Renormalization-group method for studying the spectra of disordered square lattices

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We present a new method for calculating the density of electronic states on a disordered square lattice. The method is based on the real-space renormalization-group technique proposed by Gonçalves da Silva and Koiller for the case of a disordered chain. It is shown that the method can give correct energy ranges and detailed structures of the spectra of disordered square lattices without much numerical work. The improvement required and the further use of the new method are discussed.

I. INTRODUCTION

Investigation of the electronic properties of disordered systems has received considerable attention over the past few decades. The classical analytical methods based on the single-site approximations,[1,2] which may be used to study both the energy spectra and the localization of the eigenstates of such systems, have the shortcomings of resulting in an average medium and hence cannot properly describe the effects of strong disorder. For example, the coherent-potential approximation (CPA),[3] usually regarded as the best of these single-site approximations, is shown to be successful only for systems with a large coordination number z ($z \geq 10$). The numerical simulation methods, such as Schmidt's exact-functional-equation method[4] and Dean's negative-eigenvalues method,[5] can be used to obtain the total integrated densities of states and to reveal the rich structures of the spectra. However, the numerical schemes are rather tedious in practice and incapable of obtaining the local densities of states and more information about the nature of the eigenstates. In recent years, various real-space renormalization-group (RSRG) methods have been developed to study the densities of states for disordered systems.[6-18] Some of these methods are based on the RSRG scheme proposed by Gonçalves da Silva and Koiller (GK).[6-16] Starting with the equation of motion for the Green's function, they obtain the densities of states from the usual relation, $\rho(E) = (-1/\pi)\text{Im}[G_{00}(E + i0^+)]$. Wiecko and Roman have proposed another successful method of calculating the densities of states using the decimation renormalization-group technique, in which they always work with real numbers.[17,18] All the RSRG methods mentioned above have the advantage of requiring much less numerical work than other possible methods. In all forms of the GK scheme, two approximations are introduced. The first one is that the configuration averages of the Green's function over the eliminated sites are used to substitute for that over all the lattice sites. The second is

that the averages of the Green's function are actually performed by averaging the renormalization coefficients. Langlois *et al.*[9] had suggested an improved RSRG method to calculate the densities of states of random binary chains, but they found that the method will give negative values in certain energy ranges. In a recent paper[16] we have shown that these unphysical negative values can be avoided in actual calculation, and this method is very efficient when used to calculate the densities of states for disordered chains accurately.

In the present work, a RSRG method based on the GK scheme is proposed to calculate the density of states of a disordered square lattice. It is well known that there is a basic difficulty in extending the RSRG method mentioned above to systems with dimensions greater than 1. This is essentially because in two- or three-dimensional systems, lattice decimations introduce more than nearest-neighbor interactions, which prevent the definition of a close and finite system of renormalizable variables. This difficulty has been surmounted in our method, in which we first transform the square lattice into an approximately equivalent chain and then treat the equivalent chain with the usual cluster-decimation method.

II. METHOD

Let us consider a random binary alloy system $A_x B_{1-x}$ as shown in Fig. 1, where each site of the square lattice is labeled with (i, I). We start with the tight-binding Hamiltonian,

$$H = \sum_{I,i} E_i(I)|i,I\rangle\langle i,I| + \sum_{\substack{I,i,J,j \\ i\neq j, I\neq J}} V_{i,j}(I,J)|i,I\rangle\langle j,J| ,$$

(1)

where $E_i(I)$ and $|i,J\rangle$ are the energy and the Wannier wave function of the atom centered at site (i,I), respectively, and $V_{i,j}(I,J)$ is the hopping integral between sites (i,I) and (j,J). We assume that $E_i(I)$ may be E_A and E_B
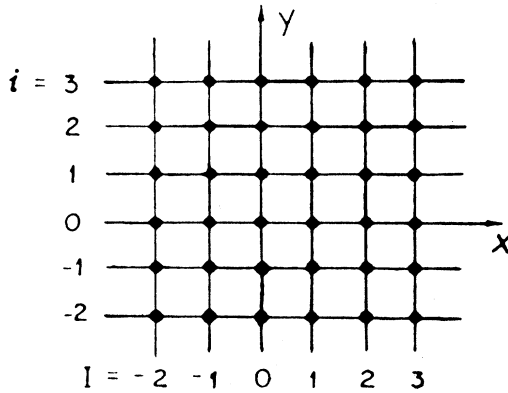
FIG. 1. Illustration for labeling the sites of the square lattice.

FIG. 2. Illustration for grouping the strip system in a cluster of N atoms.

with probabilities x and $1-x$, respectively, and $V_{i,j}(I,J)$ equals a nonzero constant V for nearest neighbors independent of the occupations and is zero otherwise.
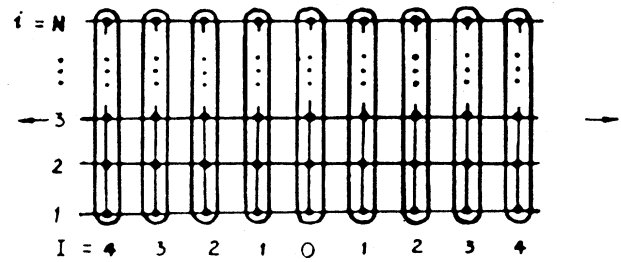
In order to make the basic idea of our method clear, we discuss first an infinite ordered strip of finite width as shown in Fig. 2. Regarding this system as an infinite chain of clusters in which each cluster consists of the N sites situated in the same array, the Hamiltonian of the system can be written in the form

$$h = \sum_I h(I) + \sum_I [h(I,I+1) + h(I,I-1)] , \qquad (2)$$

where

$$h(I) = \sum_{i=1}^{N} E_i(I)|i,I\rangle\langle i,I| + \sum_{i=1}^{N-1} V|i,I\rangle\langle i+1,I|$$
$$+ \sum_{i=1}^{N} V|i,I\rangle\langle i-1,I| \qquad (3)$$

describes the Ith cluster, and

$$h(I,I\pm1) = \sum_{i=1}^{N} V|i,I\rangle\langle i,I\pm1| \qquad (4)$$

describes the hopping between nearest clusters. The equation of motion for the Green's function,

$$g(Z-h) = 1 \quad (Z = E + i\eta, \ \eta \to 0) , \qquad (5)$$

can be expressed in the matrix form

$$[Z - h(I)]g(I,0) = \delta(I,0) + h(I,I-1)g(I-1,0)$$
$$+ h(I,I+1)g(I+1,0)$$
$$I = -\infty, \ldots, 0, \ldots, \infty \qquad (6)$$

where $g(I,J)$ is a $N \times N$ matrix defined as

$$g_{i,j}(I,J) = \langle i,I|g|j,J\rangle . \qquad (7)$$

Equation (6) is of exactly the same form as that for a single chain with only nearest-neighbor hoppings obtained by Koiller et al.[7] Therefore, it is easy to obtain the recursion relations for renormalization by using the cluster-decimation technique.[9,10,13] Without loss of generality, only the terms involving the center cluster ($I=0$) are given here:

$$h^{(k+1)}(0) = h^{(k)}(0) + h^{(k)}(0,-1)[Z-h^{(k)}(-1)]^{-1}h^{(k)}(-1,0) + h^{(k)}(0,1)[Z-h^{(k)}(1)]^{-1}h^{(k)}(1,0) , \qquad (8)$$

$$h^{(k+1)}(0,\pm1) = h^{(k)}(0,\pm1)[Z-h^{(k)}(\pm1)]^{-1}h^{(k)}(\pm1,\pm2) . \qquad (9)$$

Here, the superscript k denotes the times of renormalization. The fixed point can be obtained as

$$\lim_{k\to\infty} h^{(k)}(0,\pm1) = 0 , \quad \lim_{k\to\infty} h^{(k)}(0) = h^*(0) = h(0) + \Sigma , \qquad (10)$$

where

$$\Sigma = \sum_{k=0}^{\infty} h^{(k)}(0,-1)[Z-h^{(k)}(-1)]^{-1}h^{(k)}(-1,0) + \sum_{k=0}^{\infty} h^{(k)}(0,1)[Z-h^{(k)}(1)]^{-1}h^{(k)}(1,0) \qquad (11)$$

is the so-called self-energy which contains all the information obtained from the strip. We can regard $h^*(0)$ as the Hamiltonian of a chain consisting of N atoms. Thus we have transformed the strip into an equivalent finite chain, as is illustrated in Fig. 3. It should be noted that there are hoppings between any two sites in the equivalent chain described by $h^*(0)$.

It is evident that the numerical work would be too much for a strip of very large N. Fortunately, it is found that the hopping term $[h^*(0)]_{i,j}$ of the equivalent chain

tends to approach zero quickly as the value of $|i-j|$ increases, as shown in Table I. Therefore, as a good approximation, only the short-range hoppings ($|i-j| < m$) need to be considered for an infinite equivalent chain with respect to an infinite square lattice, and these short-range hopping terms can be approximately determined from the $N \times N$ matrix $h^*(0)$ by taking $N = m$. Thus the Hamiltonian of the equivalent chain with respect to an infinite square lattice can be approximately written as
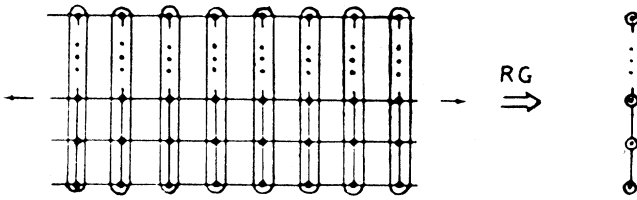
FIG. 3. Schematic representation of the effect of the RG transformation in x direction.

$$H_{i,i+j}^{equ} = H_{i+j,i}^{equ}$$

$$= \begin{cases} [h^*(0)]_{F[(1/2)(m-j)+1],\, F[(1/2)(m-j)+1]+j}, & j < m \\ 0, & j \geq m \end{cases} \tag{12}$$

where $F(x)$ stands for the integral part of x. It should be noted that such a definition is in favor of minimizing the boundary effect introduced by the finite value of m.

Now we have an infinite chain approximately equivalent to a square lattice. The approximation is determined by the value of m. The infinite chain can be exactly treated with the cluster-decimation method. Dividing the system into a chain of clusters consisting of m atoms, as shown in Fig. 4, we get a chain with only nearest-neighbor cluster hopping. Hence, H^{equ} can be expressed as

$$H^{equ} = \sum_m H^{equ}(M) + \sum_M [H^{equ}(M,M+1)$$

$$+ H^{equ}(M,M-1)], \tag{13}$$

where

$$H^{equ}(M)_{i,j} = H^{equ}_{(M-1)m+i,\,(M-1)m+j}, \tag{14}$$

$$H^{equ}(M,M+1)_{i,j} = H^{equ}_{(M-1)m+i,\,Mm+j}, \tag{15}$$

$$H^{equ}(M,M-1)_{i,j} = H^{equ}_{(M-1)m+i,\,(M-2)m+j}. \tag{16}$$

Since Eq. (13) has exactly the same form as that of Eq. (2), we can easily get the following renormalization recursion relations for the equivalent chain:
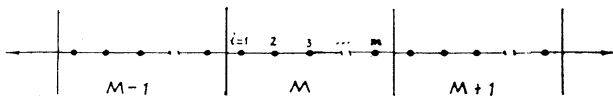

FIG. 4. Illustration for relabeling the approximately one equivalent chain.

TABLE I. The values of $h^*(0)_{F[(1/2)(m-j)+1],\,F[(1/2)(m-j)+1]+j}$ for $m=8$, $\eta=0.02$, and $V=1$, where $j < m$ and $F(x)$ stands for the integral part of x.

j	$E=0$ Real Part	$E=0$ Imag. Part	$E=1$ Real Part	$E=1$ Imag. Part	$E=2$ Real Part	$E=2$ Imag. Part	$E=3$ Real Part	$E=3$ Imag. Part	$E=4$ Real Part	$E=4$ Imag. Part
0	0.0	1.3	5.8×10^{-1}	1.2	1.3	8.7×10^{-1}	2.1	4.9×10^{-1}	3.3	3.2×10^{-2}
1	-2.8×10^{-2}	0.0	-5.3×10^{-1}	5.5×10^{-1}	-9.5×10^{-1}	6.2×10^{-1}	-1.3	4.3×10^{-1}	-1.3	9.9×10^{-3}
2	0.0	-4.0×10^{-1}	3.2×10^{-1}	-2.1×10^{-1}	2.7×10^{-1}	1.0×10^{-1}	2.3×10^{-2}	2.6×10^{-1}	-1.1×10^{-1}	7.2×10^{-3}
3	-1.2×10^{-2}	0.0	-1.4×10^{-1}	-9.5×10^{-2}	7.3×10^{-2}	-1.1×10^{-1}	1.0×10^{-1}	1.0×10^{-1}	-5.5×10^{-3}	5.2×10^{-3}
4	0.0	-6.6×10^{-2}	-9.9×10^{-2}	7.2×10^{-2}	-7.3×10^{-2}	-6.0×10^{-2}	6.7×10^{-2}	-2.4×10^{-2}	-2.9×10^{-2}	3.6×10^{-3}
5	-5.5×10^{-3}	0.0	3.5×10^{-2}	-1.2×10^{-2}	-7.2×10^{-2}	8.1×10^{-2}	3.9×10^{-3}	-3.6×10^{-2}	-1.6×10^{-2}	2.6×10^{-3}
6	0.0	-1.9×10^{-2}	-2.1×10^{-2}	-3.3×10^{-2}	2.6×10^{-2}	2.2×10^{-2}	-3.4×10^{-2}	-1.7×10^{-2}	-9.0×10^{-3}	1.6×10^{-3}
7	-2.2×10^{-3}	0.0	-4.5×10^{-2}	4.1×10^{-2}	8.3×10^{-3}	-9.9×10^{-3}	-3.7×10^{-2}	-4.9×10^{-2}	-5.1×10^{-3}	1.0×10^{-3}

$$(H^{\mathrm{equ}})^{(k+1)}(0)=(H^{\mathrm{equ}})^{(k)}(0)+(H^{\mathrm{equ}})^{(k)}(0,-1)[Z-(H^{\mathrm{equ}})^{(k)}(-1)]^{-1}(H^{\mathrm{equ}})^{(k)}(-1,0)$$

$$+(H^{\mathrm{equ}})^{(k)}(0,1)[Z-(H^{\mathrm{equ}})^{(k)}(1)]^{-1}(H^{\mathrm{equ}})^{(k)}(1,0) \ , \tag{17}$$

$$(H^{\mathrm{equ}})^{(k+1)}(0,\pm1)=(H^{\mathrm{equ}})^{(k)}(0,\pm1)[Z-(H^{\mathrm{equ}})^{(k)}(\pm1)]^{-1}(H^{\mathrm{equ}})^{(k)}(\pm1,\pm2) \ . \tag{18}$$

In addition, we can obtain the fixed point

$$\lim_{k\to\infty}(H^{\mathrm{equ}})^{(k)}(0)=(H^{\mathrm{equ}})^*(0) \tag{19}$$

from $\lim_{k\to\infty}(H^{\mathrm{equ}})^{(k)}(0,\pm1)=0$.

The density of states for an infinite ordered square lattice can be calculated by

$$\rho(E)=-\frac{1}{m\pi}\lim_{\eta\to0^+}\mathrm{Im}\,\mathrm{Tr}[Z-(H^{\mathrm{equ}})^*(0)]^{-1} \ . \tag{20}$$

Figure 5 shows the density of states calculated with different values of m compared with the exact result for an ordered square lattice. It is shown that our calculated results converge to the exact results rapidly as the value of m increases.

The method presented here is obviously not necessary for studying ordered systems; its importance lies in studying disordered systems for which no analytical result can be derived. The key problem for using the method to study disordered systems is to choose a proper approximation for performing configurational averages. Here we adopt the GK scheme[6,10,15] for simplicity.

For a strip of random binary alloy $A_x B_{1-x}$, as shown in Fig. 2, each cluster has 2^N possible configurations, since the site energy may be E_A and E_B, with probabilities x and $1-x$, respectively. The probability for a cluster in the ξth configuration, which contains n A atoms is

$$P_\xi=x^n(1-x)^{N-n} \ . \tag{21}$$

The recursion relations for renormalization of the disordered strip can be written as

$$h_\xi^{(k+1)}(0)=h_\xi^{(k)}(0)+\sum_{\xi'}P_{\xi'}\{h^{(k)}(0,-1)[Z-h_\xi^{(k)}(-1)]^{-1}h^{(k)}(-1,0)+h^{(k)}(0,1)[Z-h_\xi^{(k)}(1)]^{-1}h^{(k)}(1,0)\} \ , \tag{22}$$

$$h^{(k+1)}(0,\pm1)=\sum_{\xi'}P_{\xi'}h^{(k)}(0,\pm1)[Z-h_\xi^{(k)}(\pm1)]^{-1}h^{(k)}(\pm1,\pm2) \ , \tag{23}$$

and the fixed point can be obtained,

$$\lim_{k\to\infty}h_\xi^{(k)}(0)=h_\xi^*(0)=h_\xi(0)+\Sigma' \ , \tag{24}$$

$$\lim_{k\to\infty}h^{(k)}(0,\pm1)=0 \ , \tag{25}$$

where

$$\Sigma'=\sum_{k=0}^\infty\sum_{\xi'}P_{\xi'}\{h^{(k)}(0,-1)[Z-h_\xi^{(k)}(-1)]^{-1}h^{(k)}(-1,0)+h^{(k)}(0,1)[Z-h_\xi^{(k)}(1)]^{-1}h^{(k)}(1,0)\} \ . \tag{26}$$

Now we can define the Hamiltonian of a disordered chain, which is approximately equivalent to the infinite disordered square lattice as

$$H_{i,i+j}^{\mathrm{equ}}=H_{i+j,i}^{\mathrm{equ}}=\begin{cases} E_i+\Sigma'_{F[(1/2)m+1],F[(1/2)m+1]}, & j=0 \\ V+\Sigma'_{F[(1/2)m+1],F[(1/2)m]}, & j=1 \\ \Sigma'_{F[(1/2)(m-j)+1],\,F[(1/2)(m-j)+1]+j}, & 1<j<m \\ 0, & j\ge m \end{cases} \tag{27}$$

where E_i can take E_A and E_B with probabilities x and $1-x$, respectively.

Similar to the discussion for the equivalent chain with respect to an ordered square lattice, the recursion relations for renormalization of the disordered equivalent chain can be obtained as

$$(H_\xi^{\mathrm{equ}})'^{(k+1)}(0)=(H_\xi^{\mathrm{equ}})'^{(k)}(0)+\sum_{\zeta'}S_{\zeta'}\{(H^{\mathrm{equ}})'^{(k)}(0,-1)[Z-(H_\xi^{\mathrm{equ}})'^{(k)}(-1)]^{-1}(H^{\mathrm{equ}})'^{(k)}(-1,0)$$

$$+(H^{\mathrm{equ}})'^{(k)}(0,1)[Z-(H_\xi^{\mathrm{equ}})'^{(k)}(1)]^{-1}(H^{\mathrm{equ}})'^{(k)}(1,0)\} \ , \tag{28}$$

$$(H^{\mathrm{equ}})'^{(k+1)}(0,\pm1)=\sum_{\zeta'}S_{\zeta'}(H^{\mathrm{equ}})'^{(k)}(0,\pm1)[z-(H_\xi^{\mathrm{equ}})'^{(k)}(\pm1)]^{-1}(H^{\mathrm{equ}})'^{(k)}(\pm1,\pm2) \ , \tag{29}$$
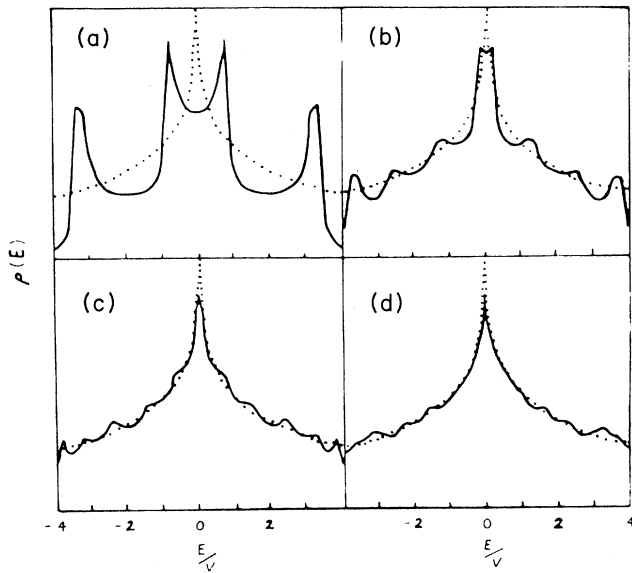
FIG. 5. Densities of states of ordered square lattice $(E_A = E_B = 0,\ V = 1)$ calculated using the RG method with (a) $m = N = 2$, $\eta = 0.1$; (b) $m = N = 4$, $\eta = 0.1$; (c) $m = N = 6$, $\eta = 0.1$; (d) $m = N = 8$, $\eta = 0.1$. The dashed line is the exact result.

where S_ζ is the probability of a cluster consisting of m equivalent atoms, as shown in Fig. 4, in the ζth configuration.

The fixed point can be finally obtained as

$$\lim_{k \to \infty} (H^{equ})'^{(k)}(0, \pm 1) = 0 \ , \tag{30}$$

$$\lim_{k \to \infty} (H_\zeta^{equ})'^{(k)}(0) = (H_\zeta^{equ})'^*(0) \ . \tag{31}$$

The average density of states for a disordered square lattice can the be calculated by

$$\rho'(E) = -\frac{1}{m\pi} \lim_{\eta \to 0^+} \mathrm{Im} \sum_\zeta S_\zeta \mathrm{Tr}[Z - (H_\zeta^{equ})'^*(0)]^{-1} \ . \tag{32}$$
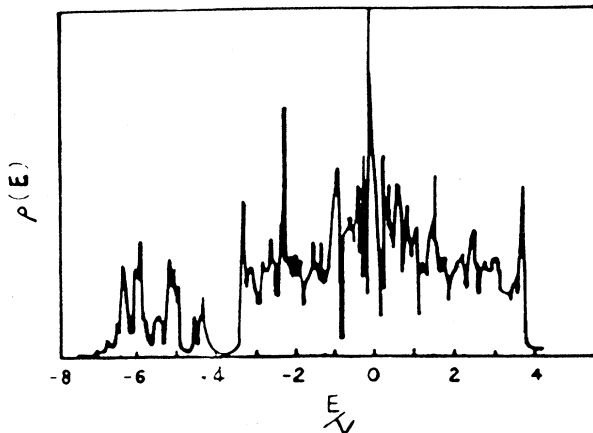

FIG. 6. Density of states of random binary alloy $(E_A = 0,\ E_B = -5,\ V = 1,\ x = 0.90)$ calculated using the new RG method with $m = N = 6$, $\eta = 0.02$.

III. NUMERICAL RESULTS
FOR DISORDERED SYSTEMS

In order to illustrate the applicability of our method in treating disordered systems, we have considered specific examples.

We have first examined a random binary alloy $A_x B_{1-x}$ with $V = 1$, $E_A = 0$, $E_B = -5$, and $x = 0.9$. Figure 6 shows the numerical results calculated with $\eta = 0.02$. As we can see, the density of states exhibits rich structures in both the majority band and the minority band. We have repeated the calculation for the same system with other values of η. It is found that the smaller η we take, the richer structures emerge in the density of states. As is well known, the structures in the density of states of a
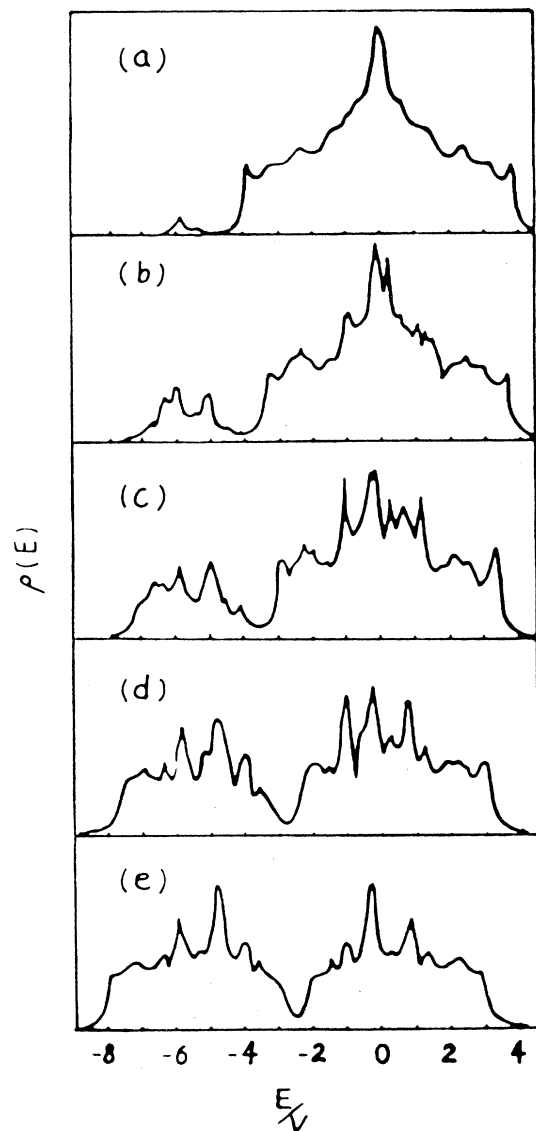

FIG. 7. Densities of states of random binary alloys $(E_A = 0,\ E_B = -5,\ V = 1)$ calculated using the new RG method with $m = N = 6$, $\eta = 0.1$ for different concentrations: (a) $x = 0.99$, (b) $x = 0.90$, (c) $x = 0.80$, (d) $x = 0.60$, and (e) $x = 0.50$.
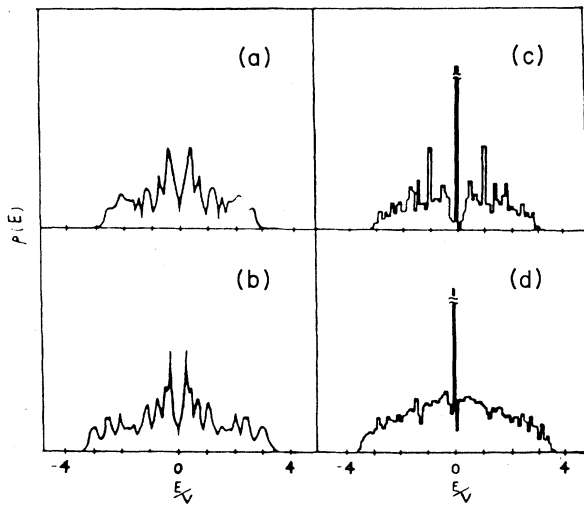
FIG. 8. Densities of states in the A subband of random binary alloys ($E_A = 0$, $E_A - E_B/V \rightarrow \infty$): (a) calculated using the RG method for $x = 0.501$ with $m = N = 6$, $\eta = 0.02$; (b) calculated using the RG method for $x = 0.715$ with $m = N = 6$, $\eta = 0.02$; (b) obtained by Kirkpatrick and Eggarter from computer simulation for $x = 0.501$; (d) obtained by Kirkpatrick and Eggarter from computer simulation for $x = 0.715$.

FIG. 9. The cluster of an isolated A atom which results in the central peak in the density of states shown in Fig. 8(c) or 8(d).

disordered system result from the compositional fluctuations. For this reason, calculations based on single-site approximations such as the CPA are not able to reveal these structures. On the other hand, the RSRG techniques enable us to approximately treat the compositional fluctuations at all length scales, thus our calculations can yield richly structured densities of states.

Figure 7 shows the calculated densities of states of a random binary alloy $A_x B_{1-x}$ with various x. In all these cases, we have set $E_A = 0$, $E_B = -5$, $V = 1$, and $\eta = 0.1$. It is shown that each of these spectra consists of two subbands, and the width of the subband corresponding to E_A (E_B) is approximately proportional to $x^{1/2}$ ($(1-x)^{1/2}$) as predicted early by Lifshitz[19] and Taylor.[20]

Finally, we have considered the case of split-band-limit $|E_A - E_B|/V \rightarrow \infty$. Figures 8(a) and 8(b) show our calculated results for $x = 0.501$ and 0.715, respectively, and Figs. 8(c) and 8(d) show the numerical simulation results obtained by Kirkpatrick and Eggarter.[21] Compared to the numerical simulation results, our calculated results are seen to be excellent in giving the energy ranges of the A subband, although there are significant differences in detail structures of the spectra.

IV. SUMMARY

We have presented a RSRG method based on the GK scheme for calculating the densities of states of disordered (or ordered) square lattices. The numerical results have manifested the efficiency of the method in giving correct energy ranges and revealing rich structures of the
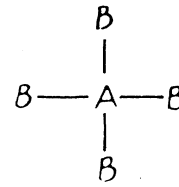
spectra of two-dimensional disordered systems. The numerical work required is not much.

It is certainly found in our numerical calculations for disordered square lattices that smaller η's lead to more peaks in the densities of states. In the GK scheme, the value of the imaginary part η of a complex energy $Z = E + i\eta$ should be taken as small as possible in principle, which means that the smaller the value of η, the more accurate the results that can be obtained in practical calculations. Therefore, all the peaks emerging in the density of states as $\eta \rightarrow 0$ should be physically relevant We think that the phenomenon of smaller η's leading to more peaks in the densities of states is probably related to the localization of eigenstates of two-dimensional disordered systems,[3,22,23] since the contributions of localized states to the densities of states should be described by δ functions in E.

The discrepancies between our calculated results and the numerical simulation results, as shown in Fig. 8, indicate that our method should be improved. These discrepancies originate from the neglect of some cluster effects which are very important in the split-band limit. For example, the peaks at $E = 0$ in Figs. 8(c) and 8(d) are just the results of the clusters in the configuration shown in Fig. 9, and these peaks do not appear in our calculations since our RG transformation cells are all in the form of chains, as shown in Fig. 10(a). We believe that the results of our method can be improved if the RG transformation cells are taken to be two-dimensional
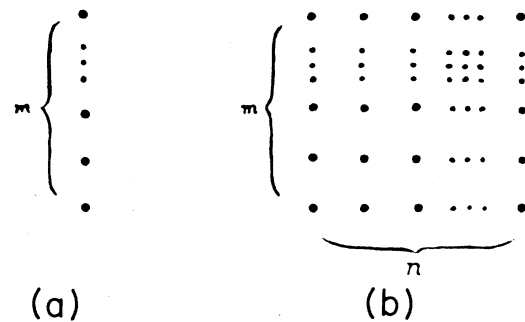

(a) (b)

FIG. 10. (a) Illustrative example for the one-dimensional cluster; (b) illustrative example for the two-dimensional cluster.

clusters, as shown in Fig. 10(b).

Finally, the present method may be extended to treat short-range order as done by Koiller et al.[7] for one-dimensional systems, and may be used to study the localization of eigenstates in two-dimensional disordered systems. We will discuss these problems in later papers.

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