas  $\gamma_1$  is the same. Equation (10) can be used to study other types of defects as well and Eq. (11) would then involve the parameters which are used to characterize that defect.

The eigenstates  $|\psi\rangle$  of the system are determined by the Schrödinger equation

$$(H_0 + H_1) |\psi\rangle = E |\psi\rangle \quad (12)$$

or

$$[I - (V_1)^{-1} G^0 H_1] |\psi\rangle = 0,$$

where  $G^0$  denotes the Green's-function matrix for the Hamiltonian  $H_0$ ,

$$G_{ij}^0 = \left\langle i \left| \frac{V_1}{E - H_0} \right| j \right\rangle.$$

$H_0$  represents a uniform chain with first- ( $V_1$ ) and second- ( $V_2$ ) neighbor interactions and the Green's functions can be obtained using the formalism of SKLT.

Since  $H_1$  is only a  $5 \times 5$  matrix, the solutions for the impurity modes can be obtained from the following  $5 \times 5$  determinantal equation:

$$\det[I - (V_1)^{-1} G^0 H_1] = 0. \quad (13)$$

If we transform to a basis which reflects the point-group symmetry of the impurity, then this equation factors into two subdeterminants  $D_s$  and  $D_a$ . The expression for  $D_s$  is quite complicated in general and gives the energies of modes which are symmetric with respect to the impurity site. The expression for  $D_a$  is simpler and gives the energies of modes which are antisymmetric with respect to the impurity site and hence have zero amplitude at the impurity.  $D_a$  has the form

$$\begin{aligned} D_a &= 1 - \rho_1(G_0^0 - G_2^0) - \rho_2(G_0^0 - G_4^0) \\ &\quad + \rho_1\rho_2[(G_0^0 - G_2^0)(G_0^0 - G_4^0) - (G_1^0 - G_3^0)^2]. \end{aligned} \quad (14)$$

In the above we have used the fact that  $G_{ij}^0 = G_{|i-j|}^0$ . In general, it is difficult to solve this equation for arbitrary values of  $A$ ,  $\rho_1$ , and  $\rho_2$  since no simple relationship exists between the various Green's functions when  $A \neq 0$ .

In the case where there are no second-neighbor interactions in the host ( $J_2 = 0$ ), the various  $G_n^0$  in (14) simplify and the local-mode energies are solutions of the following cubic equation:

$$\begin{aligned} 8\rho_2\lambda^3 + (-4\rho_2^2 - 8\rho_1\rho_2)\lambda^2 \\ + (2\rho_1 - 4\rho_2 + 4\rho_1\rho_2^2 + 2\rho_1^2\rho_2)\lambda - \rho_1^2 - (\rho_1\rho_2 - 1)^2 = 0, \end{aligned} \quad (15)$$

where

$$\lambda = (E - \varepsilon)/(2V_1). \quad (15)$$

Figure 2 indicates the regions in the  $\rho_1$ - $\rho_2$  plane where the antisymmetric modes can appear. If  $\rho_2=0$ , then there is only one solution given by

$$\lambda = (\rho_1^2 + 1) / (2\rho_1) \quad (16)$$

provided  $|\rho_1| > 1$ .

As mentioned above,  $D_s$  is generally quite complicated and requires a numerical solution. However, if  $S=S'$  (i.e.,  $\rho_i = \epsilon_i = -\gamma_i$ ), then the symmetric modes are obtained as the solutions of a quartic equation. In the next section we describe how our rescaling approach can be used to obtain these same results in a very direct way.

#### IV. SCALING TREATMENT OF DEFECTS

In this section we discuss the impurity problem of Sec. III from the point of view of the rescaling method. Although one can write down the scaling expressions for the complete second-neighbor problem and calculate any  $G_{ij}$ , we restrict ourselves here to the case of the "extended defect" discussed at the end of the preceding section, namely the case where the impurity has both first- and second-neighbor interactions while the host has only first-neighbor interactions. The advantage of this case is that the expressions become particularly simple and it also provides an excellent comparison with the conventional approach discussed in Sec. III.

A particular  $G_{ij}$  for this problem can be evaluated by choosing the site  $i$  as reference and "eliminating" the neighboring sites progressively. If we choose the impurity site 0 as the site of interest, then the expressions for the renormalized site energies and couplings given by the expressions in (5) reduce to

$$\begin{aligned} \epsilon'_0 &= \epsilon_0 + 2V_{01}^2 / (E - \epsilon_1), \\ \epsilon'_1 &= \epsilon_2 + V_1^2 / (E - \epsilon_1) + V_1^2 / (E - \epsilon), \\ \epsilon'_2 &= \epsilon' = \epsilon + 2V_1^2 / (E - \epsilon), \\ V'_{01} &= V_{01}V_1 / (E - \epsilon_1) + V_{02}, \\ V'_1 &= V_1^2 / (E - \epsilon), \\ V'_{02} &= 0, \end{aligned} \quad (17)$$

where 1 and 2 refer to the effective first and second neighbors of site 0 at each stage. In addition, we must also consider the renormalization of the inhomogeneous terms  $Z_{ij}$ . For the calculation of  $G_{00}$ , only  $Z_{00}$  is needed since in the present case of  $A=0$  it does not change from its initial value of unity. To calculate  $G_{01}$ , however, we require both  $Z_{01}$  and  $Z_{11}$  and these terms satisfy

$$\begin{aligned} Z'_{01} &= Z_{01} + Z_{11}V_{01} / (E - \epsilon_1), \\ Z'_{11} &= Z_{11}V_1 / (E - \epsilon_1), \end{aligned} \quad (18)$$

with the initial condition  $Z_{ij} = \delta_{ij}$ . The other  $G_{0j}$  may be evaluated similarly but involve larger numbers of inhomogeneous terms. Figure 3 shows the results for  $G_{00}$  and  $G_{01}$  for the following choice of impurity parameters:  $\rho_1 = \epsilon_1 = -\gamma_1 = 3$  and  $\rho_2 = \epsilon_2 = -\gamma_2 = 2.5$ . The real and imaginary parts of the  $G_{ij}$  are obtained by introducing a small positive imaginary part into the energy  $E$ . The local modes are found at the values of  $\lambda$  where the real part of the  $G$ 's diverge. Since  $G_{00}$  and  $G_{01}$  involve the impurity site, the divergence of these  $G$ 's describe the symmetric modes. In order to locate the antisymmetric modes, we must take site 1 as reference and then calculate  $G_{11}$ . The

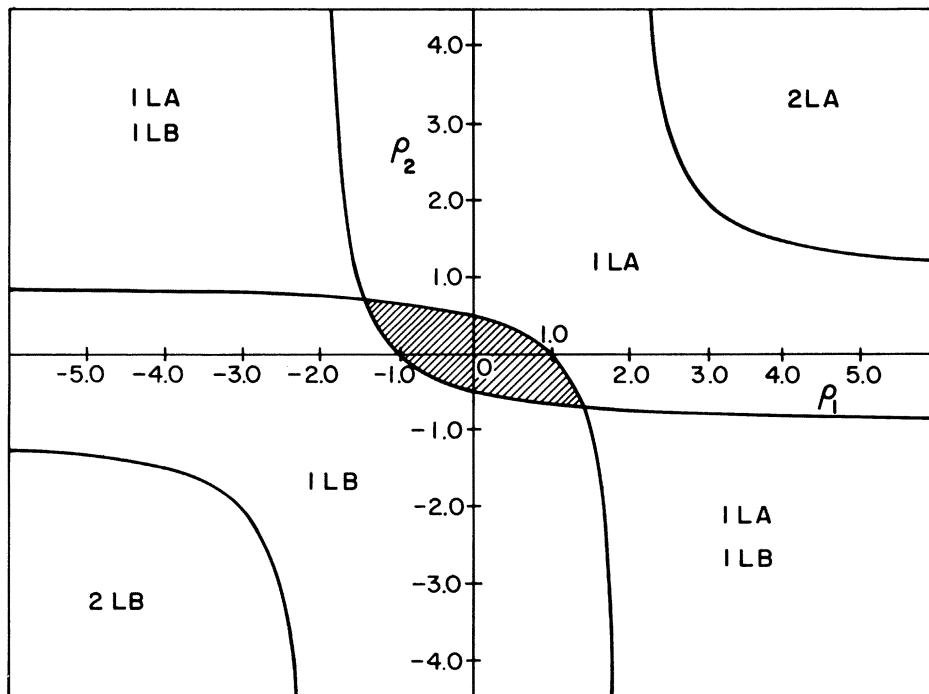


FIG. 2. Regions in the  $\rho_1$ - $\rho_2$  plane where localized (antisymmetric) modes appear. LA refers to localized above the band and LB refers to localized below the band. There are no localized antisymmetric modes in the central shaded region.

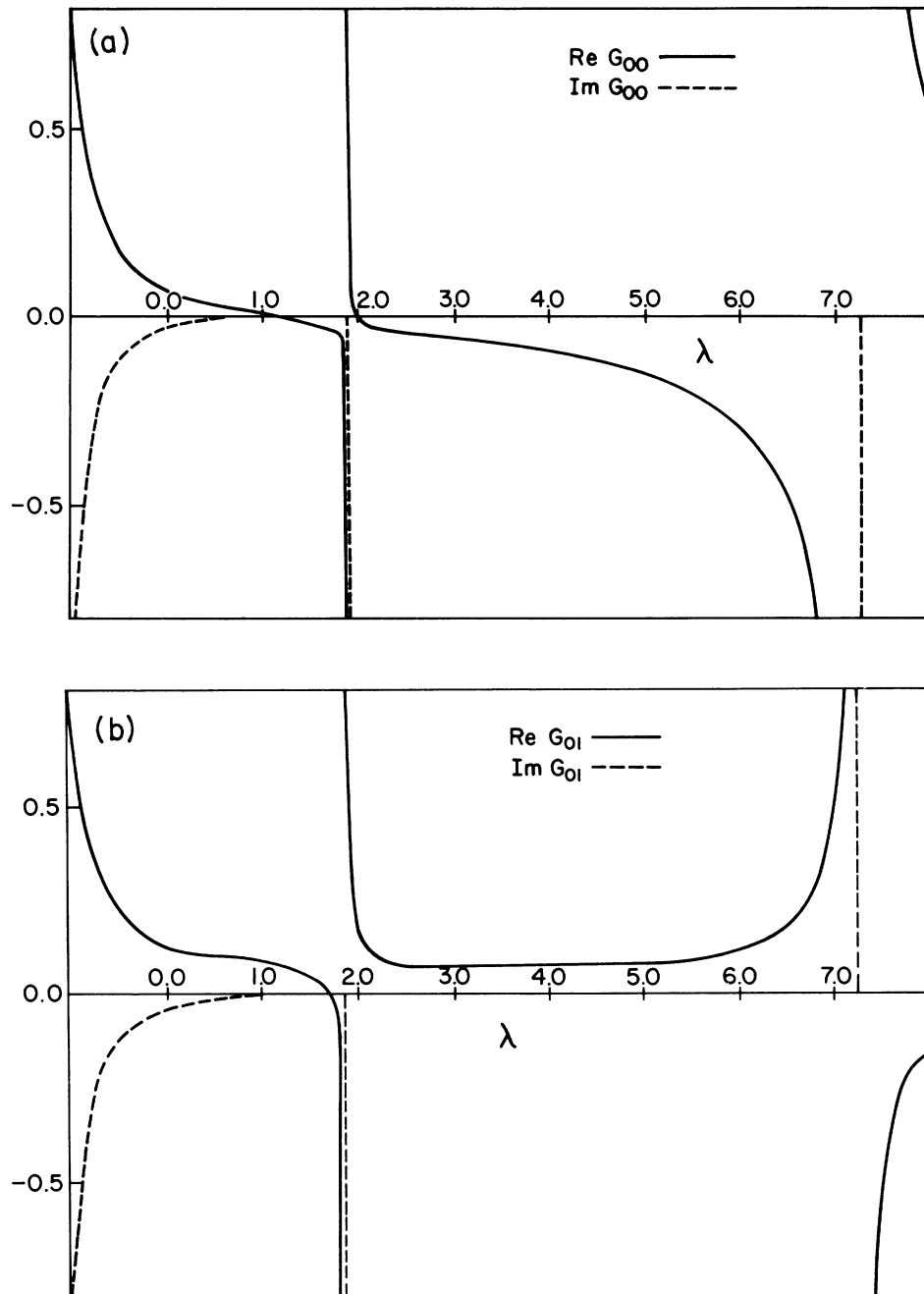


FIG. 3. (a) Real and imaginary parts of  $G_{00}$  in units of  $2V_1$  for  $\rho_1=\epsilon_1=-\gamma_1=3$  and  $\rho_2=\epsilon_2=-\gamma_2=2.5$ . The vertical dashed lines represent delta functions at the positions of the symmetric modes. The band of extended states of the host is in the range  $|\lambda| < 1$ . (b) Real and imaginary parts of  $G_{01}$  in units of  $2V_1$  for  $\rho_1=\epsilon_1=-\gamma_1=3$  and  $\rho_2=\epsilon_2=-\gamma_2=2.5$ . The vertical dashed lines represent delta functions at the positions of the symmetric modes. The band of extended states of the host is in the range  $|\lambda| < 1$ .

results for  $G_{11}$  are shown in Fig. 4. Note that  $G_{11}$  diverges at values of  $\lambda$  which correspond to both types of local modes. For the given values of  $\rho_1$  and  $\rho_2$  we observe two antisymmetric modes in agreement with Fig. 2. It is easily verified that the values of  $\lambda$  where the  $G$ 's diverge are solutions to either the cubic or quartic equations discussed in the preceding section. For values of  $|\lambda| < 1$  (within the band of extended states of the host) the  $G_{ij}$  converge after about 25 iterations. Outside the band, only about 7 iterations are required. Thus the location of the

local modes can be found with a minimum of calculation.

The rescaling transformation can be expressed in terms of any suitable set of parameters which describe the system. In the present case, the "deviation" parameters  $\rho_i$ ,  $\epsilon_i$ , and  $\gamma_i$  introduced in the preceding section are a more convenient set for obtaining information about the nature of the impurity modes. In terms of these parameters the above equations can be rewritten as follows:

$$\lambda' = 2\lambda^2 - 1, \quad (19a)$$

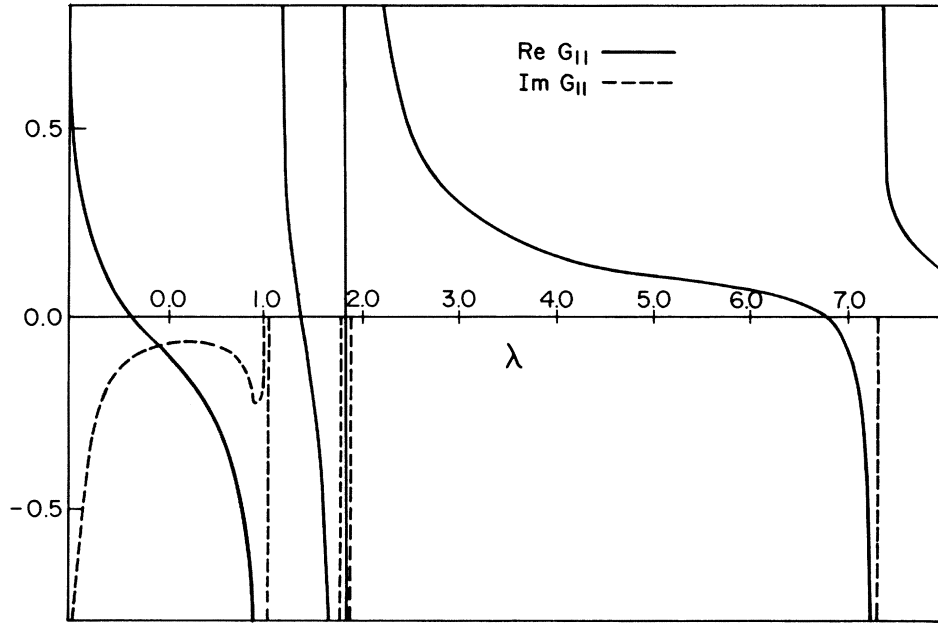


FIG. 4. Real and imaginary parts of  $G_{11}$  in units of  $2V_1$  for  $\rho_1=\epsilon_1=-\gamma_1=3$  and  $\rho_2=\epsilon_2=-\gamma_2=2.5$ . The vertical dashed lines represent delta functions at the positions of both the antisymmetric and symmetric modes. The modes alternate from symmetric to antisymmetric beginning at the highest mode.

$$\rho_1' = \frac{\rho_1}{2\lambda - \rho_1} + 2\lambda\rho_2, \quad (19b)$$

$$\rho_2' = 0, \quad (19c)$$

$$\gamma_1' = \frac{2\lambda(1+\gamma_1)}{2\lambda - \rho_1} - 1 + 2\lambda\gamma_2, \quad (19d)$$

$$(\epsilon_1' + \epsilon_2') = 2\lambda(\epsilon_1 + \epsilon_2) + \frac{2\lambda(1+\gamma_1)^2}{2\lambda - \rho_1} - 1, \quad (19e)$$

$$\gamma_2' = 0, \quad (19f)$$

where  $\lambda$  is defined as in Eq. (15).

We observe that the first three equations are decoupled from the remaining three and thus their behavior under iteration can be studied independently. This decoupling is similar to the factorization of the determinantal equation in the preceding section. The antisymmetric impurity mode solutions only depend upon the parameters  $\rho_1$  and  $\rho_2$  and thus the first three equations in (19) are sufficient to study these modes.

The first equation (19a) only involves the parameters of the host and its behavior under iteration characterizes the uniform ferromagnet. If  $|\lambda| > 1$ , then  $\lambda$  iterates to a sink at infinity. However, if  $|\lambda| < 1$ , then  $\lambda$  behaves chaotically under iteration. These two types of behavior are characteristic of the regions outside and inside the band of extended states of the magnetic excitations.  $|\lambda| = 1$  is an unstable fixed point which describes the band edge. We refer the reader to SKLT for a more detailed discussion of the uniform case.

The next two equations [(19b) and (19c)] describe the impure system and their behavior under iteration can be used to locate the regions of energy in which the localized modes associated with the impurity appear. For a mode to appear outside the band of extended states of the host,

we must have  $|\lambda| > 1$  and thus  $\lambda$  iterates to infinity. However,  $\rho_1'$  in (19b) displays two different possible types of behavior under iteration. It either approaches zero or infinity and the latter occurs only if the initial value of  $\lambda$  corresponds to the position of the local mode. When  $\lambda$  is a solution of the cubic equation (15) we can combine (19b) and (19c) and write them as

$$\alpha' = 2\alpha, \quad (20)$$

where

$$\alpha = \ln \left| \frac{1}{2\lambda - \rho_1} + \rho_2 \right|$$

and  $\alpha'$  is the same function of the primed quantities. If  $\alpha < 0$  then  $\alpha'$  iterates to  $-\infty$  whereas if  $\alpha > 0$  then it iterates to  $+\infty$ . Thus the unstable fixed point  $\alpha^* = 0$  separates these two types of behavior. A local mode is characterized by  $\alpha' \rightarrow +\infty$  which corresponds to both  $\lambda$  and  $\rho_1$  approaching  $+\infty$ . Solutions of the cubic equation which correspond to negative values of  $\alpha$  do not describe local mode solutions and correspond to  $\lambda \rightarrow +\infty$  but  $\rho_1 \rightarrow 0$ . The fixed point  $\lambda^* = \infty$ ,  $\rho_1^* = \infty$  is only accessible if the initial value of  $\lambda$  is a root of the cubic equation and  $\alpha > 0$ .

Each antisymmetric mode requires a critical value of the parameters  $\rho_1, \rho_2$  before it appears. Since these modes first appear at the band edges of the host ( $|\lambda| = 1$ ), the local modes appear whenever

$$\left| \frac{1}{2 - \rho_1} + \rho_2 \right| > 1,$$

which coincides with the solid lines in Fig. 2. The scaling form for  $\alpha$  in (20) is identical to that of the inverse lattice

spacing and hence  $\alpha$  can be identified as the inverse localization length for the local mode. In the nearest-neighbor case ( $\rho_2=0$ ), we simply have  $\alpha=\ln|1/\rho_1|$  in agreement with the standard treatment of this problem.<sup>4</sup>

The symmetric modes can also be discussed in a similar fashion but the expressions are more complicated. It is easier to evaluate the various  $G_{ij}$  directly using the general expressions in (5) and determine the location and symmetry of the local modes from their divergent behavior.

## V. SUMMARY AND CONCLUSIONS

In this paper we have described a real-space rescaling approach for the calculation of the spectral properties of a randomly disordered tight-binding model Hamiltonian on a 1D chain. Although we restricted the range of interaction to first and second neighbors and used a scaling factor of 2 (eliminating every other site) a general transformation can be obtained for any range of interaction and any scaling factor. Real-space methods have been used previously<sup>5-8</sup> for disordered tight-binding models, but the ability to handle longer-ranged interactions is crucial for the application of these techniques to higher dimensional lattices. For these lattices, the elimination procedure causes the effective range of interaction to increase under iteration and it is necessary to use a transformation which is valid for arbitrary range. We have derived an exact

transformation for the problem of a single defect in the two-dimensional square lattice and these results will be reported elsewhere.

The expressions in Sec. II can be used to study systems with an arbitrary number of defects exactly. However, for a finite concentration of defects, a suitable averaging procedure<sup>5,8,9</sup> should be used on the parameters in these expressions. We are currently studying this question.

Several other techniques are available for calculating the local Green's functions of disordered systems, notably the recursion method used by Haydock<sup>10</sup> and co-workers. In contrast to that method the present approach does not involve a preliminary transformation of the initial Hamiltonian to a tridiagonal (nearest-neighbor) form and the concomitant numerical problems of nonorthogonality.<sup>10,11</sup> Stein and Krey<sup>12</sup> have used a rescaling method in the study of Anderson localization in combination with the recursion method. However, our approach is a direct attack on the identical disordered Hamiltonian and does not rely on the tridiagonal form.

## ACKNOWLEDGMENTS

We wish to thank P. D. Loly for a critical reading of the manuscript and helpful suggestions. This research has been supported by the Natural Sciences and Engineering Research Council of Canada.

<sup>1</sup>B. W. Southern, A. A. Kumar, P. D. Loly, and A.-M. S. Tremblay, *Phys. Rev. B* **27**, 1405 (1983).

<sup>2</sup>E. N. Economou, in *Green's Functions in Quantum Physics*, Vol. 7 of *Springer Series in Solid State Sciences*, edited by M. Cardona, P. Fulde, and H.-J. Queisser (Springer, New York, 1979).

<sup>3</sup>T. Wolfram and J. Callaway, *Phys. Rev.* **130**, 2207 (1963).

<sup>4</sup>R. M. White, *Quantum Theory of Magnetism* (McGraw-Hill, New York, 1970), pp. 178-188.

<sup>5</sup>D. Schmeltzer and R. Beserman, *Phys. Rev. Lett.* **47**, 860 (1981).

<sup>6</sup>D. Schmeltzer, *Phys. Rev. B* **25**, 3915 (1982).

<sup>7</sup>C. E. T. Goncalves da Silva and B. Koiller, *Solid State Commun.* **40**, 215 (1981).

<sup>8</sup>R. B. Stinchcombe, *Phys. Rev. Lett.* **50**, 200 (1983).

<sup>9</sup>J.-M. Langlois, A.-M. S. Tremblay, and B. W. Southern, *Phys. Rev. B* **28**, 218 (1983).

<sup>10</sup>R. Haydock, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1980), Vol. 35, p. 215.

<sup>11</sup>S. Kirkpatrick, in *Disordered Systems and Localization*, Vol. 149 of *Lecture Notes in Physics*, edited by C. Castellani, C. Di-Castro, and L. Peliti (Springer, New York, 1981), p. 280.

<sup>12</sup>J. Stein and U. Krey, *Solid State Commun.* **27**, 1405 (1978).