Onset of many-body chaos and thermalization in finite systems of interacting particles

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The Fermi-Pasta-Ulam (FPU) model

\[ x''_n = \left( x_{n+1} - 2x_n + x_{n-1} \right) + \beta \left( x_{n+1} - x_n \right)^3 - \left( x_n - x_{n-1} \right)^5 \]

\[ x''_n = \left( x_{n+1} - 2x_n + x_{n-1} \right) + \alpha \left( x_{n+1} - x_n \right)^2 - \left( x_n - x_{n-1} \right)^2 \]

Fig. 1.1. The one-dimensional lattice of the FPU problem.

Resolution of the FPU paradox: The border of chaos

Analytical result for the border of chaos:

\[ 3 \beta_{cr} \frac{E}{N} \approx \left\{ \begin{array}{ll}
\frac{3 \sqrt{\Delta k}}{k} ; & k \ll N \\
\frac{3 \pi^2 \Delta k}{N^2} \left( \frac{k}{N} \right)^2 ; & N - k \ll N
\end{array} \right\} \]

F.M.Izrailev and B.V.Chirikov
Report INP (1965);

Numerical confirmation: F.M.Izrailev, A.I.Khisamutdinov, B.V.Chirikov,

Special Issue: CHAOS 15 (2005).
Comments to the classical thermalization

1. We do not need ergodicity for thermalization!
2. Onset of chaos – dependence on $N$, and strength of interaction!
3. Dependence on initial conditions!!
4. Two different situations: finite $N$ and thermodynamic limit $N \rightarrow \infty$
Chaos and thermalization in nuclei and atoms


In particular, the reduced density matrix operator was analyzed numerically for individual eigenstates, and compared with analytical average over number of chaotic states.
Chaotic eigenstates as the condition for thermalization


FIG. 7. Orbital occupation numbers in Au$^{24+}$ calculated numerically from Eq. (7) at excitation energies $E = 1, 4.5, 9.5, 17$ and 27.5 a.u. (solid circles), and the Fermi-Dirac distributions (solid line) with temperature $T$ and chemical potential $\mu$ chosen to give best fits of the numerical data.

In order to define the temperature for each selected eigenstate $|\alpha\rangle$ let us consider its occupation number distribution (OND),

$$n_s^\alpha = \langle \alpha | \hat{n}_s | \alpha \rangle = \sum_k |C_k^\alpha|^2 \langle k | \hat{n}_s | k \rangle. \quad (9)$$

As one can see, the OND (9) consists of two ingredients: the probabilities $|C_k^\alpha|^2$ and the occupation numbers $\langle k | \hat{n}_s | k \rangle$ related to the basis states of $H_0$. The latter are just integer numbers 0, 1, 2, ...$N$ depending on how many bosons occupy the single-particle level $s$ with respect to the many-body state $|k\rangle$. If the eigenstate $|\alpha\rangle$ of $H$ con-
Quantum chaos in isolated systems of interacting particles

\[ \hat{H} = \hat{H}_0 + \hat{V} \]

- $\hat{H}_0$ - “non-perturbed” part (describes the non-interacting particles/quasi-particles)
- $\hat{V}$ - interaction between particles, or, with an external field

Two-Body Interaction Model

\[ H = \sum_{k}^{m} \epsilon_k a_k^+ a_k + \frac{1}{2} \sum_{kqpr} V_{kqpr} a_k^+ a_q^+ a_p a_r \]

\(|k\rangle, |q\rangle, |p\rangle, |r\rangle\) single-particle states

\(V_{kqpr}\) two-body matrix elements (random or dynamical)

\(m\) number of single-particle states

\(n\) number of particles ("quasi-particles")

\(\epsilon_k\) energy of single-particle states

\(H\) is considered in the many-particle basis of \(H_0\)

\(H_0 = \sum_{k}^{M} \epsilon_k a_k^+ a_k\)

\(H_0\) determines the basis in which the dynamics occurs

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Chaos and relaxation dynamics in 1/2-spin models

model 1 integrable

\[ H_1 = H_0 + \mu V_1, \]
\[ H_0 = \sum_{i=1}^{L-1} J \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right), \]
\[ V_1 = \sum_{i=1}^{L-1} J S_i^z S_{i+1}^z \]

model 2 non-integrable

\[ H_2 = H_1 + \lambda V_2, \]
\[ V_2 = \sum_{i=1}^{L-2} J \left[ (S_i^x S_{i+2}^x + S_i^y S_{i+2}^y) + \mu S_i^z S_{i+2}^z \right]. \]

\[ \lambda_{cr} \approx 0.5 \]
- for transition from Poisson to Wigner-Dyson


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FIGURE 1. (Color online) Sparsity of off diagonal matrix elements. Each point represents a non-zero matrix element. Here we consider $N = 4$ particles in $M = 7$ levels.
Many-body chaos: Basic relations

\[ H = H_0 + V \]

\[ |\alpha\rangle = \sum_k C_k^\alpha |k\rangle \quad |k\rangle = \sum_\alpha C_k^\alpha |\alpha\rangle \]

\[ H_0 |k\rangle = E_k^0 |k\rangle \quad H |\alpha\rangle = E^\alpha |\alpha\rangle \]

Strength function (LDOS):

\[ F^\alpha(E) = \sum_k |C_k^\alpha|^2 \delta(E - E_k^0) \]

F-function:

\[ F_k(E) = \sum_\alpha |C_k^\alpha|^2 \delta(E - E^\alpha_k) \]

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FIG. 2 (color online). Typical localized (top) and extended (bottom) eigenstates for model 1 (left) and model 2 (right).
FIG. 2. (a)–(d) Probability $P_k(t)$ at different times $t$ in the unperturbed basis $|k\rangle$: (a) $t = 0.025$, (b) $t = 0.075$, (c) $t = 0.5$, and (d) $t = 5$. (e)–(h) Plot of $n_s(t)$ versus single-particle energies $\epsilon_s$ at (e) $t = 0.025$, (f) $t = 0.075$, (g) $t = 0.5$, and (h) $t = 5$. In (d) the envelope of the stationary distribution is shown by the black curve. The initial state is $\Psi_0 = |10104000000\rangle$, where integer numbers are numbers of bosons occupying the $s$ level. The dynamics is shown for $N = 6$, $M = 11$, and $V = 0.4$. For this value of $V$ the eigenstates are strongly chaotic [23,24].
effective number \( N_{pc}(t) \) of principal components of the wave function,

\[
N_{pc}(t) = 1/ \sum_{k} |\langle k | e^{-iHt} | j_0 \rangle|^4,
\tag{2}
\]

known in the literature as the \emph{participation ratio}.

In terms of eigenvalues and many-body eigenstates of the Hamiltonian \( H \) the participation ratio can be presented as

\[
N_{pc}(t) = \left\{ \sum_{k} \left[ P_k^d + P_k^f(t) \right]^2 \right\}^{-1},
\tag{3}
\]

where

\[
P_k^d = \sum_{\alpha} |C_{k_0}^\alpha|^2 |C_k^\alpha|^2
\tag{4}
\]

and

\[
P_k^f(t) = \sum_{\alpha \neq \beta} C_{k_0}^\alpha C_k^{\alpha \ast} C_{k_0}^\beta C_k^{\beta \ast} e^{-i(E^\beta - E^\alpha)t}
\tag{5}
\]

are the diagonal and off-diagonal parts of

\[
P_k(t) = |\langle k | \psi(t) \rangle|^2 = \sum_{\alpha, \beta} C_{k_0}^{\alpha \ast} C_k^\alpha C_{k_0}^\beta C_k^{\beta \ast} e^{-i(E^\beta - E^\alpha)t}.
\tag{6}
\]
Exponential increase of NPC

TBRI model:

Spin model:

Cascade model

\[ \frac{dW_0}{dt} = -\Gamma W_0, \]

\[ \frac{dW_1}{dt} = \Gamma W_0 - \Gamma W_1, \]

\[ \ldots \]

\[ \frac{dW_k}{dt} = \Gamma W_{k-1} - \Gamma W_k, \]

\[ \ldots \]

\[ W_0 = \exp(-\Gamma t), \]

\[ W_n = \frac{(\Gamma t)^n}{n!} \exp(-\Gamma t) = \frac{(\Gamma t)^n}{n!} W_0. \]

value of the connectivity $\mathcal{K}$, in [51] the following approximate expression has been obtained,

\[ N_{pc}(t) = \exp\left[2\Gamma \left(1 - \frac{1}{\sqrt{\mathcal{K}}}\right)t\right]. \quad (9) \]
Semi-analytical approach: Main results

\[
\frac{dW_0}{dt} = -\Gamma(W_0 - W_0^\infty),
\]

\[
\frac{dW_1}{dt} = -\Gamma(W_1 - W_1^\infty) + \Gamma(W_0 - W_0^\infty),
\]

Assuming a Gaussian shape for both the density of states and the LDOS [36], we show that the maximal value of \( N_{pc}^\infty \) is

\[
N_{pc}^{\text{max}} = \eta \sqrt{1 - \eta^2 D}
\]

(12)

where \( \eta = \Gamma / \sigma \sqrt{2} \) and \( \sigma \) is the width of the density of states (see details in SM [36]). For \( M \sim 2N \) and for \( M, N \gg 1 \) one gets the estimate

\[
t_S \sim \frac{N}{\Gamma} = Nt_\Gamma.
\]

(13)
Fermi-particles, summary

![Graph showing a linear relationship between \( \Gamma t_s \) and \( N \).](image)
Figure 7: The plot in the left column, $l_{ipr} vs. t$, is the growth of the number of principal components in time and in the left column, $W_0 vs. t$, the decay of the survival probability for a system of Fermi particles with $N = 7$, $M = 14$, $V = 0.4$. The dashed lines are the exponential fitting. The horizontal lines are the corresponding time scales. The orange line is the maximal number of principal components given by (22). The average over 9 different unperturbed initial states in the middle of the spectrum has been performed.
Many-body systems

\[ \mathcal{V}_E(t) = \mathcal{V}_E(0)e^{2\Gamma t} \sim \mathcal{V}_E(0)e^{h_{KS} t} \]

- Kolmogorov-Sinai entropy
Quantum chaos in a completely integrable non-random model

\[ H = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i<j}^{N} \delta(x_i - x_j). \]  

This many-body Hamiltonian describes \( N \) bosons with \( \delta \)-function interaction in one dimension, called the Lieb–Liniger model. This is a physical realistic model in quantum degenerate gases with s-wave scattering potential. In

One-Dimensional Bose System

\[ H = \sum_{k=-M}^{M} \varepsilon_k \hat{n}_k + \frac{g}{2L} \sum_{k.q.p.r} \hat{a}_k^+ \hat{a}_q^+ \hat{a}_p \hat{a}_r \delta(k + q - p - r) \]

where

- \( L \) -- length of a ring;
- \( n = \frac{N}{L} \) -- density of bosons
- \( N \) -- number of bosons
- \( \hat{n}_k = \hat{a}_k^+ \hat{a}_k \) and \( |k\rangle \) -- single-particle levels with \( \varepsilon_k = \frac{4\pi^2 k^2}{L^2} \)

It is known that \( n / g \to \infty \) corresponds to the mean-field regime

and \( n / g \to 0 \) is the Tonks-Girardeau regime

Transition occurs at \( n / g \approx 1 \)


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Structure of the H-matrix
Let us fix the total momentum $M = 1$

$N = 9$ particles and $l = 13$ states
Thermodynamic entropy vs. diagonal entropy

\[ S^0_{\text{diag}} + \ln\left(\Delta H/\Delta H_0\right) \]

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Thermodynamic entropy vs. diagonal entropy

Thermodynamic entropy versus diagonal entropy.—The onset of thermalization in the quench dynamics is characterized by a simple relation between two entropies, $S_{th}$ and $S_{diag}$. Here $S_{th} = \ln \mathcal{V}(E)$ is the thermodynamic entropy characterizing the system after its relaxation to equilibrium. It can be estimated from $\mathcal{V}(E) \simeq \langle N_{pc} \rangle \delta_0$, where $\delta_0 = \Delta_{H_0} / D$ is the unperturbed energy spacing, $\Delta_{H_0}$ is the effective width of the energy spectrum of $H_0$ and $D$ is the dimension of the many-body Hilbert space.

$$S_{diag}^{j_0} = - \sum_{\alpha} |C_{j_0}^\alpha|^2 \ln |C_{j_0}^\alpha|^2.$$
On computing non-equilibrium dynamics following a quench

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Thank you for your attention!
Many-body chaos

Fig. 35. Picture illustrating the compound nucleus idea, as presented by N. Bohr in 1936. In a neutron-nucleus collision the constituent nucleons are viewed as billiard balls and the nuclear binding as a shallow basin (taken from [112]).
“Quantum chaos” in deterministic systems


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Chaotic eigenstates as the condition for thermalization

L.D. Landau and E.M. Lifshitz:

† It may again be mentioned that, according to the fundamental principles of statistical physics, the result of the averaging is independent of whether it is done mechanically over the exact wave function of the stationary state of the system or statistically by means of the Gibbs distribution. The only difference is that in the former case the result is expressed in terms of the energy of the body, and in the latter case as a function of its temperature.

There is a one-to-one correspondence between sets of quantum number and sets of rapidities, defined via the logarithmic Bethe equations

$$\lambda_j R = 2\pi I_j - 2 \sum_{l=1}^{N} \arctan \left( \frac{\lambda_j - \lambda_l}{c} \right),$$  \hspace{1cm} (8)

These states have momentum $P(\{\lambda\}_N)$ and energy $E(\{\lambda\}_N)$ given by

$$P(\{\lambda\}_N) = \sum_{j=1}^{N} \lambda_j, \hspace{1cm} E(\{\lambda\}_N) = \sum_{j=1}^{N} \lambda_j^2.$$  \hspace{1cm} (3)

FIG. 2. The magnetization, $M_1$, plotted against energy for each of energy eigenstates (small dots) for (a) a nonintegrable Hamiltonian and (b) an integrable Hamiltonian; the solid curves represent the microcanonical average of the magnetization as functions of energy, and the large dots show the equilibrium values approached in numerical experiments performed with a variety of initial states. The associated error bars represent an estimate of the typical fluctuations from equilibrium.
Chaos and thermalization on the level of individual eigenstates


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Out-of-time-order correlator (OTOC)

\[ \mathcal{O}_{s,s+1}(t) = \langle \kappa_0 | [\hat{n}_s(t), \hat{n}_{s+1}(0)]^2 | \kappa_0 \rangle. \]

FIG. 4: Evolution of the four-point correlator \( \mathcal{O}_{s,s+1}(t) \) for \( s = 5 \). Dashed line is the analytical prediction (15). Horizontal line corresponds to Eq. (16). Dotted line is the fit for \( t > 0.07 \) (outside perturbative regime), giving the \( t^{2.5} \) dependence. Initial state is \( \Psi_0 = |00006000000\rangle \) and \( N = 6, M = 11, V = 0.4 \).
Ehrenfest’s Theorem, Ehrenfest Time

3. S.A.Kheifets and V.V.Sokolov, Preprint 80-133, INP Novosibirsk (1980);

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FIG. 4 (color online). Structure of eigenstates in the energy shells for model 1 (left) and model 2 (right) obtained by averaging over 5 states in the middle of the energy band. Solid curves correspond to the Gaussian form of the energy shell.
Structure of $V$ in the unperturbed many-particles basis

$N = 6$ particles and $l = 13$ states
FIG. 8. Matrix of squared components of the eigenstates

\[ |C_n^\alpha|^2 \]

model 1

|\[C_n^\alpha\]|^2

model 2

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FIGURE 6. (Color online) Structure of the eigenstates of $H$ in the unperturbed energy representation. First column: $V = 0.04$, energy $E^\alpha = 28.67$ (a1), $E^\alpha = 18.17$ (a2), $E^\alpha = 11.6$ (a3); Second column: $V = 0.1$, energy $E^\alpha = 28.51$ (b1), $E^\alpha = 17.88$ (b2), $E^\alpha = 11.27$ (b3); Third column: $V = 0.4$, energy $E^\alpha = 25.93$ (c1), $E^\alpha = 13.24$ (c2), $E^\alpha = 6.05$ (c3).