Matrix continued-fraction calculation of localization length

H. M. Pastawski, J. F. Weisz, and S. Albornoz
Instituto de Desarrollo Tecnológico para la Industria Química, Universidad Nacional del Litoral, Consejo Nacional de Investigaciones Científicas y Técnicas, Guemes 3450, 3000 Santa Fe, República Argentina

(Received 29 October 1982; revised manuscript received 1 March 1983)

A matrix continued-fraction method is used to study the localization length of the states at the band center of a two-dimensional crystal with disorder given by the Anderson model and with incommensurate charge-density waves. For the disordered case it is found that exponentially localized states, which scale according to the work of MacKinnon and Kramer, become weakly localized as the disorder becomes weaker, and there is some critical disorder for which the localization length does not saturate with the width of the strips, which confirms the results found by Pichard and Sarma. Weakly localized states are also found in one dimension for $W/V \lesssim 1$. In the case of a crystal with a modulation that is incommensurate in one direction and commensurate in the other, the localization in the first direction behaves in a similar fashion as that found by Aubry, Sokoloff, and others for the one-dimensional chain, that is, approximately the same critical modulation strength is found: $W_c/V=2$. If the modulation is incommensurate in two perpendicular directions, there appears a tendency of increasing localization lengths as the width of two-dimensional strips is increased and an intermediate regime develops between the insulating and metallic regions.

I. INTRODUCTION

Many interesting physical systems may be modeled by a Hamiltonian representing a linear chain with nearest-neighbors interaction which has the form

$$\hat{H}=\sum_i E_i \,|\, i\rangle\langle i \,|\, + V_{i,i+1} \,|\, i\rangle\langle i+1 \,|\, + V_{i+1,i} \,|\, i+1\rangle\langle i \,|\, , \tag{1}$$

where index i denotes a site with an energy E_i and $V_{i,i+1}$ is the hopping matrix element. The corresponding Green's function is

$$\hat{G}(E)=(E\hat{I}-\hat{H})^{-1} , \tag{2}$$

where $\hat{I}$ is the identity operator and E is a scalar.

In a local scheme, we can write

$$G_{00}(E)=\langle 0 \,|\, \hat{G}(E) \,|\, 0\rangle=\frac{1}{E-E_0-\Sigma_{00}(E)} . \tag{3}$$

Localization in disordered systems has been studied by expanding the self-energy Σ in an infinite renormalization perturbation series[1,2] which is difficult to handle. However, a tractable expression of the self-energy Σ_{00} may be found as the sum of two terms of the form

$$\Sigma_{00}(E)=\Delta_{00}^{-}(E)+\Delta_{00}^{+}(E) .$$

Each of these terms accounts for the effect of sites to the left or to the right of $|0\rangle$, respectively, and have a continued-fraction expression[3,4]:

$$\Delta_{00}^{\pm}=\cfrac{|V_{0,\pm1}|^2}{E-E_{\pm1}-\cfrac{|V_{\pm1,\pm2}|^2}{E-E_{\pm2}-\cfrac{|V_{\pm2,\pm3}|^2}{E-E_{\pm3}-\cdots}}} . \tag{4}$$

In order to clarify the meaning of this expansion we may put $E_{\pm(N+1)}=\infty$ and see that the self-energy $\Sigma_{00}^{(N)}(E)$ calculated with N sites to each side of $|0\rangle$ provides the exact self-energy for such a finite chain. If we work entirely within the realm of real numbers and have a system for which the continued fraction converges in L steps to the right (left) for a certain eigenenergy E, it means that there is an eigenvector which has an expansion in a finite number of local states. We may interpret the convergence length L as a measure of such a localization length. This follows from the criteria that states are localized when the self-energy is real and extended otherwise. It is clear, for example, that if the self-energy is not real then convergence is not obtained.

The continued-fraction expansion has been widely used in solving the density of states (DOS) and localization of one-dimensional charge-density waves[5–7] (CDW's) and Anderson disordered[8] systems. In studying higher-dimensionality systems there are various ways of proceeding. In one of these,[9] it is usual to reduce the model Hamiltonian to the form (1) using a recursion method which provides an algorithm for reducing a Hamiltonian to a tridiagonal form which can then be handled as in a one-dimensional system. However, we do not follow this procedure, but instead make use of the fact that the Hamil-

tonian in a tight-binding representation appears in a block-tridiagonal form.

Thus in Sec. II we carry out a straightforward generalization of (3) and (4) as a matrix continued fraction (MCF) where $G_{00}(E)=\langle 0|\hat{G}(E)|0\rangle$ becomes a matrix, the state $|0\rangle$ representing a set of states in a layer perpendicular to the length of the chain.

In Sec. III we use the MCF formalism in evaluating the localization length in a two-dimensional Anderson disordered system. We show the results for the statistics of the localized states and find the regimes for exponentially and weakly localized states. Results seem to be in accord with those obtained by Pichard and Sarma[10] using a transfer-matrix approach.

In Sec. IV we study the tight-binding model for CDW systems and show by numerical computation that for two-dimensional CDW systems, the localization properties are not very different from those of a one-dimensional chain (as studied by Sokoloff,[5] Bulka,[7] Soukoulis and Economou,[11] and others).

II. MATRIX CONTINUED FRACTIONS

In order to calculate the local DOS and localization length in systems with a dimensionality higher than 1, we will use the fact, already pointed out by Butler,[12] that the resolvent or Green's function of a linear operator represented by a matrix, which is tridiagonal in blocks, permits a continued-fraction-like expansion.

Such a Hamiltonian has the form (1) where now the state $|i\rangle$ represents the set of N_i states associated with the index i; E_i is a $(N_i\times N_i)$ matrix representing the Hamiltonian matrix elements among states in the same set and $V_{i,i+1}$ is a $(N_i\times N_{i+1})$ matrix which connects successive sets of states.

Equation (2) for the Green's function is still valid and a particular block on the diagonal $G_{00}=\langle 0|\hat{G}|0\rangle$ may be written in a manner analogous to (3),

$$G_{00}(E)=[E-E_{00}-\Sigma_{00}(E)]^{-1}, \tag{5}$$

where $\Sigma_{00}=\Delta_{00}^{-}+\Delta_{00}^{+}$ is a matrix representing the self-energy and

$$\Delta_{ii}^{\pm}=V_{i,i\pm1}(E-E_{i\pm1,i\pm1}-\Delta_{i\pm1,i\pm1}^{\pm})^{-1}V_{i\pm1,i}. \tag{6}$$

These formulas may be deduced following Wu *et al.*[4] with the caution that the product of matrices may be noncommutative. The validity of Eqs. (4)—(6) is not restricted by the dimensionality of blocks.

For the case in which the $V_{i,i+1}$ matrices are of the form $V_{ij}=v\delta_{ij}$ (and hence commute) then the usual recursion formulas[13] of continued-fraction theory, namely

$$Q^{(n)}=A_nQ^{(n-1)}+Q^{(n-2)}$$

and

$$P^{(n)}=A_nP^{(n-1)}+P^{(n-2)}$$

with

$$Q^{(1)}=A_1,\quad A_n=\frac{(E-E_n)(-1)^n}{v},\quad P^{(1)}=I,$$

$$Q^{(0)}=I,\quad P^{(0)}=0$$

can be used to find successive convergents $\Delta^{(n)}=(Q^{(n)})^{-1}P^{(n)}$. However, even though this method is much faster than continually inverting matrices as in (6), it is found to be numerically unstable. Thus, we used (6) directly in our calculations.

If the matrix self-energy may be calculated accurately after L steps of iteration with (6) this length can be considered to be the maximum localization length of a state with energy E, in the neighborhood of the $|0\rangle$ set of states. It should be noted that the calculations of Σ_{00} are always referred to the same original site $|0\rangle$, thus in calculating each new convergent the continued fraction must be recalculated. Convergence of the continued fraction is obtained when the difference between successive convergents approaches zero.

There are two different methods which are very successful in evaluating the mean localization length in disordered systems. It is important to emphasize the differences between them and the MCF approach. The main idea is to calculate some property characteristic of the whole system which, if the system is large enough, will depend on the strength of the disorder and on the sample dimensions, but not on the particular configuration used in the calculation. In the method of MacKinnon and Kramer this property is the transmittance between the two ends of the finite strip (bar), which in the limit of very long length was the asymptotic property

$$\mathrm{Tr}\,|\langle 0|G(E)|N\rangle|^2=e^{-2(N-1)/\lambda}\quad (N\to\infty).$$

In the other method, that of Pichard and Sarma, the transfer matrices T_i up to the Nth slice are evaluated to find the transfer matrix of the whole strip (bar):

$$T^N=T_NT_{N-1}\cdots T_2T_1,$$

whose minimum eigenvalue $\gamma_{\min}$ has the asymptotic property

$$\gamma_{\min}\propto e^{-N/\lambda}\quad (N\to\infty).$$

In both methods $\lambda=\lambda(W,E)$ is a statistical measure of the localization length. As a mean property, it may be evaluated as accurately as needed by taking N sufficiently large, the results being configuration independent.

On the other hand, our method is based on a different idea. Given a particular configuration and a given layer which we call $|0\rangle$, we ask how large must a cluster be in order to reproduce correctly the local properties at layer $|0\rangle$ and its neighborhood. The MCF expansion of the site self-energy $\Sigma_{00}(E)$ gives us an idea of localization of an eigenstate of energy E in this region and also permits the evaluation of local density of states from G_{00} (an example is given in Sec. IV). Of course, for a different cluster the localization length may not be the same. Moreover, the convergence of these local properties do not necessarily follow any well-defined law. In particular, certain configurations will have very large localization lengths. Our method permits the study of the statistical distribution of the localization lengths among the different configurations.

III. ANDERSON DISORDERED LATTICE

A. General considerations

In this section we will consider the usual tight-binding Hamiltonian

$$\hat{H}=\sum_{\vec{R}} E_{\vec{R}}\,|\vec{R}\rangle\langle\vec{R}| + \sum_{\substack{\vec{R},\vec{R}' \\ \text{(nearest neighbor)}}} V_{\vec{R},\vec{R}'}(|\vec{R}\rangle\langle\vec{R}'|+|\vec{R}'\rangle\langle\vec{R}|)\,, \quad (7)$$

where $\vec{R}$ are sites in a square lattice forming a strip of width M and infinite length ($D=2$) or sites in a cubic lattice forming an infinite bar ($D=3$) of cross section M^2.

Following Anderson[1] the energies $E_{\vec{R}}$ are assumed to be equidistributed in the interval $[-\frac{1}{2}W, \frac{1}{2}W]$ and for simplicity we take the hopping parameter V to be the same in all directions.

Hamiltonian (7) is tridiagonal in blocks so we can calculate the matrix self-energy $\Sigma_{00}=\Delta_{00}^{-}+\Delta_{00}^{+}$ of the $|0\rangle$ layer with expression (6). The convergence of the M^{D-1} dimensional matrix continued fraction might require lengthy calculations, so we introduce an additional assumption; the norm of the difference between successive convergents decreases exponentially, namely

$$||\Delta_{00}^{(N)}-\Delta_{00}^{(N-1)}||\sim\exp(-N/\lambda) \quad (8)$$

with

$$\lambda=\lambda(E,W/V)\sim L$$

and

$$||A||=\max\left[\sum_j |A_{ij}|\right].$$

This expression is expected to work well for a one-dimensional chain with uncorrelated disorder and exponentially localized states. Although we were not able to prove it for the proposed generalization, it fits well the numerical data for disorder which is not too weak and we will interpret this fact as evidence of exponential localization. There is a compromise between the number of points used to fit (8) and the time (proportional to N^2) required to calculate the N convergents; for this reason we perform only 50 iteration steps before fitting the data with the exponential.

For each set of parameters $(E,M,D,W/V)$ the averages of λ and $1/\lambda$ have been computed by taking an ensemble of 100 systems. This size of the ensemble has been selected in order to maintain the variance of $\langle\lambda\rangle_{\text{av}}$ and $\langle 1/\lambda\rangle_{\text{av}}$ to less than 5% of the mean.

The probability distribution of λ and $1/\lambda$ proved to be well defined so that there is no problem in finding the mean. At this point there may be some doubt as to whether it is appropriate to calculate a value representative of the exponential localization length by examining the mean of the distribution of λ or that of $1/\lambda$. We give the results of averaging λ: $\langle L\rangle_{\text{av}}\cong 10\langle\lambda\rangle_{\text{av}}$. It can be easily shown from the Schwartz inequality that $\langle\lambda\rangle_{\text{av}}\geq\langle 1/\lambda_{\text{av}}\rangle^{-1}$ so that the other possibility for averaging would give a somewhat smaller localization length. We find that both expressions give results which are qualitatively similar.

B. One-dimensional results

When calculating the exponential localization length of one-dimensional systems we found that when there is a strong disorder, Eq. (8) is very accurate for all systems in the ensemble, but as the disorder becomes weaker there appear systems with increasing frequency which do not satisfy (8) and show very low correlation coefficients in adjusting the data to the exponential, thus we adopted the criteria of discarding systems with a correlation coefficient below 0.75. Unless explicitly stated, in no case do we show results for $\langle\lambda\rangle_{\text{av}}$ if more than $\frac{1}{3}$ of the systems were discarded.

In Fig. 1 we show a histogram for the localization lengths of 200 one-dimensional systems with a weak-disorder parameter ($W/V=1.2$). Figure 1(a) shows the λ values obtained by writing (8) with correlation coefficients larger than 0.75. The other systems with lower correlation coefficients are plotted in Fig. 1(b). This shows qualitatively that the systems with low correlation coefficients (not exponentially localized) have larger localization lengths.

In Fig. 2 we plot the mean localization length for $E=0$ as a function of disorder parameter (W/V). The open circles represent averages over ensembles where more than $\frac{1}{3}$ of the systems should be discarded. The closed circles satisfy the usual one-dimensional result, namely

$$\lambda=\lambda_0\frac{1}{(W/V-W_c/V)^{\nu}},\quad W_c=0,\quad \nu=2\,. \quad (9)$$

For an analytic discussion of these results see the works of Thouless and Kirkpatrick,[14] Weisz *et al.*,[6] or Sarker.[15]

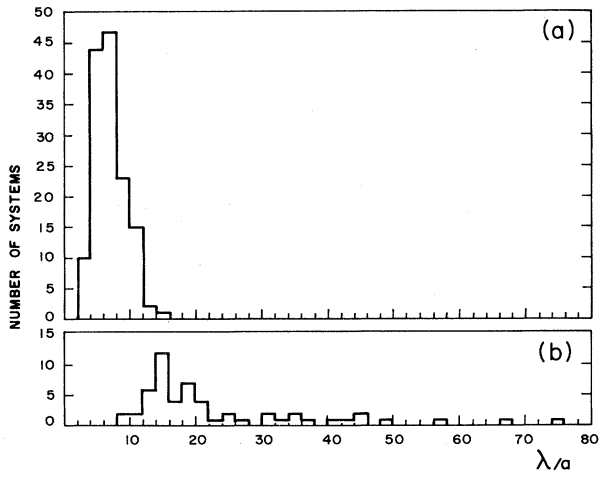

FIG. 1. Histograms showing the distribution of exponential localization length λ for 200 systems for $M=1$, $W/V=1.2$, and $E=0$. Systems in (a) have a correlation coefficient higher than 0.75; the others are represented in (b).

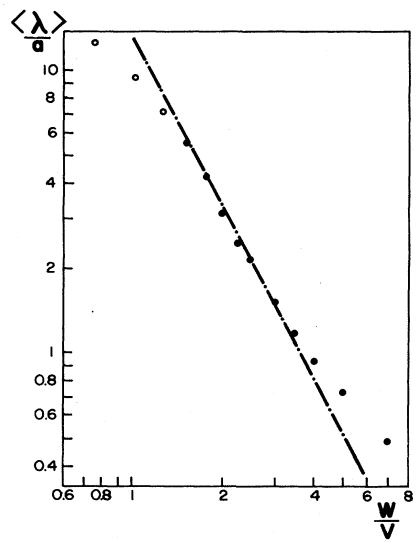

FIG. 2. Mean exponential localization length ($\langle\lambda\rangle_{av}$) for $E=0$ as a function of disorder (W/V) for a one-dimensional chain. Open circles are used for the averages where more than $\frac{1}{3}$ of the ensemble was discarded. The solid line has a slope -2.

C. Two-dimensional results

The same calculations were performed in two dimensions for a strip of width 10 and results are shown in Fig. 3. Equation (9) again represents quite well the behavior of exponential localization length with the same parameters $W_c=0$ and $\nu=2$. This shows that one-dimensional behavior is maintained for strips of finite width.

We also studied how the mean of exponential localization length evolves when the dimensionality of systems is increased varying M from 1 to 12 for $W/V=14,10,8,7,6,5,4$. The results shown in Fig. 4(a) are apparently those found by MacKinnon and also satisfy the one-parameter scaling found by this author. However, because the number of systems for which the exponential fit is good decreases as the width is increasing, as shown in Fig. 4(b), the procedure of using the exponential fit becomes invalid. We interpret this situation as a breakdown of exponential localization. Instead, we used the criteria that convergence is obtained when $||\Delta_L-\Delta_{L-1}||\leq 10^{-4}$; the graphs of L vs M for $W/V=6$ became linear up to $M=35$. However, for values of $W/V=10$ the saturating behavior could still be observed. It was difficult to obtain very good statistics with this latter method as only a few systems could be considered; however, there was every indication that the linear behavior was present if the disorder is weak. We have also shown in Fig. 4(b) how the number of systems for which the exponential fit is satisfactory steadily decreases as the width is increasing for $W/V\leq 8$. Thus there is clearly a regime where weak localization sets in. This is in accord with results of Pichard and Sarma. The MCF also seems to provide results similar to that of Pichard and Sarma for the three-dimensional case, but since it requires a great deal of machine time, we are not able to present them yet.

Our result that there is a linear behavior of L with M for states at $E=0$ for weak diagonal disorder may bring to mind the results of Soukoulis *et al.*,[16] who find the linear behavior at $E=0$ for a model with off-diagonal disorder. This brings up the question as to whether localization with diagonal disorder is similar to localization with off-diagonal disorder, after all. It appears, though, that there remains a strong qualitative difference between our results with diagonal disorder and those of Soukoulis

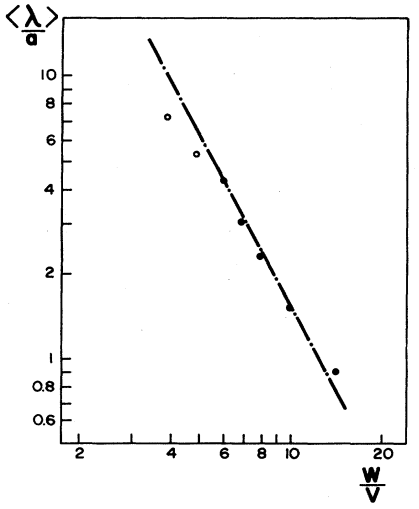

FIG. 3. Mean localization length as function of disorder (W/V) for a strip of width 10. The open circles are used for the averages where more than $\frac{1}{3}$ of the ensemble was discarded. The solid line has slope -2.

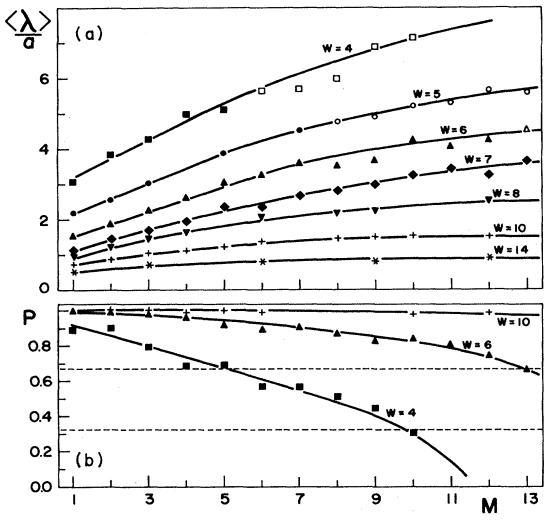

FIG. 4. (a) Mean exponential localization length $\langle\lambda\rangle$ as a function of the strip width M, (b) the proportion P of systems with exponential localization against M, both for $E=0$ and various values of W/V.

et al.[16] with off-diagonal disorder. Indeed their linear (nonexponential) behavior for $E=0$ persisted right up to the strongest disorder parameter that they used. This contrasts with our work where we can indeed talk about exponentially localized states, and saturating behavior for the localization length, provided the disorder is strong enough. This fact is not surprising if we think that although a larger width in the distribution of the respective parameters has a localizing tendency in both cases, the largest off-diagonal matrix elements would tend to favor extended states, while larger values of diagonal disorder tend to favor localized states. It is known, for example, that models of off-diagonal disorder which emphasize smaller values of V are the most likely to lead to localization at the band center.[17]

Another difference is that we fail to see a significant qualitative change using values of E chosen to the band center. This is in accord with the arguments used by Soukoulis *et al.*[16] since the diagonal disorder is known to remove the Van-Hove logarithmic singularity at $E=0$ of the two-dimensional crystal.[18]

Another consideration is that we deliberately do not mention a power-law localization. At this point it should be remembered that our method yields different information to that of methods used in Refs. 10, 16, and 19 (see discussion in Sec. II). Thus in their work a single iteration sequence, if made long enough, will yield an average localization within a given error. In our method, however, we are able to calculate localization lengths for particular clusters, and we obtain very different lengths for different configurations. In the limit of strong disorder the exponential fit (8) is valid and we obtain agreement with previous work[10,19] upon averaging a large number of configurations. In the weak-disorder limit, however, these lengths fluctuate so much that the data from individual configurations do not follow a given law. Thus instead of trying to fit a power-law behavior to the data, we preferred to examine the distribution of the weakly localized states. Our conclusion was that the long tail in the distribution of the weakly localized states appears to imply that there is a certain fraction of the ensemble with larger localization length than any given length. This is not surprising if one thinks that a certain subset of the configurations are nearly ordered.

Our calculations for $E\neq 0$ close to the band center indicate that for strong disorder the states remain exponentially localized, as expected. For weaker disorder different clusters have widely different localization lengths and one may mention a proportion P of exponentially localized states. Then since this proportion increases smoothly as one moves toward the band edge, one cannot consider the notion of an abrupt mobility edge to be valid in these systems. Haydock[20] has also found weakly localized states near the band center.

IV. TWO-DIMENSIONAL LATTICES WITH INCOMMENSURATE POTENTIALS

A. General considerations

The properties of electronic wave functions of CDW systems have been modeled with a one-dimensional tight-binding Hamiltonian with a periodic potential representing the distortion (e.g., Sokoloff, Bulka, and Soukoulis and Economou). If the modulation is incommensurate with the lattice, the system does not possess translational order, and unlike the one-dimensional random disordered chains, a mobility edge may arise separating extended states from localized ones.

At certain temperatures electrostatic repulsion among neighboring chains in the same plane may produce a locking of the relative phase from chain to chain in an angle of π.

In this section we study the localization of electrons in such a two-dimensional case by considering Hamiltonian (7) where $\vec{R}$ now denotes a position in a rectangular lattice with basis vector $\vec{a}_1$ and $\vec{a}_2$, that is

$$\vec{R}=n\vec{a}_1+m\vec{a}_2, \quad n,m \text{ integers}$$

and the matrix elements are defined in terms of a wave vector

$$\vec{Q}=Q_1\frac{\vec{a}_1}{a_1}+Q_2\frac{\vec{a}_2}{a_2},$$

$$E_{\vec{R}}=W\cos(\vec{Q}\cdot\vec{R})=W\cos(nQ_1a_1+mQ_2a_2), \tag{10a}$$

$$V_{\vec{R}\,\vec{R}'}=\begin{cases} V_1 & \text{if } \vec{R}-\vec{R}'=\pm\vec{a}_1 \\ V_2 & \text{if } \vec{R}-\vec{R}'=\pm\vec{a}_2 \\ 0, & \text{otherwise}. \end{cases} \tag{10b}$$

The modulation is only included in the diagonal term $E_{\vec{R}}$. If a_iQ_i is a rational multiple of π the periodicity of the lattice is commensurable with the CDW along that direction and incommensurable otherwise. For the sake of simplicity we take $V_1=V_2=V$; the modulation in the $\vec{a}_2$ direction is taken to be either commensurate ($a_2Q_2=\pi$) or incommensurate ($a_2Q_2=3$), and in the $\vec{a}_1$ direction it is taken to be incommensurate ($Q_1a_1=2$ and 3).

As Hamiltonian (7) is block tridiagonal we studied the localization of the wave function using the two methods which pemit a matrix continued-fraction expansion of the self-energy.

One method is to study the behavior of L when the dimensionality is increased, as we did in Sec. II; this is obtained by considering a strip of width ranging from 1 to 12.

The other possibility is to use the periodicity in direction $\vec{a}_2$ by applying the Bloch theorem to the strip of infinite width. This simplifies the problem to that of two interacting one-dimensional chains for each k state. The reduced Hamiltonian is then

$$H'_k=\begin{bmatrix} \vdots & & & \\ \cdots & \Lambda^k_{n-1} & V_{n-1,n} & 0 \\ & V_{n,n+1} & \Lambda^k_n & V_{n,n+1} \\ & 0 & V_{n+1,n} & \Lambda^k_{n+1} \quad \cdots \\ & & & \vdots \end{bmatrix}, \tag{11}$$

where

$$-\frac{\pi}{2a_2} < k \leq \frac{\pi}{2a_2}$$

and

$$V = \begin{bmatrix} V_1 & 0 \\ 0 & V_1 \end{bmatrix},$$

$$\Lambda_n^k = \begin{bmatrix} W\cos(Q_1 n) & V_1 + V_2 e^{ika_2} \\ V_1 + V_2 e^{-ika_2} & -W\cos(Q_1 n) \end{bmatrix}.$$

In both cases we calculate the localization length L as the number of steps required for convergence of the MCF expansion of the self-energy. The local DOS may be calculated as

$$n_i(E) = -\frac{1}{\pi} \lim_{\delta \to 0^+} \langle i \mid \hat{G}(E + i\delta) \mid i \rangle$$

to permit the identification of localized states in the CDW induced gap.

B. Results

In Fig. 5 we show the localization in the middle of the band $E = 0$ for a strip with modulation which in the principal direction has a wavelength close to three lattice spacings ($Q_1 a_1 = 2$). It should be noted that for the commensurate case with $Q_1 a_1 = 2\pi/3$ there is a finite DOS at $E = 0$ and the situation does not change much for the incommensurate case ($Q_1 a_1 = 2$). The plots correspond to widths 1, 2, 4, 6, and 12. The open circles represent the case where there is a commensurate modulation of period 2 in transverse direction ($Q_2 a_2 = \pi$) while the closed circles represent a charge-density wave which is incommensurate in two perpendicular directions ($Q_2 a_2 = 3$).

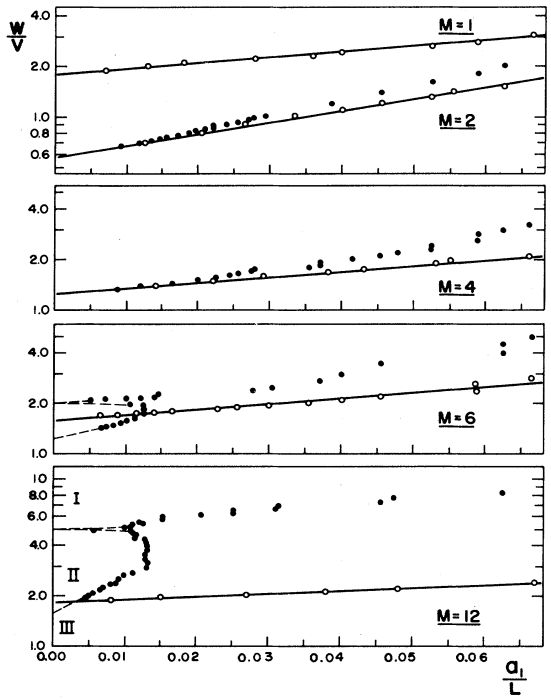

FIG. 5. Localization length L for $E = 0$ for strips widths 1, 2, 4, 6, and 12 with incommensurate modulation along the principal axis ($Q_1 a_1 = 2$) and either commensurate ($Q_2 a_2 = \pi$, open circles) and incommensurate ($Q_2 a_2 = 3$, closed circles) along the lateral direction. The insulating (I), intermediate (II), and metallic (III) phases are shown for $M = 12$.

All graphs show a critical modulation strength for which the states become localized. This critical "disorder" is decreased when new chains are added beside a single one and then rises again to nearly the one-dimensional value when there are more than eight chains ($M = 8$), simulating a two-dimensional system. The Aubry[21] formula for localization

$$1/L = \ln(W/V_1) + \text{const} \tag{12}$$

fits the numerical results very well for any value of the width and for all modulation strengths which are not too strong.

The result that the localization length in a two-dimensional CDW is similar to that of a linear chain for the case $Q_2 a_2 = \pi$ may be easily understood by analyzing the reduced Hamiltonian (11). There are two quantum numbers k which represent extreme situations: $k = 0$ and $k = \pi/(2a_2)$. For $W = 0$ and $k = 0$ the Hamiltonian (11) represents a pair of coupled linear chains which can be uncoupled by transforming to a pair of symmetric and antisymmetric wave functions whose spectra is then centered at $V_1 + V_2 = 2V$ and $-2V$, respectively, and broadened about those values with width $4V_1 = 4V$ because of the interactions along the a_1 direction. If $k = \pi/2a_2$ then H_k' is uncoupled independently of W and the two uncoupled spectra are centered at $E = 0$. As a modulation $W \neq 0$ appears, the $E = 0$ states corresponding to the $k = 0$ wave vector become localized since they are located just at the border of the bands centered at $+2V$ and $-2V$. However, the $k = \pi/2a_2$ states with energy $E = 0$ are still extended and are the last to be localized; this occurs when $W/V = 2$ as found by Aubry for the one-dimensional chain. The matrix continued fraction will converge for $E = 0$ when the last state becomes localized so the calculation provides a maximum localization length. In this sense the mobility edge for this case must be defined as separating a region where all states are localized (for all k values) for the energy region where both localized and extended states are present.

From Fig. 5 it can be seen that as modulation in transverse direction becomes incommensurate ($Q_2 a_2 = 3$), there is a region of long localization lengths (W is a little above the critical value) where the Aubry relation (12) is satisfied. The slope of the linear part (large values of L) increases above that of the commensurate case as the width of the strip increases although the critical value of modulation remains nearly the same.

For a one-dimensional chain with a commensurate modulation of period 2 ($Q_1 a_2 = \pi$) there is a gap in the middle of the spectrum. If the modulation becomes incommensurate ($Q_1 a_1 = 3$), a narrow extended band appears, which is exactly centered at $E = 0$, inside this gap.

Bulka[7] also found this band by considering a modulation of the off-diagonal matrix elements. The width of this narrow band decreases with increasing W and disappears at $W_c/V \gtrsim 1.3$ as shown in Fig. 6.

Using the same modulation we studied, the localization length at E equals 0 for various strip widths. The dependence of L on W did not follow Eq. (12) in this case, although they show the critical point at $W=W_c$. The application of MCF to the reduced Hamiltonian (11) for representative k's agreed with the results for the wide strip.

The problem of two- and three-dimensional incommensurate structures has been discussed by Sokoloff.[5] In this work the existence of an intermediary region between metallic and insulating behavior is mentioned. It may be tentatively concluded from our results that just such an intermediate is developing, separated from the others by two critical values of the modulation. This behavior is shown in Fig. 5 for $M=12$ where those phases are labeled I, II, and III. It should be noted that this intermediate phase only forms for the incommensurate case (in the transverse direction) and not for the commensurate case.

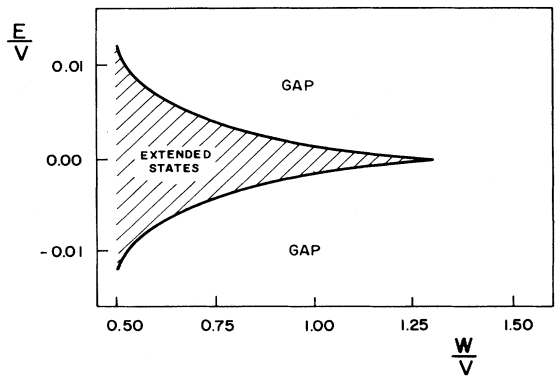

FIG. 6. Behavior of the narrow band inside the gap of an incommensurate ($Q_1a_1=3$) one-dimensional CDW as a function of the modulation strength (W/V).

V. CONCLUSIONS

We have shown that the MCF method is useful in calculating the localization length as well as the DOS in various systems with dimensionality higher than 1. This information is complementary to that provided by methods of Refs. 10, 16, and 19.

When applied to the case of a strip with rectangular disorder the results confirm those of MacKinnon, for exponentially localized states only. However, we find that the states are not always exponentially localized. In fact, the longest localization lengths come from weakly localized states, which are expected to play an important role in the conduction process. This breakdown of exponentially localized states occurs both as the width is increased and disorder is decreased; in one dimension it occurs for sufficiently small disorder ($W/V \leq 1$). Thus the histograms obtained for the two-dimensional systems were similar to that shown in one dimension [Figs. 1(a) and 1(b)]. This result also seems to be in general agreement with the conclusion of Chitanvis and Leath.[22] A transition around $W/V=6$ has of course been noted previously by a number of authors, see for example, Stein and Krey,[23] though the detailed nature of this transition has been under discussion.

The results for the CDW modulation for the two-dimensional strips were similar to those of the one-dimensional results. In particular, the critical value of the modulation does not change very much. However, in the case of an incommensurate CDW in two perpendicular directions the slope of the $1/L$ vs $\ln W/V$ curves appears to increase as the width of the strips increases indicating a tendency towards the localization. Also a fine structure appears in the localization length for stronger values of modulation, and an intermediate region develops between the insulating and conducting regimes.

ACKNOWLEDGMENTS

We wish to acknowledge valuable conversations with C. Balseiro, N. Cohan, A. López, J. Simonin, and M. Weissmann, and correspondence with A. MacKinnon. We would also like to thank M.C.G. Passeggi for his discussions and constant encouragement in the course of this work. This work was performed with the financial support of Consejo Nacional de Investigaciones Científicas y Téchnicas.

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