Anderson localization and the Fermi-Pasta-Ulam paradox

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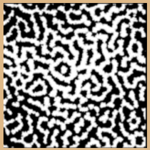
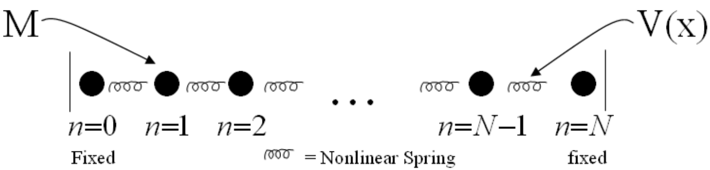


1. Introduction

1.1. The Fermi-Pasta-Ulam paradox (1955)

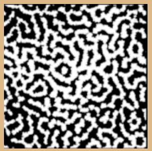
1.1.1. Molecular dynamics

Los Alamos (1953-1954): Enrico Fermi, John Pasta, and Stan Ulam decided to use the most powerful computer, the MANIAC-1 (Mathematical Analyzer Numerical Integrator And Computer), to study the equipartition of energy expected from statistical mechanics in simplest classical model of a solid: a $I - D$ chain of equal mass particles coupled by nonlinear springs:



$$V(x) = \frac{1}{2}kx^2 + \frac{1}{3}ax^3 + \frac{1}{4}bx^4. \quad (1)$$

Key conclusion: "The results show very little, if any, tendency toward equipartition of energy among the degrees of freedom."



1.1.2. FPU recurrence

Localization in the k-space of normal modes or the energy localization:

> **Energy, initially placed in a low-frequency normal mode of the linear problem, stayed almost completely locked within a few neighbor modes, instead of being distributed among all modes of the system.**

982 266. – *Studies of non Linear Problems*

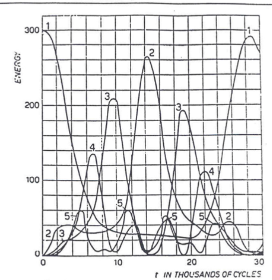
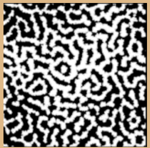


Fig. 1. – The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. N = 32; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.

[E. Fermi, J. Pasta, and S. Ulam, Los Alamos, Report No. LA-1940, 1955; also in *Collected Papers of Enrico Fermi*, edited by E. Segre (University of Chicago Press, Chicago, 1965), Vol. II, p. 978]

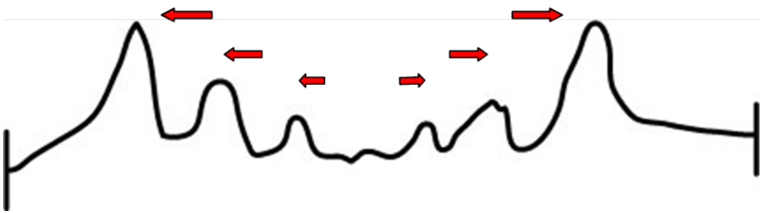


1.1.3. FPU and solitons

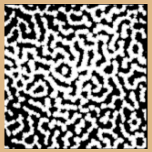
First alternative explanation of the FPU paradox: the integrability of nonlinear equations.
late 50s - early 60s: Multiple scale analysis in formal continuum limit $a \to 0$ (since discrete models are harder to treat analytically than continuum theories).
KdV-equation:

$$u_t + uu_x + u_{xxx} = 0. \tag{2}$$

Amplitude, shape and velocity interdependent: characteristic of nonlinear wave-solitons retain identities in interactions.



Initial pulse (typically low mode) breaks up into (primarily) a few solitons. Number and size of solitons depends on initial condition.

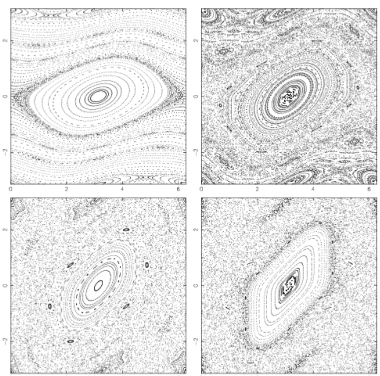


1.1.4. Dynamical (deterministic) chaos

Second alternative explanation of the FPU paradox: existence of a stochasticity threshold.
[F. M. Izrailev and B.V. Chirikov, Institute of Nuclear Physics (Novosibirsk, USSR, 1965); Dokl. Akad. Nauk SSSR 166, 57 (1966)]
The Taylor-Chirikov Standard map:
The Poincare map for the kicked rotator

$$p_{n+1} = p_n + K\sin(x_n),$$
$$x_{n+1} = x_n + p_{n+1},\ \ mod\,(2\pi).$$

n - discrete time



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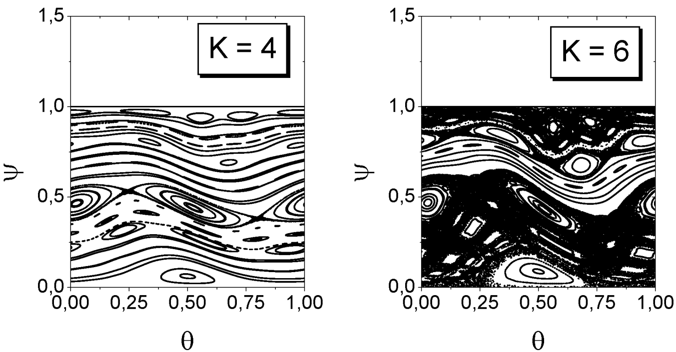
Keywords: Ergodicity, integrability, stability of motion and chaos.

> If nonlinearity is below a stochasticity threshold, the dynamics of the system remains similar to unperturbed system for large time scales. For strong nonlinearity the overlap of nonlinear resonances leads to strong dynamical chaos, destroying the FPU effect.

Initial conditions and 'phase transitions':



Bounded tokamap [V.N. Kuzovkov and O. Dumbrajs (2007)]

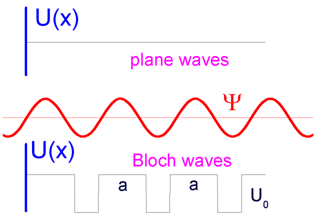
1.2. The Anderson localization (1958)

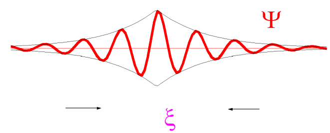
1.2.1. Localization length

Possibility of electron localization for a random system, provided that the degree of disorder is sufficiently large.

Absence of diffusion of waves in a random medium.

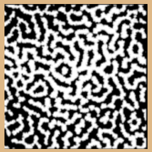
[P.W. Anderson, Phys. Rev. 109, 1492 (1958)]





Typical wave functions of localized state with localization length ξ

Transition between a metal and an insulator = metal-insulator transition (MIT)



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1.2.2. Tight-binding model

Quantum tight-binding model with diagonal disorder (Schrödinger equation):

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

ε_n - random potentials

The nature of electronic states in the Anderson model depends strongly on spatial dimension D.

- In one dimension (1-D) all states are localized at any level of disorder
- For $D = 2$ all states are localized at any level of disorder (the conclusion of the scaling theory)
- Metal-insulator transition occurs for $D > 2$ if the disorder is sufficiently strong

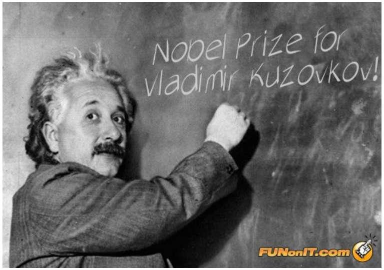
[E. Abrahams, P.W. Anderson, D.C. Licciardello, and T.V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979)]

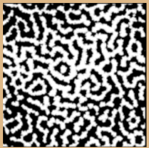
1.3. The FPU problem vs the Anderson localization problem

- Anderson localization problem $\Longleftrightarrow$ FPU effect in (modified) dynamical system
- Delocalized states $\Longleftrightarrow$ FPU recurrence
- Localized states $\Longleftrightarrow$ FPU thermalization

Enrico Fermi, Nobel Prize in Physics (1938)

Philip W. Anderson, Nobel Prize in Physics (1977)





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2. (Analytical) theory vs (numerical) experiment

2.1. Numerical analysis

2.1.1. "From first principles"?

[P. Markoš, Acta physica slovaca, 56, 561 (2006)]

> **The big advantage of the numerical simulation is that it can relatively easy analyze statistical properties of any quantity of interest. No averaging is necessary in the course of calculations. All mean values can be calculated "from first principles". This cannot be done analytically.**

Numerical methods.

We are not able to describe metal-insulator transition analytically. What remains is numerical simulations

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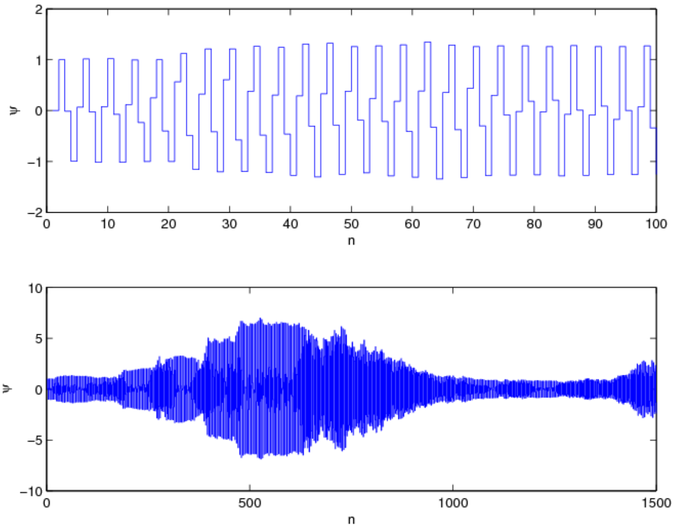
2.1.2. Example: Cauchy problem

The Schrödinger equation for the 1-D Anderson model as a recursive relation (n - discrete time):

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

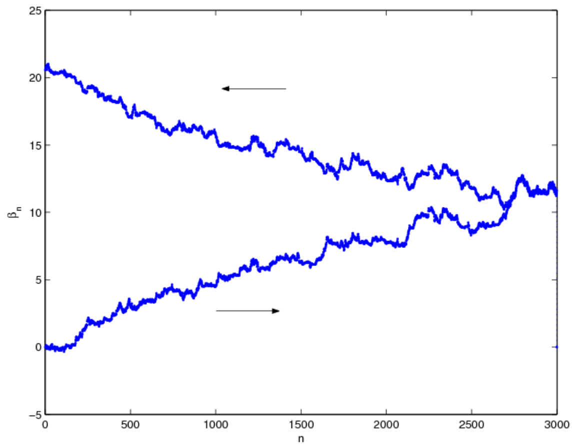
The Cauchy problem with the *fixed initial conditions* for ψ_1 and ψ_0.



2.1.3. Reversibility

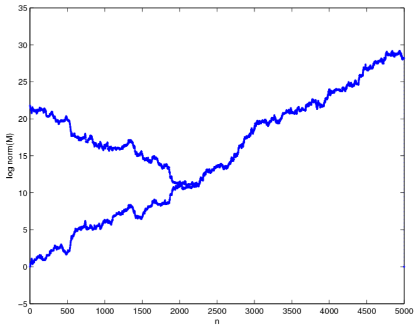
$$\Longrightarrow \psi_{n+1} = (E - \varepsilon_n)\psi_n - \psi_{n-1}.$$

$$\Longleftarrow \psi_{n-1} = (E - \varepsilon_n)\psi_n - \psi_{n+1}.$$

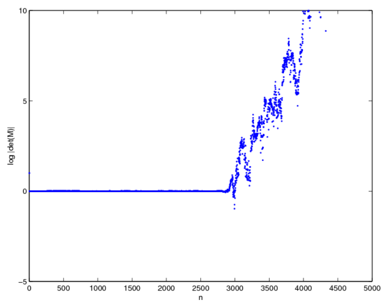


$$\beta_n = \frac{1}{2}\ln(\psi_{n+1}^2 + \psi_n^2)$$

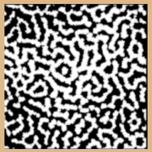
2.1.4. Transfer Matrix



$norm(M)$



$\det(M)$



2.2. Analytical theory

2.2.1. Causality principle

[L. Molinari. J.Phys.A: Math. Gen. 25, 513 (1992)]

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

Is is easy to see that:

- ψ_2 **is a function of** ε_1**,**
- ψ_3 **is a function of** ε_2**,**ε_1**,**
- ψ_{n+1} **is a function of** $\varepsilon_n, \ldots, \varepsilon_2$**,**$\varepsilon_1$ **(causality).**

So both amplitudes ψ_n **and** ψ_{n-1} **on the rhs of equation are statistical independent of** ε_n **and can be averaged separately (causality principle):**

$$\langle\psi_{n+1}\rangle = E\langle\psi_n\rangle - \langle\psi_{n-1}\rangle,$$
$$\langle\psi^2_{n+1}\rangle = (E^2 + \langle\varepsilon^2_n\rangle)\langle\psi^2_n\rangle - 2E\langle\psi_n\psi_{n-1}\rangle + \langle\psi^2_{n-1}\rangle,$$

etc.

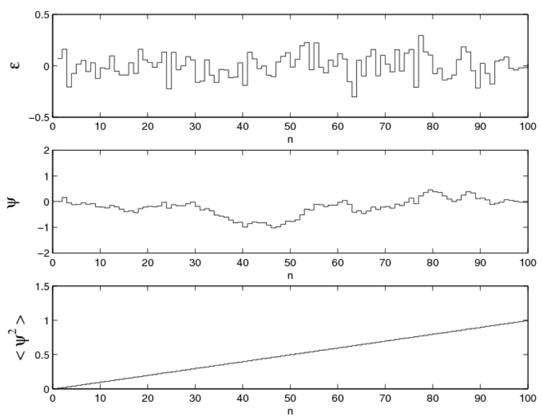
2.2.2. Diffusion and divergence

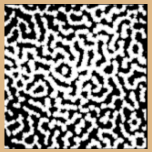
Random walks and normal diffusion.

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

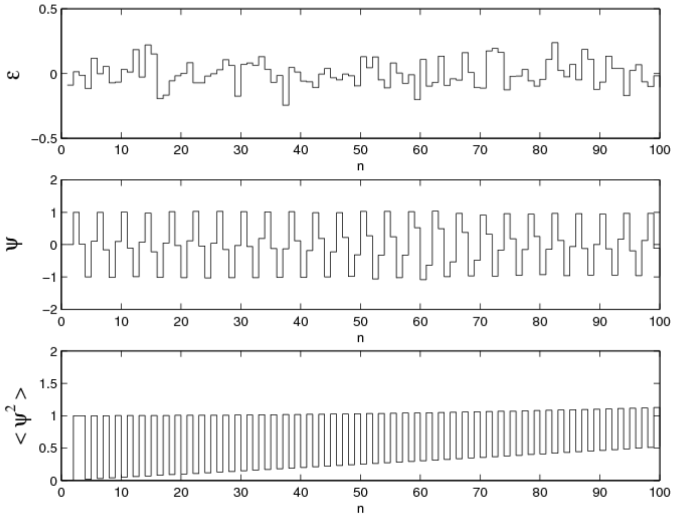
$$\langle \psi_n^2 \rangle = \langle \psi_0^2 \rangle + \sigma^2 n.$$

$\sigma^2 = \langle \varepsilon_n^2 \rangle$





2.2.3. Localization as generalized diffusion



The diffusion motion is characterized by divergences, e.g. for the mean time when the system returns to the initial state. To detect the diffusion, it is *sufficient* to demonstrate the divergence of the second moment of the amplitude and to establish its law of time-dependence.

3. Anderson localization and classical Hamiltonian map

3.1. Classical Hamiltonian map for one-dimensional case

3.1.1. Classical phase space (p, q)

[F.M. Izrailev and A.A. Krokhin, Phys.Rev.Lett., 82, 4062 (1999)]

The representation of quantum tight-binding model with diagonal disorder

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

in terms of classical two-dimensional Hamiltonian map.
Definitions: $q_n = sign(E)\psi_n$, $p_n = sign(E)\left(\psi_{n+1} - \psi_n\right)$

$$\begin{aligned} p_{n+1} &= p_n - \omega^2 q_n - \varepsilon_n q_n, \\ q_{n+1} &= q_n + p_{n+1}. \end{aligned}$$

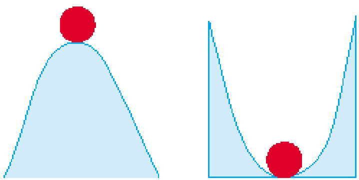
3.1.2. Bounded and unbounded trajectories

Kicked-oscillator Hamiltonian

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

$\omega^2 = 2 - \lfloor E \rfloor$.

It defines the system with unperturbed Hamiltonian of oscillator which is affected by a periodic sequence of kicks (δ-pulses) with the period Δt.



- $\lfloor E \rfloor > 2$ **(outside the band) - unstable mode**
- $\lfloor E \rfloor < 2$ **(inside the band) - stable mode**

3.1.3. Localized and delocalized states

Unperturbed system ($\varepsilon_n \equiv 0$). Trajectories in the classical phase space:

- $|E| > 2$ (outside the band) - unbounded
- $|E| < 2$ (inside the band) - bounded

Localized states - statistically unbounded trajectories in the classical phase space.

- Stable mode - bounded first moment $|\langle q_n \rangle| < \infty$ for $n \to \infty$
- Delocalized states - bounded second moment, $\langle q_n^2 \rangle < \infty$
- Localized states - unbounded second moment, $\langle q_n^2 \rangle \to \infty$ for $n \to \infty$

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3.2. Classical Hamiltonian map for D-dimensional case

3.2.1. Cauchy problem for the Schrödinger equation

The semi-infinite system, or infinite system with a boundary, where the index $n \equiv m_D \geq 0$, but all $m_j \in (-\infty, \infty)$, $j = 1, 2, \ldots, p$, with

$$p = D - 1.$$

We combine indices in the vector $\mathbf{m} = \{m_1, m_2, \ldots, m_p\}$. The boundary which is the layer $n = 0$ defines the preferential direction (the axis n).

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

Summation over $\mathbf{m}'$ includes the nearest neighbours of the site $\mathbf{m}$.
The on-site potentials $\varepsilon_{n,m}$ are independently and identically distributed. We assume hereafter existence of the two first moments,

$$\langle \varepsilon_{n,\mathbf{m}} \rangle = 0,$$
$$\left\langle \varepsilon^2_{n,\mathbf{m}} \right\rangle = \sigma^2,$$

where the parameter σ characterizes the disorder level.

3.2.2. Fourier transform

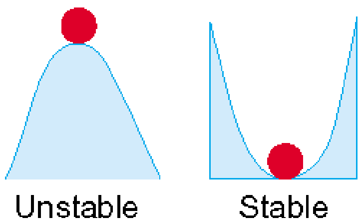
$$\varepsilon_n(\mathbf{k}) = \sum_{\mathbf{m}} \varepsilon_{n,\mathbf{m}} e^{i\mathbf{k}\mathbf{m}},$$

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

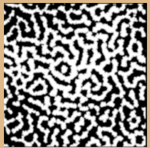
Schrödinger equation

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

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



- $|\mathcal{L}(\mathbf{k})| > 2$ **(outside the band) - unstable mode**
- $|\mathcal{L}(\mathbf{k})| < 2$ **(inside the band) - stable mode**



3.2.3. Diffusion and localization

- **Initial conditions - ONLY stable modes**
- **Bounded first moment** $\lfloor \langle \psi_n(\mathbf{k}) \rangle \rfloor < \infty$ **for** $n \to \infty$
- **Delocalized states - bounded second moment,** $\langle Q_n^2 \rangle < \infty$
- **Localized states - unbounded second moment,** $\langle Q_n^2 \rangle \to \infty$ **for** $n \to \infty$

Q^2-Definition

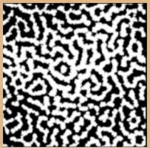
$$Q_n^2 \equiv U_n = \int \frac{d^p\mathbf{k}}{(2\pi)^p} \langle \lfloor \psi_n(\mathbf{k}) \rfloor^2 \rangle.$$

Unperturbed system ($\sigma = 0$):

$$U_n^{(0)} < \infty \;\; for \, n \to \infty.$$

Z-transform:

$$U(z) = \sum_{n=1}^{\infty} \frac{U_n}{z^n}.$$



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3.2.4. Localization operator $H(z)$

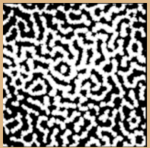
$$U(z) = H(z)U^{(0)}(z).$$

Convolution property

$$U_n = \sum_{l=0}^{n-1} h_l U_{n-l}^{(0)}.$$

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

The concept of the localization operator $H(z)$ is a general and abstract description of the problem of localization. Instead of analyzing wave functions, it is sufficient to analyse properties of $H(z)$ by means of the theory for functions of complex variables.
Knowledge of the fundamental characteristics of the system - the localization operator $H(z)$ - permits to determine the phase diagram of the system (regions of localized and delocalized solutions), as well as the localization length.



3.2.5. Exact solution and intuition

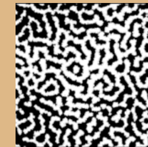
Stochastically interactions of all modes:

$$\int \frac{d^p \mathbf{k}_1}{(2\pi)^p} \varepsilon_n(\mathbf{k}-\mathbf{k}_1)\psi_n(\mathbf{k}_1).$$

- Thermalization
- $\Longrightarrow$ statistically unbounded trajectories in the classical phase space
- $\Longrightarrow$ Localized states

Is there a delocalization for all dimensions?

One man could be tried in Britain for bigamy but was saved by his advocate proving that his client had three wives. (G.C. Lichtenberg)



3.3. The FPU problem vs the Anderson localization problem

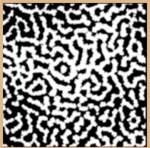
3.3.1. Nonlinearity vs Noise

FPU:

- Nonlinear equations
- Stochasticity via nonlinearity
- Only stable modes
- Stochasticity threshold
- Phase transition: **FPU recurrence** vs **Thermalization**

Anderson localization:

- Linear equations
- Stochasticity via noise (random potentials)
- Stable and unstable modes
- Disorder threshold.
- Phase transition: **Coherent dynamics** (only stable modes) vs **Thermalization** (all modes)



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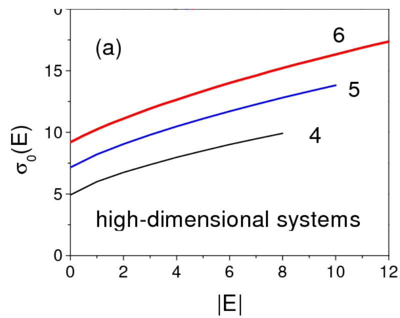
3.3.2. Stochasticity threshold vs disorder threshold

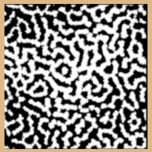
[V.N. Kuzovkov and W. von Niessen, Eur. Phys. J. B, 42, 529 (2004)]
High-dimensional systems ($D \geq 4$) for $\lfloor E \rfloor \leq 2D$ (the old band):



[H. Kunz and B. Souillard, J.Phys. (Paris) Lett. 44, 503 (1983)]

> **The effect of statistical fluctuations cause a change of regime at $D = 4$, for $D > 4$ there should not exist a phase transition.**

Is Gibbs statistics true for $D > 4$?



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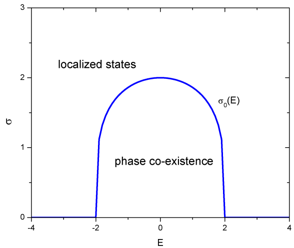
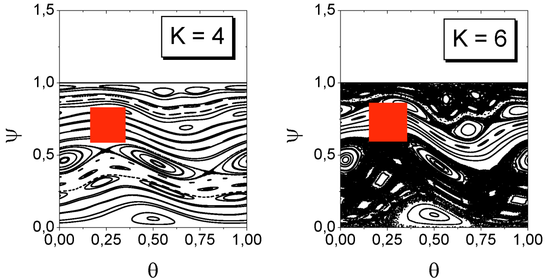
[V.N. Kuzovkov, W. von Niessen, V. Kashcheyevs and O. Hein, J. Phys.: Condens. Matter, 14, 13777 (2002)]

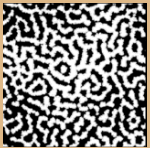
Low-dimensional systems ($D = 2, 3$):



Phase diagram for ensemble of random potentials



Ensemble of initial conditions for dynamical systems



3.3.3. FPU recurrence vs delocalized states

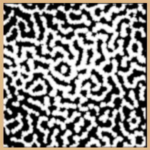
[V.N. Kuzovkov, W. von Niessen, V. Kashcheyevs and O. Hein, J. Phys.: Condens. Matter, 14, 13777 (2002)]

Convolution property

$$U_n = \sum_{l=0}^{n-1} h_l U_{n-l}^{(0)}.$$

Example: For $D = 2$ and $E = 0$ (band centre)
Localization operator h_n^- is bounded oscillating function,

$$h_n^- = \delta_{n,0} + 2\tan(\phi)\sin(2\phi n),$$
$$2\sin(\phi) = \sigma.$$



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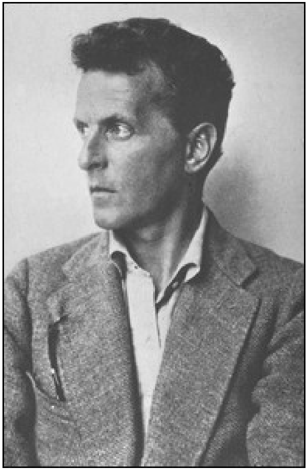
4. Conclusion

L. Wittgenstein



The cognition process consists in the replacement of rough mistakes by more refined mistakes.