Role of the initial conditions in the FPU problem

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Antonio Ponno

University of Padova, Italy
www.math.unipd.it/~ponno

most of results from a preprint - under review, JSP - in collaboration with G. Benettin (Padova) and R. Livi (Firenze)
To begin with...
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THANKS!
Outline part I

Historical foreword: motivations
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2. Model, relevant quantities, numerics
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3. Numerical results
Theory I: “clean” results
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- Resonant normal form construction: *FG-truncation* of the Korteweg-de Vries equation

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  - Time-scales

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- **Aim of the work:** numerical test of the ergodic hypothesis on simple models of quasi-integrable Hamiltonian systems having a large number of degrees of freedom.

- **Unexpected result:** for the examined systems, time-averages of relevant quantities do not approach the expected value (w.r. to the supposed ergodic measure) within the integration time.

- The motivation of the study goes back to previous works of Poincaré and Fermi himself on the subject.
Study the *prototype* Hamiltonian problem

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H_N(q, p) = \sum_{j=0}^{N-1} \left[ \frac{p_j^2}{2} + \frac{r_j^2}{2} + \alpha \frac{r_j^3}{3} + \beta \frac{r_j^4}{4} \right]
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(2) Model, relevant quantities, numerics

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\[ M_0/N \ll 1 \quad ; \quad E_N = H_N(q(0), p(0)) = N\epsilon \]
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\[k = 1, \ldots, N - 1\] (dispersion relation)
\[ H_N(z, z^*) = \sum_{k=1}^{N-1} \omega_k |z_k|^2 + \frac{2\alpha}{3\sqrt{N}} \sum_{k_1, k_2, k_3=1}^{N-1} \Delta_{k_1, k_2, k_3} \prod_{s=1}^{3} \sqrt{\omega_{k_s}} \text{Re}(z_{k_s}) \]
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\[ \Delta_{k_1, k_2, k_3} = \delta_{k_1, k_2+k_3} + \delta_{k_2, k_1+k_3} + \delta_{k_3, k_1+k_2} - \delta_{k_1+k_2+k_3, 2N} \]
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- a *metastable state*, or “quasi-state” characterized by an exponentially decaying energy spectrum - 
  \[ E_k \sim C \left( \frac{k}{N} \right)^p e^{-\gamma(\epsilon)k/N} \] - persists for very long times.
INITIAL DATA:

\[ z_k(0) = \frac{A_k \omega_k + i B_k}{\sqrt{2} \omega_k} \quad , \quad E_k(0) = \frac{B_k^2 + \omega_k^2 A_k^2}{2} \]
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An interesting example:

\[ z_k(0) = \sqrt{\frac{N\varepsilon}{M_0 \omega_k}} \cdot e^{-i \phi_k}, \quad E_k(0) = \frac{N\varepsilon}{M_0} \]

\((k = 1, \ldots, M_0, \text{ zero otherwise})\) with different choices of the initial phases \(\phi_k\).
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One defines the (normalized, time-averaged) modal energy spectrum:

\[
\frac{\bar{E}_k(t)}{\varepsilon} = \frac{1}{\varepsilon t} \int_0^t E_k(s) ds \quad \text{vs.} \quad k/N
\]
Figure: Snapshots of a modal energy spectrum: $N = 1024$, $\varepsilon = 2.5 \cdot 10^{-4}$, 10% of modes initially excited, random phases; notice the persistence of the exponential tail
The effective number $M(t)$ of active modes at time $t$ is measured by a Boltzmann-Shannon-like counter:

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Effective density \( f(t) \) of active modes:

\[
f(t) = \frac{M(t)}{N} = \frac{e^{S(t)}}{N}
\]

\( \mathcal{P}_k = 1/N \) at equilibrium, and \( f_{eq} = 1 \).
Effective density $f = \frac{M}{N}$ of active modes vs. time; $N = 1024$, $\varepsilon = 2.5 \cdot 10^{-4}$ and $\varepsilon = 10^{-3}$, $f(0) = 0.1$
Initial excitation of $M_0$ low-frequency, consecutive normal modes with the same energy. Two kinds of choices for their phases.
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- **Random phases**: $\phi_k$'s i.i.d. random variables with uniform density in $[0, 2\pi]$ ($k = 1, \ldots, M_0$).
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- **Coherent phases**: either $\phi_k$’s all equal, or regularly spaced ($\phi_k = \phi_1 + (k - 1)\psi$).
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Does it matter at all?
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Does it matter at all? Look at an example:
Figure: Effective density $f = \frac{M}{N}$ of active modes vs. time; $N = 1024$, $\varepsilon = 2.5 \cdot 10^{-4}$, $f(0) = 0.1$ ($M_0 = 102$); six different choices of phases
Independently of phases one finds the following two phenomenological scaling laws satisfied by the effective density of active modes $f(t, N, \varepsilon, M_0)$:
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Independently of phases one finds the following two phenomenological scaling laws satisfied by the effective density of active modes $f(t, N, \varepsilon, M_0)$:

(S1) \[ f(\lambda^{-3/4} t, \lambda^{-1/4} N, \lambda \varepsilon, M_0) = \lambda^{1/4} f(t, N, \varepsilon, M_0) \]

(S2) \[ f(\mu^{3/2} t, \mu N, \varepsilon, M_0) = f(t, N, \varepsilon, M_0) \]

where $\lambda, \mu > 0$. 
Independently of phases one finds the following two phenomenological scaling laws satisfied by the effective density of active modes $f(t, N, \varepsilon, M_0)$:

\begin{align*}
\text{(S1)} & \quad f(\lambda^{-3/4}t, \lambda^{-1/4}N, \lambda\varepsilon, M_0) = \lambda^{1/4}f(t, N, \varepsilon, M_0) \\
\text{(S2)} & \quad f(\mu^{3/2}t, \mu N, \varepsilon, M_0) = f(t, N, \varepsilon, M_0)
\end{align*}

where $\lambda, \mu > 0$.

(S1) can be predicted exactly from KdV scaling; (S2) has no clear explanation (but for some a fortiori heuristic estimate).
(3) Numerical results

Figure: Check of scaling (S1); $\lambda_j = 2^{-j+2}, j = 0, \ldots 7$, $\varepsilon_{\text{ref}} = 2.5 \cdot 10^{-4}$, $N_{\text{ref}} = 4096$; random phases.
Figure: Check of scaling (S1); $\lambda_j = 2^{-j+2}, j = 0, \ldots, 7$, $\varepsilon_{ref} = 2.5 \cdot 10^{-4}$, $N_{ref} = 4096$; equal phases: kick-like initial condition.
Figure: Check of scaling (S2); $\mu_j = 2^j, j = 0, \ldots 4$, $\varepsilon = 2.5 \cdot 10^{-4}$, $N_{\text{ref}} = 1024$, $M_0 = 26$ random phases.
Figure: Check of scaling (S2); $\mu_j = 2^j$, $j = 0, \ldots, 4$, $\varepsilon = 2.5 \cdot 10^{-4}$, $N_{\text{ref}} = 1024$, $M_0 = 26$ equal phases: zero initial velocities.
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\[ f(t, N, \varepsilon, M_0) = \varepsilon^{1/4} \mathcal{F}(\varepsilon^{3/8} N^{-3/2} t, M_0) \]

where \( \mathcal{F} \) is a suitable function of two variables depending on the choice of the phases.
FIRST CONCLUSION

Combining the scaling laws (S1) and (S2) together, one gets

$$f(t, N, \varepsilon, M_0) = \varepsilon^{1/4} F(\varepsilon^{3/8} N^{-3/2} t, M_0)$$

where $F$ is a suitable function of two variables depending on the choice of the phases.

In other words: if $M_0$ is kept fixed - independent of $N$ - then $f \sim \varepsilon^{1/4}$ on a time-scale $\tau_1 \sim N^{3/2} \varepsilon^{-3/8}$. 
In the case of finite density $f_0 = M_0/N$ of modes initially excited, the dependence of $\mathcal{F}$ on $M_0$ is strongly affected by the initial choice of the phases.
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- **Random phases:**

\[
    f(t, N, \varepsilon, M_0) = \varepsilon^{1/4} G(\varepsilon^{3/8} f_0^{3/2} t) \quad (RP)
\]
In the case of finite density $f_0 = M_0/N$ of modes initially excited, the dependence of $\mathcal{F}$ on $M_0$ is strongly affected by the initial choice of the phases. One finds:

- Random phases:

$$ f(t, N, \varepsilon, M_0) = \varepsilon^{1/4} G(\varepsilon^{3/8} f_0^{3/2} t) \quad (RP) $$

i.e. $f \sim \varepsilon^{1/4}$ on a t.s. $\tau_1 \sim \varepsilon^{-3/8} f_0^{-3/2} > \varepsilon^{-3/4}$. 
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Figure: Check of scaling (RP), two values of $\varepsilon$, four values of $N$. 
Figure: Check of scaling (CP); left: $\phi_k = \pi/2$; right: $\phi_k = k\pi/2$
CONCLUSION:
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- The FPU scenario with extended initial excitations and random phases might persist in the thermodynamic limit.
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- The FPU scenario with extended initial excitations and random phases might persist in the thermodynamic limit.
- No t.d. limit persistence is expected to be possible with extended excitations and coherent phases.
Mode-coupling is ruled by the selector

\[ \Delta_{k_1, k_2, k_3} = \delta_{k_1+k_2, k_3} + \delta_{k_2+k_3, k_1} + \delta_{k_3+k_1, k_2} - \delta_{k_1+k_2+k_3, 2N} \]

with corresponding processes

\[ \omega_{k_1} + \omega_{k_2} \simeq \omega_{k_3 = k_1+k_2} \]

small denominators: forbidden to low modes
Resonant normal form construction

STRA TEGY
Resonant normal form construction

**STRATEGY**

\[(q, p)_{FPU} \xrightarrow{\text{Perturbation theory}} (\xi, \xi^*)_{FPU}\]

\[U_{KdV} \xleftarrow{\text{analyticity}} (u, u^*)_{FG-KdV} \xrightarrow{\text{reconstruction}} \]

Normal form
Perform the canonical rescaling \((z, t, H_N) \mapsto (\zeta, \tau, K_N)\) defined by

\[
\zeta_k = \frac{z_k}{N \sqrt{2\epsilon}}, \quad \tau = \frac{t}{2N}, \quad K_N = \frac{H_N}{N\epsilon}
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where \(0 < \epsilon = \varepsilon + O(\varepsilon^{3/2})\). Define \(\mu = \alpha\sqrt{\epsilon}\), \(L = 2N\sqrt{\mu}\) (\(\alpha > 0\) w.l.g.) and expand \(\omega_k\).
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\[
K_N(\zeta, \zeta^*) = \sum_{k=1}^{N-1} (2\pi k)|\zeta_k|^2 + \mu W(\zeta, \zeta^*) + O(\mu^2)
\]
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\]

where

\[
W = -\sum_{k=1}^{N-1} \frac{(2\pi k)^3}{24L^2} |\zeta_k|^2 + \frac{2}{3} \sum_{k_1, k_2, k_3=1}^{N-1} \Delta_{k_1, k_2, k_3} \prod_{s=1}^{3} \sqrt{2\pi k_s} \operatorname{Re}(\zeta_{k_s})
\]

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Role of the initial conditions in the FPU problem
Unperturbed \((\mu = 0)\) motion: \(\zeta = e^{-i2\pi J \tau} \zeta(0),\) 1-periodic in time, 
\(J = \text{diag}(1, \ldots, N - 1)\) (i.e. \(\zeta_k = e^{-i2\pi k \tau} \zeta_k(0))\).
Unperturbed ($\mu = 0$) motion: $\zeta = e^{-i2\pi J_\tau} \zeta(0)$, 1-periodic in time, $J = \text{diag}(1, \ldots, N-1)$ (i.e. $\zeta_k = e^{-i2\pi k\tau} \zeta_k(0)$).

**Proposition (Averaging)**

There exists a canonical transformation $(\zeta, \zeta^*) \mapsto (\xi, \xi^*)$, $\mu$-close to the identity, such that

$$K_N(\xi, \xi^*) = \sum_{k=1}^{N-1} (2\pi k)|\xi_k|^2 + \mu \overline{W}(\xi, \xi^*) + O(\mu^2)$$

where

$$\overline{W}(\xi, \xi^*) = \int_0^1 W(e^{-i2\pi J_\tau} \xi, e^{i2\pi J_\tau} \xi^*) \, d\tau$$

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Role of the initial conditions in the FPU problem
Introducing the time-dependent transformation to noncanonical co-rotating coordinates

\[(\xi, \tau, K_N) \mapsto (u, T, \overline{W} + O(\mu))\]

\[u = \sqrt{2\pi J} \ e^{i2\pi J \tau \xi}, \quad T = \mu \tau\]
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the resonant normal form Hamiltonian of the FPU system is

\[
\overline{W}(u, u^*) = -\sum_{k=1}^{N-1} \frac{(2\pi k)^2}{24L^2} |u_k|^2 + \frac{1}{4} \sum_{k_1, k_2, k_3=1}^{N-1} \delta_{k_1+k_2+k_3}(u_{k_1}^* u_{k_2}^* u_{k_3} + c.c.)
\]

up to a remainder \(O(\mu)\).
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\]

up to a remainder $O(\mu)$. The equations of motion are

\[
\frac{d u_k}{dT} = -i(2\pi k) \frac{\partial \overline{W}}{\partial u_k^*}
\]
Proposition

The Hamilton equations of $\overline{W}(u, u^*)$ coincide with the Fourier-Galerkin truncation to the first $N - 1$ modes of the KdV equation

$$U_T = \frac{1}{24L^2} U_{XXX} + \frac{1}{2} U U_X, \quad X \in \mathbb{T}(= \mathbb{R}/\mathbb{Z})$$

with initial datum satisfying: $\int_0^1 U \, dX = 0$, $\int_0^1 U^2 \, dX = 2$
Proposition

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Thus the KdV equation in the small dispersion regime ($L \propto N \epsilon^{1/4}$ very large) ”formally” describes the dynamics of the FPU problem on the time-scale $t \sim N/\sqrt{\epsilon}$ (recall that $T = t \sqrt{\epsilon}/N$).
The Fourier-Galerkin projection operator $P^N$ is defined by

$$(P^N U)(X, T) = \sum_{k=-N+1}^{N-1} \hat{U}_k(T) e^{-i2\pi kX}.$$
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Define

$$u^N(X, T) \equiv \sum_{k=1}^{N-1} u_k e^{-i2\pi kX} + u_k^* e^{i2\pi kX}$$
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One has

$$\overline{W} = - \frac{1}{48L^2} \int_0^1 (u^N_X)^2 dX + \frac{1}{12} \int_0^1 (u^N)^3 dX$$
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and

$$\frac{du_k}{dT} = -i(2\pi k) \frac{\partial \overline{W}}{\partial u_k^*} \iff u^N_T = \partial_X \mathbf{P}^N \left( \frac{\delta \overline{W}}{\delta u^N} \right)$$
Recall that \( U_T = \frac{1}{24L^2} U_{XXX} + \frac{1}{2} U U_X \) and \( L \propto N \epsilon^{1/4}, \; T \propto \sqrt{\epsilon t / N} \).
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$$\epsilon \to \lambda \epsilon, \quad N \to \lambda^{-1/4} N, \quad t \to \lambda^{-3/4} t$$

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leaves the KdV equation invariant. Based on Cauchy estimates, for the effective density of active modes \( f = M / N \) one expects

\[
 f \propto \frac{L}{N} = \epsilon^{1/4} \quad \overset{(*)}{\Rightarrow} \quad f \rightarrow \lambda^{1/4} f
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leaves the KdV equation invariant. Based on Cauchy estimates, for the effective density of active modes $f = M/N$ one expects

$$
f \propto \frac{L}{N} = \varepsilon^{1/4} \quad \Rightarrow \quad f \rightarrow \lambda^{1/4} f
$$

which implies

$$
f(\lambda^{-3/4} t, \lambda^{-1/4} N, \lambda \varepsilon, M_0) = \lambda^{1/4} f(t, N, \varepsilon, M_0)
$$
Theorem (Kappeler-Pöschel 07)

Consider the KdV equation \( U_T = \delta U_{XXX} + \frac{1}{2}UU_X \).

If the initial datum \( U(X,0), X \in \mathbb{T} \), is analytic in the (maximal) complex strip \( \{ |\text{Im}(z)| \leq a \} \), then there exists \( 0 < \rho(\delta) \leq 1 \) s.t. the corresponding solution \( U(X, T) \) is analytic in the complex strip \( \{ |\text{Im}(z)| \leq a\rho(\delta) \} \) for any \( T \in \mathbb{R} \).
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That is to say: analytic initial data evolve into global solutions which are analytic in a possibly narrower but finite-width strip.
Regularity of solutions

**Theorem (Kappeler-Pöschel 07)**

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That is to say: analytic initial data evolve into global solutions which are analytic in a possibly narrower but finite-width strip.

No estimate of \( \rho(\delta) \) available: we are interested in the limit \( \delta \to 0! \)
Consider the KdV equation $U_T = \frac{1}{24L^2} U_{XXX} + \frac{1}{2} UU_X$. 
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By the TKP thm \( U(z, T) \) analytic in \( \{|\text{Im}(z)| \leq \sigma(T; L)\} \).
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Define

\[
\mathcal{M}(T; L) \equiv \max_{\text{Re}(z) \in [0,1], |\text{Im}(z)| = \sigma(T; L)} |U(z, T)| ;
\]

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Role of the initial conditions in the FPU problem
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Define

$$\mathcal{M}(T; L) \equiv \max_{\text{Re}(z) \in [0,1]} |U(z, T)| ;$$

then (Cauchy)

$$\frac{1}{24L^2} U_{XXX} \leq \frac{\mathcal{M}}{4L^2\sigma^3} , \quad \frac{1}{2}UU_X \leq \frac{\mathcal{M}^2}{2\sigma}$$
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\[
\frac{1}{24L^2} U_{XXX} \leq \frac{M}{4L^2 \sigma^3} \quad , \quad \frac{1}{2} U U_X \leq \frac{M^2}{2 \sigma} \]

Notice that as \( L \to \infty \) the KdV eqn approaches the Burgers-Hopf eqn \( U_T = \frac{1}{2} U U_X \), whose solutions display vertical slopes in a finite critical time \( T_c = O(1) \).
HEURISTIC ARGUMENTS:

- for any fixed $T > T_c$, $\sigma(T; L) \to 0$ as $L \to \infty$;
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- for any fixed $T > T_c$, $\sigma(T; L) \to 0$ as $L \to \infty$;
- requiring, in the limit, constant ratio of the above Cauchy upper bounds yields

$$\sigma(T; L) \sim \frac{c(T)}{L} \quad (L \to \infty)$$

where $c(T) > \overline{c} > 0 \ \forall T \in \mathbb{R}$ due to the KP thm.
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- m.e.s.: \( E_k(T) = |\hat{U}_k(T)|^2 \leq C e^{-2\sigma|k|} \leq C e^{-\frac{2c|k|}{N_{\varepsilon}^{1/4}}} \);
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- d.a.m.: $f \propto \frac{1}{N\sigma} \propto \varepsilon^{1/4}$
$U(X, T)$: solution of the KdV eqn with in.dat. $U(X, 0)$;
Asymptotic reconstruction

$U(X, T)$: solution of the KdV eqn with in.dat. $U(X, 0)$;

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**Theorem (Kalisch 05)**

Suppose $U(X, 0) \in \mathcal{H}^{a_0, s}$, where $a_0 > 0$ and $s > 0$; then, for any fixed $T > 0$ there exist two positive constants $\lambda(T)$ and $a(T)$ s.t.

$$\sup_{t \in [0, T]} \| U(\cdot, t) - u_N(\cdot, t) \|_{L^2} \leq \lambda(T) \frac{e^{-a(T)N}}{N^{s-1}}$$
Asymptotic reconstruction

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\sup_{t \in [0, T]} \| U(\cdot, t) - u_N(\cdot, t) \|_{L^2} \leq \lambda(T) \frac{e^{-a(T)N}}{N^{s-1}}
$$

That is to say: $u^N$ and $U$ can be made arbitrarily close on any fixed time-interval if $N$ is large enough.
Heuristic estimates of $f$ are based on the dispersion-nonlinearity balance in the KdV equation written in Fourier space:
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$$\frac{1}{L^2} \hat{U}_{xxx} \approx \frac{1}{2} \hat{U}U_x$$
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\[
\frac{1}{L^2} \hat{U}_{XXX} \approx \frac{1}{2} \hat{U} \hat{U}_X
\]

i.e.

\[
\frac{k^2}{N^2 \sqrt{\varepsilon}} \approx \frac{(\hat{U} * \hat{U})_k}{\hat{U}_k}
\]
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i.e.

$$\frac{k^2}{N^2 \sqrt{\varepsilon}} \approx \frac{(\hat{U} \ast \hat{U})_k}{\hat{U}_k}$$

The r.h.s. is evaluated on the initial condition

$$U(X, 0) = \frac{2}{\sqrt{M_0}} \sum_{k=1}^{M_0} \cos(2\pi kX + \phi_k)$$
One gets

\[ \frac{k^2}{N^2 \sqrt{\varepsilon}} \approx \left\{ \begin{array}{c} \sqrt{M_0} \\ O(1) \end{array} \right\} \quad (CP) \quad (RP) \]
Coherence effects

One gets

\[ \frac{k^2}{N^2 \sqrt{\varepsilon}} \approx \begin{cases} \sqrt{M_0} & (CP) \\ O(1) & (RP) \end{cases} \]

Thus

\[ f \approx \frac{k_c}{N} \approx \begin{cases} (M_0 \varepsilon)^{1/4} = (f_0 E)^{1/4} & (CP) \\ \varepsilon^{1/4} & (RP) \end{cases} \]
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This is a rough, though eventually correct, explanation of the observed dependence of the dynamics on the phases.
Time scales are evaluated by comparing the time-derivative term with the linear one in the KdV equation, recalling that
\[ t = \left( \frac{N}{\sqrt{\varepsilon}} \right) T: \]
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which, evaluated at \( f \approx k_c/N \), yields

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\[ \tau \approx \begin{cases} (M_0 \varepsilon)^{-3/4} = (f_0 E)^{-3/4} & (CP) \\ \varepsilon^{-3/4} & (RP) \end{cases} \]

both being lower bounds to \( \tau_1 \)!
Conclusions: open problems

- Rigorous estimate of $\sigma(T; L)$ - perhaps a possibility, in a paper by Venakides
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- Second stage of the story: breakdown of KdV approximation and estimate of the time-scale to equipartition - difficult