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The localization transition in the Aubry model through maps

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Résumé. — L'équation de mouvement pour le modèle d'Aubry unidimensionnel est étudiée à l'aide d'une application 3-d qui couple le paramètre de modulation γ avec la densité d'états intégrée k . Nous présentons des résultats numériques pour l'énergie $E = 0$ et pour γ et k constants en fonction du potentiel V . Pour $V = 2$ la transition de localisation se manifeste par le passage d'une courbe bien définie à un nuage de points. La complexité des courbes augmente lorsqu'on approche par en dessous la valeur critique. Nous définissons un rayon moyen pour la projection sur le plan x - y de l'application 3-d et nous montrons numériquement qu'il converge vers une constante finie pour $V < 2$. D'autre part, son comportement critique est analysé pour un γ égal au nombre d'or. Finalement, nous discutons des résultats antérieurs sur la chaîne désordonnée.

Abstract. — The equation of motion for the wave function of the 1-d Aubry model is analyzed through a 3-d map which couples the modulation parameter γ and the integrated density of states k . Numerical results are presented for constant γ and k for energy $E = 0$ as a function of the potential strength V . The localization transition is found at $V = 2$ as the disappearance of a well defined curve into a cloud of points. The curves grow in complexity when approaching the critical value from below. We define a mean radius for the xy -plane projection of the 3-d map and we show numerically that it converges to a finite constant for $V < 2$. Also, its critical behavior is analyzed for V equal to the golden mean. Comments are made on previous results concerning disordered chains.

1. Introduction.

The effect of a quasiperiodic potential on the Schrödinger equation has been investigated in the last few years with considerable interest [1]. These systems are intermediate between the periodic perfect crystal and the random or disordered solid. They arise in incommensurate structures [2]; in the band calculation of electrons in a 2d crystal in a magnetic field [3]; in superconducting networks [4]; and in the electronic structure of quasicrystals [5].

One of the most studied models in this area is the Harper or almost-Mathieu equation [3, 6]

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which describes a linear chain under a cosine quasiperiodic potential in the tight-binding approach :

$$\psi_{n+1} + \psi_{n-1} + V \cos(2\pi\gamma n) \psi_n = E\psi_n \quad (1)$$

where ψ_n is the amplitude of the wave function at site n ; V is the strength of the potential, and γ is the modulation which can take rational or irrational values. For this model Aubry and André [6] have shown that a transition from extended to localized states takes place when V 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 equation (1) has the same form with the change of $V \rightarrow 4/V$. For irrational values of γ (with the exception of Liouville numbers which are of measure zero) [6-8] the spectrum is absolutely continuous and the states are extended for $V < V_c = 2$; there is a point spectrum and localized states for $V > V_c$, and for $V = V_c$ the spectrum is singular continuous and the states are critical. If γ is rational ($\gamma = p/q$) the solutions of (1) are extended states which satisfy Bloch's theorem.

The aim of this paper is to illustrate the Aubry transition to localization within the framework of dynamical systems. Here, we explore the problem empirically by computer calculations. Although what we will show is too pictorial, it gives, in our opinion, an interesting insight on the way the transition takes place. Recently, the study of tight-binding equations like (1) through the use of dynamical maps has started to be explored. For example, a map for the trace of transfer matrices has been widely used for the Fibonacci chain by Kohmoto and coworkers [5]. A map, similar to the one we will analyze in the next section, was used by Luck and Petritis [9] to study the eigenmodes of the vibrations of a one dimensional quasicrystal, and by Kostadinov and Nachev [10] to study the 1d off-diagonally disordered chain; these authors obtain some striking results.

2. The map.

Equation (1) is usually formulated in terms of the transfer matrix $M(n)$:

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \begin{pmatrix} E - V \cos 2\pi\gamma n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} = M(n) \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}. \quad (2)$$

From the point of view of dynamical systems, this is a 2d linear non-autonomous map (i.e. it depends on the «time» n) which is measure preserving in the phase space defined by (ψ_{n+1}, ψ_n) because $\det(M(n)) = 1$. We write it as an autonomous map by expanding the dimension of the phase space in the usual way :

$$\begin{aligned} x_{n+1} &= (E - V \cos 2\pi z_n) x_n - y_n \\ y_{n+1} &= x_n \\ z_{n+1} &= z_n + \gamma \pmod{1} \end{aligned} \quad (3)$$

Now, the new 3d map is non-linear and we will study it through its projections in the planes (x, y) and (y, z) . The projection of (3) in the (x, y) -plane leads to equation (2) and this map has been studied by Luck and Petritis [9], and by Kostadinov and Nachev [10], for the models mentioned above. The projection in (y, z) was shown in the paper of Ostlund and Pandit [11] for an extended state in the Aubry model.

For a complete understanding of (3) we first analyze in detail the case when $V = 0$. Here, the dynamical system decouples into two independent maps :

$$\begin{aligned} x_{n+1} &= Ex_n - y_n \\ y_{n+1} &= x_n \end{aligned} \quad (4)$$

and

$$z_{n+1} = z_n + \gamma \mid \text{mod } 1 \quad (5)$$

The map of equation (4) has a fixed point for $(0, 0)$ which is elliptic for $|E| < 2$ (band states) and hyperbolic for $|E| > 2$. It is also integrable with the constant of motion :

$$I = x^2 + y^2 - 2 E x y \quad (6)$$

which is determined by the energy E and the initial conditions (x_0, y_0) . Analyzing (6) one sees that once the initial conditions are specified, the map of equation (4) gives points which lie on a circle for $E = 0$; on an ellipse with axes at an angle $\pi/4$ with respect to $y = 0$ for $0 < |E| < 2$; on two parallel lines for $|E| = 2$, and on two hyperbolas for $|E| > 2$. These are the invariant curves of the map (i.e. the curves which are invariant through the iteration of (4)).

The map of equation (4) can be converted into a circular map with :

$$\begin{aligned} x' &= x - E/2 y \\ y' &= (1 - E^2/4)^{1/2} y \end{aligned} \quad (7)$$

for $|E| < 2$. In these new variables the orbits are circular with radius equal to the constant of motion I and consequently equation (4) can be reduced to a single map in the angle variable :

$$w_{n+1} = w_n + k \mid \text{mod } 1 \quad (8)$$

with $k = \frac{1}{2\pi} \cos^{-1}(E/2)$ and $w_n = \frac{1}{2\pi} \cos^{-1}(x'_n)$. This is the well-known circle map [12] with winding number k . For k rational ($k = p/q$) it has orbits which close on themselves after a finite number of iterations (q) of the mapping, and thus are periodic given q points on the circle [12]. And for k irrational the orbits fill densely the circle, and thus are ergodic [12].

Therefore the map in (4) has the same behavior, namely, for $k = p/q$ it takes discrete q values and for k irrational it fills an ellipse and the values of ψ_n are arbitrary and dense. In particular for the special case of $E = 0$, which corresponds to $k = 1/4$, the transformation (7) is the identity, and we get four points in the (x, y) plane once the initial conditions are given.

Now we return to the map corresponding to the Aubry model (Eq. (3)). After the preceding analysis we can visualize this mapping as a coupling of two circle maps whose respective winding numbers are k and γ . This coupling does not alter the circular map for z_n but couples it to the map for (x_n, y_n) through the potential strength V . In this way, the dynamical map takes into account the competition between the period of the lattice and the period of the incommensurate potential. Due to the presence of the coupling we have to recalculate k which is now the winding number of the (x, y) projection of (3) :

$$k = \frac{1}{2\pi} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \text{Im} \left[\ln \left(\frac{y_n}{x_n} \right) \right] \quad (9)$$

and which corresponds to one half of the integrated density of states of the chain [11, 13].

Our aim is to analyze the delocalization transition in the Aubry model by numerical iteration of the mapping (3) at fixed winding numbers γ and k as function of V . Since k enters the map through the energy E we have, in general, to know the function $E(k)$ for each value of V . But this is a complicated and unknown function which must be estimated numerically [11]. Therefore, for simplicity, we decided to restrict ourselves to the only case in which we

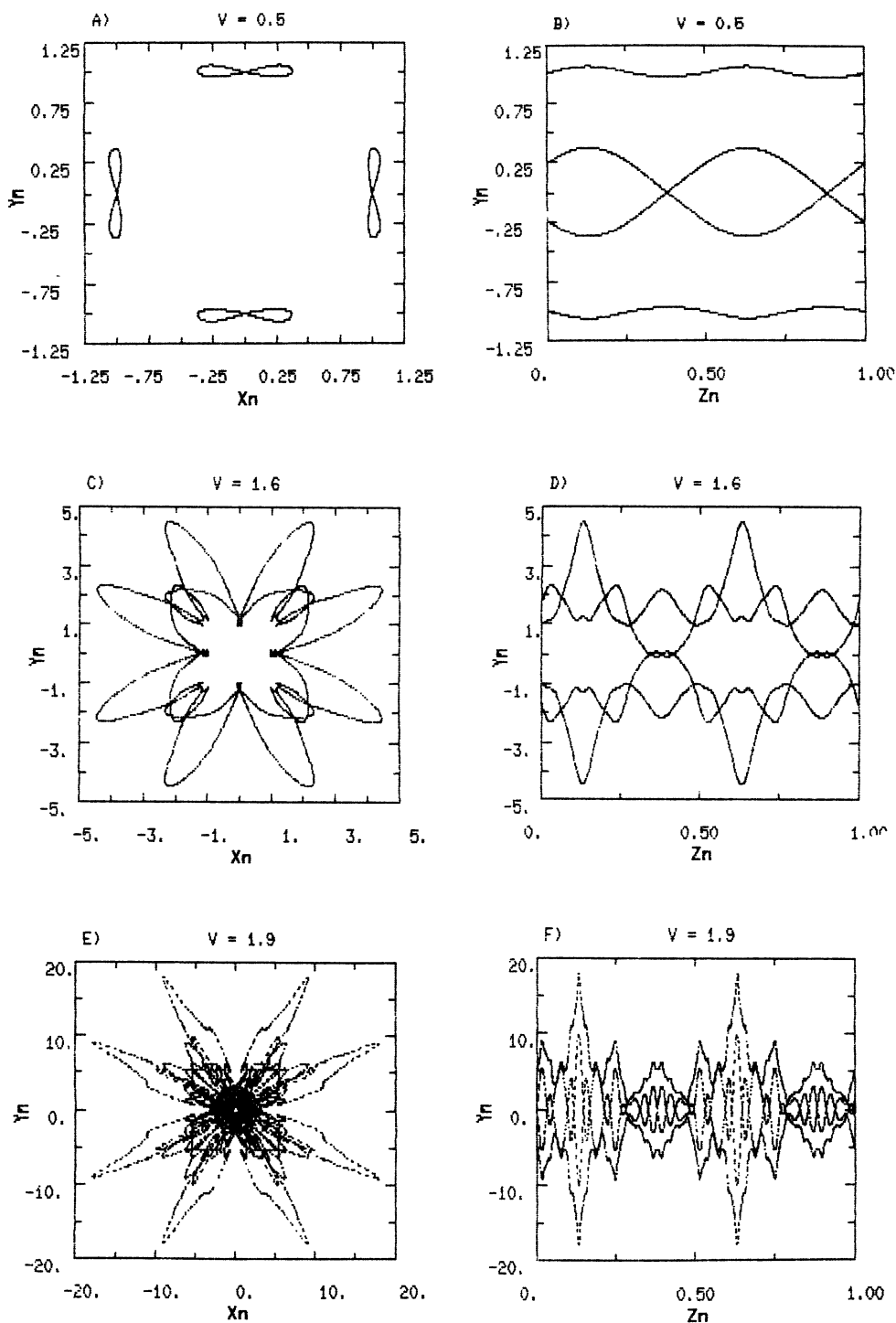


Fig. 1. — Projections of the map of equation (3) for extended states for different values of the potential strength V for $\gamma = (\sqrt{5} - 1)/2$, $k = 1/4$: (a) xy projection and (b) yz projection for $V = 0.5$ up to 3 000 iterations; (c) xy projection and (d) yz projection for $V = 1.6$ up to 6 000 iterations; (e) xy projection and (f) yz projection for $V = 1.9$ up to 12 000 iterations.

know exactly the relation between E and k . This happens for $E = 0$, which corresponds to $k = 1/4$ for every value of V as it is known for this model [1, 6, 7, 11].

Then we iterate the map (3) for $E = 0$ with the initial condition $(x_0, y_0, z_0) = (c, 0, 0)$ which physically corresponds to a semi-infinite chain. In figures 1-3 we show the projections (x, y) and (y, z) for different values of V for the case of $\gamma = (\sqrt{5} - 1)/2$, the golden mean. We found that :

i) For $V < 2$ the points of the iterated map seem to lie on well defined curves in each projection, as can be seen from figure 1. This suggests that there exists an invariant set for the mapping and that it has a constant of motion that is complicated to define. Due to the $k = 1/4$ value of the winding number the curves on the (x, y) projection are symmetric for rotations in $\pi/2$. The complexity of these curves grows with V . For small values of V the four isolated points of the circle map for $V = 0$ are transformed into four little topknots in the (x, y) plane and the corresponding horizontal lines for $V = 0$ (two of them superposed at $y = 0$) are transformed into four wavy lines (now the two central curves are separated) in the

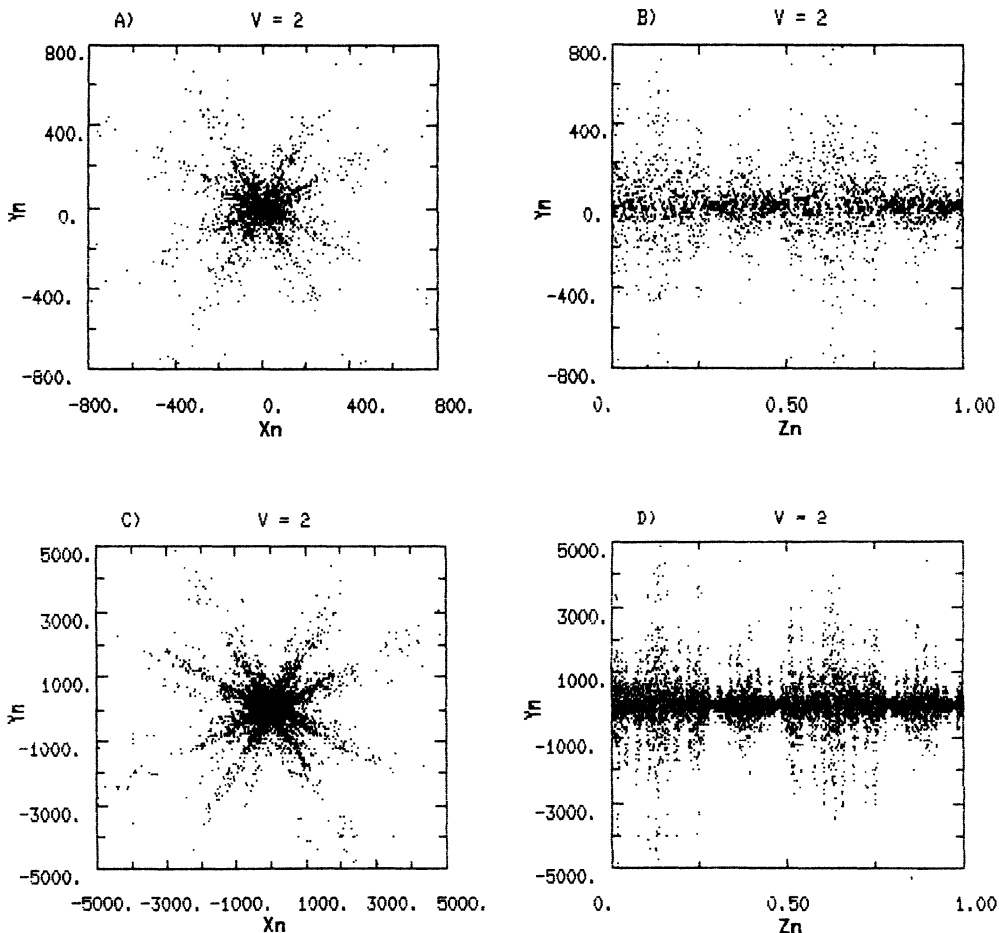


Fig. 2. — Projections of the map of equation (3) for a critical state ($V = 2$) for $\gamma = (\sqrt{5} - 1)/2$, $k = 1/4$: (a) xy projection and (b) yz projection up to 3 000 iterations ; (c) xy projection and (d) yz projection up to 12 000 iterations.

(y, z) plane (see Fig. 1a and 1b). When V increases these topknots grow in size, develop structure, cross each other, and form a connected figure (Fig. 1c and 1d). The number of intersections of the curves continues increasing with V in both planes giving increasingly complicated drawings (Fig. 1e and 1f). Also the region of phase space through which we get points on the curves grows with V . The effect of varying c in the initial condition is just to change the scale in the curves in both planes. However, by changing γ we have found that the shape of the orbits varies forming different beautiful drawings but in all cases the points lie on curves.

ii) For $V = 2$ (the critical value) the curves disappear and the planes (x, y) and (y, z) get filled by a cloud of points (clearly in Fig. 2a and 2b it is not possible to draw a curve through these points) with some regions more densely populated than the others. As the number of iterations grows the cloud extends in the space and then the orbit becomes unbounded (2c and 2d).

iii) For $V > 2$ the map takes exponentially growing values and in a log-log plot of (x, y) we get an unbounded cloud over a line (Fig. 3a). For a localized state we expect to have in the (x, y) plane a spot at the origin with a few points away, corresponding to an exponentially decreasing wave function. But due to the fact that there is also an exponentially growing solution in equation (1), it predominates through rounding errors in the iteration of the map giving the diverging picture we show in figure 3a and 3b.

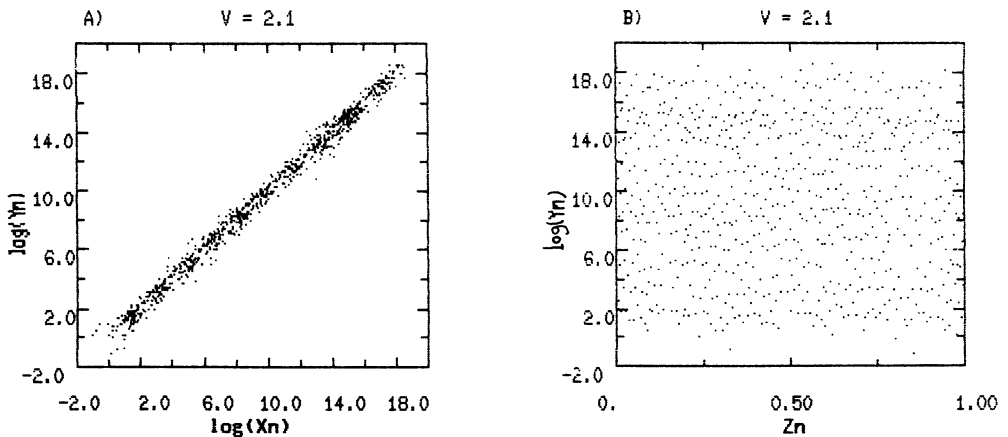


Fig. 3. — Projections of the map of equation (3) for a localized state : $V = 2.1$, for $\gamma = (\sqrt{5} - 1)/2$, $k = 1/4$: (a) xy projection and (b) yz projection up to 2 000 iterations.

All this suggests that the localization transition in the Aubry model happens as a growth of complexity of a certain integral of motion until it finally disappears at the critical value $V = 2$. This transition clearly corresponds to the disappearance of the quasi-Bloch extended states of the model.

These results are reminiscent of KAM theorem [14] in the sense that for small values of the perturbation (i.e. for $V < 2$) the invariant curves are not destroyed and when the perturbation grows sufficiently (i.e. $V \geq 2$) they disappear. In this direction, the ideas of KAM theory were used by Dinaburg and Sinai [15] to analyze the Schrödinger equation with a weak quasiperiodic potential.

3. The mean radius.

We want to study in a more quantitative way how the disappearance of the constant of motion takes place. To do this we first remember that for $V = 0$ the constant of motion is given by the radius of the circular orbit (at $E = 0$). For $V \neq 0$ we intend to extend this concept defining a mean radius by averaging up to N iterations the distance to the origin of each point in the (x, y) plane :

$$\rho(N) = \left(\frac{1}{N} \sum_{n=1}^N r_n^2 \right)^{1/2} \quad (10)$$

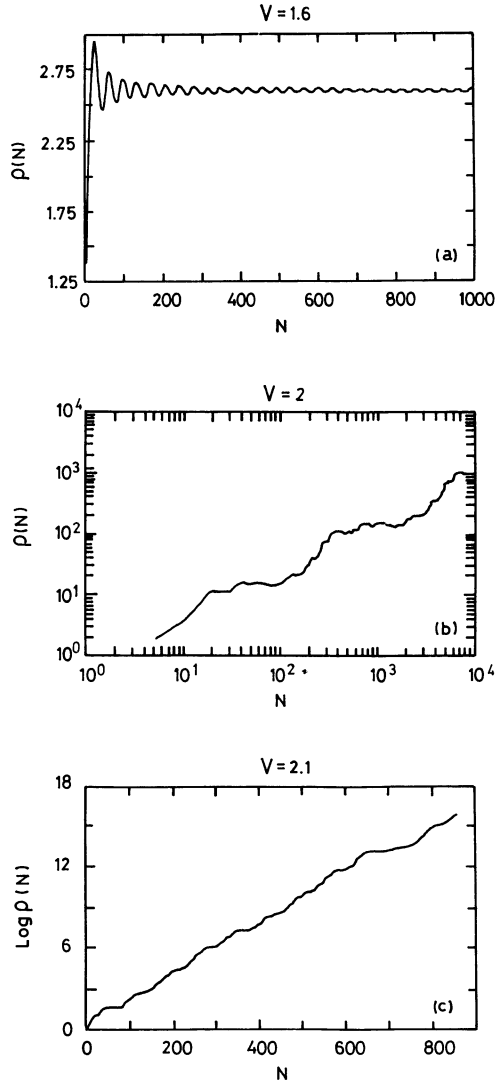


Fig. 4. — Behavior of the mean radius $\rho(N)$ as a function of the number N of iterations for $\gamma = (\sqrt{5} - 1)/2$, $k = 1/4$: (a) extended state, $V = 1.6$, see the convergence of the limit $\bar{\rho} = \rho(\infty)$; (b) critical state, $V = 2$, power law growing of $\rho(N)$; (c) localized state, $V = 2.1$, exponential growing of $\rho(N)$.

with $r_n = (x_n^2 + y_n^2)^{1/2}$. This can be related to the normalization A of the wave function by :

$$A = \left(\sum_{n=1}^N |\psi_n|^2 \right)^{1/2} \quad (11)$$

$$\rho^2(N) = 2 \frac{A^2}{N}$$

where $A \neq 1$ (because we obtain the wave function by iteration of (2) with fixed initial conditions).

We found by numerical inspection that for $V < 2$ the limit :

$$\bar{\rho} = \lim_{N \rightarrow \infty} \rho(N) \quad (12)$$

converges to a finite constant (see Fig. 4a) and we take this as an evidence for the existence of a constant of motion. Meanwhile for $V > 2$ we have found that the numerical evaluation of $\rho(N)$ can be fitted by an exponential law (see Fig. 4c) :

$$\rho(N) \sim e^{\alpha N} \quad (13)$$

with α the inverse of the localization length, and therefore the limit (12) is ∞ (there is no constant of motion). For the critical strength $V_c = 2$ we have found numerically that the averaged radius has an envelope with a power law growing (see Fig. 4b) :

$$\rho(N) \sim N^\beta. \quad (14)$$

Also we have seen that the values of $\bar{\rho}$ increase as V tends to its critical value $V_c = 2$ from below. These results lead us to study by numerical computations the growing of $\bar{\rho}$ as a function of $V_c - V$. In figure 5 we show a log-log plot of these variables for $\gamma = (\sqrt{5} - 1)/2$ (the golden mean). In this case we can fit a power law behaviour :

$$\bar{\rho} \sim (V_c - V)^{-\nu} \quad (15)$$

giving a critical index $\nu = 0.782$. However for different values of γ we have found a variety of situations in the behavior of $\bar{\rho}$ against $V_c - V$ which will be studied in detail elsewhere.

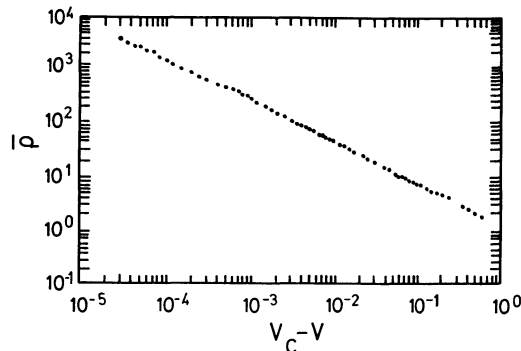


Fig. 5. — Critical behavior of $\bar{\rho}$ as V tends to $V_c = 2$ for $\gamma = (\sqrt{5} - 1)/2$, $k = 1/4$.

4. Discussion.

The results we have obtained in section 2 can be interpreted with the following argument. One can analyze in the (x, y) projection of the mapping (Eq. (2)) the condition for the fixed point $(0, 0)$ to be locally elliptic at each iteration n (for $E = 0$) :

$$\begin{aligned} |\operatorname{tr} M(n)| &< 2 \\ |\cos 2 \pi z_n| &< 2/V. \end{aligned} \quad (16)$$

For $V < 2$ equation (16) is always satisfied, thus at every iteration $(0, 0)$ is an elliptic point, which explains the fact that the orbits are bounded in this case. The condition for local hyperbolicity is :

$$|\cos 2 \pi z_n| > 2/V. \quad (17)$$

Therefore, for $V > 2$ we get some points locally hyperbolic, their number increasing with V . The appearance of hyperbolic points for $V > 2$ could explain the breaking of the integral of motion we have shown in section 2. However this is not sufficient to prove localization as can be seen if we extend the above argument for every energy E . The general condition to have elliptic points is :

$$|E - V \cos 2 \pi z_n| < 2 \quad (18)$$

which is always satisfied for :

$$|E| < 2 - V. \quad (19)$$

But we know that all the states are extended for $V < 2$ [6], then it is possible to have bounded orbits with some locally hyperbolic points. The condition (19) coincides with the mobility edges found by Sokoloff [16] within a quasiclassical theory of equation (1) for $\gamma \ll 1$. This was investigated by Dy and Ma [7] who showed that (19) separates classically extended states from quasilocalized ones, that is, states which are classically localized but become extended by quantum tunneling.

The opposite of (18) gives the condition for points always hyperbolic :

$$|E| > 2 + V \quad (20)$$

which coincides with the condition to have no states in equation (1).

Finally we want to make some comments of how the point of view of section 2 could be applied for random chains. In this case the tight-binding equation is :

$$\psi_{n+1} + \psi_{n-1} + V \varepsilon_n \psi_n = E \psi_n \quad (21)$$

where ε_n is a random variable with probability distribution :

$$\rho(\varepsilon_n) = \begin{cases} 1/2 & |\varepsilon_n| < 1 \\ 0 & |\varepsilon_n| > 1 \end{cases} \quad (22)$$

and V is now the disorder strength. We can rewrite (21) as a three dimensional mapping :

$$\begin{aligned} x_{n+1} &= (E - Vz_n) x_n - y_n \\ y_{n+1} &= x_n \\ z_{n+1} &= f(z_n) \end{aligned} \quad (23)$$

where $f(x)$ is a stochastic map with the probability distribution (22). The (x, y) projection of the mapping is the usual matrix transfer formulation of the problem and is similar to the mapping of Kostadinov and Nachev [10]. Now we can think that what we have is a coupling between a circular map with winding number k (the map of Eq. (4)) and a stochastic map $z_{n+1} = f(z_n)$. The effect of this map is to introduce noise into the ellipses of the circular map through the perturbation V . For small V it transforms ellipses into elliptical clouds such as those seen in reference [10]. There, the authors have interpreted them as « quasiextended » states. When the number of iterations grows the curves will slowly move in a random fashion performing a random walk between ellipses (as can be seen in Fig. 3 of Ref. [10]) but finally the points will diffuse to infinity, as we have checked numerically. This final diverging behavior is what is expected for a weakly localized state. This is the interpretation of the results of Kostadinov and Nachev [10] which we think is more appropriate than their claims of the existence of these « quasiextended » states. This mapping for a random chain has the same kind of behavior as a four dimensional map consisting of two weakly coupled standard maps studied by Froeschlé [18] in the last decade. He took initial conditions in the region of invariant curves of one of the maps and in the chaotic region of the other, and he obtained a set of drawings very similar to that of reference [10], due to the coupling of these two maps.

In conclusion, we have reinterpreted the Aubry model as a coupling of two circular maps. We have studied these maps for the special case of $E = 0$ and we have seen that the delocalization transition takes place as a disappearance of a certain integral of motion. We have related the existence of this constant of motion to the existence of a mean radius for the (x, y) map for $V < V_c$. Usually the localization problem has been studied through the behavior of the Lyapunov exponent of the transfer matrix product of equation (2) [1, 6]. This permits to study how the transition occurs coming from $V > V_c$ values, but it is not useful to the study of the transition from below V_c (because the Lyapunov exponent is zero for extended states). The existence of the mean radius permits to perform this analysis and a previous result was presented in section 3. It remains for future investigation a more detailed study of its critical behavior.

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