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Classical representation of the one-dimensional Anderson model

F M Izrailev†‡, S Ruffo§¶ and L Tessieri‖¶

† Instituto de Física, Universidad Autónoma de Puebla, Apdo. Postal J-48, Col. San Manuel, Puebla, Pue. 72570, Mexico
‡ Budker Institute of Nuclear Physics, Novosibirsk 630090, Russia
§ Dipartimento di Energetica 'Sergio Stecco', Università degli Studi di Firenze, Via di Santa Marta, 3 50139 Firenze, Italy
‖ Dipartimento di Fisica, Università degli Studi di Firenze, Largo E. Fermi, 2 50125, Firenze, Italy

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Abstract. A new approach is applied to the one-dimensional Anderson model by using 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 centre and at the edge of the energy band, where standard perturbation theory fails. Approximate analytical expressions for strong disorder are also obtained.

1. Introduction

Recently, in [1], treating one-dimensional (1D) tight-binding models with diagonal disorder in terms of classical Hamiltonian maps was suggested. 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 more transparent way, by making reference to the properties of the dynamics of the noisy Hamiltonian map into which the model is transformed.

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

$$\psi_{n+1} + \psi_{n-1} = (\epsilon_n + E)\psi_n \tag{1}$$

with ϵ_n standing for the diagonal potential and E for the energy of an eigenstate, can be written in the form of a two-dimensional (2D) Hamiltonian map

$$\begin{aligned} x_{n+1} &= x_n \cos\mu - (p_n + A_n x_n)\sin\mu \\ p_{n+1} &= x_n \sin\mu + (p_n + A_n x_n)\cos\mu. \end{aligned} \tag{2}$$

Here, the variables (p_n, x_n) play the role of the momentum and the 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 $|\epsilon| \leqslant W/2$, with variance $\langle\epsilon^2\rangle = \sigma^2 = W^2/12$. Between two successive kicks, the rotation in the

¶ Also at: INFN, Firenze, Italy.

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phase space is given by the eigenstate energy, $E = 2\cos\mu$. In such a representation, amplitudes ψ_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, θ_n) according to the standard transformation, $x = r\sin\theta$, $p = r\cos\theta$. The corresponding map, therefore, has the form

$$\begin{aligned} r_{n+1} &= r_n D_n \\ \sin\theta_{n+1} &= D_n^{-1}(\sin(\theta_n - \mu) - A_n \sin\theta_n \sin\mu) \\ \cos\theta_{n+1} &= D_n^{-1}(\cos(\theta_n - \mu) + A_n \sin\theta_n \cos\mu) \end{aligned} \tag{3}$$

where

$$D_n = \sqrt{1 + A_n \sin(2\theta_n) + A_n^2 \sin^2\theta_n}. \tag{4}$$

The localization length l is defined by the standard relation

$$l^{-1} = \lim_{N\to\infty} \left\langle \frac{1}{N} \sum_{n=0}^{N-1} \ln\left|\frac{x_{n+1}}{x_n}\right| \right\rangle = \overline{\left\langle \ln\left|\frac{x_{n+1}}{x_n}\right| \right\rangle} \tag{5}$$

where the overbar represents time average and the brackets represent the average over different disorder realizations. The contributions to l^{-1} can be split into two terms

$$l^{-1} = \overline{\left\langle \ln\left(\frac{r_{n+1}}{r_n}\right) \right\rangle} + \overline{\left\langle \ln\left|\frac{\sin\theta_{n+1}}{\sin\theta_n}\right| \right\rangle}. \tag{6}$$

The second term on the r.h.s. is negligible because it is the average of a bounded quantity. It only becomes important when the first term is also 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 θ_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

$$l^{-1} = \int P(\epsilon) \int_0^{2\pi} \ln(D(\epsilon, \theta))\rho(\theta)\,\mathrm{d}\theta\,\mathrm{d}\epsilon \tag{7}$$

where $P(\epsilon)$ is the density of the (uncorrelated) distribution of ϵ_n, and $\rho(\theta)$ represents the invariant measure of the 1D map for the phase θ, see (3). We use the fact that $\rho(\theta)$ does not depend on the specific sequence ϵ_n, but can depend on the moments of $P(\epsilon)$, particularly on its second moment σ^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].

2. 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 ϵ_n must go to zero faster than μ (how much faster is determined by the properties of the Hamiltonian map). Retaining only terms up to $O(A_n^2)$ in the map (3) for θ_n one finds

$$\theta_{n+1} = \theta_n - \mu - A_n \sin^2\theta_n + A_n^2 \sin^3\theta_n \cos\theta_n \qquad \bmod 2\pi \tag{8}$$

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

The expression (7) for l^{-1} can be written in the weak disorder limit explicitly,

$$l^{-1} = \frac{1}{2\sin^2\mu} \int \epsilon^2 P(\epsilon)\,\mathrm{d}\epsilon \int_0^{2\pi} \rho(\theta)\left(\tfrac{1}{4} - \tfrac{1}{2}\cos(2\theta) + \tfrac{1}{4}\cos(4\theta)\right)\mathrm{d}\theta \tag{9}$$

which is valid over all the spectrum except at the band edge, where the additional contribution in (6) is present (see below). In fact, standard perturbation theory [6] corresponds to the assumption that $\rho(\theta)$ is constant. Thus, one easily obtains

$$l^{-1} = \frac{\sigma^2}{8\sin^2\mu} = \frac{W^2}{96\left(1 - \frac{E^2}{4}\right)}. \tag{10}$$

This expression was found to work quite well over all energies, but, surprisingly, numerical experiments [7] showed a small but clear deviation at the band centre. One had to explain why standard perturbation theory fails at the band centre, while it is correct everywhere else. Non-standard perturbation theory methods were devised in [4, 5], where the correct value for l^{-1} at the band centre was obtained and, moreover, a different scaling with disorder was discovered at the band edge [5]. However, these methods hide the physical origin of the discrepancy behind mathematical difficulties. Here we are able, by looking at the properties of map (8), to understand both the physical nature of the discrepancy at the band centre and the different scaling at the band edge. Moreover, our derivation is much simpler mathematically and more straightforward (this can already be seen from the very simple derivation of expression (10)).

2.1. The band centre

In order to derive analytically the correct expression for l^{-1} at the band centre $E = 0$, one has to find the exact expression for the invariant probability measure $\rho(\theta)$. The latter arises from map (8) specialized to the value $\mu = \pi/2$. For vanishing disorder the trajectory is a period 4, specified by the initial angle θ_0. For a weak disorder any orbit diffuses around the period 4, with an additional drift in θ. 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)

$$\theta_{n+4} = \theta_n + \xi_n^{(1)} \sin^2\theta_n + \xi_n^{(2)} \cos^2\theta_n - \frac{\sigma^2}{2}\sin(4\theta_n) \tag{11}$$

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 equation (11) mixed terms of the kind $\epsilon_n\epsilon_m$ ($m \neq n$) and approximated $(\xi_n^{(1)})^2$ and $(\xi_n^{(2)})^2$ by their common variance $2\sigma^2$, which is meaningful in a perturbative calculation at first order in ϵ_n.

Thus, the invariant distribution can be determined analytically in the continuum limit where $\theta_{n+4} - \theta_n$ is replaced with $\mathrm{d}\theta$ and the random variables $\xi_n^{(1)}, \xi_n^{(2)}$ with the Wiener variables $\mathrm{d}W_1, \mathrm{d}W_2$ with properties

$$\langle \mathrm{d}W_i \rangle = 0$$
$$\langle \mathrm{d}W_i\,\mathrm{d}W_j \rangle = 2\delta_{ij}\sigma^2\,\mathrm{d}t \qquad i, j = 1, 2$$

obtaining the Ito equation

$$d\theta = dW_1 \sin^2\theta + dW_2 \cos^2\theta - \frac{\sigma^2}{2}\sin(4\theta)\,dt. \tag{12}$$

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

$$\frac{\partial P}{\partial t}(\theta, t) = \frac{\sigma^2}{2}\frac{\partial}{\partial\theta}(\sin(4\theta)P(\theta, t)) + \frac{\sigma^2}{4}\frac{\partial^2}{\partial\theta^2}[(3+\cos(4\theta))P(\theta, t)]. \tag{13}$$

The stationary solution $\rho(\theta)$ of equation (13), satisfying the conditions of periodicity $\rho(0) = \rho(2\pi)$ and normalization $\int_0^{2\pi}\rho(\theta)\,d\theta = 1$, is

$$\rho(\theta) = \left(2\boldsymbol{K}\left(\frac{1}{\sqrt{2}}\right)\sqrt{3+\cos(4\theta)}\right)^{-1} \tag{14}$$

where $\boldsymbol{K}$ 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.

By inserting formula (14) into (9) at $\mu = \pi/2$ we find

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

This result agrees perfectly with the one obtained in [5, 9], although it is derived here using 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 α irrational, but does not work for the band centre. Moreover, if one would consider observables which contain higher harmonics than those present in the formula for l^{-1} (9), one would obtain 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 $\alpha = \frac{1}{2}$, which corresponds to the band centre. It is clear from formula (8), that the only energy value for which a contribution owing to the modulations in the measure $\rho(\theta)$ is present in the inverse localization length l^{-1}, is the band centre $\alpha = \frac{1}{2}$. This is because in equation (9) only second- and fourth-order harmonics must be averaged, and only for $\alpha = \frac{1}{2}$ the fourth harmonic occurs in $\rho(\theta)$. This is of course only true in the small disorder limit.

2.2. 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 as we made in the previous section, the map (8) reduces to

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

where δ^2 is the variance of the noise ϵ_n. For vanishing disorder and $\mu \to 0$ the orbits are fixed points. Moving away from the band edge produces a quasiperiodic 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

$$\frac{\partial P}{\partial t}(\theta, t) = \frac{\partial}{\partial\theta}\left[\left(\mu - \frac{\delta^2}{\mu^2}\sin^3\theta\cos\theta\right)P(\theta, t)\right] + \frac{\delta^2}{2\mu^2}\frac{\partial^2}{\partial\theta^2}(\sin^4\theta P(\theta, t)). \tag{17}$$

There are in this case two small quantities: the noise ϵ_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 timescale of the drift term in (17) is unique and, moreover, it coincides with the diffusion timescale, being $1/\mu$. We can thus rescale time $\tau = t\mu$ and obtain the following stationary Fokker–Planck equation,

$$\frac{\partial}{\partial\theta}[(k - \sin^3\theta\cos\theta)\rho(\theta)] + \frac{1}{2}\frac{\partial^2}{\partial\theta^2}(\sin^4\theta\,\rho(\theta)) = 0 \tag{18}$$

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

$$\rho(\theta) = \frac{f(\theta)}{\sin^2\theta}\left[C + \int_0^\theta \mathrm{d}x\,\frac{2J}{f(x)\sin^2 x}\right] \tag{19}$$

where

$$f(\theta) = \exp(2k(\tfrac{1}{3}\cot^3\theta + \cot\theta)) \tag{20}$$

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

$$J^{-1} = \frac{\sqrt{8\pi}}{k^{2/3}}\int_0^\infty \mathrm{d}x\,\frac{1}{\sqrt{x}}\exp\left(-\frac{x^3}{6} - 2k^{2/3}x\right). \tag{21}$$

As mentioned in section 1, in the evaluation of the inverse localization length given by (6) we must now take into account both terms on the r.h.s., thus we arrive at the expression

$$l^{-1} = \overline{\left\langle \ln\left|D_n\frac{\sin\theta_{n+1}}{\sin\theta_n}\right|\right\rangle}. \tag{22}$$

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

$$l^{-1} = -\mu\overline{\langle\cot\theta_n\rangle} = -2\mu\int_0^\pi \cot\theta\rho(\theta)\,\mathrm{d}\theta. \tag{23}$$

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

$$l^{-1} = \frac{(\delta^2)^{1/3}}{2}\frac{\int_0^\infty \mathrm{d}x\,x^{1/2}\exp\left(-\frac{x^3}{6} - 2k^{2/3}x\right)}{\int_0^\infty \mathrm{d}x\,x^{-1/2}\exp\left(-\frac{x^3}{6} - 2k^{2/3}x\right)} \tag{24}$$

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

$$l^{-1} = \frac{6^{1/3}\sqrt{\pi}}{2\Gamma(\frac{1}{6})}(\delta^2)^{1/3} = 0.289\ldots(\delta^2)^{1/3}. \tag{25}$$

It is interesting to observe that a similar scaling law was also found for chaotic billiards (stadia and oval ones) when looking at the behaviour 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 which in billiards measures the distance from integrability, with the intensity of the disorder $\sqrt{\delta^2}$ in the Anderson model.

In this section we have seen 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 behaviour of the localization length in the weak disorder limit, and the non-standard corrections to such a theory both at the band centre 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 centre case, the procedure is mathematically more straightforward than those previously used [4, 5].

3. 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 quite a 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 θ. 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 equation (7), initially over the phase θ,

$$\frac{1}{4\pi}\int_0^{2\pi} \ln(1 + A\sin(2\theta) + A^2\sin^2\theta)\,\mathrm{d}\theta = \frac{1}{2}\ln\left(1+\frac{A^2}{4}\right) \qquad A^2 = \epsilon^2/\sin^2\mu \tag{26}$$

and after, over the disorder ϵ,

$$l_w^{-1} = \frac{1}{2}\int P(\epsilon)\ln\left(1+\frac{\epsilon^2}{4\sin^2\mu}\right)\mathrm{d}\epsilon = \frac{1}{2}\ln\left(1+\frac{W^2}{16\sin^2\mu}\right) + \frac{\arctan\left(\frac{W}{4\sin\mu}\right)}{\frac{W}{4\sin\mu}} - 1. \tag{27}$$

Direct numerical simulations show that this expression gives quite a good agreement with the data for the disorder $W \leqslant 1$–3 inside the energy range $|E| \leqslant 1.85$. Therefore, the above expression can serve as a generalization of the weak disorder formula (10), since it is also valid for the relatively strong disorder $W \approx 1$. However, for very strong disorder $W \gg 1$, equation (27) gives incorrect results. The reason behind this is that in this case the invariant measure $\rho(\theta)$ is strongly non-uniform, hence expression (26) is no longer valid.

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

$$|E - \epsilon_n| > 2 \tag{28}$$

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

$$\lambda_n^{(1,2)} = \tfrac{1}{2}\left((E-\epsilon_n) \pm \sqrt{(E-\epsilon_n)^2 - 4}\right) \tag{29}$$

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 λ_+ of these two eigenvalues, by neglecting the region $|E-\epsilon| < 2$,

$$l_s^{-1} = \langle \ln|\lambda_+|\rangle = \int \ln\left(\tfrac{1}{2}\left(x+\sqrt{x^2-4}\right)\right)\mathrm{d}x = F(z_1) + F(z_2). \tag{30}$$

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

$$F(z) = \frac{2}{W}\left(z\ln\left(z+\sqrt{z^2-4}\right) - \sqrt{z^2-4} - z\ln 2\right). \tag{31}$$

This expression fits the data more accurately than the known expression for the localization length in the limit of a very strong disorder,

$$l_s^{-1} = \ln \frac{W}{2} - 1. \tag{32}$$

4. Concluding remarks

In section 2 we showed how to derive an exact expression for the localization length in the weak disorder limit, using the properties of a noisy circle map (8). In particular, at the centre of the energy band, a small correction to the localization length obtained by standard perturbation theory is needed, owing to the contribution of the fourth 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 quantities other 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 [5] of the localization length and of the density of states is performed after shifting the energy $E \to E + x$ 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 for the derivation of the localization length near the centre of the band. Moreover, we can also understand why the shift has to be, as in [5], of the order of the variance of the disorder. In fact, the method 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 α is too large, the orbit becomes quasiperiodic. In this case the modulation of the invariant measure which results in the non-trivial contribution to the localization length, is lost.

The method used here works perfectly for models with uncorrelated and finite variance disorder. However, the Hamiltonian map approach has been originally applied to the dimer model [2], for which there are strong short-range correlations in the potential. There are many other models with correlated disorder which are treated by different methods, one of which is based on the transfer matrix techniques, which also uses 2D maps or the so-called 'generalized Poincare map' [11]. Other well known models, which are treated by different mapping and transfer matrix techniques, are the Fibonacci Schrödinger operators (see, for example, the seminal papers [12]). One can indeed expect that the approach based on equations (3) and (4) can also serve as a starting point for the study of models with correlated potentials, such as almost periodic potentials, the Fibonacci potential, etc. Recent results which relate correlations in the potential with the occurence of delocalized states [13] show the effectiveness of the Hamiltonian map approach.

Finally, it is interesting to note that the 1D map (8) can be compared with the Arnold map [14]

$$\theta_{n+1} = \theta_n - a + b \sin\theta_n \qquad \mod 2\pi. \tag{33}$$

If we approximate A_n^2 with its average, it is then tempting to associate the parameter a to our parameter μ, 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 increasingly narrow 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 quasiperiodic. Trajectories inside the tongues of our model 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 in our model is also quasiperiodic and the invariant measure is flat.

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