

## Hamiltonian map approach to resonant states in paired correlated binary alloys

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The origin of resonant states in tight-binding models with correlated disorder is analyzed using an approach based on classical Hamiltonian maps. In this method, extended states correspond to bounded trajectories in the phase space of a parametrically excited linear oscillator, where the external force corresponds to the site potential of the original model. We pay particular attention to the nearly resonant states of the random dimer model. We also discuss the case of a general  $N$ -mer model.

### I. INTRODUCTION

In one-dimensional tight-binding-type models an infinitesimal amount of disorder renders all eigenstates localized.<sup>1,2</sup> This property, in models without any short-range order, leads to the absence of electronic propagation in the lattice. On the other hand, it is generally known that in quasi-one-dimensional polymers, the presence of disorder might not necessarily lead to a complete lack of conduction.<sup>3,4</sup> In Ref. 4 in particular, various organic disordered systems were quoted with electrical properties. The presence of extended states in such systems (that lead to electronic propagation) can be understood when, in the disordered tight-binding model there exists short-range order.<sup>3-9</sup> The prototypical case is that of the random dimer model<sup>3,4</sup> (RDM), where (in the context of a tight-binding Hamiltonian) pairs of adjacent energy levels are assigned at random, leading to two-site correlations in an otherwise random model. The presence of correlations in RDM results in the diffusive and superdiffusive electronic propagation for specific values of energies.

Since for infinite samples fully delocalized states appear only for specific energy values, there is no Anderson transition in the usual sense (see, also Ref. 7). However, a large number of transparent states occur for any finite sample size; this number was found to be proportional to the square root of the length of the sample.<sup>3,4</sup> This fact is related to the divergence of the localization length in infinite samples when energy approaches the resonant value.<sup>5,6</sup>

In the present paper we address the issue of the spectrum of RDM and extensions from a point of view different to those used in Refs. 2-8. In particular, we use a Hamiltonian map approach and transform the original correlated random tight-binding model into a two-dimensional map which corresponds to classical linear oscillator with a parametrical perturbation given in the form of periodic delta kicks.<sup>10</sup> The amplitudes of these kicks are defined by the site potential of the given tight-binding model. As a result, extended states are essential-

ly represented by the bounded trajectories in the phase space of the Hamiltonian map. This approach gives quite an effective and simple tool for understanding specific properties of eigenstates as well as for deriving some analytical expressions which have been found before in a different way.<sup>3-9</sup> In particular, one can easily see the meaning of fully transparent states for the general case when  $N$  sites are correlated.

### II. RESONANT STATES: HAMILTONIAN MAP APPROACH

#### A. Time-dependent linear map

Our starting point is the usual Schrödinger equation in the tight-binding approximation in one dimension:

$$i \frac{dc_n(t)}{dt} = \epsilon_n c_n(t) + c_{n+1}(t) + c_{n-1}(t), \quad (1)$$

where  $c_n(t)$  is the probability amplitude for an electron to be at site  $n$  and  $\epsilon_n$  is the local site energy. The eigenvalue problem is obtained by making the transformation  $c_n(t) = \exp(-iEt)x_n$  which results in the equation

$$x_{n+1} + x_{n-1} = v_n x_n, \quad (2)$$

with  $v_n = E - \epsilon_n$ . We cast Eq. (2) in the form of a two-dimensional map, i.e.,

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} v_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix}, \quad (3)$$

where the substitution  $y_n = x_{n-1}$  is made. While Eq. (3) is equivalent to the tight-binding Eq. (2), it nevertheless provides with an alternative interpretation, viz., that of a two-dimensional dynamical system. In this picture an eigenstate of Eq. (2) can be seen as a "trajectory" of the map of Eq. (3). Straightforward diagonalization of this map leads to

$$\lambda_n^\pm = \frac{v_n \pm i\sqrt{4-v_n^2}}{2} = e^{\pm i\mu_n}, \quad (4)$$

where the phase  $\mu_n$  is introduced by the relation  $v_n = 2 \cos \mu_n$ . One can easily see that for  $|v_n| < 2$  the map results in a simple rotation with the phase  $\mu_n$ . Consequently, the stability condition for the trajectories of Eq. (3) has the form

$$|E - \epsilon_n| < 2. \quad (5)$$

In order to specialize the general Eq. (3) for the random dimer case we must take pairs of random site energies, i.e.,  $\epsilon_n = \epsilon_{n+1} = \epsilon_1$  or  $\epsilon_2$ . To understand the origin of the resonant states, reported in Ref. 3, we consider the sequence  $\epsilon_n$  which consists of one dimer only, i.e., where all the values of  $\epsilon_n$  are equal to  $\epsilon_1$  except two values for which we have  $\epsilon_m = \epsilon_{m+1} = \epsilon_2$ . From Eq. (4) one can see that this unique dimer with energy  $\epsilon_2$  does not influence the trajectories of the map of Eq. (3) when the total phase advance  $\mu_m + \mu_{m+1} = 2\mu_m$  through the dimer is equal to  $\pi$  or  $2\pi$ . Since the latter value  $\mu_m = \pi$  is forbidden due to the stability condition of Eq. (5), the resonant energy  $E_{cr}$  is defined by  $\mu_m = \pi/2$  giving  $E_{cr} = \epsilon_2$ . As a result, for the general case of randomly distributed dimers  $\epsilon_1$  and  $\epsilon_2$  there are two resonant values

$$E_{cr} = \begin{cases} \epsilon_1 \\ \epsilon_2 \end{cases} \quad (6)$$

for which dimers of the first type  $\epsilon_1$  or of the second  $\epsilon_2$  have no influence on the transparent states. One should note that in the case of only one type of dimer, say  $\epsilon_2$ , the transparent states appear for only one value  $E_{cr} = \epsilon_2$ .

Based on the above analysis, it is easy to understand that in the general case of  $N$ -mer (two values  $\epsilon_1$  and  $\epsilon_2$  appear in blocks of length  $N$ ) the resonant energy is defined by the following condition:

$$\mu = \frac{\pi}{N}, \frac{2\pi}{N}, \frac{3\pi}{N}, \frac{4\pi}{N}, \dots, \frac{(k+1)\pi}{N}, \quad (7)$$

$$k = 0, 1, 2, \dots, N-2.$$

For example, for trimers the resonant energies are given by the relations

$$E_{cr} - \epsilon_{1,2} = 2 \cos \mu_m, \quad \mu_m = \frac{\pi}{3}, \frac{2\pi}{3}, \quad (8)$$

which result in four values for  $E_{cr}$ :

$$E_{cr} = \epsilon_1 - 1; \epsilon_1 + 1; \epsilon_2 - 1; \epsilon_2 + 1 \quad (9)$$

(see also Ref. 8).

We now use a different approach<sup>10</sup> suggested for tight-binding models of type (3). The idea is to use an alternative two-dimensional Hamiltonian map, instead of the map of Eq. (3). For this, the new variable  $p_{n+1} = x_{n+1} - x_n$  is introduced which plays a role of the momentum in the discrete Hamiltonian equations

$$p_{n+1} = p_n + f_n x_n, \quad (10)$$

$$x_{n+1} = x_n + p_{n+1}.$$

The above map can be easily obtained from Eq. (2) by making the substitution for  $p_{n+1}$  and  $p_n$ . In this repre-

sentation the amplitude  $f_n$  of the linear force depends on the discrete time  $n$  as follows:

$$f_n = E - 2 - \epsilon_n, \quad (11)$$

where  $f_n$  is determined by the disorder site energy  $\epsilon_n$  of the underlying tight-binding model. It is important to note that the eigenvalues  $\lambda_n$  of the map, Eq. (10), are defined by the same condition given in Eq. (5) as for the map of Eq. (3). The corresponding Hamiltonian for the map of Eq. (10) has the form

$$H(p, x, t) = \frac{p^2}{2} + \frac{x^2}{2} \delta_1(t), \quad \delta_1(t) \equiv - \sum_{n=-\infty}^{\infty} f_n \delta(t-n), \quad (12)$$

where the potential is given in the form of  $\delta$  kicks with time-dependent amplitudes [here  $\delta(t-n) \equiv \delta_{t,n}$  equals 1 for  $t=n$  and 0 otherwise]. The analysis of the Hamiltonian map (10) turns out to be very instructive for understanding the structure of resonant states.

In the simplest case of the complete order, i.e.,  $\epsilon_n = \epsilon_1$  for all  $n$ , [constant force  $f_n = f$  in (10)] the motion is represented by an ellipse in the phase space  $(p, x)$  with the orientation defined by  $\epsilon_1$ . If the sequence of constant energies  $\epsilon_n = \epsilon_1$  is interrupted only once at a given site  $m$  with a local energy  $\epsilon_m = \epsilon_2$ , then the result in the phase space is the following: All trajectory points for  $n < m$  fall on a given ellipse in the phase space, at  $n = m$  there is a kick to larger or smaller amplitudes and the remaining points for  $n > m$  fall on a different ellipse but with the same orientation as the original one [Fig. 1(a)]. If now the second site with energy different from  $\epsilon_1$  is placed next to the one at the  $m$ th site, i.e.,  $\epsilon_{m+1} = \epsilon_2$  it is possible to have a reversal of the effect of the first kick from the energy  $\epsilon_2$  at site  $m$ . This happens when  $\epsilon_m = \epsilon_{m+1}$  and the total phase advance after the two kicks is  $\mu = \mu_m + \mu_{m+1} = \pi$  [Fig. 1(b)]. This condition for the phase advance is a generalized resonant condition that leads to a propagating state. When a random mixture of dimers with energy  $\epsilon_2$  is embedded in the chain with energy  $\epsilon_1$  we obtain a phase-space trajectory similar to the one in Fig. 1(c). We observe the two ellipses corresponding to  $\epsilon_1$  and  $\epsilon_2$  values. The second ellipse is formed by points occurring every time the first site of a dimer is encountered in the map.

From the above consideration, it is easy to understand that similar resonant states may exist even for a more complicated case of slightly correlated sequences of  $\epsilon_n$  of any length  $M$ . The only condition is that the total sum  $\sum_{n=1}^M \mu_n$  of phase shifts has to be equal to  $m\pi$  for any sequence with  $m$  integer. In this case, the trajectory always goes back to the ellipse in the phase space, which is associated with the perfect lead to the left and to the right of the scattering potential.

## B. Parametric linear oscillator

Another representation of the original model of Eq. (2) is similar to the map of Eq. (10) but more convenient for the analysis of localization length.<sup>10</sup> It is easy to show

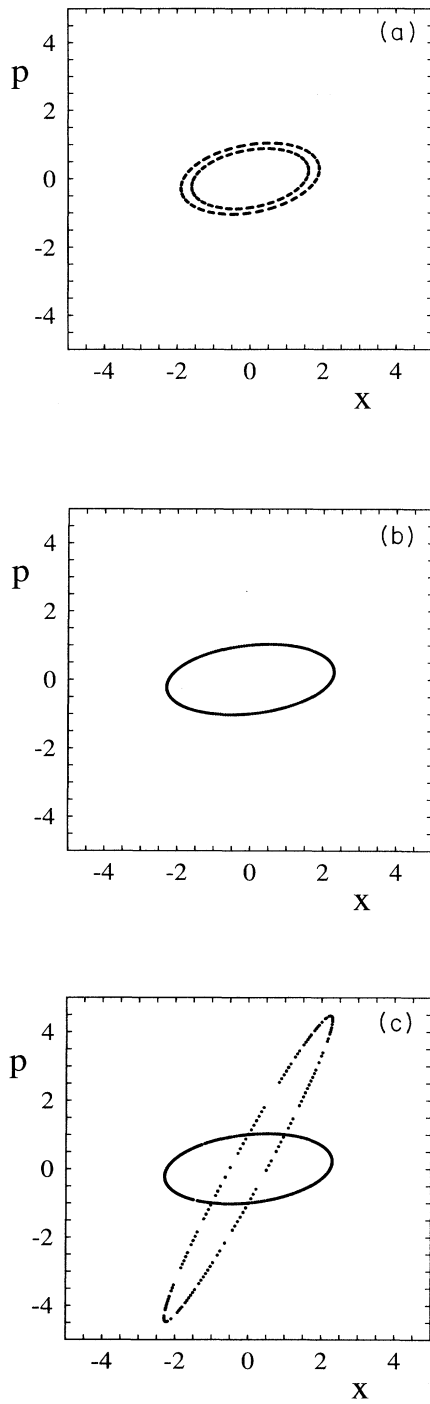


FIG. 1. The phase space of the map (10) for  $p_0=x_0=1$ . (a) One value of  $\epsilon_2$  in the sequence  $\epsilon: \dots \epsilon_1 \epsilon_1 \epsilon_1 \epsilon_2 \epsilon_1 \epsilon_1 \epsilon_1 \dots$  for  $E=1.7$ ;  $\epsilon_1=0$ ;  $\epsilon_2=1.8$ . We note that one point is outside of the ellipse representing the kick to the  $\epsilon_1$  trajectory by  $\epsilon_2$ . (b) Two values of  $\epsilon_2$  (one dimer) in the sequence  $\epsilon: \dots \epsilon_1 \epsilon_1 \epsilon_1 \epsilon_2 \epsilon_2 \epsilon_1 \epsilon_1 \epsilon_1 \dots$  for  $\epsilon_1=0$ ;  $E=\epsilon_2=1.8$ . We note that there is a point inside the ellipse representing the kick to the  $\epsilon_1$  trajectory by the first  $\epsilon_2$  value. The second  $\epsilon_2$  value kicks the trajectory back to the ellipse. (c) dimer of type  $\epsilon_2$ , randomly (with probability  $Q=0.5$ ) distributed in the sequence  $\epsilon$  for  $\epsilon_1=0$  and  $E=\epsilon_2=1.8$ .

that two successive maps

$$\tilde{p}_n = p_n + A_n x_n, \tag{13}$$

$$\tilde{x}_n = x_n$$

and

$$p_{n+1} = \tilde{p}_n \cos \mu_0 - \tilde{x}_n \sin \mu_0, \tag{14}$$

$$x_{n+1} = \tilde{p}_n \sin \mu_0 + \tilde{x}_n \cos \mu_0,$$

can be written in the form of the relation (2)

$$x_{n+1} + x_{n-1} = (2 \cos \mu_0 + A_n \sin \mu_0) x_n. \tag{15}$$

Comparing with (2) one can establish the correspondence

$$E = 2 \cos \mu_0, \quad A_n = -\frac{\epsilon_n}{\sin \mu_0} \tag{16}$$

between the parameters  $E, \epsilon_n$  in the original model (2) and the parameters  $\mu_0, A_n$  of the map (13) and (14). The latter has clear meaning, i.e., the map (13) corresponds to an instant linear kick of the strength  $A_n$  resulting in the change of the momentum  $p_n$  and the map Eq. (14) describes the free rotation in the phase plane  $(p, x)$  defined by the angle  $\mu_0$ . One can see that such a map can be associated with the Hamiltonian of a linear oscillator with a periodic parametrical perturbation:

$$\tilde{H} = \frac{\mu_0 p^2}{2} + \frac{\mu_0 x^2}{2} - \frac{1}{2} x^2 \tilde{\delta}_1(t), \quad \tilde{\delta}_1(t) \equiv \sum_{n=-\infty}^{\infty} A_n \delta(t-n), \tag{17}$$

which may be treated analytically.

It is interesting to note that the one-dimensional map of the type (13) and (14) is well known in accelerator physics (see, e.g., Ref. 11). It describes the motion of a charged particle subjected to periodic linear kicks due to thin magnetic lenses or due to beam-beam interaction, when neglecting nonlinear terms. In such an application, the quantity  $\mu$  has the meaning of the phase shift of betatron oscillations between two successive kicks. In the case of kicked noise [ $\tilde{p}_n = p_n + A_n$  in Eq. (13)] the problem is analytically solved in Ref. 12.

For the above dimer defined by two values of  $\epsilon_1, \epsilon_2$ , without the loss of generality, one can put  $\epsilon_1=0$ . As a result, the motion corresponding to  $\epsilon_n=\epsilon_1$  is represented by the circle in the phase plane  $(p, x)$  and resonant behavior appears when, after numbers of kicks with  $\epsilon_n=\epsilon_2$ , the trajectory comes back to this circle. Some examples with different values of  $\epsilon_2$  are given in Figs. 2 and 3 for  $E=\epsilon_2$  and  $E=\epsilon_1=0$ .

### C. Nearly resonant states

The above representation of the given quantum model of Eq. (2) allows for the study of global properties of eigenstates. In particular, the resonant delocalized states correspond to a bounded motion described by the maps of Eqs. (10), (13), and (14). Localized states, on the other hand, are represented by unbounded trajectories which

go away from the origin of the phase space  $(p, x)$ . This is well illustrated in Fig. 4 for the case of random dimers with nonresonant values of energy  $E$ . The exponential increase of a distance from the origin ( $p = x = 0$ ) can be related to the localization length of the eigenstate. To study the dependence of the localization length  $l$  for nearly resonant states, it is useful to pass to action-angle variables  $(r, \theta)$  for the map of Eqs. (13) and (14):

$$x = r \cos\theta, \quad p = r \sin\theta. \tag{18}$$

As a result, one can obtain the following map for the action  $r$ :

$$r_{n+1}^2 = r_n^2 D_n^2, \quad D_n^2 = (1 + A_n^2 \cos^2 \theta_n + A_n \sin 2\theta_n), \tag{19}$$

where the transformation for  $\cos\theta_n$  and  $\sin\theta_n$  is given by the relations

$$\begin{aligned} \cos\theta_{n+1} &= D_n^{-1} \{ \cos(\theta_n + \mu_0) - A_n \cos\theta_n \sin\mu_0 \}, \\ \sin\theta_{n+1} &= D_n^{-1} \{ \sin(\theta_n + \mu_0) + A_n \cos\theta_n \cos\mu_0 \}. \end{aligned} \tag{20}$$

The relations of Eqs. (19) and (20) can be used instead of

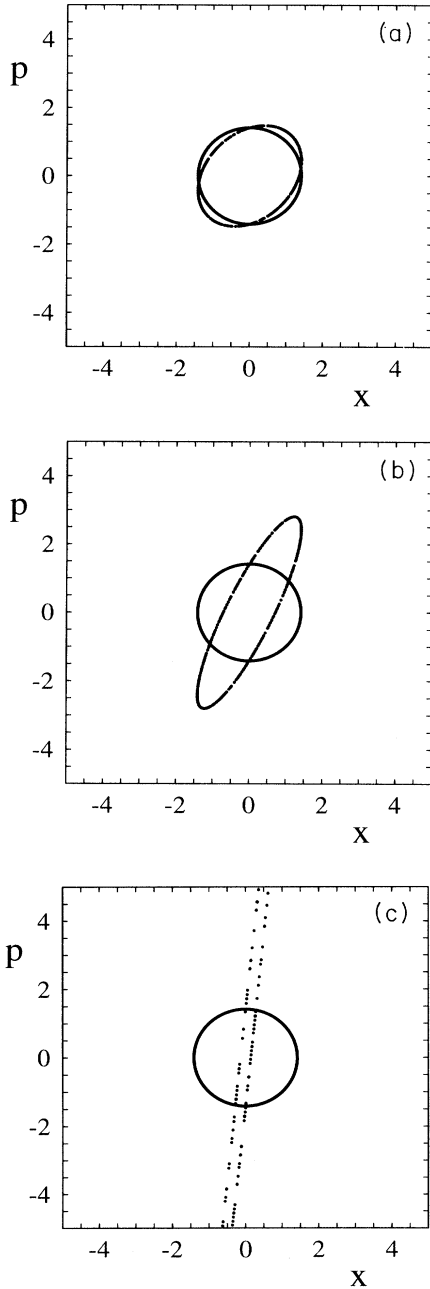


FIG. 2. The phase space of the map (13)–(14) for  $p_0 = x_0 = 1$  and  $Q = 0.5$ ;  $\epsilon_1 = 0$ . (a)  $E = \epsilon_2 = 0.3$ ; (b)  $E = \epsilon_2 = 1.3$ ; (c)  $E = \epsilon_2 = 1.96$ . The length  $N$  of sequence  $\epsilon$  is equal to  $N = 1000$ .

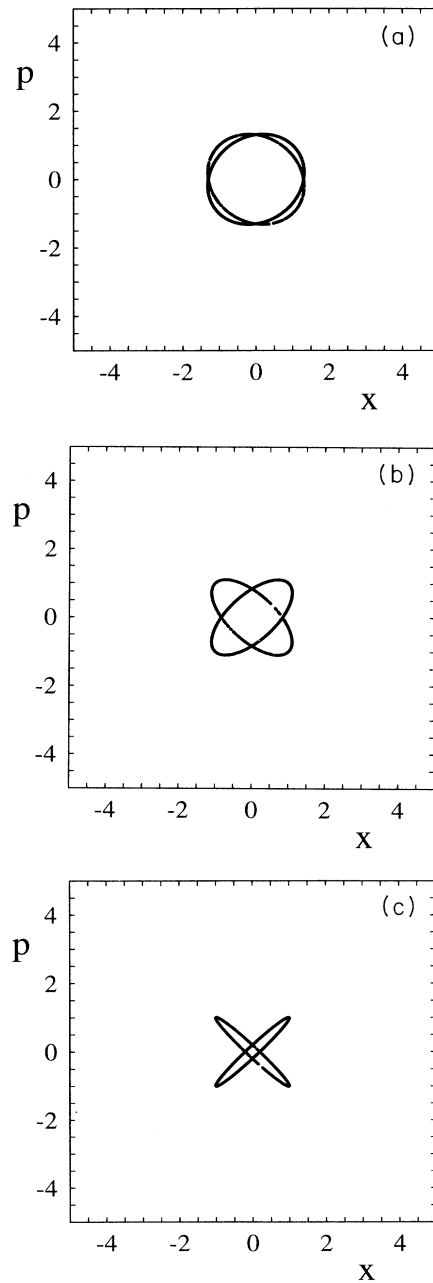


FIG. 3. The same as in Fig. 2 for  $E = \epsilon_1 = 0$ . (a)  $\epsilon_2 = 0.3$ ; (b)  $\epsilon_2 = 1.3$ ; (c)  $\epsilon_2 = 1.96$ .

the common transfer-matrix approach for the determination of the localization length. The latter can be found from the Lyapunov exponent  $\gamma$  which is defined as

$$\gamma = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \ln \left( \frac{r_{n+1}}{r_n} \right), \quad (21)$$

where the ratio  $r_{n+1}/r_n = D_n$  is given by (19). Due to

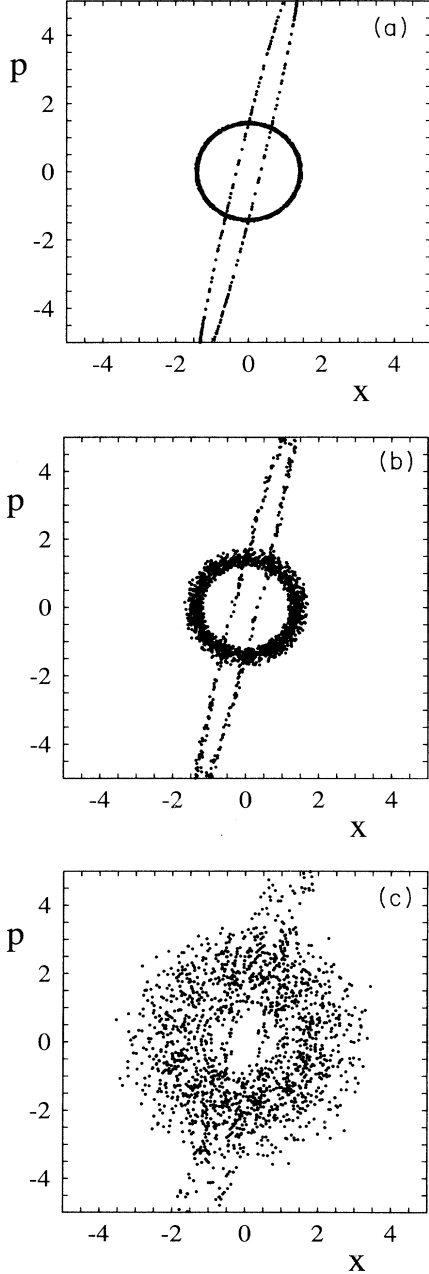


FIG. 4. Nearly resonant states; the same as in Fig. 2 for different  $E$ . Comparing with the resonant states shown in Figs. 2 and 3, nearly resonant states correspond to the unbounded (for  $n \rightarrow \infty$ ) motion with a slow spread of the points in the phase space. (a)  $E=1.799$ ;  $\epsilon_2=1.8$ ; (b)  $E=1.790$ ;  $\epsilon_2=1.8$ ; (c)  $E=1.771$ ;  $\epsilon_2=1.8$ .

correlations in the sequence  $\theta_n$ , expression (21) cannot be evaluated directly. However, it is possible to construct an effective map for two successive kicks of the single map (19) and neglect the correlations between the phases  $\theta_{n+2}$  and  $\theta_n$  near the resonance  $E = E_{cr} - \delta \approx E_{cr}$ . One can show that the two-step map has the form

$$r_{n+2}^2 = r_n^2 [1 - W F_1(\theta_n) + 2\delta W F_2(\theta_n)], \quad (22)$$

where  $W = A_n \delta / \sin \mu_0$  and functions  $F_1, F_2$  are given by

$$F_1(\theta_n) = \sin^2 \theta_n - \sin^2(\theta_n + \mu_0) \quad (23)$$

and

$$F_2(\theta_n) = \sin \theta_n \sin(\theta_n + \mu_0). \quad (24)$$

Near the resonance,  $\delta \ll 1$ , the Lyapunov exponent can be estimated by making use of expansion in  $W$  with the successive averaging over  $\theta_n$ . As a result, one can get

$$\gamma \approx \frac{Q}{4} \frac{\delta^2 \cos^2 \mu_0}{\sin^2 \mu_0}, \quad (25)$$

where the factor  $Q$  stands for the probability for the dimer of the second kind (with energy  $\epsilon_2$ ), to appear. From the above expression the dependence of the localization length on the distance  $\delta$  (with  $\delta \ll 1$ ) from the resonance can be easily found for two extreme cases. The first one corresponds to the case when the value of  $\epsilon_2$  is far enough from the stability border  $E_b = 2$ . If the distance  $\Delta = E_b - \epsilon_2 \equiv 2 - \epsilon_2$  is large compared to  $\delta = \epsilon_2 - E$ , then the estimate for the localization length  $l = \gamma^{-1}$  has the form

$$l \sim \frac{\Delta}{\delta^2}, \quad \text{for } \delta \ll \Delta \ll 1 \quad (26)$$

due to the relation  $2 \cos \mu_0 = E = \epsilon_2 - \delta$ . In the other limit, case  $\epsilon_2 = 2$ , we have

$$l \sim \frac{1}{\delta}, \quad \text{for } \delta \ll 1, \Delta = 0. \quad (27)$$

The above dependencies of the localization length  $l$  on the parameter  $\delta \ll 1$  have also been found through a different approach in Refs. 5 and 6 (see also Ref. 9).

### III. CONCLUSIONS

We have studied a one-dimensional tight-binding model with binary on-site disorder randomly assigned every two sites. For such a model it was found<sup>3,4</sup> that there exist special energies  $E_{cr}$  at which transparent states appear. We recover the above results using the approach based on the classical Hamiltonian maps. Moreover, we generalized our results for a  $N$ -mer case (see also Ref. 8) giving a simple expression for the resonant values of energy. In the suggested approach, resonant delocalized states correspond to a bounded motion, while localized states are represented by unbounded trajectories in the phase space  $(p, x)$ . Making use of expansion in the vicini-

ty of the resonance we give an analytical expression (25) for the Lyapunov exponent for the nearly resonant states. From this expression one can obtain that in the limit  $\delta \ll \Delta \ll 1$  the localization length diverges as  $l \sim \Delta/\delta^2$ ; in the other limit,  $\delta \ll 1$  and  $\Delta = 0$ , the dependence is  $l \sim 1/\delta$  in perfect agreement with Refs. 5, 6, and 9. Important aspects of fluctuations of the transmission coefficient for nearly resonant states are discussed in Ref. 13.

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