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The Anderson localization problem, the Fermi–Pasta–Ulam paradox and the generalized diffusion approach

V N Kuzovkov

Institute of Solid State Physics, University of Latvia, 8 Kengaraga, LV—1063 Riga, Latvia

E-mail: kuzovkov@latnet.lv

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Abstract
The goal of this paper is twofold. First, based on the interpretation of a quantum tight-binding model in terms of a classical Hamiltonian map, we consider the Anderson localization (AL) problem as the Fermi–Pasta–Ulam (FPU) effect in a modified dynamical system containing both stable and unstable (inverted) modes. Delocalized states in the AL are analogous to the stable quasi-periodic motion in FPU, whereas localized states are analogous to thermalization, respectively. The second aim is to use the classical Hamilton map for a simplified derivation of *exact* equations for the localization operator $H(z)$. The latter was presented earlier (Kuzovkov *et al* 2002 *J. Phys.: Condens. Matter* **14** 13777) treating the AL as a generalized diffusion in a dynamical system. We demonstrate that counter-intuitive results of our studies of the AL are similar to the FPU counter-intuitivity.

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1. Introduction

Half a century ago, two celebrated papers were published temporally close to each other, which gave birth to two fundamental directions of theoretical physics. In 1955, the Fermi–Pasta–Ulam (FPU) paradox was formulated [1, 2], which suggested the nonequipartition of energy among normal modes of an anharmonic atomic chain. This phenomenon is closely connected with the problems of ergocidity, integrability, chaos and stability of motion [2, 3]. A few years later, in 1958, Anderson [4] suggested the possibility of electron localization (Anderson localization (AL)) in a random system, provided that the disorder is sufficiently large. This idea is one of the foundations for understanding the electronic properties of disordered systems [5]. From a more general point of view, this idea implies the absence of wave diffusion in a random medium as a universal feature of stochastic processes. Unlike the AL problem, where the stochasticity was explicitly introduced into consideration through random potentials, the FPU considers the stochasticity as a nontrivial effect in the dynamics of nonlinear systems, since strong chaotic behavior can be observed even in a system with several degrees of freedom.

Despite the fact that the FPU paradox can be reformulated analogously to the AL problem in terms of waves (interaction of normal modes that are characterized by their wave number k), their conceptual similarity has not been seen so far. In fact, *localization*, even when mentioned in the FPU literature, is not associated with disorder; usually this means that the energy initially placed in a low-frequency normal mode k_0 of the linear problem stays almost completely locked within a few modes neighboring the k_0 mode. The localization in k-space of normal modes [6] or analogous energy localization in the FPU chain [7] is typically considered here. Sometimes the AL and FPU are mentioned together, but as *independent* and even competing processes. In particular, energy transport in binary isotropically disorded nonlinear FPU chains was considered [8] with the competition between localization (a *disorder* effect) and mode transitions (a *nonlinearity* effect). Note also that a close connection between the nonlinear dynamics and the AL was established for nonlinear systems with a much smaller number of degrees of freedom than in the FPU problem. Thus, it was shown that the quantum kicked rotor model [9, 10] can be mapped onto the AL model. On the other hand, the quantum kicked rotor serves as the starting point of a systematic analysis of the quantum dynamics for classically chaotic dynamical systems. In [11], the connection

between the AL and the Kolmogorov–Arnold–Moser theory is discussed.

Our purpose is to establish a *close connection* between the two fundamental problems. That is, the AL is nothing but the FPU effect in a modified dynamical system with interacting normal modes. Besides, the delocalized states in the AL problem are analogous to the stable quasi-periodic motion (recurrence in the FPU problem) and, respectively, the localized states are similar to the *thermalization* (motion instability) in the FPU. Our FPU modification includes: (i) nontrivial change of the mode ensemble. In the FPU without interactions all normal modes are stable. In contrast, in the AL both stable and unstable (*inverted*) modes also exist. (ii) A modified mode interaction: the stochasticity in the AL is introduced directly, through random forces *linear* in coordinates, and rather indirectly, through nonlinear terms in the dynamical equations.

A critical comparison of the AL problem and the FPU paradox is all the more useful since the former turned out to be also a paradox. Indeed, in recent years, the conflicting situation was established that (a) experimental results contradict the generally accepted theory [5, 12], whereas (b) the analytical theory contradicts numerical simulations [13, 14]. Despite such a clear conflict, the results of our *exact* analytical theory [15–17] (see also [18] (anisotropic systems) and [19] (the system in an external magnetic field) for more details) are considered as highly unexpected in the Anderson community [20–23] since they contradict the generally accepted results of the scaling theory [24] and numerical modeling [13]. In particular, doubts are expressed about our conclusion on the existence of the metal–insulator transition in the two-dimensional (2D) disordered system of noninteracting electrons (which does not contradict real experimental data [5, 12]) and that the Anderson transition is of the first order (localized and conducting state coexist). The latter statement is a clear example of a counter-intuitive prediction. The appearance of highly unexpected results is typical for such counter-intuitive (paradox) problems such as the AL and FPU.

In this paper, we employ the main results of our analytical method [15–17] and treat the AL as generalized diffusion in a dynamical system. The random forces impose random walk amplitudes (the dynamics is bounded in the phase space for unperturbed system), which can lead to the diffusion divergence. The diffusion problem with random forces linear in the coordinates can be exactly solved. Moreover, the diffusion concept permits one to connect the AL and FPU problems. As is well known [10], the equations for nonlinear dynamical systems can under certain conditions describe pseudo-random walks, which leads to the diffusion behavior and diffusion increase in mean energy (i.e. divergence).

We shall also employ the interpretation of the Schrödinger equation (quantum tight-binding model) in terms of the classical Hamiltonian map [25–27]. As a result, the problem can be reformulated in terms of interacting mode dynamics, which opens the opportunity for the detailed comparison of AL with FPU. It should be stressed that the ideas [25–27] allow one to considerably simplify the mathematical formalism used earlier [15–17]. This is important in light of recent criticism [20, 22] that the *engineering language* (signal theory) of the mentioned formalism (input and output signals, filter function, etc) is new for the AL community. In this paper, we suggest a compact derivation of the main feature of the disordered system—the localization operator $H(z)$ [17].

The structure of this paper is as follows. In section 2.1 we explain how the 1D tight-binding model with diagonal disorder can be presented in terms of the classical 2D Hamiltonian map for normal or inverted oscillators. In section 2.2, we present the equations for arbitrary dimensions. We show that delocalized states, in general, correspond to the statistically bounded trajectories, whereas localized states correspond to unbounded trajectories, respectively. The trajectory type depends on the excited mode (normal or inverted). We show in section 2.3 that statistically unbounded trajectories can be treated in terms of a *generalized diffusion*, with exactly predictable properties. As a result, we arrive in section 2.4 at the definition of the localization operator $H(z)$. In section 3, a possible comparison of the AL and FPU problems is discussed. It is shown that the AL treatment in terms of the classical Hamiltonian map results in a paradox, demonstrating the counter-intuitive nature of this problem. The results [15–17] are compared with those for the FPU and their detailed similarities are analyzed.

2. Anderson localization and the classical Hamiltonian map

2.1. The Cauchy problem and the classical Hamiltonian map for the 1D case

As is well known, in order to determine the Lyapunov exponent γ (which is the inverse of the localization length, $\xi = 1/\gamma$) and the phase diagram (the areas of the localized and delocalized states), the Cauchy problem with fixed initial conditions has to be solved [13, 15, 22, 28]. For illustration, the 1D Schrödinger equation with random potentials ε_n can be presented as a recursive relation

$$\psi_{n+1} = E\psi_n - \psi_{n-1} - \varepsilon_n\psi_n. \tag{1}$$

The treatment of one of the spatial coordinates as a temporal variable (discrete time n) is a standard approach in chaos theory [29] which opens the way to the dynamical interpretation. Taking into account the so-called *causality principle* [15, 17], the latter equation permits an exact stochastic analysis. The idea of the causality principle could be illustrated for the 1D Anderson model (this is also true for *higher dimensions*). Indeed, it is easy to see that in the Cauchy problem (with fixed initial conditions for ψ_1 and ψ_0), equation (1), ψ_2 is a function of ε_1, ψ_3 is a function of ε_2, ε_1, etc (a *causality*). That is, both amplitudes ψ_n and ψ_{n-1} on the rhs of equation (1) are statistically independent of ε_n and can be averaged separately (causality principle):

$$\langle\psi_{n+1}\rangle = (E - \langle\varepsilon_n\rangle)\langle\psi_n\rangle - \langle\psi_{n-1}\rangle, \tag{2}$$

$$\langle\psi_{n+1}^2\rangle = (E^2 - 2E\langle\varepsilon_n\rangle + \langle\varepsilon_n^2\rangle)\langle\psi_n^2\rangle - 2(E - \langle\varepsilon_n\rangle)\langle\psi_n\psi_{n-1}\rangle + \langle\psi_{n-1}^2\rangle. \tag{3}$$

The causality principle can be used only (a) for the recursive relation for the Cauchy problem and (b) when on-site

potentials are independently distributed ($\langle \varepsilon_n \varepsilon_{n'} \rangle = \sigma^2 \delta_{n,n'}$) but not for the Dirichlet problem, correlated potentials, etc.

To study the origin of localized/delocalized states, we use a simple approach [25–27] based on the interpretation of a quantum tight-binding model, equation (1), with diagonal disorder in terms of the classical 2D Hamiltonian map. The difference equation (1) is reduced to a discrete transform with a simple physical interpretation. Let us write the second-order equation as a set of two first-order equations. Assume that $q_n = \psi_n$ and $p_n = \psi_{n+1} - \psi_n$ for $E \geqslant 0$; whereas $q_n = -\psi_n$ and $p_n = -(\psi_{n+1} - \psi_n)$ as $E < 0$. The obtained equation set reads

$$p_{n+1} = p_n - \omega^2 q_n - \varepsilon_n q_n, \tag{4}$$

$$q_{n+1} = q_n + p_{n+1}, \tag{5}$$

where $\omega^2 = 2 - |E|$.

As is shown [29], the discrete transform (4) and (5) can be connected with the equivalent differential equation of the Hamilton dynamics with the Hamiltonian (kicked oscillator)

$$\mathcal{H} = \frac{p^2}{2} + \frac{\omega^2 q^2}{2} + \frac{\varepsilon(t) q^2}{2} \sum_n \delta(t - n\Delta t). \tag{6}$$

It defines the system with the unperturbed Hamiltonian for an oscillator affected by a periodic sequence of kicks (δ-pulses) with the period Δt. Discrete transform arises when magnitudes of the coordinate and impulse are considered with a discrete time increment Δt and correspondingly with a discrete time index n (discrete time).

Depending on the sign of ω^2, there exist two cases. For $|E| < 2$, corresponding to the solutions inside the band in the unperturbed system, we obtain a normal (stable) oscillator with $\omega^2 > 0$. In contrast, the energies outside the band, $|E| \geqslant 2$, are associated with inverted (unstable) oscillators with $\omega^2 \leqslant 0$. Without disorder $\varepsilon_n \equiv 0$ and delocalized quantum states correspond to a normal oscillator and trajectories bounded in the classical (p, q) space as $n \to \infty$ [26]. Simple characteristics of the dynamical system q_n^2 or p_n^2 are bounded, respectively. In contrast, an inverted oscillator describes non-physical solutions outside the band, which are now unbounded in the classical phase space; the q_n^2 magnitude is divergent as $n \to \infty$.

When disorder is introduced, the situation changes qualitatively. Random kicks for a normal oscillator lead to random amplitude walks. The oscillatory motion remains since the average $\langle q_n \rangle$ remains bounded as $n \to \infty$. For a random amplitude walk, long trajectories in the classical phase space (p, q) are possible, which can be treated as diffusion [17]. This is characterized by a typical parameter divergence: $\langle q_n^2 \rangle \to \infty$ as $n \to \infty$. Since these trajectories correspond in 1D to the localized states, these can be considered as statistically unbounded. In the case of the inverted oscillator the amplitude increases exponentially (in the model with Hamiltonian equation (6)) between successive kicks, but the force linear in coordinates is able to change a coordinate sign. Note that this divergence is observed not only at true random potentials (as in our case) but also under weaker conditions, e.g. [11] (quasi-periodic potentials having two basic frequencies).

Use of the diffusion terminology is quite justified here. Indeed, to detect the diffusion, it is sufficient to demonstrate the divergence of the second moment of the amplitude q_n and to establish its time dependence, the function $f(n)$ in $\langle q_n^2 \rangle = f(n)$. The divergence of the second moment defines the conditions of the diffusion appearance. For a *normal diffusion* the mean square displacement is linear in time, $\langle q_n^2 \rangle \propto n$. This come from the fact that the random perturbation ε_n is *additive* in the equation of the Brownian motion (random walk problem) [17]. The notion of an *anomalous diffusion* [30, 31] derives from the fact that the mean square displacement may be anomalously diffusive, $\langle q_n^2 \rangle \propto n^\alpha$ ($\alpha \neq 1$), i.e. nonlinear in time (power-law divergence). The quantity $\langle q_n^2 \rangle = \langle \psi_n^2 \rangle$ in equation (1) was calculated analytically [15, 28]: $\langle q_n^2 \rangle \propto \exp(2\gamma n)$ with $\gamma \geqslant 0$ for an arbitrary E value, provided $\sigma > 0$. This is so because equation (4) contains the product of ε_n and q_n (multiplicative noise), which determines the exponential character of the divergence. In this case, *generalized diffusion* takes place. The appearance of the localization in the approach based on equation (1) is equivalent to the appearance of diffusion. Respectively, the well-known statement that in one dimension all states are localized at any level of disorder is equivalent to the statement on the diffusion character of all solutions of equation (1) in 1D for $\sigma \neq 0$.

2.2. Classical Hamiltonian map for the D-dimensional case

The above-discussed statement of the problem can be naturally generalized for an arbitrary dimension D; this idea was mentioned but not realized in [27]. The phase diagram of the system with a metal–insulator transition should be obtained in the thermodynamical limit (the infinite system). Let us consider the semi-infinite system, or an infinite system with a boundary, where the index $n \equiv m_D \geqslant 0$, but all $m_j \in (-\infty, \infty)$, $j = 1, 2, \ldots, p$, with $p = D - 1$. We combine indices in the form of a vector $\mathbf{m} = \{m_1, m_2, \ldots, m_p\}$. The boundary that is the layer $n = 0$ defines the preferred direction (the axis n).

The Schrödinger equation can be rewritten as a recursion equation (in terms of the discrete time n)

$$\psi_{n+1,\mathbf{m}} = (E - \varepsilon_{n,\mathbf{m}})\psi_{n,\mathbf{m}} - \psi_{n-1,\mathbf{m}} - \sum_{\mathbf{m}'} \psi_{n,\mathbf{m}'}. \tag{7}$$

Summation over $\mathbf{m}'$ runs over the nearest neighbors of the site $\mathbf{m}$. The on-site potentials $\varepsilon_{n,m}$ are independently and identically distributed. We assume hereafter the existence of the two first moments, $\langle \varepsilon_{n,\mathbf{m}} \rangle = 0$ and $\langle \varepsilon_{n,\mathbf{m}}^2 \rangle = \sigma^2$, where the parameter σ characterizes the disorder level.

Let us perform the Fourier transform:

$$\varepsilon_n(\mathbf{k}) = \sum_{\mathbf{m}} \varepsilon_{n,\mathbf{m}} e^{i\mathbf{km}}, \tag{8}$$

$$\psi_n(\mathbf{k}) = \sum_{\mathbf{m}} \psi_{n,\mathbf{m}} e^{i\mathbf{km}}. \tag{9}$$

The relation for similar random quantities, $\langle \varepsilon_{n,\mathbf{m}} \rangle = 0$, $\langle \varepsilon_{n,\mathbf{m}} \varepsilon_{n',\mathbf{m}'} \rangle = \sigma^2 \delta_{n,n'} \delta_{\mathbf{m},\mathbf{m}'}$, leads to

$$\langle \varepsilon_n(\mathbf{k}) \rangle = 0, \tag{10}$$

$$\langle \varepsilon_n(\mathbf{k}) \varepsilon_{n'}^*(\mathbf{k}') \rangle = (2\pi)^p \sigma^2 \delta_{n,n'} \delta(\mathbf{k} - \mathbf{k}'). \tag{11}$$

As a result of the Fourier transform, the Schrödinger equation (7) transforms into the equation set for the mode dynamics, enumerated by the index **k**,

$$\psi_{n+1}(\mathbf{k}) = \mathcal{L}(\mathbf{k})\psi_n(\mathbf{k}) - \psi_{n-1}(\mathbf{k}) - \int \frac{\mathrm{d}^p\mathbf{k}_1}{(2\pi)^p}\varepsilon_n(\mathbf{k}-\mathbf{k}_1)\psi_n(\mathbf{k}_1). \quad (12)$$

Here

$$\mathcal{L}(\mathbf{k}) = E - 2\sum_{j=1}^{p=D-1}\cos(k_j), \quad (13)$$

with fixed initial conditions $\psi_0(\mathbf{k})$ and $\psi_1(\mathbf{k})$.

A comparison of equation (12) with its 1D analogue, equation (1), demonstrates that the dynamics of the multi-dimensional system can be reduced to the dynamics of the multi-oscillatory system. The frequencies of these oscillators are defined by the relation $\omega(\mathbf{k})^2 = 2 - |\mathcal{L}(\mathbf{k})|$. That is, one can distinguish, as before, normal oscillators with $|\mathcal{L}(\mathbf{k})| < 2$ and inverted oscillators with $|\mathcal{L}(\mathbf{k})| \geqslant 2$. As we have shown [17], the condition $|\mathcal{L}(\mathbf{k})| < 2$ without perturbation corresponds to delocalized states inside the band; and in contrast, $|\mathcal{L}(\mathbf{k})| \geqslant 2$ corresponds to the solution outside the band. In other words, the connection between the classical oscillator type (normal or inverted) and the quantum-mechanical solution also remains for arbitrary dimensions. However, there is also an important difference between the 1D and *N*D systems: in the former case, the energy magnitude uniquely determines the oscillator type. The terms with a random force describe only the oscillator's stochastic self-interaction, due to its linear dependence, $-\varepsilon_n q_n$ in equation (4), the oscillator cannot be stopped, i.e. $q = p = 0$ is not fulfilled.

In contrast, in the multi-dimensional case the energy E no longer uniquely determines the system's state, the fixed initial conditions $\psi_0(\mathbf{k})$ and $\psi_1(\mathbf{k})$ define simultaneously the type and number of initially excited oscillators, among which can be found both normal and inverted oscillators. The integral in equation (12) corresponding to a random force describes now the stochastic interaction between oscillators. That is, knowledge of the 1D system is *not* sufficient for the description of multi-dimensional systems; as we demonstrate below, fundamentally new effects arise here.

Using the *causality principle* [15, 17], the equation for the first momentum of a random amplitude $\langle\psi_n(\mathbf{k})\rangle$ is quite trivial:

$$\langle\psi_{n+1}(\mathbf{k})\rangle = \mathcal{L}(\mathbf{k})\langle\psi_n(\mathbf{k})\rangle - \langle\psi_{n-1}(\mathbf{k})\rangle. \quad (14)$$

It is easy to see that for unstable modes, $|\mathcal{L}(\mathbf{k})| \geqslant 2$, even the first moments are divergent, $|\langle\psi_n(\mathbf{k})\rangle| \to \infty$, as $n \to \infty$. Its analogue in the classical phase space (p, q) corresponds to unbounded trajectories.

Since we associate the appearance of localized states with unbounded trajectories for classical oscillators, it is easy to formulate the necessary (but not sufficient) condition for the appearance with disorder of the delocalized states: the initial conditions should correspond to excitation of normal oscillators only, i.e. the amplitudes $\psi_0(\mathbf{k})$ and $\psi_1(\mathbf{k})$ are nonzero only for modes with $|\mathcal{L}(\mathbf{k})| < 2$. This coincides with the statement in [17] based on different ideas. Under this condition the dynamics of the first moments is bounded for all modes, $|\langle\psi_n(\mathbf{k})\rangle| < \infty$ as $n \to \infty$. However, this condition is not sufficient, since the localized states, as was illustrated for the 1D case, correspond in general to *statistically unbounded trajectories*, $\langle|\psi_n(\mathbf{k})|^2\rangle \to \infty$ as $n \to \infty$. That is, the search for the sufficient condition for the existence of the delocalized states is reduced to the solution of equations for the *second moments* of the random amplitudes [15, 17].

2.3. Equations for second moments

Divergence of the second moments is a typical diffusion behavior; an observation of such a diffusion dynamics directly indicates the presence of the localized states, and vice versa. An easy criterion of a diffusion is the behavior of the squared coordinate for all oscillators

$$U_n = \int \frac{\mathrm{d}^p\mathbf{k}}{(2\pi)^p}\langle|\psi_n(\mathbf{k})|^2\rangle. \quad (15)$$

To detect the generalized diffusion in the 1D case, it was sufficient to demonstrate the divergence of the second moment of the amplitude, $\langle q_n^2\rangle$, and to establish its time dependence as $n \to \infty$ (section 2.1). Now in the *N*D case it is sufficient to prove divergence of all second moments $\langle|\psi_n(\mathbf{k})|^2\rangle$ or divergence of the function U_n.

Let us define the second moments by the relations:

$$x_n(\mathbf{k}) = \langle|\psi_n(\mathbf{k})|^2\rangle = \langle\psi_n(\mathbf{k})\psi_n^*(\mathbf{k})\rangle, \quad (16)$$

$$y_n(\mathbf{k}) = \frac{1}{2}[\langle\psi_n(\mathbf{k})\psi_{n-1}^*(\mathbf{k}) + \psi_n^*(\mathbf{k})\psi_{n-1}(\mathbf{k})\rangle]. \quad (17)$$

One obtains

$$U_n = \int \frac{\mathrm{d}^p\mathbf{k}}{(2\pi)^p}x_n(\mathbf{k}). \quad (18)$$

Using the causality principle (see details in [15, 17])) for equation (12), one immediately obtains for the nonzero average quantities

$$\langle|\psi_{n+1}(\mathbf{k})|^2\rangle = \mathcal{L}^2(\mathbf{k})\langle|\psi_n(\mathbf{k})|^2\rangle + \langle|\psi_{n-1}(\mathbf{k})|^2\rangle - \mathcal{L}(\mathbf{k})\langle[\psi_n(\mathbf{k})\psi_{n-1}^*(\mathbf{k}) + \psi_n^*(\mathbf{k})\psi_{n-1}(\mathbf{k})\rangle + \int\int \frac{\mathrm{d}^p\mathbf{k}_1}{(2\pi)^p}\frac{\mathrm{d}^p\mathbf{k}_2}{(2\pi)^p}\langle\varepsilon_n(\mathbf{k}-\mathbf{k}_1)\varepsilon_n^*(\mathbf{k}-\mathbf{k}_2)\rangle \times \langle\psi_n(\mathbf{k}_1)\psi_n^*(\mathbf{k}_2)\rangle. \quad (19)$$

Taking into account properties of random potentials, equation (10), one obtains for $n \geqslant 1$

$$x_{n+1}(\mathbf{k}) = \mathcal{L}^2(\mathbf{k})x_n(\mathbf{k}) + x_{n-1}(\mathbf{k}) - 2\mathcal{L}(\mathbf{k})y_n(\mathbf{k}) + \sigma^2 U_n. \quad (20)$$

Note that the last term in equation (20) does not depend on **k**, i.e. the noise equally affects *all* modes. The noise intensity is described by $\sigma^2 U_n$, where U_n was defined in equation (18). Analogously, the complementary equation is derived as

$$y_{n+1}(\mathbf{k}) + y_n(\mathbf{k}) = \mathcal{L}(\mathbf{k})x_n(\mathbf{k}). \quad (21)$$

Let us perform now the Z-transform:

$$X(z, \mathbf{k}) = \sum_{n=1}^{\infty}\frac{x_n(\mathbf{k})}{z^n}, \quad (22)$$

$$Y(z,\mathbf{k}) = \sum_{n=1}^{\infty} \frac{y_n(\mathbf{k})}{z^n}, \tag{23}$$

$$U(z) = \sum_{n=1}^{\infty} \frac{U_{\mathrm{n}}}{z^n}. \tag{24}$$

Taking into account equation (18), one easily obtains

$$U(z) = \int \frac{\mathrm{d}^p\mathbf{k}}{(2\pi)^p} X(z,\mathbf{k}). \tag{25}$$

The Z-transform of equations (20) and (21) leads to the relations containing the initial conditions

$$[z - z^{-1} - \mathcal{L}^2(\mathbf{k})]X(z,\mathbf{k}) + 2\mathcal{L}(\mathbf{k})Y(z,\mathbf{k}) = x_1(\mathbf{k}) + z^{-1}x_0(\mathbf{k}) + \sigma^2 U(z), \tag{26}$$

$$(z+1)Y(z,\mathbf{k}) - \mathcal{L}(\mathbf{k})X(z,\mathbf{k}) = y_1(\mathbf{k}). \tag{27}$$

It is easy to find that

$$\frac{(z-1)}{(z+1)}[(z+1)^2/z - \mathcal{L}^2(\mathbf{k})]X(z,\mathbf{k}) = \lambda(z,\mathbf{k}) + \sigma^2 U(z), \tag{28}$$

where $\lambda(z,\mathbf{k}) = 2\mathcal{L}(\mathbf{k})y_1(\mathbf{k})/(z+1) + x_0(\mathbf{k}) + x_1(\mathbf{k})/z$. Taking into account the definition (25), equation (28) is the integral equation, but with a simple structure. The function $\lambda(z,\mathbf{k})$ can be easily expressed through $\psi_0(\mathbf{k})$ and $\psi_1(\mathbf{k})$.

2.4. Localization operator

Let us assume initially that $\sigma = 0$, i.e. there is no disorder in equation (28), and use the relevant solution $X^{(0)}(z,\mathbf{k})$ for the calculation of the squared coordinate, equation (25). Thus, one obtains

$$U^{(0)}(z) = \frac{(z+1)}{(z-1)} \int \frac{\mathrm{d}^p\mathbf{k}}{(2\pi)^p} \frac{\lambda(z,\mathbf{k})}{[(z+1)^2/z - \mathcal{L}^2(\mathbf{k})]}. \tag{29}$$

For $\sigma \neq 0$, the solution reads

$$U(z) = H(z)U^{(0)}(z). \tag{30}$$

Here $H(z)$ is the localization operator

$$\frac{1}{H(z)} = 1 - \sigma^2 \frac{(z+1)}{(z-1)} \times \int \frac{\mathrm{d}^p\mathbf{k}}{(2\pi)^p} \frac{1}{[(z+1)^2/z - \mathcal{L}^2(\mathbf{k})]}. \tag{31}$$

Using the convolution property for the Z-transform [15, 17], one obtains

$$U_n = \sum_{l=1}^{n} U_l^{(0)} h_{n-l}, \tag{32}$$

where h_n is the result of the inverse Z-transform of the localization operator $H(z)$.

As was mentioned, the necessary condition for the existence in the presence of disorder of the delocalized states is the presence at the initial time of normal (stable) modes only. In this case $U_{\mathrm{n}}^{(0)}$ corresponds to the stable dynamics of the unperturbed problem and thus is bounded in the index n: $U_{\mathrm{n}}^{(0)} < \infty$ as $n \to \infty$. In turn, the sufficient condition for the delocalized states is the *absence* of the (diffusion) U_{n} divergence: $U_{\mathrm{n}} < \infty$ as $n \to \infty$. As soon as $U_{\mathrm{n}} \to \infty$, as $n \to \infty$, this indicates the localized states.

The convergence or divergence of U_n is not dependent on the properties of the unperturbed solutions. The problem is reduced to a study of the asymptotic behavior ($n \to \infty$) of the h_n coefficients in the linear transformation, equation (32) [15]. This does not need calculation of the coefficients h_n but, by means of analytical methods, analysis of the localization operator $H(z)$ as a function of the complex variable z. Therefore, the physical problem of the localized/delocalized states is reduced to the mathematical search for the poles of the function $H(z)$ of the complex variable [15, 16].

In particular, it was shown [15, 16] that the localization operator $H(z)$ is a non-analytic function of the complex variable z. The unit circle $|z| = 1$ divides the complex plane into two analytic domains: the interior and the exterior of the unit circle. The inverse Z-transform is quite generally defined via countour integrals in the complex plane

$$h_n = \frac{1}{2\pi \mathrm{i}} \oint H(z) z^n \frac{\mathrm{d}z}{z}. \tag{33}$$

This definition is only possible in an analytic domain and does not always represent a solution that can be physically interpreted [15, 16]. In this way, multiple solutions can result in the formal analysis of the problem. The first solution $H_+(z)$ describes the localized states. It is defined outside the unit circle and always exists. The second solution $H_-(z)$ describes delocalized states. It is defined inside the unit circle. The coexistence of the two solutions (if any) was physically interpreted [15–17] as the coexistence of two *phases*—an insulating and a metallic one.

Note that the same result can be obtained using, instead of the total squared coordinate, equation (18), the total squared momentum as a criterion of the diffusion dynamics

$$V_n = \int \frac{\mathrm{d}^p\mathbf{k}}{(2\pi)^p} \langle |\psi_{n+1}(\mathbf{k}) - \psi_n(\mathbf{k})|^2 \rangle. \tag{34}$$

After simple transformations, one obtains

$$V(z) = H(z)V^{(0)}(z) \tag{35}$$

whose structure is similar to that of equation (30), the definition of the localization operator $H(z)$ also remains, equation (31), whereas $V^{(0)}(z)$ is the squared momentum of the unperturbed system.

The expression for the localization operator $H(z)$ was derived by us earlier [15, 16]. However, the nontraditional *engineering language* was used (such as input/output signals, filter function, etc). As we demonstrated above, the derivation can be considerably simplified, since in the system of interacting modes the asymptotic behavior of the total squared coordinate U_n serves as a natural indicator of the presence/absence of diffusion in the system's dynamics. Therefore, reformulation of the Schrödinger equation (the quantum tight-binding model) in terms of the classical Hamiltonian map permits us to retain the basic definitions of the alternative approach [15–17], but opens up the additional possibility of a new interpretation of the results obtained earlier, which we discuss in the next section.

3. The Fermi–Pasta–Ulam problem versus the Anderson localization problem

3.1. Stability and thermalization

It is generally believed that an increase in space dimension greatly increases the system's stability with respect to disorder. Thus, there is without doubt the presence of a metal–insulator transition in the 3D case. It is believed that the effect of statistical fluctuations changes the regime at $D = 4$ [32, 33]; no phase transitions are expected for $D > 4$. The 2D system marks the *borderline* between high and low dimensions [34]. However, all these conclusions derive from the phenomenological scaling theory of localization [24]. The alternative point of view with different classifications of high and low dimensions has been presented by us in [16]. In general, this confirms the system stability in higher dimensions.

An advantage of our interpretation of the AL in terms of classical dynamics of stochastically interacting oscillators is that it causes the statement on the relation between system stability and space dimension to be not so obvious. Indeed, for the energy range inside the old band $|E| \leqslant 2D$, where normal modes certainly exist, simultaneously the inverted modes with $|\mathcal{L}(\mathbf{k})| \geqslant 2$ are also always possible. A change of the space dimensions D affects the weights of these states, but their *complete* disappearance is impossible. That is, this problem can be resolved only by means of the exact analytical solution.

On the other hand, the *instability* mechanism for multi-dimensional systems ($D > 1$) in terms of oscillators is quite obvious. Even assuming that at the beginning only normal modes are excited, stochastic interaction inavoidably excites also neighboring, in particular, inverted modes. In other words, *thermalization* of all modes takes place. It is important to stress that *all* modes—normal and inverted ones—contribute to the localization operator $H(z)$, irrespective of which modes were excited in the beginning. The inverted mode dynamics in the classical phase space (p, q) corresponds to unbounded trajectories which do not correspond to the delocalized states. However, an immediate conclusion suggests itself that all solutions of the dynamical problem—independent of the space dimension and disorder level—correspond only to the localized states. Such a paradox conclusion demonstrates clearly that the problem under consideration is counter-intuitive.

In our opinion, the AL paradox has much in common with the FPU problem [1, 3]. To show their close similarity, let us summarize here the main results.

Numerical simulations of a chain of harmonic oscillators coupled with a quadratic or cubic nonlinearity show that the energy, initially placed in a low-frequency normal mode of the linear problem, stays almost completely locked *within a few neighbor modes* (or *quasi-modes* [3]), instead of being distributed among *all modes of the system*. Recurrence of energy to the originally excited mode is also observed. The nonlinear effects are significant and cannot be neglected.

Two alternative explanations of the FPU paradox were suggested [3]: the integrability of nonlinear equations and dynamical (deterministic) chaos. The second approach points to the existence of a *stochasticity threshold* in the FPU problem. If the nonlinearity is below a stochasticity threshold, the dynamics of the system remains similar to that of the unperturbed system for large time scales. For a strong nonlinearity the overlap of nonlinear resonances leads to a strong dynamical chaos, destroying the FPU effect. Namely in this case the intuitive thermalization occurs.

Therefore, in the standard FPU statement, nonlinear effects play a *key role* being responsible for stochasticity: the motion of a nonlinear dynamical system even with a few degrees of freedom can exhibit chaotic behavior. On the other hand, nonlinearity of the dynamic equations prevents their analytical analysis. A number of questions remain open. In particular, the main results are obtained for systems with a few degrees of freedom, the behavior of the system is not known in the thermodynamic limit, when the number of degrees of freedom goes to infinity.

In our interpretation of the Schrödinger equation in terms of the classical Hamiltonian map, stochasticity is introduced through on-site potentials, which are random variables. Therefore, there is no longer the need to solve nonlinear equations. For the Cauchy problem with fixed initial conditions, where the *causality principle* can be applied [15, 17], this problem can be solved *exactly analytically* (see section 2.4), both for finite-size systems and its thermodynamic limit. Unlike the FPU problem with counter-intuitive solution, the classical interpretation of the AL problem is more complicated due to the unobvious dynamics of the inverted modes.

We will consider below the delocalized states in the quantum mechanical problem as statistically stable quasi-periodic motion, in terms of the classical Hamiltonian map, with excitations spreading only over a few neighbor modes (of the initially excited normal modes). Such a dynamics is bounded. The localized states are interpreted as diffusion dynamics with statistically unbounded trajectories. In the FPU problem this means thermalization with an excitation spreading over *all* modes.

3.2. Stochasticity threshold versus disorder threshold

As was noted in [3], the existence of a *stochasticity threshold* in the FPU is a nonlinear effect. For a strong nonlinearity the overlap of nonlinear resonances leads to a dynamical chaos, destroying the FPU recurrence. As a result, fast convergence to thermal equilibrium arises. The problem of the nonlinearity prevents its detailed analytical study. The stochasticity threshold depends on the type of nonlinearity, and space dimension; the thermodynamic limit is also unclear. Compared to this situation, the dynamical interpretation of the Schrödinger equation has obvious advantages permitting an exact analytical solution. It is expected that in the stochastic AL problem the relevant stochasticity threshold transforms into the *disorder threshold*.

When comparing the two problems, one has to keep in mind that the AL was formulated as a statistical problem with an ensemble of random potential realizations. Thus, it is convenient to reformulate the FPU as a statistical problem. Introducing the stochasticity parameter K (nonlinearity coefficient [29]), the type of dynamical trajectories is defined by the initial conditions. In other words, in the nonlinear dynamic problem the stochasticity parameter is not a unique

factor determining the dynamics. For example, the behavior of the FPU system depends strongly on whether low- or high-frequency modes are initially excited [3]. The number of excited modes seems also to be important for the dynamics.

As is well known, in such problems the phase space is divided into regions with qualitatively different types of motion, and these regions are separated by barriers. If initial conditions were chosen in the region corresponding to a stable quasi-periodic motion, this dynamics corresponds to the recurrent behavior as in the FPU experiment and is classified as the dynamics below the stochasticity threshold. In another region an instability of motion exists for a wide range of the initial conditions (the dynamics above the stochasticity threshold). The trajectory will flow away due to Arnold diffusion. The value of the stochasticity parameter K determines the borders of these regions.

Let us now define some domain in phase space and an ensemble of the initial conditions therein. If, for a given K, a whole domain chosen falls into some region, all trajectories in this ensemble reveal the same dynamics—stable quasi-periodic motion or dynamical chaos (single-phase domain)—otherwise an ensemble reveals trajectories of different kinds (two-phase domain). In the latter case, trivial *co-existence* of the two phases (or two *dynamics*, in a statistical sense) takes place. A change of the stochasticity parameter K in a given ensemble leads to the phase transitions. It is easy to show that in our statistical problem, phase transitions from single-phase to hetero-phase (phase co-existence) dominate, and vice versa, since these transitions correspond to the boundary motion of the regions. Transitions from one single-phase system to another single phase are also possible since variation in the K parameter in the phase space can induce spontaneous creation of new regions with a different dynamics.

The Schrödinger equation in terms of the classical Hamiltonian map does not depend so strongly on the initial conditions. In fact, these determine only the quantity defined by equation (29), whereas the existence of localized/delocalized states is defined entirely by the localization operator $H(z)$, equation (31), which does not depend at all on the initial conditions [15–17]. The physical reason for this is obvious. The ensemble of different trajectories in the AL can be created already for fixed initial conditions by means of the ensemble of random potential realizations. For these realizations, even qualitatively different trajectories in the classical phase space occur. There is no reason to believe that the disorder parameter σ uniquely defines the trajectory types. It can be assumed that some random potentials (called *coherent realization*) correspond to the solutions $\psi_n(\mathbf{k})$ close to average values $\langle\psi_n(\mathbf{k})\rangle$ (the *delocalization* regime). For these realizations excitation of neighbor modes also occurs; however, at the next discrete time steps n these modes return to an equilibrium position, $\psi_n(\mathbf{k}) = 0$ (the recurrent behavior). In other words, only their *virtual* dynamics around equilibrium with limited amplitude takes place. For other potential realizations (the *localization* regime) thermalization occurs and the recurrent behavior disappears. The main physical question—whether these two regimes have comparable statistical contributions—requires us to draw the phase diagram [15–17].

Since a detailed AL study in the thermodynamic limit for an arbitrary space dimension D has already been published by us [16], we restrict ourselves here to the interpretation of the result from the point of view of the disorder threshold. As was shown [16], for $D \geqslant D_0 = 4$ the spectrum of wave function fluctuations changes, as well as the convergence of the integral in equation (31). The spatial dimension $D_0 = 4$ was also discussed in [32, 33]; however, the conclusion was drawn therein that this is an upper critical dimension for localization, so no phase transitions are expected for $D > 4$. In other words, no localized states can exist here. Since the appearance of the localized states in the dynamical version of the Schrödinger equation (12) means *thermalization* (i.e. energy transfer from initially excited modes to all other modes), the analogue of the above-mentioned result [33] in the FPU is a very strong statement on the existence of entirely recurrent states and no convergence to the thermal equilibrium in dynamical systems for $D > 4$. That is, the Gibbs statistics would not be applicable for high-dimensional systems. However, this statement is not based on exact solutions and looks very suspicious to us. Thus, let us consider the alternative idea.

According to our work [16], for $D \geqslant D_0 = 4$ the problem is fundamentally simplified: for all energies inside the old band $|E| \leqslant 2D$ (where only the delocalized states exist) there is a disorder threshold $\sigma_0(E)$. There is no thermalization for $\sigma < \sigma_0(E)$, but only delocalized states, characterized by the (formal) Lyapunov exponent $\gamma \equiv 0$. For $\sigma \geqslant \sigma_0(E)$ thermalization occurs, all states are exponentially localized with a certain $\gamma(\sigma, E)$. As noted in [15, 16, 17], the Lyapunov exponent γ can be treated in the AL problem as the *long-range order* parameter: the two different phases reveal different γ values, $\gamma \equiv 0$ (delocalized states) and $\gamma \neq 0$ (localized states, respectively). A similar relation occurs in other systems, such as ferromagnets (order parameter magnetization) and ferroelectrics (order parameter polarization). The order parameter is zero for one phase and nonzero for another phase. A sharp separation in the phase diagram of the localized and delocalized states recalls the second-order phase transition, where phases cannot coexist. However, the phase transition here is not of the second order, since γ reveals step-like changes at the disorder threshold. As the space dimension D increases, the system stability increases with respect to disorder, but thermalization in principle *cannot* completely disappear.

For the case $2 \leqslant D \leqslant 3$ (the low-dimensional case [16]) the problem becomes more complicated; the energy threshold $E_0 = E_0(D)$ also arises. The delocalized states disappear even under infinitesimal disorder on the boundaries of the old band, $E_0 \leqslant |E| \leqslant 2D$. In other words, only thermalization is possible in this energy range. There is no analogue of the FPU recurrence here. In the region $|E| \leqslant E_0$ the disorder threshold $\sigma_0(E)$ again appears, e.g. for $D = 2$ $E_0 = 2$ and $\sigma_0(E) = 2(1 - \sigma^2/E_0^2)^{1/4}$ [15]), but its sense changes. If disorder σ exceeds the threshold, only the localized states exist (full thermalization). As $\sigma < \sigma_0(E)$, the disorder parameter σ no longer separates uniquelly the localized and delocalized states, since *phase co-existence* takes place [15–17]. In other words, in the ensemble of different disorder potential realizations in this region *both* localized and delocalized solutions can arise with comparable probabilities. As a result

of phase co-existence, phase transition in low-dimensional systems should be considered as a first-order transition. As was said above, this nontrivial result has a direct analogy in the statistical version of the FPU problem.

In the 1D case the analogy between the AL and FPU problems disappears; the Schrödinger equation corresponds here to a *single* oscillator only and thermalization has no longer any meaning. Note, however, that historically the FPU problem arose during the numerical simulations of a 1D chain of oscillators [1, 3]. The localization in 1D means diffusion excitation in one degree of freedom with specific disorder effects. This is not surprising: when presenting the Schrödinger equation in the form of equation (12), one of the spatial coordinates in the D-dimensional system was interpreted as a discrete time variable, respectively, the Hamiltonian dynamics is treated for oscillator systems in a $p = D - 1$ space dimension. That is, the AL problem in a space dimension D should be compared with the FPU with a lower space dimension, $p = D - 1$.

3.3. FPU recurrence versus delocalization

For the sake of illustration, we restrict ourselves to the case of the band center $E = 0$ for the 2D system. For this particular case for the delocalized states ($H(z) = H_{-}(z)$) we calculated analytically [15] the inverse Z-transform, equation (33), and found the coefficients h_n in equation (32). Equation (32) can be transformed:

$$U_n - U_n^{(0)} = 2\tan(\phi)\sum_{l=1}^{n-1} U_l^{(0)} \sin(2\phi(n-l)). \qquad (36)$$

Equation (36) is valid only for $\sigma \leqslant 2$, provided $2\sin(\phi) = \sigma$ [15].

It is easy to note that the solution for a disordered system derives from that for the ordered system with the help of the sinusoidal modulation. Taking into account that the full squared coordinate $U_n^{(0)}$ is a sum of oscillating quantities (normal modes), the solution for the perturbed problem U_n is a quasi-periodic motion. That is, one observes a direct analogue of the recurrent behavior in the FPU systems.

The 2D case for the AL corresponds to the 1D dynamics (classical Hamiltonian map). Note that the FPU paradox was established for the first time, namely for the 1D system [1, 2]. If the recurrent behavior takes place for the 1D FPU, and this is generally accepted as a reliable fact, there are no strong grounds to reject our conclusion on the delocalized states in the 2D AL, since these states are analogous to the 1D quasi-periodic motion in FPU.

4. Conclusion

The AL and the FPU problems are complementary: the counter-intuitive result in one of these problems has its analogue in the other problem. A stable quasi-periodic motion (the recurrent behavior) in the FPU corresponds to the existence of the delocalized states in the AL problem. The thermalization effect in FPU has an analogue in the localized states in the AL. We have shown here a deep analogy between the two problems using the quantum tight-binding model in terms of a classical Hamiltonian map.

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