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The discrete, non-translational Schrödinger-like 1–d problem. An overview

F. LEMA* AND C. WIECKO*
Centro Atómico Bariloche
8400 S.C. de Bariloche, Río Negro, Argentina

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ABSTRACT. We describe the current approach to a set of linear coupled equations with "random" coefficients. These are thought of as models for superlattices when charge effects are ignored or reduced to a one-electron situation. Other formally analogous models from solid state physics are quoted as well. Historical evolution of model "potentials" is presented. Current methods are also outlined together with our own novel method of decimation with real frequencies, which has been used to derive almost all of our results, some of which are presented at the end, as an illustration of the current questions in this field. Mainly, we approach the eigenvalue-eigenvector problem, but for space reasons the transport properties are not discussed. However, we do discuss multifractal analysis, as a tool for characterization. Extensions to higher dimensions are only mentioned slightly. We stress the pedagogical interest of the field as an introduction to theoretical research which does not require large computational facilities.

RESUMEN. Describimos cómo resolver un sistema de ecuaciones lineales acopladas con coeficientes "al azar". Se toman como modelos para superredes cuando se pueden ignorar efectos de carga o reducir a un problema de un electrón. Se mencionan otras aplicaciones dentro de la física del sólido. Se presenta la evolución histórica de los "potenciales" modelo. Se discuten los métodos más antiguos de resolución junto con nuestro método más nuevo de decimación con frecuencias reales. Esto se ha usado para derivar casi todos nuestros resultados, algunos de los cuales se presentan al final, como ilustración de los problemas que se pueden estudiar en el campo. Discutimos casi exclusivamente el problema de encontrar los autovalores y los autovectores, pero por razones de espacio, omitimos las propiedades de transporte. Sin embargo discutimos el análisis multifractal como herramienta de caracterización. Sólo muy brevemente mencionamos extensiones a dimensiones mayores que uno. Remarcamos el interés pedagógico del campo como una introducción a la investigación en física teórica que no requiere grandes facilidades computacionales.

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1. INTRODUCTION

Basically, the problem to be discussed is the linear, discrete, nearest-neighbor connected set of equations with coefficients that are either random, or built from some formation rule or vary as a function non-commensurate with the lattice sites. It can be called the non-translational discrete Schrödinger type problem. Because of the lack of translational symmetry we cannot Fourier transform. The above mentioned topic should be a chapter of the theory of disorder, although it is not clearly pointed out in current literature on

*Fellow of the Consejo Nacional de Investigaciones Científicas y Técnicas of Argentina.

the subject [1-3]. Most of the discussions here are concerned with 1–d equations, however, we will point out few extensions to higher dimensions.

Connection with physics comes from studies of superlattices, mainly where now, due to the beam epitaxy technique [4], different arrangements can be formed with a special type of "disorder" along one direction.

Several physical systems of current interest can be described by these linear models: crystals containing modulating periodic potentials of a period different from that of the underlying lattice, either commensurate or incommensurate with it [5], electrons in 2–d square lattice in a perpendicular magnetic field [6], the Schrödinger equation with arbitrary potential of atomic type (through the construction of the Poincaré maps of the problem) [7], superconductive networks (through the De Gennes-Alexander theory) [8]) etc.

As for superlattices the experimental realization has been achieved in various ways. Apart from periodic hetero-structures [4,9] a Fibonacci chain [10] and a hierarchical arrangement [11] have been discussed. Also magnetic properties can be studied with magnetic superlattices when the quantum Ising model in traverse magnetic field is used [12].

We present here an introductory overview of the field, giving several currently used examples of "disorder" or non-translational "potential". We discuss the current methods, together with the method of decimation that we have applied in one particular way and that we have used quite successfully in the field [13-15].

We present briefly what is expected to be calculated, illustrate some of the questions, etc. We also discuss the multifractal analysis and use it as a tool to characterize different regimes. We present here some of our results and give references to related literature.

As far as methods are concerned we became very interested in that of decimation which in 1–d is exact and, at least with our procedure [13-15] allows excellent solutions for non-translational problems. Most authors use it through Green's functions formulation where the complication of imaginary parts arises. At least in 1–d decimation can solve bigger samples than direct diagonalization, having besides other advantages over the direct diagonalization of the states.

We have extended it to 2–d [16] but *ad-hoc* approximations are needed and it requires more computation. At present, we study the possibility of using it with a many body term in nontrivial mean-field approximation [17]. This type of problem, we think, has many model applications in solid state physics. For example, in Ref. [16] we deal with superconductivity through the mean field negative U Hubbard model. We could also think, perhaps, of charge effects in superlattices [18]. So, to our knowledge, the field is open.

The overview is organized as follows: In Sect. 2 we present the problem as the discrete Schrödinger equation in 1–d and we also give the equations for some formally analogous problems from solid state physics such as phonons, low-temperature magnons, the tight-binding electrons and the superconducting networks. In Sect. 3 we present and discuss, in a historical way, some currently studied "potentials" for disorder such as the binary alloy, the Anderson model of localization, the Aubry model, the quasicrystal model through the Fibonacci chain, the Tue-Morse sequential model and the hierarchical model. In Sect. 4 we discuss the numerical solutions; first the traditional methods of direct diagonalization, the transfer matrix approach and the continuous fraction method. Then we develop in some detail the new method of decimation, based on the renormalization-group-ideas, and

especially our novel approach to it. In Sect. 5 we introduce the concept of multifractality as a tool for the classification, by dimension, of a set formed by the wave-functions of the above mentioned models. In Sect. 6 we show some of our numerical results for wave-functions, integrated densities of states and multifractal singularity distribution function $f(\alpha)$ in order to show connections between those quantities and collaborate in solving some polemical results. All this was obtained with our procedure of decimation, so it is also a proof of the efficiency of this method with the cases where there are other available results. We finish briefly, summing up with some conclusions.

We see this job as a kind of pedagogical overview in order to show possibilities in the area. It is specially useful as a starting point for research in the solid state field, specially where large computers are not available.

The overview is mostly based on Lic. F. Lema's Master Thesis work (Bariloche, Dec. 91, unpublished) (in Spanish) where more details can be found.

2. THE DISCRETE 1–D SCHRÖDINGER PROBLEM AND OTHER ANALOGIES IN SOLIDS

a) The 1-d Schrödinger equation for one-particle

This is the basic formulation. We write the one particle Schrödinger equation 1–d

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x). \tag{1}$$

We now set a lattice of spacing a. We discretize the operator as follows:

$$-\frac{\hbar^2}{2m}\left(\frac{\frac{\psi(x+a)-\psi(x)}{a} - \frac{\psi(x)-\psi(x-a)}{a}}{a}\right) + V(x)\psi(x) = E\psi(x). \tag{2}$$

The discrete limit of this notation has to be analyzed in detail. However, for the local potentials used here, we can generalize the problem in the following discrete equation (taking it as a starting point):

$$-tf_{n+1} + \epsilon_n f_n - tf_{n-1} = Ef_n. \tag{3}$$

This is a basic set of linear equations with "random" diagonal coefficients. We are interested in determining the eigenenergies E and the eigenfunctions f_n. This is called "diagonal disorder". In other applications we can also make t site-dependent (off diagonal disorder).

b) Normal modes

For normal modes we postulate the temporal dependence e^{iwt} and have

$$(\phi_{ll} - w^2 M_\ell I)\cdot u_l + \sum_{l'\neq l}\phi_{ll'}\cdot u_{l'} = 0, \tag{4}$$

where M_ℓ is the mass on site ℓ and $\phi_{\ell\ell'} = \phi(R_\ell - R_{\ell'})$ is the force constant. With only nearest neighbor interaction we have the formal equivalence with Eq. (3):

$$\frac{1}{M_l}\phi_{l,l+1} \cdot u_{l+1} + \frac{1}{M_l}\phi_{ll} \cdot u_l + \frac{1}{M_l}\phi_{l,l-1} \cdot u_{l-1} = \omega^2 u_l \tag{5}$$

where u_l is the displacement from the equilibrium position under the action of elastic forces as defined above. In 1–d, it was studied for example in Ref. [14].

c) The magnetic excitations

Those are currently described by the Heisenberg Hamiltonian

$$H = -\frac{1}{2}\sum_{ll'} J_{ll'} S_l \cdot S_{l'}, \tag{6}$$

where J is the magnetic exchange constant.

Let us suppose the ferromagnetic case, with $S_l^{(Z)} < S$. We write down the equation of motion for the operators $S_l^{(\pm)}$ in Heisenberg representation:

$$i\hbar\frac{\partial S_l^{(-)}}{\partial t} = -2\sum_{l'\neq l}\left[J''_{ll'} S_l^{(-)} S_{l'}^{(Z)} - J_{ll'}^{\perp} S_{l'}^{(-)} S_l^{(Z)}\right]. \tag{7}$$

If we suppose that each $S_l^{(-)}$ behaves as $e^{i\omega t}$ and for almost ordered system (low temperature solution) we obtain

$$\left(2S\sum_{l'\neq l} J''_{ll'} - \hbar\omega\right) S_l^{(-)} - 2S\sum_{l'\neq l} J_{ll'}^{\perp} S_{l'}^{(-)} = 0 \tag{8}$$

For only nearest neighbors:

$$\left[2S(J''_{l,l+1} + J''_{l,l-1}) - \hbar\omega\right] S_l^{(-)} - 2SJ_{l,l+1}^{\perp} S_{l+1}^{(-)} - 2SJ_{l,l-1}^{\perp} S_{l-1}^{(-)} = 0. \tag{9}$$

d) The electrons on the lattice

In the tight binding approximation, the lattice contribution with a potential that is the linear superposition of atomic potentials $V_l(r - R_l)$, where R_l is the ionic position:

$$V(r) = \sum_l V_\ell(r - R_l). \tag{10}$$

We now write down the Schrödinger equation, with a solution given as a linear combination of atomic orbitals:

$$\varphi(r) = \sum_{l,\alpha} u_l^{(\alpha)} \phi_l^{\alpha}(r - R_l). \tag{11}$$

We get a set of equations for the coefficients $u_l^{(\alpha)}$:

$$\left(\epsilon_l^{(\alpha)} - E\right) u_l^{(\alpha)} + \sum_{l' \neq l} \sum_{\beta} V_{ll'}^{(\alpha,\beta)} u_{l'}^{(\beta)} = 0. \tag{12}$$

The $V_{ll'}^{(\alpha,\beta)}$ are the overlap integrals between the different orbitals and the potential. For nearest neighbor overlaps only (narrow bands) we get

$$\left(\epsilon_l^{(\alpha)} - E\right) u_l^{(\alpha)} + \sum_{\beta} \left(V_{l,l+1}^{(\alpha,\beta)} u_{l+1}^{(\beta)} + V_{l,l-1}^{(\alpha,\beta)} u_{l-1}^{(\beta)}\right) = 0. \tag{13}$$

This is the classical equation from the field of Anderson localization [19].

e) Superconducting networks

This description [8] starts with the linearized Ginzburg-Landau equations for nets of thin wires, which behave as weak links joining the nodes of the network. On a 1–d branch which joins nodes a, b and has length $l = L/\xi$ (ξ the coherence length) the order parameter reads

$$\psi(s) = \frac{\exp(i\gamma_{as})}{\sin l} \left[\psi_a \sin(l - s) + \psi_b \exp -i\gamma_{ab}) \sin s\right], \tag{14}$$

where ℓ is the linear coordinate along the branch from a; $\gamma_{as} = \frac{2\pi}{\varphi_0} \int_a^s \vec{A}(l')\, dl'$ with $\vec{A}$ the vector potential of the applied field, φ_0 is the flux quantum and $\varphi_a = |\psi_a| e^{i\alpha}$ and $\psi_b = |\varphi_b| e^{i\beta}$ are the values of ψ at a, b.

When the quantum mechanical current associated with the order parameter is implemented with a generalized Kichhoff current law, one obtains linear equations for the order parameter at the nodes, where compatibility conditions lead to the phase diagram.

For example, for a geometry of infinite length ladder, the equations are

$$\begin{aligned} 3\cos l\psi_n^{\uparrow} - e^{i\gamma}\psi_{n-1}^{\uparrow} - e^{-i\gamma}\psi_{n+1}^{\uparrow} - \psi_n^{\downarrow} &= 0, \\ 3\cos l\psi_n^{\downarrow} - e^{-i\gamma}\psi_{n-1}^{\downarrow} - e^{i\gamma}\psi_{n-1}^{\downarrow} - \psi_n^{\uparrow} &= 0, \end{aligned} \tag{15}$$

where n indicates the node, $\uparrow\downarrow$ refer to the branch and $2\gamma = 2\pi\varphi/\varphi_0$. The solutions are of the form $\psi_n^{\alpha} = f_q^{\alpha} e^{iqn}$ ($\alpha = \uparrow\downarrow$).

This is again an eigenvalue-eigenvector problem with $\cos \ell$ as energy parameter. The phase diagram is given by the minimum ℓ as a function of γ.

The problem was studied for several geometries [22]. It is in this model that we first applied our decimation method [22].

3. THE POTENTIALS

a) Introduction

Superlattices is a topic of growing interest, including nowadays possible extensions to magnetic-nonmagnetic and to superconducting-normal ones. Of course these last problems have to be studied with a different formalism. However, they have in common the property that translational invariance is absent only in one-direction: that of a deposition of the materials. There has been enormous progress in fabrication techniques of microstructures by such techniques as molecular beam epitaxy.

We give here examples of mathematical models currently found in present day literature which relate with semiconductor superlattices or are otherwise of interest as theoretical models, perhaps not yet explored experimentally.

The potentials can be presented globally as a "diagonal model" for disorder. Starting with the generalization [Eq. (3)]

$$V_{n,n+1}f_{n+1} + \epsilon_n f_n + V_{n-1,n}f_{n-1} = Ef_n, \tag{16}$$

and taking

$$V_{l,l+1} = V_{l,l-1} = V = 1$$

(energy unit), we get the "diagonal disorder model"

$$f_{l+1} + \epsilon_l f_l + f_{l-1} = Ef_l, \tag{17}$$

where ϵ_l is the potential on the lattice site l and E is the eigenvalue.

b) The binary alloy

Historically, the first model for "diagonal disorder" consisted in taking two types of site components ϵ_A and ϵ_B, with concentration as a probability for each species. The regime goes continuously, starting from the very dilute case (the "impurity" model, solved usually in k-space language through a scattering potentials technique, in the limits of one defect, which is exactly solvable [23]). to the intermediate case, for which the CPA approximation has been developed [1,2] and the very dense case which almost joins the next model (multiple-component alloy model). Although these two models can presumably be in different universality classes.

The regular intercalated elements A and B are called quantum wells problem in the literature of semiconductors such as for example GaAs [17]. However, nowadays, some kind of random deposition can also be generated experimentally. We are aware of recent

deposition with the Fibonacci sequence [48]. The main problem in matching theoretical potentials with experimental results is that of diffusion in realistic samples [49].

c) The Anderson model

This is the model with random diagonal elements on each site taken from some probability distribution, $P(\epsilon_l)$. It is the kind of thermodynamical limit of the multi-component alloy model, from the previous section.

Historically the Anderson probability distribution was the box distribution

$$P(\epsilon) = \begin{cases} \dfrac{1}{W} & \text{for } -\frac{W}{2} \leq \epsilon \leq \frac{W}{2} \\ 0, & \text{otherwise,} \end{cases} \tag{18}$$

where W is the disorder parameter (kind of characterization of the strength of disorder).

Other distributions used are: the Gaussian

$$P_W^{\mathrm{G}}(\epsilon) = \left(\frac{1}{\sqrt{2\pi}W} e^{-\epsilon^2/2W^2} \right) \tag{19}$$

and the Lorentzian $P(\epsilon) = \frac{1}{4}\frac{\gamma}{\epsilon^2+\gamma^2}$, which can be exactly solved. Anderson was the first to discuss the possibility of localized states in disordered systems in spite of the already known local mode states in impurity models.

d) The Aubry model

After the idea of random disposition of the "diagonal" parameter the idea of a modulating function distribution with the possibility of incommensurate periodicity with the lattice arised.

The model most studied was the Aubry one [24], which reads

$$\epsilon_\ell = \lambda \cos(2\pi q l), \tag{20}$$

where λ is the strength of the potentials, q is the modulation and l the position.

There is a transition in parameter space. Aubry and André [24] have shown that a transition from extended to localized states takes place when λ increases from values less than 2 to values bigger than 2. The proof of Aubry and André is based on self-duality, which means that the Fourier transform of the tight binding equation with that potentials has the same form with the change of $\lambda \to 4/\lambda$. For irrational values of γ the states are extended for $\lambda < \lambda_c = 2$; there is a point spectrum and localized states for $\lambda > \lambda_c$ and for λ_c the spectrum is singular continuous and the states are critical. If γ is rational, $\gamma = p/q$, the solutions are extended and satisfy Bloch's theorem. The Aubry model [24] and the modified Soukoulis-Economou model [5] both present a strange and new "packet-states". The resistances and the transitions through the energies of these special state present

regular oscillatory in magnitude behaviour with the length of the sample [47,44]. This was first suggested by Sokoloff [50]. It can be perhaps of technological interest for resistance devices.

e) Fibonacci chain

The next step was to build the potentials through some kind of "inflation" rule, which in principle does not mean the inflation symmetry. The Fibonacci chain was applied to a physical problem of quasicrystals which are solids with crystallographically forbidden symmetry. Experimental realizations are being achieved [48]. There, the rule is

$$A \to AB, \qquad B \to A, \tag{21}$$

starting with a set $\{S_0\} = A$ like a zero generation.

It is simple to verify that

$$\{S_{j+1}\} = \{S_j, S_{j-1}\}. \tag{22}$$

The eigenvalue ϵ of the chain in the n–generation, will be that of the chains in higher generations n.

The number of atoms in generation n will be given by the Fibonacci number F_n which follows the rule

$$\begin{aligned} F_n &= F_{n-1} + F_{n-2}, \\ F_0 &= 1, \quad F_1 = 2. \end{aligned} \tag{23}$$

f) The Tue-Morse model [26]

Another example which has appeared recently in current literature is the sequential model formed by the rule

$$A \to AB, \qquad B \to BA, \tag{24}$$

starting with $\{S_0\} = A$ as generation.

We verify here that

$$\{S_{j+1}\} = \{S_j, \bar{S}_j\} \tag{25}$$

where $\bar{S}_j$ means to interchange A with B in S_j.

Due to that, if $\epsilon_A = -\epsilon_B$ (antisymmetric), the potential ϵ_l is odd with respect to the center of the chain (Lema Master Thesis, Bariloche, 1991). The size of the chains in generation n is ℓ^n.

One difference with respect to the Fibonacci chain, consists in the fact that the analogical model cannot be characterized by a finite number of irrationals (as appear in the continuous fraction expansion for the self energy).

g) The hierarchical potentials [11]

This chain can be constructed as follows: If k is a maximum integer value so that n is divisible by 2^k then $\epsilon_n = -U_e R^k$ where U_0 is the strength of a potentials and R the position of a vector. If we consider that the size of the sample is $2^m - 1$, then ϵ_l is even with respect to the center.

The hierarchical's potentials eigenvalues can be mapped on a tree, similar to the pure tight-binding model [11,29].

This situation is similar to the Sherrington-Kirkpatrick model of spin glasses [29] for the spin configuration which are also hierarchical as a function of the order parameter. It is even possible to draw a close analogy between both models which was suggested by one of us [30]. The hierarchical potentials is of interest from the theoretical point of view. It can be thought in some sense as a "model" for going from an insulator towards a metal although this is a preliminary remark. We think it will play an important role in a developing field of biological physics *e.g.* neural networks [29]).

4. THE NUMERICAL SOLUTION METHODS

We shall comment on three "traditional methods", namely: the direct diagonalization, the transfer matrix and the continuous fraction methods and we shall then present our original method, the Roman-Wiecko Decimation (DRW) [13-15]

a) Direct diagonalization

The direct diagonalization depends strongly on computational facilities. As mentioned in Ref. [31] with the aid of an available subroutine in the EISPAC subroutine library and by access to a suitably large computing facility (for example Cray supercomputers) it is practical to diagonalize a tridiagonal matrix for N of order 10^4, specially if one is satisfied with computation of the eigenvalues only. Accurate computation of the eigenstates is a considerably greater time-consuming procedure. Localized or extended states are determined by inspection.

b) The transfer matrix [1]

In this procedure we start with the tight binding equation

$$t_{n-1,n}\psi_{n-1} + \epsilon_n \psi_n + t_{n,n+1}\psi_{n+1} = 0 \tag{26}$$

as

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T_n^{(1)} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \quad \text{with} \quad T_n^{(1)} = \begin{pmatrix} \epsilon_n/t_{n+1} & t_{n-1}/t_{n+1} \\ 1 & 0 \end{pmatrix}, \tag{27}$$

where ψ_n is the wave function at site n, t is the hopping parameter and $\epsilon_n = E - \epsilon'_n$ with

E the eigenvalue. The complete set is resumed as the products of transfer matrices

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T^{(n)} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = \left(\prod_{i=1}^{n} T_i^{(1)} \right) \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \tag{28}$$

Starting with a suitable initial condition for ψ_0 and ψ_1 we calculate the localization length λ defined as

$$\lambda^{-1} = \lim_{N \to \infty} \frac{1}{N} \psi_N. \tag{29}$$

If $\lambda > 0$ we are in the gap region or have a localized state (which is indistinguishable in the method, so it has to be complemented with the explicit calculation of the density of states by some standard method such as Dean's [32]). If $\lambda > 0$ the region is extended.

c) The continuous fraction method

It was developed by Economou and Cohen [33]. It goes through the formalism of one-particle Green's functions defined as

$$G(E) = \langle 0|(E - H)^{-1}|0\rangle = \underbrace{\frac{1}{E - \epsilon_n - \Sigma}}_{b_0}, \tag{30}$$

where $|0\rangle = \psi_{(x)}$ denotes the Wannier orbital on site x. Σ is expressed in terms of a pair of infinite continued fraction K_+ and K_-. Thus if

$$K_+ = -\frac{1}{b_1 - \frac{1}{b_2}}, \tag{31}$$

with K defined as the continued fraction obtained upon replacing b_n by b_n, a basic result is that:

$$\sum(E) = -(K_+ + K_-). \tag{32}$$

Two criteria were established:

1. Either K_+ or K_- diverge for a given energy and the solutions are necessarily extended.
2. if both K_+ and K_- converge, either there is a non normalizable eigenstate or there exists a localized eigenstate.

The continued fraction converges if

$$K_+ = \lim_{n \to \infty} \left(\frac{P_n}{Q_n} \right), \tag{33}$$

with $u_n = b_n u_{n-1} - u_{n-2}$ subject to the initial values $P_{-1} = 1$, $P_0 = 0$, $Q_{-1} = 0$, $Q_0 = 1$.

d) DRW: Roman-Wiecko decimation.
A unified method for eigenvalues and wave-function [13–15,34]

The more recent method was proposed based on the renormalization-group decimation idea [35,36]. In those references it is formulated through the Green's functions technique. The density of states is obtained through the standard relation $N(w) = -\frac{1}{\Pi}\,\mathrm{Im}\,G(w + i\eta)$, $\eta \to 0$. Ref. [35] makes an early and unnecessary approximation by changing the site-dependent configuration by some mean values.

We have developed [13–15] the RG decimation method directly for the set of equations for the wave-function [Eq. (26)]. This has the advantage that we always deal with real frequencies. (The introduction of imaginary parts apart from numerical complications, obscures the distinction between localized and extended states.) The approaches as used in Ref. [36] distinguish localized from extended solutions only by the number of steps needed for convergence to a fixed point and complements it with direct inspections of the wave-functions.

Our procedure gives direct criteria for the extended, localized and gap states (even tentatively for band-edges) as is stated below.

Our procedure is the following [13-15]. Starting with the initial equation of motion for a given site [Eq. (26)], the variables for the n.n (odd sites) are replaced by their values from the equation associated with them [equivalent to Eq. (4)]. The number of degrees of freedom is reduced in one half and the form conserving equation for the doubled lattice is derived. After r iterations the chain of spacing 2^r is reached with the corresponding form concerning the set of equations

$$t^{(r)}_{n-k}\psi_{n-k} + t^{(r)}_{n,n+k}\psi_{n+k} = \epsilon^{(r)}_n\psi_n,$$

when $k = 2^r$ and the recursion relations are

$$\begin{aligned} \epsilon^{(r+1)}_n &= \left(\epsilon_n - \frac{t^2_{n,n-k}}{\epsilon_{n-k}} - \frac{t^2_{n,n+k}}{\epsilon_{n+k}}\right)^{(r)}, \\ t^{r+1}_{n\pm 2k,n\pm k} &= -\left(\frac{t_{n\pm 2k,n\pm k}t_{n\pm k,n}}{\epsilon_{n\pm k}}\right)^{(r)}. \end{aligned} \tag{34}$$

In our procedure the decimation is performed exactly on a given configuration (stored in the machine). No configurational averages are performed as in Ref. [35]. The capacity of a Vax machine for this approach allows 15 iterations ($\simeq 2^{16}$ atoms in a chain).

The main point of the procedure related with localization comes from the study of how the coefficients ϵ_n and $t_{n,n+\delta}$ behave upon iteration at a given energy. We have found [13-15] that:

1. An oscillatory behavior of both coefficients characterizes extended states.
2. Convergence of $t_{n,n+\delta}$ towards zero and of ϵ_n towards *non-zero* value characterize a *gap* [no solution of a set of Eq. (30)].

3. Convergence of *both* coefficients towards *zero* characterizes a localized solution (the only way to have a non-trivial solution once $t \to 0$ which happens for a localized state with iteration).
4. Convergence of the energy coefficient towards zero can *also* characterize a "packet state" with infinite localization length, determined by direct inspection of the wave function.
5. Convergence of $\epsilon_n \to 0$ when t_n just changes from saturation to oscillation is a "practical" criterium for band edges.

The method can be efficiently implemented through a short program which analyzes the behavior of the coefficients at the highest available iteration as a function of energy. Criteria for estimating density of states are given in Refs. [13–15]. The method is therefore very systematic and precision can be adequated to the interest in each particular region of the spectrum once an overall view is performed. Convergence in general is very quick. The calculation is entirely performed with real numbers.

So far, our concern was with the eigenvalues. However, if Eq. (26) is simply iterated with the eigenvalue found from decimation, in the case of a localized state, both the decreasing and the increasing solutions appear as was observed in Ref. [14].

Here we have found the way around it in order to obtain directly only the normalizable solution [34].

We chose the origin site 0. Then the equations

$$t_{-1}\psi_{-1} + \epsilon_0\epsilon_0 + t_1\psi_1 = 0 \qquad (35a),$$

$$t_1\psi_0 + \epsilon_1\psi_1 + t_2\psi_2 = 0 \qquad (35b),$$

$$t_2\psi_1 + \epsilon_2\psi_2 + t_3\psi_3 = 0 \qquad (35c),$$

define the infinite matrix. We replace Eq. (35c) in (35b) to eliminate ψ_1 obtaining one equation connecting ψ_0, ψ_2 and ψ_3; repeating the procedure $(n-1)$ times one has

$$t_{+1}\psi_0 + a_n\psi_n + b_n\psi_{n+1} = 0. \qquad (36)$$

And similarily to the left:

$$t_{-1}\psi_0 + a_{-n}\psi_{-n} + b_{-n}\psi_{-(n+1)} = 0, \qquad (37)$$

with the following recursion relations:

$$\begin{aligned} a_n &= -\frac{\epsilon_n}{t_n}a_{n-1} + b_{-1} \\ b_n &= -\frac{t_{n+1}}{t_n}a_{n-1} \end{aligned} \qquad (n \geq 1), \qquad (38)$$

with the initial values $a_0 = -t_1$ and $b_0 = 0$. Likewise, recursion relations can be written for negative n.

The full wave function is determined as follows. Iterate Eqs. (36) and (37) and by imposing periodic boundary conditions at a "far away" site N, solve the system by taking $\psi_0 = 1$. Going back from $n = \pm N$ to $n = \pm 1$ using Eqs. (36) and (37) (the values for $a_{\pm n}$ have been previously stored) our method calculates ψ_n and matches both solutions using Eq. (35a) by adjusting the eigenvalue. A similar procedure has been proposed independently in Ref. [32].

In Ref. [35] several iterations were needed to match the equations. Recently [37] we have discovered that the eigenvalue found by decimation for the central site, the zero site, matches the equations directly with great numerical precision in the case of localized states and also for the critical states.

5. THE CHARACTERIZATION BY DIMENSION. MULTIFRACTAL ANALYSIS

Euclidean, integer dimension characterizes continuously derivable geometrical sets. The fractional dimension was made popular by Mandelbrot [38] and nowadays it has been incorporated to the study of such non-analytical curves as the wave-functions in non-translational invariant potentials [39]. Initially it has been stated as mass scaling of the wave function [40,34,42,42]. The more complete multifractal analysis was introduced by Kadanoff *et al.* [43].

Fractality is close to the concept of self-similarity or dimensional dilution symmetry [28]. To introduce the concept we take boxes of size l and cover the volume l^D. We will need for that N_l boxes. Now, if we reduce the box size l which is the change in N_l in order to cover the whole volume, we get

$$N_l \sim l^{-d} \quad \text{for} \quad l \to 0 \quad \text{with} \quad d \geq 0. \tag{39}$$

We can get:

d integer	euclidean object
d noninteger	fractal object.

We define d as a Hausdorff dimension of a set. This is the extension of the concept of dimension in the sense of measure.

For the multifractal analysis we cover our set again with boxes of size l. We can have $f(x)$ (≥ 0 for all x) as the density of probability associated with each x. We calculate the integrated probability $P_i(l)$ in each box i as

$$P_i = \int_{x_i - l/2}^{x_i + l/2} f(x)\, dx. \tag{40}$$

For $l \to 0$ we suppose the asymptotic behavior

$$P_i(l) \sim \ell^{\alpha'} \tag{41}$$

(α' the power of the singularity at point x_i).

We now want to obtain the Hausdorff dimension $f(\alpha')$ of each subset. The number of boxes to cover the subset with the power of singularity $\alpha \leq \alpha' \leq \alpha + d\alpha$ will be, for $l \sim 0$

$$N_{\alpha'} \sim l^{-f(\alpha')}. \tag{42}$$

We evaluate the auxiliary function

$$\chi(q) = \lim_{q \to 0} Z(q, l) = \lim_{l \to 0} \sum_i [p_i(l)]^q. \tag{43}$$

We can write as an integration over α'

$$Z(q, l) = \int d\alpha' \, g(\alpha') l^{q\alpha' - f(\alpha')}. \tag{44}$$

As $l \to 0$, the integral is dominated by the minimum value of $[q\alpha' - f(\alpha')]$. For each q, we have $\alpha(q)$ that minimizes this expression. So we get a scaling law, for $l \to 0$:

$$Z(q, l) \sim l^{Z(q)}. \tag{45}$$

Therefore,

$$Z(q) = q\alpha(q) - f(\alpha(q)). \tag{46}$$

We get the conditions for the minimum value:

$$\frac{d}{d\alpha'}[q\alpha' - f(\alpha')]\bigg|_{\alpha'=\alpha(q)} = 0, \quad \frac{d^2}{d(\alpha')^2}[q\alpha' - f(\alpha')]\bigg|_{\alpha'=\alpha(q)} \leq 0. \tag{47}$$

We deduce that

$$\begin{aligned} f'(\alpha(q')) &= q, \\ f''(\alpha(q')) &\leq 0. \end{aligned} \tag{48}$$

In literature, the generalized dimension appears as

$$D_q = \frac{Z(q)}{q - 1}. \tag{49}$$

If $f(\alpha)$ is a distribution of values we get a multifractal curve.

6. Some results

In the type of approach we propose in this overview it is of interest to characterize each "model" in terms of the localization properties of the spectrum and of the eigenstates.

Our experience is mostly numerical although the field has also been attracted by rigorous mathematicians. Also transport properties [45] are of great interest, although we do not comment on that here. However, the statics and the dynamics are highly related. For example, we have found in the past [44] that high precision in the eigenvalue is crucial for good description of the transmission and the resistances.

The three basic types of eigenfunctions are illustrated in Ref. [46] for the Aubry model. In the past we have found the new function called "connected packets" which corresponds to the extended region but it is very peculiar [47]. It is shown in Fig.1. This packet structure, although in a hierarchical manner, also appears in the critical states of the Fibonacci chain model and the Tue-Morse model. We show it in Figs. 2 and 3 respectively. This structure strongly influences the transport properties.

Also in the localized region, packet structure appears once we suppress the exponential. We show it in Fig. 4 for the Anderson model.

To illustrate this we comment on a question we have explored lately. It is whether we can connect these packet structures with multifractal behavior, also taking into account the integrated density of states as a function of energy.

It is currently believed that critical states are related to singular continual spectra (some kind of devil's staircase for the integrated density of spectra). It is also believed that they are multifractals.

In Fig. 5 we show these magnitudes for the Fibonacci. However, in the localized regime there is the controversy about multifractality of the Anderson model wave-functional. We have compared the binary alloy which, although pure-point, has a spectrum full of gaps, with self-similar, peaks in the density of states with the Anderson model, where the spectrum is pure-point but dense. In Fig. 6 we show both model's integrated densities of states.

The multifractal analysis for both, shown in Fig. 6, indicates structure. Although in the case of the Anderson model the spread in α is very small. The spread in the binary alloy, on the other hand , is compared to the Fibonacci chain. Size analysis on the Anderson model is not conclusive due to limitations in the available computer memory.

7. CONCLUSIONS

In this overview, we have tried to present in a pedagogical and introductory manner the field of the "Theory of Disorder" mapped into non-translational, discrete, 1–d Schrödinger equation. Although we have presented in some detail our unified method of decimation for the eigenvalues and eigenfunctions which has the advantage of high precision with low numerical cost, we have not mentioned extensions to 2–d problems and the transport properties that are of practical interest.

We have also discussed the novel topic of multifractal analysis that can be applied to such sets as wave functions and also used for its characterization. From our experience we think that this field is very appropriate for people starting research in physics. We hope to raise some interest among young scientists, specially in the Latin American area. This type of research can be performed with quite modest computational facilities and, nevertheless, publishable results can be obtained and the intellectual capability exercised.

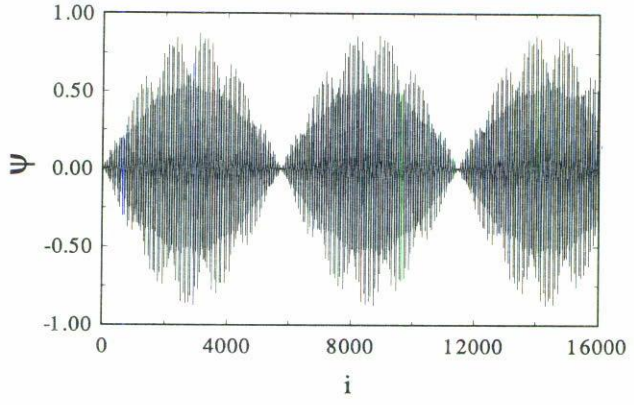

FIGURE 1. The wave-function for the Aubry-chain as a function of position ("extended packets" wave function).

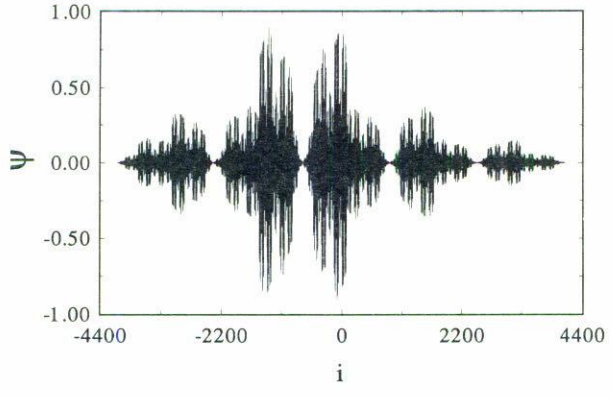

FIGURE 2. The wave-function for the Fibonacci chain as a function of position ("critical" wave-function) Ref. 46.

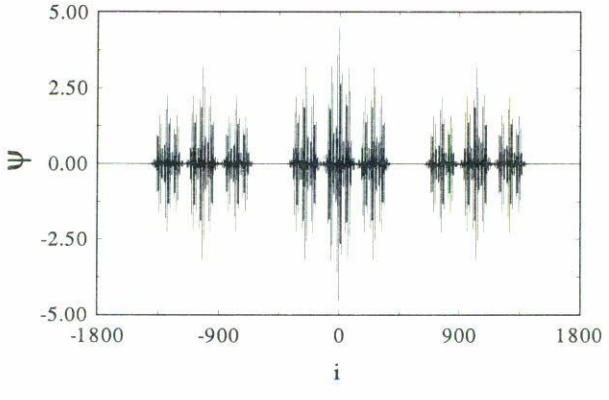

FIGURE 3. The wave function for the Tue-Morse model as a function of position (hierarchical packets).

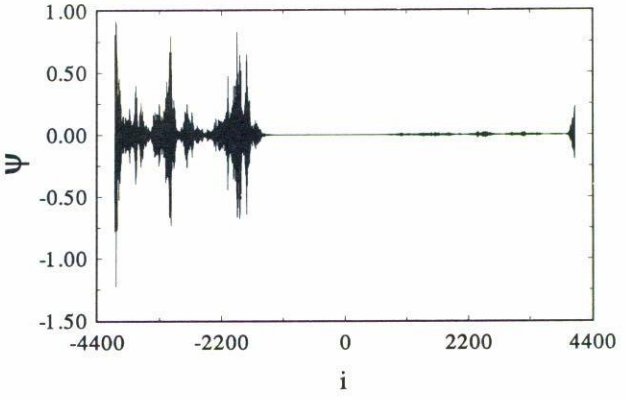

FIGURE 4. The wave-function (without the exponential decay) for the Anderson model as a function of position.

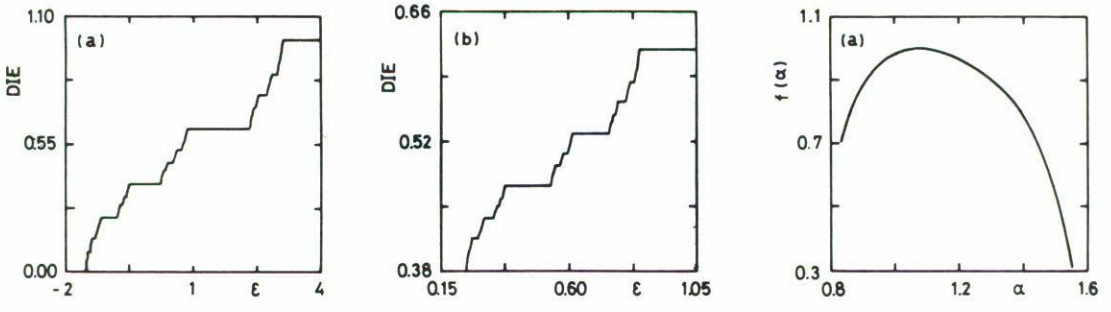

FIGURE 5. Fibonacci chain: the integrated density of states a) and its dilution amplified symmetry character b); c) the multifractal $f(\alpha)$ distribution.

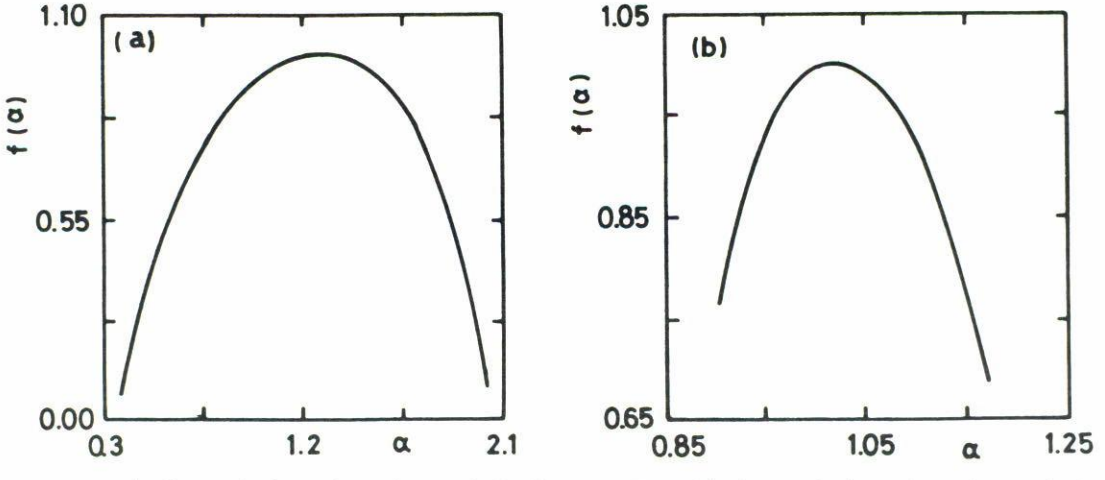

FIGURE 6. a) the multifractal analysis of the binary alloy; b) the multifractal analysis of the Anderson model.

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