Kinetic theory of (lattice) waves

Jani Lukkarinen

based on joint works with

Herbert Spohn (TU München), Matteo Marcozzi (U Geneva), Alessia Nota (U Bonn), Christian Mendl (Stanford U), Jianfeng Lu (Duke U)

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Part I

Time-correlations in stationary states of the discrete NLS

Setup for the rigorous result

- **Finite lattice:** \( L \geq 2, \quad \Lambda = \{0, 1, \ldots, L - 1\}^d \)

- **Periodic BC:** \textit{All arithmetic \ mod \ L}

- **Dual lattice:** \( \Lambda^* = \{0, \frac{1}{L}, \ldots, \frac{L-1}{L}\}^d \)

- **"Integration"** = finite sum:
  \[
  \int_{\Lambda^*} dk \ f(k) := \frac{1}{|\Lambda|} \sum_{k \in \Lambda^*} f(k)
  \]

- **"Dirac delta"** = finite sum:
  \[
  \delta_{\Lambda}(k) := |\Lambda| \mathbb{1}_{\{k \ mod \ 1 = 0\}}
  \]

- **Fourier transform:** \((x \in \Lambda, \ k \in \Lambda^*)\)
  \[
  \hat{f}(k) = \sum_{y \in \Lambda} f(y) e^{-i2\pi k \cdot y} \quad \Rightarrow \quad f(x) = \int_{\Lambda^*} dk' \hat{f}(k') e^{i2\pi k' \cdot x}
  \]
Evolution equations

Discrete nonlinear Schrödinger equation

\[ i \frac{d}{dt} \psi_t(x) = \sum_{y \in \Lambda} \alpha(x - y) \psi_t(y) + \lambda |\psi_t(x)|^2 \psi_t(x) \]

- \( \psi_t : \Lambda \to \mathbb{C}, \quad t \in \mathbb{R} \)
- \( \lambda > 0 \) (defocusing)
- Harmonic coupling determined by \( \alpha : \mathbb{Z}^d \to \mathbb{R} \).
- \( \alpha \) has finite range (for instance, nearest neighbour)
- We assume also \( \alpha(-x) = \alpha(x) \)
Conservation laws

Hamiltonian function

\[ H_\Lambda(\psi) = \sum_{x,y \in \Lambda} \alpha(x - y)\psi(x)^*\psi(y) + \frac{1}{2}\lambda \sum_{x \in \Lambda} |\psi(x)|^4 \]

- Relate \( q_x, p_x \in \mathbb{R} \) to \( \psi \) by \( \psi(x) = \frac{1}{\sqrt{2}}(q_x + ip_x) \)
- NLS equivalent to the Hamiltonian equations
  \[ \dot{q}_x = \partial_{p_x} H_\Lambda, \quad \dot{p}_x = -\partial_{q_x} H_\Lambda \]
- Thus \( H_\Lambda(\psi_t) \) is conserved
- By explicit differentiation, also \( \sum_x |\psi_t(x)|^2 \) is conserved
Initial state

Probability distribution of $\psi = \psi_0$ (Grand canonical ensemble)

$$\frac{1}{Z_{\beta,\mu}^\lambda} e^{-\beta (H_\Lambda(\psi) - \mu \|\psi\|^2)} \prod_{x \in \Lambda} [d(\text{Re} \psi(x)) d(\text{Im} \psi(x))]$$

- Define $\omega : \mathbb{T}^d \to \mathbb{R}$ by $\omega = \mathcal{F}_{x \to k} \alpha$.

- We consider only $\beta > 0$ and $\mu < \min_k \omega(k)$
  $\Rightarrow$ Also the Gaussian measure at $\lambda = 0$ is well-defined

- $Z_{\beta,\mu}^\lambda > 0$ is the normalization constant

- Let $\mathbb{E}$ denote expectation over the initial data
The solution $\psi_t$ exists and is unique for all $t \in \mathbb{R}$ with any initial data $\psi_0 \in \mathbb{C}^\Lambda$. (conservation laws)

Initial state is stationary: $\mathbb{E}[F(\psi_t)] = \mathbb{E}[F(\psi_0)]$

Also invariant under periodic translations:

$\mathbb{E}[F(\tau_x \psi)] = \mathbb{E}[F(\psi)]$, $\ (\tau_x \psi)(y) = \psi(y + x)$

Translations commute with the time-evolution:

$\tau_x \psi_t = \tilde{\psi}_t|_{\tilde{\psi}_0 = \tau_x \psi_0}$

“Gauge invariance”: similar invariance properties hold for translations of total phase, $\psi_0(x) \mapsto e^{i\varphi} \psi_0(x), \varphi \in \mathbb{R}$.

Thus, for instance, $\mathbb{E}[\psi_t] = 0, \mathbb{E}[\psi_t \psi_t] = 0,$

$\mathbb{E}[\psi_t(x')^* \psi_t(x)] = \mathbb{E}[\psi_0(0)^* \psi_{t-t'}(x-x')]$
Fix test-functions $f, g \in \ell_2$, and assume they have finite support.

**Observable**

$$Q^\lambda_{\Lambda}(\tau) := \mathbb{E}\left[\langle \hat{f}, \hat{\psi}_0 \rangle^* \langle e^{-i\omega^\lambda \tau \lambda^{-2}} \hat{g}, \hat{\psi}_{\tau \lambda^{-2}} \rangle\right]$$

Under additional assumptions on the decay of equilibrium correlations and on the dispersion relation:

**Theorem**

There is $\tau_0 > 0$ such that for all $|\tau| < \tau_0$

$$\lim_{\lambda \to 0} \lim_{\Lambda \to \infty} Q^\lambda_{\Lambda}(\tau) = \int_{\mathbb{T}^d} dk \, \hat{g}(k)^* \hat{f}(k) W(k) e^{-\Gamma_1(k)|\tau| - i\tau \Gamma_2(k)}$$

Jani Lukkarinen

Kinetic theory of lattice waves
Summary of the main result

- **Loosely**: for all not too large $t = \mathcal{O}(\lambda^{-2})$,

  \[ \mathbb{E}[\hat{\psi}_0(k')^*\hat{\psi}_t(k)] \approx \delta_\Lambda(k' - k) W(k) e^{-i\omega^\lambda_{\text{ren}}(k)t} e^{-|\lambda^2 t|\Gamma_1(k)} \]

- $W(k) = (\beta(\omega(k) - \mu))^{-1} = \text{covariance function for } \lambda = 0$

- $\omega^\lambda_{\text{ren}}(k) = \omega(k) + \lambda R_0 + \lambda^2 \Gamma_2(k)$

- $\Gamma_1(k) \geq 0$

  $\Rightarrow k$-space correlation decays exponentially in $t$, as dictated by $e^{-|\lambda^2 t|\Gamma_1(k)}$.

- Nearest neighbour couplings ($\omega_{\text{nn}}(k) = c - \sum_{\nu=1}^{d} \cos(2\pi k\nu)$) satisfy all of our assumptions if $d \geq 4$
\( \Gamma_j(k) \) are real, and \( \Gamma(k) = \Gamma_1(k) + i\Gamma_2(k) \) is given by

\[
\Gamma(k_1) = 2 \int_0^\infty dt \int_{(\mathbb{T}^d)^3} dk_2 dk_3 dk_4 \delta(k_1 + k_2 - k_3 - k_4) \\
\times e^{it(\omega_1 + \omega_2 - \omega_3 - \omega_4)} (W_2 W_3 + W_2 W_4 - W_3 W_4)
\]

with \( \omega_i = \omega(k_i), \ W_i = W(k_i) \).

\[
\Rightarrow \quad \Gamma_1(k_1) = 2\pi \frac{1}{W(k_1)^2} \int_{(\mathbb{T}^d)^3} dk_2 dk_3 dk_4 \delta(k_1 + k_2 - k_3 - k_4) \\
\times \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) \prod_{i=1}^4 W(k_i)
\]

\( 2\Gamma_1(k) \geq 0 \) coincides with the loss term of the linearisation of \( \mathcal{C}_{NL} \) around \( W \).

Can be “derived” following the same recipe as for kinetic equations (more later...)
Main tool to handle non-Gaussian initial data
Moments to cumulants formula

Cumulant expansion

For any index set \( I \),

\[
\mathbb{E}\left[ \prod_{i \in I} \hat{\psi}_0(k_i, \sigma_i) \right] = \sum_{S \in \pi(I)} \prod_{A \in S} \left[ \delta_{\Lambda} \left( \sum_{i \in A} k_i \right) C_{|A|}(k_A, \sigma_A) \right],
\]

where the sum runs over all partitions \( S \) of the index set \( I \).

Here truncated correlation (cumulant) functions are

\[
C_n(k, \sigma) := \sum_{x \in \Lambda^n} \mathbb{1}_{\{x_1=0\}} e^{-i2\pi \sum_{i=1}^n x_i \cdot k_i} \mathbb{E}\left[ \prod_{i=1}^n \psi_0(x_i, \sigma_i) \right]^{\text{trunc}}
\]

and for any random variables \( a_1, \ldots, a_n \)

\[
\mathbb{E}\left[ \prod_{i=1}^n a_i \right]^{\text{trunc}} := \kappa[a_1, \ldots, a_n] = \partial_{\eta_1} \cdots \partial_{\eta_n} \ln \mathbb{E}[e^{\sum_i \eta_i a_i}] \bigg|_{\eta=0}
\]
Assumption: decay of initial correlations

\( \ell_1 \)-clustering of the equilibrium measure

- For sufficiently small \( \lambda \) and for all \( n \geq 4 \) the truncated correlation functions (\textit{cumulants}) should satisfy

\[
\sup_{\Lambda, \sigma \in \{\pm 1\}^n} \sum_{x \in \Lambda^n} \mathbb{1}_{\{x_1 = 0\}} \left| \mathbb{E} \left[ \prod_{i=1}^n \psi_0(x_i, \sigma_i)^{\text{trunc}} \right] \right| \leq \lambda c_0^n n!
\]

- For \( n = 2 \) should have

\[
\sum_{\|x\|_\infty \leq L/2} \left| \mathbb{E}[\psi_0(0)^* \psi_0(x)] - \mathbb{E}[\psi_0(0)^* \psi_0(x)]_{L=\infty}^{\lambda=0} \right| \leq \lambda 2 c_0^2
\]

- Proven in [Abdesselam, Procacci, and Scoppola, 2009]

- Estimates imply that \( \|C_n\|_\infty < \infty \)

  \( \Rightarrow \) cumulant expansion encodes all singularities in \( k_i \)

- The rest is “just” analysis of oscillatory integrals...
Part II

Asymptotic independence, evolution of cumulants, and kinetic theory

Goal: Kinetic theory of homogeneous DNLS

Assume that the initial state is translation invariant, "gauge invariant" and with fast decay of correlations.

Then there always is $\tilde{w}_t(x)$ such that

$$\mathbb{E}[\psi_t(x')^*\psi_t(x)] = \tilde{w}_t(x' - x)$$

Kinetic conjecture: $W_\tau = \lim_{\lambda \to 0} \lim_{\Lambda \to \infty} (\mathcal{F} \tilde{w}_{\tau\lambda}^{-2})$ solves a homogeneous non-linear Boltzmann–Peierls equation

$$\partial_\tau W_\tau(k) = C_{NL}[W_\tau(\cdot)],$$

$$C_{NL}[h](k_1) = 4\pi \int_{(T^d)^3} dk_2 dk_3 dk_4 \delta(k_1 + k_2 - k_3 - k_4) \times \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) [h_2 h_3 h_4 - h_1 (h_2 h_3 + h_2 h_4 - h_3 h_4)]$$
Observation: If $y, z$ are independent random variables we have

$$E[y^n z^m] = E[y^n]E[z^m] \neq 0$$

whereas the corresponding cumulant is zero if $n, m \neq 0$. 
**Observation:** If \( y, z \) are independent random variables we have\[
\mathbb{E}[y^n z^m] = \mathbb{E}[y^n] \mathbb{E}[z^m] \neq 0
\]
whereas the corresponding cumulant is zero if \( n, m \neq 0 \).

Consider a random lattice field \( \psi(x), x \in \mathbb{Z}^d \), which is (very) strongly mixing under lattice translations:

Assume that the fields in well separated regions become asymptotically independent as the separation grows.

- Then \( \kappa[\psi(x), \psi(x + y_1), \ldots, \psi(x + y_{n-1})] \rightarrow 0 \) as \( |y_i| \rightarrow \infty \).
  
  How fast? \( \ell_1 \)- or \( \ell_2 \)-summably?

- Not true for corresponding moments: \( \mathbb{E}[|\psi(x)|^2|\psi(x + y)|^2] \)
Call the field $\ell_p$-clustering if

$$\sup_{x \in \mathbb{Z}^d} \sum_{y \in (\mathbb{Z}^d)^{n-1}} |\kappa[\psi(x), \psi(x + y_1), \ldots]|^p < \infty, \forall n.$$ 

- If $1 \leq p \leq 2$, can take Fourier-transform in $y$ 
  $\Rightarrow$ functions $F^{(n)}(x, k)$, $L^\infty$ in $x \in \mathbb{Z}^d$ and $L^2$-integrable for $k \in (\mathbb{T}^d)^{n-1}$.

- $\ell_1$-clustering implies that $F^{(n)}(x, k)$ is continuous and uniformly bounded ($\Rightarrow$ helps in nonlinearities)

- Many examples of $\ell_1$-clustering thermal Gibbs states, e.g., discrete NLS [Abdesselam, Procacci, Scoppola]
As before, consider \textit{deterministic evolution} of $\psi_t$, with \textit{random initial data} for $\psi_0$.

- Cumulants are \textit{multilinear} and \textit{permutation invariant}

$$\Rightarrow \partial_t \kappa[\psi_t(x_\ell)_{\ell=1}^n] = \sum_{\ell=1}^n \kappa[\partial_t \psi_t(x_\ell), \psi_t(x_{\ell'})_{\ell' \neq \ell}]$$

- Solution? How to iterate into a closed hierarchy?
- Computations often simplified by using Wick polynomial representation of $\partial_t \psi_t$
Consider the DNLS with *initial data* for $\psi_0$ which is

- $\ell_1$-*clustering*

- *Gauge invariant*: $\psi_0(x) \sim e^{i\theta} \psi_0(x)$ for any $\theta \in \mathbb{R}$
  $\Rightarrow$ also $\psi_t$ will then be gauge invariant.

- *Slowly varying in space*: the cumulants vary only slowly under spatial translations

Then, for instance, $(x, y) \mapsto \mathbb{E}[\psi_0(x)^* \psi_0(x + y)]$ is slowly varying in $x$ and $\ell_1$-summable in $y$.

- Denote

  $$W_t(x, k) = \sum_{y \in \mathbb{Z}^d} e^{-i2\pi k \cdot y} \mathbb{E}[\psi_t(x)^* \psi_t(x + y)]$$

- In the spatially homogeneous case, $W_t(x, k) = W_t(k) = \text{Wigner function}$ (as defined in earlier works)
Higher order Wigner functions

\( \psi_t(x, +1) = \psi_t(x) \) and \( \psi_t(x, -1) = \psi_t(x)^* \)

If \( \ell_p \)-clustering is preserved by the time-evolution, should study

Order-\( n \) “Wigner functions”:
\[ x \in \mathbb{Z}^d, \, k \in (\mathbb{T}^d)^{n-1}, \, \sigma \in \{\pm 1\}^n \]

\[ F_t^{(n)}(x, k, \sigma) = \sum_{y \in (\mathbb{Z}^d)^{n-1}} e^{-i2\pi k \cdot y} \kappa[\psi_t(x, \sigma_1), \psi_t(x + y_1, \sigma_2), \ldots, \psi_t(x + y_{n-1}, \sigma_n)] \]

1. Now \( W_t(x, k) = F_t^{(2)}(x, k, (-1, 1)) \)
2. Its derivative involves only \( W \) and \( F^{(4)} \)
3. Compute also the derivative of \( F^{(4)} \) and “solve” both by integrating out the free evolution (in Duhamel form)
4. Insert \( F^{(4)} \) result into \( W \), and check/argue that the remaining \( F^{(4)} \) and \( F^{(6)} \) can be ignored for \( t^{-1}, \lambda \ll 1 \)
With $\omega(k) = \hat{\alpha}(k)$ and $\rho_t(x) = \mathbb{E}[|\psi_t(x)|^2] = \int dk \ W_t(x, k)$,

$$\partial_t W_t(x, k) = -i \sum_z \alpha(z) e^{i 2\pi k \cdot z} (W_t(x, k) - W_t(x - z, k))$$

$$-i 2\lambda \sum_z (\rho_t(x + z) - \rho_t(x)) \int dk' e^{i 2\pi z \cdot (k' - k)} W_t(x, k')$$

$$-i \lambda \int dk'_1 dk'_2 \left( F_t^{(4)}(x, k'_1, k'_2, k - k'_1 - k'_2) - F_t^{(4)}(x, k'_1, k'_2, k) \right)$$
With $\omega(k) = \hat{\alpha}(k)$ and $\rho_t(x) = \mathbb{E}[|\psi_t(x)|^2] = \int dk \ W_t(x,k)$, 

$$
\partial_t W_t(x,k) = -i \sum_z \alpha(z) e^{i2\pi k \cdot z} (W_t(x,k) - W_t(x-z,k))
$$

$$
- i2\lambda \sum_z (\rho_t(x+z) - \rho_t(x)) \int dk' \ e^{i2\pi z \cdot (k' - k)} W_t(x,k')
$$

$$
- i\lambda \int dk'_1 dk'_2 \left( F^{(4)}_t(x, k'_1, k'_2, k - k'_1 - k'_2) - F^{(4)}_t(x, k'_1, k'_2, k) \right)
$$

$$
\approx -\frac{1}{2\pi} \nabla_k \omega(k) \cdot \nabla_x W_t(x,k) + 2\lambda \nabla_x \rho_t(x) \cdot \frac{1}{2\pi} \nabla_k W_t(x,k) + \lambda^2 C_{NL}[W_t(x,\cdot)](k)
$$

- $O(\lambda)$ term is of Vlasov–Poisson type

- The first two terms vanish for spatially homogeneous states

- Using the same recipe in Part I yields $\Gamma(k)$
Part III

Kinetic theory of the onsite FPU-chain (DNKG) with pre-thermalization

Pre-thermalization = quasi-thermalization

The system is thermalized but with “wrong” equilibrium states (e.g. extra conservation laws)

- Happens if there are quasi-conserved observables with very long equilibration times (e.g. with relaxation times of order $e^L$ for system size $L$)

- Problematic, since may interfere with relaxation of the “true” conservation laws:

  For instance, if diffusive, $L^2 \ll e^L$ for system $L \gg 1$
We consider a chain of classical particles with nearest neighbour interactions, *dynamics* defined by

The Hamiltonian

\[
H = \sum_{j=0}^{N-1} \left[ \frac{1}{2} p_j^2 + \frac{1}{2} q_j^2 - \frac{1}{2} \delta (q_{j-1} q_j + q_j q_{j+1}) + \frac{1}{4} \lambda q_j^4 \right]
\]

- \( \lambda \geq 0 \) is the *coupling constant* for the *onsite anharmonicity*.
- If \( \lambda = 0 \), the evolution is explicitly solvable using *normal modes* whose *dispersion relations* are \( \pm \omega(k) \) with

\[
\omega(k) = (1 - 2\delta \cos(2\pi k))^{1/2}
\]

- The parameter \( 0 < \delta \leq \frac{1}{2} \) controls the *pinning onsite potential*.
- This model is expected to have (diffusive) *normal heat conduction* for \( \lambda, \delta > 0 \).
From a solution \((q_i(t), p_i(t))\) define

**Phonon fields**

\[
\hat{a}_t(k, \sigma) = \frac{1}{\sqrt{2\omega(k)}} [\omega(k)\hat{q}(k, t) + i\sigma\hat{p}(k, t)] , \quad \sigma \in \{\pm 1\}
\]

\[
\Rightarrow \quad \frac{d}{dt}\hat{a}_t(k, \sigma) = -i\sigma\omega(k)\hat{a}_t(k, \sigma)
\]

\[
-\sigma\lambda \sum_{\sigma' \in \{\pm 1\}^3} \int_{(\Lambda^*)^3} d^3 k' \delta_{\Lambda}(k - \sum_{j=1}^3 k'_j) \prod_{\ell=0}^3 \frac{1}{\sqrt{2\omega(k'_{\ell})}} \prod_{j=1}^3 \hat{a}_t(k'_j, \sigma'_j)
\]

- Here \(k \in \Lambda^* := \{-\frac{1}{2} + \frac{1}{N}, \ldots, \frac{1}{2} - \frac{1}{N}, \frac{1}{2}\}\) for a finite periodic chain of length \(N (= |\Lambda^*|)\)
Assume a **spatially homogeneous state** and consider the corresponding **Wigner function**

\[
 w_t(k; L) := \int_{\Lambda^*} dk' \langle \hat{a}_t(k')^* \hat{a}_t(k) \rangle = \sum_{y \in \Lambda} e^{-i2\pi y \cdot k} \langle a_t(0)^* a_t(y) \rangle
\]

We expect ("**kinetic conjecture**") that then the following limit exists

\[
 W_\tau(k) = \lim_{\lambda \to 0} \lim_{L \to \infty} w_{\lambda^{-2}\tau}(k; L)
\]

- Describes evolution of covariances for large lattices \((L \to \infty)\) at **kinetic time-scales** \((t = \lambda^{-2}\tau = O(\lambda^{-2}))\)
In addition, the limiting Wigner functions should satisfy the following *phonon Boltzmann equation*

\[
\frac{\partial}{\partial t} W(k_0, t) = 12\pi \lambda^2 \sum_{\sigma \in \{\pm 1\}^3} \int_{\mathbb{T}^3} d^3k \prod_{\ell=0}^{3} \frac{1}{2\omega_{\ell}}
\]

\[
\times \delta(k_0 + \sum_{j=1}^{3} \sigma_j k_j) \delta\left(\omega_0 + \sum_{j=1}^{3} \sigma_j \omega_j\right)
\]

\[
\times \left[ W_1 W_2 W_3 + W_0 (\sigma_1 W_2 W_3 + \sigma_2 W_1 W_3 + \sigma_3 W_1 W_2) \right]
\]

- Here \( W_i = W(k_i, t), \quad \omega_i = \omega(k_i) \)
- For chosen *nearest neighbour interactions*, the collision \( \delta \)-functions have solutions only if \( \sum_{j=1}^{3} \sigma_j = -1 \)
Boltzmann–Peierls equation

Kinetic equation (spatially homogeneous initial data)

\[
\frac{\partial}{\partial t} W(k_0, t) = \frac{9\pi}{4} \chi^2 \int_{\mathbb{T}^3} d^3 k \frac{1}{\omega_0 \omega_1 \omega_2 \omega_3} \\
\times \delta(\omega_0 + \omega_1 - \omega_2 - \omega_3) \delta(k_0 + k_1 - k_2 - k_3) \\
\times \left[ W_1 W_2 W_3 + W_0 W_2 W_3 - W_0 W_1 W_3 - W_0 W_1 W_2 \right]
\]

- Stationary solutions are

\[
W(k) = \frac{1}{\beta'(\omega(k) - \mu')}
\]

- \(\mu'\) results from number conservation which is broken by the original evolution (then expect \(\mu' = 0\))
**Microsystem**

\[ w_t(k) = \int dk' \langle a_t(k')^* a_t(k) \rangle \]

\[ \downarrow \]

\[ \partial_\tau W_\tau(k) = C[W_\tau](k) \]

\[ \downarrow \]

\[ \partial_\tau S[W_\tau] = \sigma[W_\tau] \]

\[ \downarrow \]

\[ \sigma[W_{\text{eq}}] = 0 \]

**Dynamics:** free evolution + \( \lambda \times \) perturbation

**Initial state:** translation invariant & “chaotic”

\[ \downarrow \text{(weak coupling)} \]

**Boltzmann equation** for \( W_\tau = \lim_{\lambda \to 0} w_\lambda^{-2\tau} \)

\[ \downarrow \]

\( S = \text{kinetic entropy} \) (H-function)

\( \sigma = \text{entropy production} \geq 0 \)

\[ \downarrow \]

\( \sigma[W_{\text{eq}}] = 0 \leftarrow W_{\text{eq}} \text{ from an equilibrium state} \)

(classifies stationary solutions)
To compare in more detail to kinetic theory, we consider several stochastic, periodic and translation invariant initial data: Then

$$W_{\text{sim}}(k, t) = \frac{1}{N} \langle |a(k, t)|^2 \rangle$$

Computing the covariance from simulated equilibrium states (one parameter, $\beta$) and fitting numerically to the kinetic formula (two parameters, $\beta', \mu'$) yields

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>1</th>
<th>10</th>
<th>100</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta'$</td>
<td>0.912</td>
<td>8.98</td>
<td>97.1</td>
<td>986.4</td>
</tr>
<tr>
<td>$\mu'$</td>
<td>-0.488</td>
<td>-0.229</td>
<td>-0.0426</td>
<td>-0.0120</td>
</tr>
</tbody>
</table>

As expected, $\beta' \approx \beta$ and $\mu' \approx 0$ for large $\beta$.
Set $N = 64$ (periodic BC), $\delta = \frac{1}{4}$ (pinning)

Consider two sets of non-equilibrium initial data:

**A) Bimodal momentum distribution ($\lambda = 1$):**

Choose an initial "temperature" $\beta_0$ and sample positions $q_j$ from the corresponding equilibrium distribution and the momenta $p_j$ from the bimodal distribution

$$Z^{-1} \exp\left[-\beta_0 (4p_j^4 - \frac{1}{2}p_j^2)\right]$$

**B) Random phase, with given initial Wigner function ($\lambda = \frac{1}{2}, 10$):**

Take a function $W_0(k)$ and compute initial $q_j$ and $p_j$ from

$$a(k) = \sqrt{NW_0(k)} e^{i\varphi(k)}$$

where each $\varphi(k)$ is i.i.d. randomly distributed, uniformly on $[0, 2\pi]$
A) Bimodal initial data

Wigner function from simulations (blue dots) vs. solving the kinetic equation (yellow triangles) starting at \( t = 500 \).
(\textit{black dashed line}) Kinetic equilibrium profile fitted to (f)
B) Random phase initial data ($\lambda = \frac{1}{2}$)

Wigner function from simulations (blue dots) vs. solving the kinetic equation (yellow triangles) starting at $t = 500$. 
(f) Expected equilibrium distribution (red dot-dashed line)
Eventual relaxation towards equilibrium? ($\lambda = 10$)

Figure: Time evolution of the density and energy differences using $\lambda = 10$ ($\Rightarrow$ kinetic time-scale $(\frac{\beta}{\lambda})^2 \approx 10$) and longer simulation time $t_{\text{max}} = 10^6$

(a) $\rho_{\text{sim}}(t) - \rho_{\text{sim}}(t_{\text{max}})$

(b) $e_{\text{sim}}(t) - e_{\text{sim}}(t_{\text{max}})$

Will this trend continue until true equilibrium values have been reached?
Open problems

Pre-thermalization: What is going on here?
   Is it 1D effect only?
   ... or finite size?
   ... or just for some initial data?

Inhomogeneous initial data:
   Does kinetic theory perform as well?
   ... with the Vlasov–Poisson term?
   Proofs and proper assumptions?

For rigorous proofs of time-correlations:
   a priori estimates for propagation of clustering for equilibrium time-correlations derived in
   Anything similar for non-stationary states?
Appendix
Outline of the proof

1. Show that it is enough to prove the result assuming $t > 0$

2. Iterate a Duhamel formula $N_0(\lambda)$ times to expand $a_t$ into a perturbation sum (we choose $N_0! \approx \lambda^{-p}$, for a small $p$)

3. There are two types of terms in the expansion:
   - **Main terms**: These will contain a finite monomial of $a_0$ whose expectation can be evaluated using the “moments to cumulants formula”.
   - **Error terms**: These will involve also $a_s$ for some $s > 0$. The expectation is estimated by a Schwarz bound and stationarity of the equilibrium measure

   $\Rightarrow$ The bound involves again only finite moments of $a_0$. 
4 Each cumulant induces linear dependencies between the wave vectors. These can be encoded in “Feynman graphs”.

5 This results in a sum with roughly \((N_0!)^2\) non-zero terms. However, most of these vanish in the limit \(\lambda \to 0\), due to oscillating phase factors.

6 Careful classification of graphs: we use a special resolution of the wave vector constraints which allows an estimation based on identifying, and iteratively estimating, certain graph motives.

7 Only a small fraction of the graphs (leading graphs) will remain. These consist of graphs obtained by iterative addition of one of the 20 leading motives.

8 The limit of the leading graphs is explicitly computable, and their sum yields the result in the main theorem.
Wick polynomials

Generating functions

\[ g_t(\lambda) := \ln g_{\text{mom},t}(\lambda), \quad g_{\text{mom},t}(\lambda) := \mathbb{E}[e^{\lambda \cdot \psi_t}]. \]

Then with \( \partial^J_{\lambda} := \prod_{i \in J} \partial_{\lambda_i}, \ y^J = \prod_{i \in J} y_i, \)

\[ \kappa[\psi_t(x)J] = \partial^J_{\lambda} g_t(0), \quad \mathbb{E}[\psi_t(x)^J] = \partial^J_{\lambda} g_{\text{mom},t}(0) \]

Define

\[ G_w(\psi_t, \lambda) = \frac{e^{\lambda \cdot \psi_t}}{\mathbb{E}[e^{\lambda \cdot \psi_t}]} \]

\[ \Rightarrow \partial_t \kappa[\psi_t(x)J] = \partial^J_{\lambda} \partial_t g_t(\lambda)|_{\lambda=0} = \partial^J_{\lambda} \mathbb{E}[\lambda \cdot \partial_t \psi_t \ G_w(\psi_t, \lambda)]|_{\lambda=0} \]

\[ = \sum_{\ell \in J} \mathbb{E}[\partial_t \psi_t(x_\ell) \partial^{J\setminus \ell}_{\lambda} G_w(\psi_t, 0)] \]

\[ \partial^J_{\lambda} G_w(\psi_t, 0) = :\psi_t(x)^J: \text{ are called Wick polynomials} \]
WP have been mainly used for Gaussian fields. They were introduced in quantum field theory where the unperturbed measure concerns Gaussian (free) fields.

**Gaussian case** has significant simplifications:

If $C_{j'j} = \kappa[y_{j'}, y_j]$ denotes the *covariance matrix*,

$$G_w(y, \lambda) = \exp[\lambda \cdot (y - \langle y \rangle) - \lambda \cdot C\lambda/2].$$

$\Rightarrow$ Wick polynomials are *Hermite polynomials*.

The resulting orthogonality properties are used in the Wiener chaos expansion and Malliavin calculus.
Truncated moments-to-cumulants formula

\[ \mathbb{E} \left[ y_{J'} : y_{J} : \right] = \sum_{\pi \in \mathcal{P}(J' \cup J)} \prod_{A \in \pi} (\kappa[y_A] \mathbb{1}_{\{A \not\subset J\}}) \] (1)

\( :y_{J} : \) are \( \mu \)-a.s. unique polynomials of order \( |J| \) such that (1) holds for every \( J' \)

Multi-truncated moments-to-cumulants formula

Suppose \( L \geq 1 \) is given and consider a collection of \( L + 1 \) index sequences \( J', J_\ell, \ell = 1, \ldots, L \). Then with \( I = J' \cup (\bigcup_{\ell=1}^{L} J_\ell) \)

\[ \mathbb{E} \left[ y_{J''} \prod_{\ell=1}^{L} : y_{J_\ell} : \right] = \sum_{\pi \in \mathcal{P}(I)} \prod_{A \in \pi} (\kappa[y_A] \mathbb{1}_{\{A \not\subset J_\ell, \forall \ell\}}) . \]
Suppose that the evolution equation of the random variables $y_j(t)$ can be written in a form

$$\partial_t y_j(t) = \sum_I M^I_j(t) :y(t)^I:$$

Then the cumulants satisfy

$$\partial_t \kappa[y(t)^I'] = \sum_{\ell \in I'} \sum_I M^I_\ell(t) \mathbb{E}[ :y(t)^I::y(t)^{I'\setminus\ell}:]$$

where the truncated moments-to-cumulants formula implies

$$\mathbb{E}[ :y(t)^I::y(t)^{I'\setminus\ell}:] = \sum_{\pi \in \mathcal{P}(I \cup (I' \setminus \ell))} \prod_{A \in \pi} (\kappa[y(t)_A] 1\{A \cap I \neq \emptyset, A \cap (I' \setminus \ell) \neq \emptyset\})$$

$$\Rightarrow \text{ evolution hierarchy for cumulants}$$
The discrete NLS equation on the lattice $\mathbb{Z}^d$ deals with functions $\psi : \mathbb{R} \times \mathbb{Z}^d \rightarrow \mathbb{C}$ which satisfy

$$i \partial_t \psi_t(x) = \sum_{y \in \mathbb{Z}^d} \alpha(x - y) \psi_t(y) + \lambda |\psi_t(x)|^2 \psi_t(x)$$

Assuming that $\mathbb{E}[\psi_t(x)] = 0$ and using the WP one gets

$$i \partial_t \psi_t(x) = \sum_{y \in \mathbb{Z}^d} \alpha(x - y) : \psi_t(y) : + 2\lambda \rho_t(x) : \psi_t(x) :$$

$$+ \lambda : \psi_t(x)^* \psi_t(x) \psi_t(x) :$$

$$\rho_t(x) = \mathbb{E}[\psi_t(x)^* \psi_t(x)] = \mathbb{E}[|\psi_t(x)|^2]$$

This splitting was called "pair truncation" in [JL, Spohn] (Part I)
Simulate a chain of $N$ particles with two heat baths (Nosé-Hoover) at ends, waiting until a steady state reached.

Measure temperature and current profiles:

$$T_i = \langle p_i^2 \rangle, \quad J = \frac{1}{N} \sum_j \langle J_{j,j+1} \rangle \approx \langle J_{i,i+1} \rangle$$

Fourier’s Law predicts that when $\Delta T \to 0$,

$$- \frac{N}{\Delta T} J \to \kappa(T,N).$$

Repeat for several $\Delta T$, and estimate $\kappa(T,N)$ from the slope.

Increase $N$ to estimate $\kappa(T) = \lim_{N \to \infty} \kappa(T,N)$. 
Simulations yield good agreement with the kinetic prediction of
\[ T^2 \kappa(T) \approx 0.28 \delta^{-3/2} \] for \( T \to 0 \), \( \delta \) small (black solid line)
Evolution of entropy

- Time evolution of entropy $S(t) = \int dk \log W(k, t)$

(b) Random phase initial data

- (blue dots) $W = \text{Wigner function measured from simulations}$
- (orange dots) $W = \text{solution to the kinetic equation, initial data from } t = 500 \text{ simulation results}$