Classical Representation of the 1D Anderson Model

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Abstract

A new approach is applied to the 1D Anderson model by making use of a two-dimensional Hamiltonian map. For a weak disorder this approach allows for a simple derivation of correct expressions for the localization length both at the center and at the edge of the energy band, where standard perturbation theory fails. Approximate analytical expressions for strong disorder are also obtained.

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I. INTRODUCTION

Recently, it was suggested to treat 1D tight-binding models with diagonal disorder in terms of classical Hamiltonian maps [1]. This approach has been successfully used in the description of delocalized states in the so-called dimer model [2], as well as for the Kronig-Penney model [3]. In this paper we show that even for the standard 1D Anderson model, this approach allows us to obtain new analytical results and reproduce known results in a much more transparent way, by making reference to the properties of the dynamics of the noisy Hamiltonian map into which the model is transformed.

As was indicated in [1,2], the discrete stationary Schrödinger equation

\[ \psi_{n+1} + \psi_{n-1} = (\epsilon_n + E)\psi_n , \]  

with \( \epsilon_n \) standing for the diagonal potential and \( E \) for the energy of an eigenstate, can be written in the form of a two-dimensional Hamiltonian map

\[ x_{n+1} = x_n \cos \mu - (p_n + A_n x_n) \sin \mu \]
\[ p_{n+1} = x_n \sin \mu + (p_n + A_n x_n) \cos \mu . \]  

Here, the variables \((p_n, x_n)\) play the role of the momentum and position of a linear oscillator subjected to linear periodic delta-kicks with the period \( T = 1 \). The amplitude \( A_n \) of the kicks depends on time according to the relation \( A_n = -\epsilon_n / \sin \mu \). For the Anderson model the distribution \( P(\epsilon) \) of the disorder is given by \( P(\epsilon) = 1/W \) for \( |\epsilon| \leq W/2 \), with variance \( \langle \epsilon^2 \rangle = \sigma^2 = W^2/12 \). Between two successive kicks, the rotation in the phase space is given by the eigenstate energy, \( E = 2 \cos \mu \). In such a representation, amplitudes \( \psi_n \) of a specific eigenstate at site \( n \) correspond to positions of the oscillator at times \( t_n = n \) and, therefore, the structure of eigenstates can be studied by investigating the time-dependence of the trajectories in the phase space \((p_n, x_n)\). In particular, localized states correspond to unbounded trajectories and, vice-versa, extended states are represented by bounded trajectories.

It is convenient to pass to action-angle variables \((r_n, \theta_n)\) according to the standard transformation, \( x = r \sin \theta, p = r \cos \theta \). The corresponding map, therefore, has the form

\[ r_{n+1} = r_n D_n \]
\[ \sin \theta_{n+1} = D_n^{-1} (\sin(\theta_n - \mu) - A_n \sin \theta_n \sin \mu) \]
\[ \cos \theta_{n+1} = D_n^{-1} (\cos(\theta_n - \mu) + A_n \sin \theta_n \cos \mu) , \]  

where

\[ D_n = \sqrt{1 + A_n \sin(2\theta_n) + A_n^2 \sin^2 \theta_n} . \]  

The localization length \( l \) is defined by the standard relation

\[ l^{-1} = \lim_{N \to \infty} \left( \frac{1}{N} \sum_{n=0}^{N-1} \ln \left| \frac{x_{n+1}}{x_n} \right| \right) = \left( \ln \left| \frac{x_{n+1}}{x_n} \right| \right) , \]  

where the overbar stays for time average and the brackets for the average over different disorder realizations. The contributions to \( l^{-1} \) can be splitted in two terms.
\[ l^{-1} = \langle \ln \left( \frac{r_{n+1}}{r_n} \right) \rangle + \langle \ln \left| \sin \frac{\theta_{n+1}}{\sin \theta_n} \right| \rangle. \]  

(6)

The second term on the r.h.s. is negligible because it is the average of a bounded quantity. It becomes important only when also the first term is small, i.e. at the band edge \( \mu \approx 0 \). Thus, apart from this limit, the localization length can be evaluated from the map (3) using only the dependence of the radius \( r_n \) on discrete time. The ratio \( r_{n+1}/r_n \) is a function only of the angle \( \theta_n \) and not of the radius \( r_n \), thus the computation of the localization length implies just the average over the invariant measure \( \rho(\theta) \), which is an advantage with respect to transfer matrix methods. Moreover, since \( r_{n+1}/r_n \) is positive, there is no need to work with complex quantities.

In a direct analytical evaluation of (5) one can, therefore, write

\[ l^{-1} = \int P(\epsilon) \int_0^{2\pi} \ln(D(\epsilon, \theta)) \rho(\theta) \, d\theta \, d\epsilon, \]

(7)

where \( P(\epsilon) \) is the density of the (uncorrelated) distribution of \( \epsilon_n \), and \( \rho(\theta) \) stands for the invariant measure of the one-dimensional map for the phase \( \theta \), see (3). We use here the fact that \( \rho(\theta) \) does not depend on the specific sequence \( \epsilon_n \), but can depend on the moments of \( P(\epsilon) \), particularly on its second moment \( \sigma^2 \) (see below). As one can see, the main problem is in the expression for \( \rho(\theta) \), which was not found explicitly even in the limit of a weak disorder, \( A_n \to 0 \) [4,5].

**II. WEAK DISORDER**

By weak disorder we mean that \( A_n \) is small. This can be arranged even at the band-edge, where the denominator \( \sin \mu \) of \( A_n \) is also small; thus the disorder \( \epsilon_n \) must go to zero faster than \( \mu \) (how much faster, it is determined by the properties of the Hamiltonian map). Retaining only terms up to \( O(A_n^2) \) in the map (3) for \( \theta_n \) one gets

\[ \theta_{n+1} = \theta_n - \mu - A_n \sin^2 \theta_n + A_n^2 \sin^3 \theta_n \cos \theta_n \mod 2\pi, \]

(8)

which coincides with formula (62) in Ref. [4].

The expression (6) for \( l^{-1} \) can be written in the weak disorder limit explicitly,

\[ l^{-1} = \frac{1}{2} \sin^2 \mu \int \epsilon^2 P(\epsilon) \, d\epsilon \int_0^{2\pi} \rho(\theta) \left( \frac{1}{4} - \frac{1}{2} \cos(2\theta) + \frac{1}{4} \cos(4\theta) \right) \, d\theta, \]

(9)

which is valid over all the spectrum except at the band edge, where the additional contribution in (3) is present (see below). In fact, standard perturbation theory [3] corresponds to the assumption that \( \rho(\theta) \) is constant. Thus, one easily obtains

\[ l^{-1} = \frac{\sigma^2}{8 \sin^2 \mu} = \frac{W^2}{96 \left( 1 - \frac{E^2}{4} \right)}. \]

(10)

This expression was found to work quite well over all energies, but, surprisingly, numerical experiments [3] showed a 4% deviation at the band center. One had to explain why standard
perturbation theory fails at the band center, while it is correct everywhere else. Non-standard perturbation theory methods were devised in Refs. [4,5], where the correct value for $l^{-1}$ at the band center was obtained and, moreover, a different scaling with disorder was discovered at the band-edge [5]. However, these methods hide behind mathematical difficulties the physical origin of the discrepancy. We are here able, by looking at the properties of map (8), to understand both the physical nature of the discrepancy at the band center and the different scaling at the band edge. Moreover, our derivation is much simpler mathematically and more straightforward (this can be already seen from the very simple derivation of the expression (10)).

A. The band center

In order to derive analytically the correct expression for $l^{-1}$ at the band center $E = 0$, one has to find the exact expression for the invariant probability measure $\rho(\theta)$. This latter arises from map (8) specialized to the value $\mu = \pi/2$. For vanishing disorder the trajectory is a period four, specified by the initial angle $\theta_0$. For a weak disorder any orbit diffuses around the period four, with an additional drift in $\theta$. Asymptotically, any initial condition gives rise to the same invariant distribution, which can now be expected to be different from constant. To find this distribution, we write the fourth iterate of the map (8)

$$\theta_{n+4} = \theta_n - \xi_n^{(1)} \sin^2 \theta_n - \xi_n^{(2)} \cos^2 \theta_n - \frac{\sigma^2}{2} \sin (4\theta_n) ,$$

(11)

where $\xi_n^{(1)} = \epsilon_n + \epsilon_{n+2}$ and $\xi_n^{(2)} = \epsilon_{n+1} + \epsilon_{n+3}$ are uncorrelated random variables with zero mean and variance $2\sigma^2$. Here, we have neglected in Eq. (11) mixed terms of the kind $\epsilon_n \epsilon_m (m \neq n)$ and approximated $\langle (\xi_n^{(1)})^2 \rangle$ and $\langle (\xi_n^{(2)})^2 \rangle$ by their common variance $2\sigma^2$, which is meaningful in a perturbative calculation at first order in $\epsilon_n$.

Thus, the invariant distribution can be determined analytically in the continuum limit where $\theta_{n+4} - \theta_n$ is replaced with $d\theta$ and the random variables $\xi_n^{(1)}, \xi_n^{(2)}$ with the Wiener variables $dW_1, dW_2$ with properties

$$\langle dW_i \rangle = 0$$

$$\langle dW_idW_j \rangle = 2\delta_{ij}\sigma^2 dt \ i,j = 1,2$$

obtaining the Ito equation

$$d\theta = -dW_1 \sin^2 \theta - dW_2 \cos^2 \theta - \frac{\sigma^2}{2} \sin (4\theta) dt .$$

(12)

To this we can associate the Fokker-Planck equation [8]

$$\frac{\partial P}{\partial t}(\theta, t) = \frac{\sigma^2}{2} \frac{\partial}{\partial \theta} (\sin(4\theta)P(\theta, t)) + \frac{\sigma^2}{4} \frac{\partial^2}{\partial \theta^2} [(3 + \cos(4\theta))P(\theta, t)] .$$

(13)

The stationary solution $\rho(\theta)$ of Eq. (13), satisfying the conditions of periodicity $\rho(0) = \rho(2\pi)$ and normalization $\int_0^{2\pi} \rho(\theta) = 1$, is
\[
\rho(\theta) = \left(2K \left(\frac{1}{\sqrt{2}}\right) \sqrt{3 + \cos(4\theta)}\right)^{-1}, \tag{14}
\]

where \(K\) is the complete elliptic integral of the first kind. One should note that the expression for the invariant measure has never been derived before, and it could turn out to be useful for obtaining observables other than \(l^{-1}\). Note that solution (14) does not depend on the strength of the random process.

Inserting formula (14) into (9) at \(\mu = \pi/2\) we get

\[
l^{-1} = \frac{\sigma^2}{8} \left(1 + \int_0^{2\pi} \rho(\theta) \cos(4\theta) \, d\theta\right) = \sigma^2 \left(\frac{\Gamma(3/4)}{\Gamma(1/4)}\right)^2 = \frac{W^2}{105.2\ldots} \tag{15}
\]

This result perfectly agrees with the one obtained in Ref. [5,9], although it is here derived with a different approach, that involves much simpler calculations.

Thouless’ standard perturbation theory result would correspond to neglect the average of the \(\cos(4\theta)\) term in (15), meaning that the stationary solution (14) is approximated with a flat distribution. This approximation works well for all energies \(E = 2 \cos \mu\), with \(\mu = \alpha \pi\) and \(\alpha\) irrational, but doesn’t work for the band-center. Moreover, if one would consider observables which contain higher harmonics than those present in the formula for \(l^{-1}\), one would get corrections to standard perturbation theory also for other rational values of \(\alpha = p/q\). In fact, numerical experiments show that the invariant measure for rationals is modulated with the main period \(T = \pi/q\) (\(p\) and \(q\) being prime to each other). The amplitude of the modulation decreases with \(q\); thus the strongest modification is obtained for \(\alpha = 1/2\), which corresponds to the band-center. It is moreover clear from formula (8), that the only energy value for which a contribution due to the modulations in the measure \(\rho(\theta)\) is present in the inverse localization length \(l^{-1}\) is the band center \(\alpha = 1/2\). This is because in Eq. (9) only second and fourth order harmonics must be averaged, and only for \(\alpha = 1/2\) the fourth harmonic occurs in \(\rho(\theta)\). This is of course true only in the small disorder limit.

B. The band edge

The neighbourhood of the band edge corresponds to \(\mu \approx 0\). If the second order noisy term \(A_n^2\) in the map (8) is replaced by its average, which is the same approximation we did in the previous Section, the map (8) reduces to

\[
\theta_{n+1} = \theta_n - \mu + \frac{\epsilon_n}{\mu} \sin^2 \theta_n + \frac{\delta^2}{\mu^2} \sin^3 \theta_n \cos \theta_n \mod 2\pi, \tag{16}
\]

where \(\delta^2\) is the variance of the noise \(\epsilon_n\). For vanishing disorder and \(\mu \to 0\) the orbits are fixed points. Moving away from the band edge produces a quasi-periodic motion and switching on the disorder gives rise to diffusion. Following the procedure of the previous Section (but here we do not have to go to the four-step map), we obtain the corresponding Fokker-Planck equation

\[
\frac{\partial P}{\partial t}(\theta, t) = \frac{\partial}{\partial \theta} \left(\mu - \frac{\delta^2}{\mu^2} \sin^3 \theta \cos \theta P(\theta, t)\right) + \frac{\delta^2}{2\mu^2} \frac{\partial^2}{\partial \theta^2} \left(\sin^4 \theta P(\theta, t)\right). \tag{17}
\]
There are in this case two small quantities: the noise $\epsilon_n$ and the distance from the band edge $\Delta = 2 - 2 \cos \mu \approx \mu^2$. Below we consider the double limit $\Delta \to 0$, $\delta^2 \to 0$. One can see that, if we keep the ratio $k = \mu^3/\delta^2$ fixed, the time scale of the drift term in (17) is unique and, moreover, it coincides with the diffusion time scale, being $1/\mu$. We can thus rescale time $\tau = t\mu$ and obtain the following stationary Fokker-Planck equation,

$$
\frac{\partial}{\partial \theta} \left( k - \sin^3 \theta \cos \theta \rho(\theta) \right) + \frac{1}{2} \frac{\partial^2}{\partial \theta^2} \left( \sin^4 \theta \rho(\theta) \right) = 0 ,
$$

which depends only on $k$. Its solution, with the same normalization and periodicity conditions as above, is

$$
\rho(\theta) = \frac{f(\theta)}{\sin^2 \theta} \left[ C + \int_0^\theta dx \frac{2J}{f(x) \sin^2 x} \right] ,
$$

where

$$
f(\theta) = \exp \left( 2k \left( \frac{1}{3} \cot^3 \theta + \cot \theta \right) \right) ,
$$

and $C, J$ are integration constants. To make $\rho$ normalizable, constant $C$ must vanish and $J$ is then fixed by the normalization condition,

$$
J^{-1} = \sqrt{\frac{8\pi}{k^{2/3}}} \int_0^\infty dx \frac{1}{\sqrt{x}} \exp \left( -\frac{x^3}{6} - 2k^{2/3}x \right) .
$$

As was mentioned in Section I, in the evaluation of the inverse localization length given by (11) we must now take into account both terms on the r.h.s.; thus, we come to the expression

$$
l^{-1} = \left\langle \ln \left| \frac{D_n \sin \theta_{n+1}}{\sin \theta_n} \right| \right\rangle .
$$

In the limit of a weak disorder and for $\mu \to 0$ one gets

$$
l^{-1} = -\mu \left\langle \cot \theta_n \right\rangle = -2\mu \int_0^\pi \cot \theta \rho(\theta) d\theta .
$$

After some straightforward calculations, with $\mu = (k\delta^2)^{1/3}$, one obtains

$$
l^{-1} = \left( \delta^2 \right)^{1/3} \frac{\int_0^\infty dx \frac{x^{1/2}}{\sqrt{x}} \exp \left( -\frac{x^3}{6} - 2k^{2/3}x \right)}{2 \int_0^\infty dx \frac{x^{-1/2}}{\sqrt{x}} \exp \left( -\frac{x^3}{6} - 2k^{2/3}x \right)} ,
$$

which coincides with expression (36) in Ref. [5]. The limits $k \to 0$ and $k \to \infty$ are then easily rederived and coincide with those in Ref. [3]. For instance, the $k \to 0$ limit gives the scaling law

$$
l^{-1} = \frac{6^{1/3} \sqrt{\pi}}{2\Gamma \left( \frac{1}{6} \right)} (\delta^2)^{1/3} = 0.289 \ldots (\delta^2)^{1/3} .
$$
It is interesting to observe that a similar scaling law was also found for chaotic billiards (stadium and oval ones) looking at the behavior of the Lyapunov exponent in the integrable limit \( [10] \). It is quite natural to associate the Lyapunov exponent with the inverse localization length, and the geometrical parameter that in billiard measure the distance from integrability, with the intensity of the disorder \( \sqrt{\delta^2} \) in the Anderson model.

We have seen in this Section that the study of the dynamics of the noisy circle map \((8)\) allows us to derive both the standard Thouless perturbation theory results for the behavior of the localization length in the weak disorder limit, and the non-standard corrections to such a theory both at the band-center and at the band edge. The advantage of our method is that the derivation of the final formula has a clear physical meaning; moreover, for the band-center case, the procedure is mathematically more straightforward than those previously used \([4,5]\).

### III. STRONG DISORDER

As is known, the analytical expression for the localization length was found only in the limiting cases of a very weak or a very strong disorder. It is interesting that relation \( (7) \) allows us to derive an approximate expression which is also good for a quite large disorder. Indeed, if the energy is not close to the band edge and the disorder is not very large, one can expect a strong rotation of the phase \( \theta \). Therefore, the invariant measure \( \rho(\theta) \) can be approximately taken as constant, \( \rho(\theta) = (2\pi)^{-1} \). For such a disorder, one can explicitly integrate Eq.\((7)\), first over the phase \( \theta \),

\[
\frac{1}{4\pi} \int_0^{2\pi} \ln \left( 1 + A \sin(2\theta) + A^2 \cos^2(\theta) \right) d\theta = \frac{1}{2} \ln \left( 1 + \frac{A^2}{4} \right); \quad A^2 = \epsilon^2 / \sin^2 \mu \quad (26)
\]

and after, over the disorder \( \epsilon \),

\[
l_w^{-1} = \frac{1}{2} \int P(\epsilon) \ln \left( 1 + \frac{\epsilon^2}{4 \sin^2 \mu} \right) d\epsilon = \frac{1}{2} \ln \left( 1 + \frac{W^2}{4 \sin^2 \mu} \right) + \frac{\arctg \left( \frac{W}{2 \sin \mu} \right)}{W} - 1 \quad (27)
\]

Direct numerical simulations show that this expression gives quite a good agreement with the data for the disorder \( W \leq 1 \div 3 \) inside the energy range \( |E| \leq 1.85 \).

For a much stronger disorder, one can use another approach. Note, that for the unstable region

\[
|E - \epsilon_n| > 2 \quad (28)
\]

of the one-step Hamiltonian map \( (3) \) both eigenvalues \( \lambda_n^{(1,2)} \) are real,

\[
\lambda_n^{(1,2)} = \frac{1}{2} \left( (E - \epsilon_n) \pm \sqrt{(E - \epsilon_n)^2 - 4} \right) \quad (29)
\]

with \( \lambda_n^{(1)} \lambda_n^{(2)} = 1 \). Therefore, for stronger disorder \( W \gg 1 \), one can compute the inverse localization length directly via the largest value \( \lambda_+ \) of these two eigenvalues, by neglecting the region \( |E - \epsilon| < 2 \),
\[ l_s^{-1} = \langle \ln |\lambda_+| \rangle = \int \ln \left( \frac{1}{2} \left( x + \sqrt{x^2 - 4} \right) \right) dx = F(z_1) + F(z_2) \]  

(30)

Here, \( x = |E - \epsilon| \) and \( z_1 = W/2 + E, \ z_2 = W/2 - E \); the function \( F \) is defined by

\[ F(z) = \frac{2}{W} \left( z \ln \left( z + \sqrt{z^2 - 4} \right) - \sqrt{z^2 - 4} - z \ln 2 \right) \]  

(31)

Note that from this expression one can easily obtain the known expression for the localization length in the limit of a very strong disorder,

\[ l_s^{-1} = \ln \frac{W}{2} - 1 \]  

(32)

IV. CONCLUDING REMARKS

We have shown in Section II how to derive exact expression for the localization length in the weak disorder limit, using the properties of a noisy circle map (8). In particular, at the center of the energy band, a small correction to the localization length obtained by standard perturbation theory is needed, which is due to the contribution of the forth harmonics in the expression for the invariant measure \( \rho(\theta) \). It is interesting that for other “resonant” values of the energy, the (weak) modulation of \( \rho(\theta) \) has no influence on the localization length. However, for other quantities than the localization length, these corrections may be important. In this sense, the exact expression (14) for the invariant measure \( \rho(\theta) \) obtained in this paper for a weak disorder, may find important applications.

We would like to point out that the calculation in Ref. [4] of the localization length and of the density of states is performed after shifting the energy \( E \rightarrow E + x \) slightly away from the “resonant” values, the size of the shift being proportional to the variance \( x \sim \sigma^2 \) for all energies except the band-edge. It is easy to see that the approach we have used here, also allows us for the derivation of the localization length near the center of the band. Moreover, we can also understand why the shift has to be, as in Ref. [4], of the order of the variance of the disorder. In fact, the recipe is that one should have \( A_n \gg x \), because, if the shift from a value of the energy corresponding to a rational value of \( \alpha \) is too large, the orbit becomes quasi-periodic. In this case the modulation of the invariant measure which results in the non–trivial contribution to the localization length, is lost.

Finally, it is interesting to note that the 1D map (8) can be compared with the Arnold map [11]

\[ \theta_{n+1} = \theta_n - a + b \sin \theta_n \mod 2\pi . \]  

(33)

If we approximate \( A_n^2 \) with its average, it is then tempting to associate the parameter \( a \) to our parameter \( \mu \), and the parameter \( b \) to \( \langle A_n^2 \rangle \). Although the modulation of the circle map (8) is a different function, and the noise is added through the term containing \( A_n \), our results show that the structure of the Arnold tongues persists (Arnold tongues are regions of the parameter space \( \{a, b\} \) where the dynamics is locked on a periodic orbit of period \( q \), the tongues become narrower and narrower as \( b \) is reduced). Indeed, inside the tongue of the Arnold map any orbit corresponds to a rational rotation number \( p/q \); outside the
tongues the motion is quasi-periodic. Trajectories inside the tongues of our model do display periodic motion with an additional diffusion, the periodic motion being responsible for the modulation of the invariant measure $\rho(\theta)$. Outside the tongue, the motion is quasi-periodic also in our model and the invariant measure is flat.

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