Kinetic theory of (lattice) waves

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based on joint works with

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Bristol 2018

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CENTRES OF EXCELLENCE IN RESEARCH

Part I

Time-correlations in stationary states of the discrete NLS

[JL and H. Spohn, *Invent. Math.* **183** (2011) 79–188]

Setup for the rigorous result

- Finite lattice: $L \geq 2\,, \quad \Lambda = \{0, 1, \ldots, L-1\}^d$
  - Periodic BC: *All arithmetic* mod L
- Dual lattice: $\Lambda^* = \{0, \frac{1}{L}, \ldots, \frac{L-1}{L}\}^d$
  - *"Integration"* = finite sum:

$$\int_{\Lambda^*} \mathrm{d}k\, f(k) := \frac{1}{|\Lambda|} \sum_{k \in \Lambda^*} f(k)$$

  - *"Dirac delta"* = finite sum:

$$\delta_\Lambda(k) := |\Lambda| \mathbb{1}_{\{k \bmod 1 = 0\}}$$

- Fourier transform: $(x \in \Lambda,\ k \in \Lambda^*)$

$$\widehat{f}(k) = \sum_{y \in \Lambda} f(y) \mathrm{e}^{-\mathrm{i}2\pi k \cdot y} \quad \Rightarrow \quad f(x) = \int_{\Lambda^*} \mathrm{d}k'\, \widehat{f}(k') \mathrm{e}^{\mathrm{i}2\pi k' \cdot x}$$

Evolution equations

Discrete nonlinear Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi_t(x) = \sum_{y\in\Lambda}\alpha(x-y)\psi_t(y) + \lambda|\psi_t(x)|^2\psi_t(x)$$

- $\psi_t : \Lambda \to \mathbb{C}, \quad t \in \mathbb{R}$
- $\lambda > 0$ (*defocusing*)
- Harmonic coupling determined by $\alpha : \mathbb{Z}^d \to \mathbb{R}$.
- α 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 ψ 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)

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

- 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
- $Z^{\lambda}_{\beta,\mu} > 0$ is the normalization constant
- Let $\mathbb{E}$ denote expectation over the initial data

Properties of the system

- The solution ψ_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:
  $\mathbb{E}[F(\tau_x\psi)] = \mathbb{E}[F(\psi)], \quad (\tau_x\psi)(y) = \psi(y+x)$
- 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, $\psi_0(x) \mapsto \mathrm{e}^{\mathrm{i}\varphi}\psi_0(x)$, $\varphi \in \mathbb{R}$.
- Thus, for instance, $\mathbb{E}[\psi_t] = 0$, $\mathbb{E}[\psi_{t'}\psi_t] = 0$,

$$\mathbb{E}[\psi_{t'}(x')^*\psi_t(x)] = \mathbb{E}[\psi_0(0)^*\psi_{t-t'}(x-x')]$$

Field-field correlation function

Fix *test-functions* $f, g \in \ell_2$, and assume they have finite support.

Observable

$$Q_\Lambda^\lambda(\tau) := \mathbb{E}[\langle \widehat{f}, \widehat{\psi}_0 \rangle^* \langle \mathrm{e}^{-\mathrm{i}\omega^\lambda \tau \lambda^{-2}} \widehat{g}, \widehat{\psi}_{\tau\lambda^{-2}} \rangle]$$

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

Theorem

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

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

Summary of the main result

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

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

- $W(k) = (\beta(\omega(k)-\mu))^{-1}$ = covariance function for $\lambda = 0$
- $\omega^\lambda_{\mathrm{ren}}(k) = \omega(k) + \lambda R_0 + \lambda^2 \Gamma_2(k)$
- $\Gamma_1(k) \geq 0$

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

- Nearest neighbour couplings ($\omega_{\mathrm{nn}}(k) = c - \sum_{\nu=1}^d \cos(2\pi k^\nu)$) satisfy all of our assumptions if $d \geq 4$

- $\Gamma_j(k)$ are real, and $\Gamma(k) = \Gamma_1(k) + \mathrm{i}\Gamma_2(k)$ is given by

$$\Gamma(k_1) = 2\int_0^\infty \mathrm{d}t \int_{(\mathbb{T}^d)^3} \mathrm{d}k_2 \mathrm{d}k_3 \mathrm{d}k_4 \delta(k_1 + k_2 - k_3 - k_4) \\ \times \mathrm{e}^{\mathrm{i}t(\omega_1+\omega_2-\omega_3-\omega_4)} (W_2 W_3 + W_2 W_4 - W_3 W_4)$$

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

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

- $2\Gamma_1(k) \geq 0$ coincides with the loss term of the linearisation of $\mathcal{C}_{\mathrm{NL}}$ 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,

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

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

- Here *truncated correlation (cumulant) functions* are

$$C_n(k,\sigma) := \sum_{x\in\Lambda^n}\mathbb{1}_{\{x_1=0\}}\mathrm{e}^{-\mathrm{i}2\pi\sum_{i=1}^n x_i\cdot k_i}\mathbb{E}\Big[\prod_{i=1}^n\psi_0(x_i,\sigma_i)\Big]^{\mathrm{trunc}}$$

and for any random variables $a_1,\ldots,a_n$

$$\mathbb{E}\Big[\prod_{i=1}^n a_i\Big]^{\mathrm{trunc}} := \kappa[a_1,\ldots,a_n] = \partial_{\eta_1}\cdots\partial_{\eta_n}\ln\mathbb{E}[\mathrm{e}^{\sum_i\eta_i a_i}]\Big|_{\eta=0}$$

Assumption: decay of initial correlations

ℓ_1-clustering of the equilibrium measure

- For sufficiently small λ and for all $n \geq 4$ the truncated correlation functions (*cumulants*) should satisfy

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

- 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

[JL and M. Marcozzi, *J. Math. Phys.* **57** (2016) 083301 (27pp)]

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

$$\partial_\tau W_\tau(k) = \mathcal{C}_{\mathrm{NL}}[W_\tau(\cdot)],$$

$$\mathcal{C}_{\mathrm{NL}}[h](k_1) = 4\pi \int_{(\mathbb{T}^d)^3} \mathrm{d}k_2 \mathrm{d}k_3 \mathrm{d}k_4 \, \delta(k_1 + k_2 - k_3 - k_4)$$

$$\times \, \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) \, [h_2 h_3 h_4 - h_1(h_2 h_3 + h_2 h_4 - h_3 h_4)]$$

Why study cumulants?

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 $n, m \neq 0$.

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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 $\kappa[\psi(x), \psi(x + y_1), \ldots, \psi(x + y_{n-1})] \to 0$ as $|y_i| \to \infty$. How fast? ℓ_1- or ℓ_2-summably?
- Not true for corresponding moments: $\mathbb{E}[|\psi(x)|^2 |\psi(x + y)|^2]$

ℓ_p-clustering states

Call the field ℓ_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 $1 \le p \le 2$, can take Fourier-transform in y $\Rightarrow$ functions $F^{(n)}(x,k)$, L^∞ in $x\in\mathbb{Z}^d$ and L^2-integrable for $k\in(\mathbb{T}^d)^{n-1}$.
- ℓ_1-clustering implies that $F^{(n)}(x,k)$ is continuous and uniformly bounded ($\Rightarrow$ helps in nonlinearities)
- Many examples of *ℓ_1-clustering* thermal Gibbs states, e.g., discrete NLS [Abdesselam, Procacci, Scoppola]

Time-evolution of cumulants?

As before, consider *deterministic evolution* of ψ_t, with *random initial data* for ψ_0.

- Cumulants are *multilinear* and *permutation invariant*

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

- Solution? How to iterate into a closed hierarchy?
- Computations often simplified by using Wick polynomial representation of $\partial_t \psi_t$

An example: Discrete NLS

Consider the DNLS with *initial data* for ψ_0 which is

- *ℓ_1-clustering*
- *Gauge invariant*: $\psi_0(x) \sim e^{i\theta}\psi_0(x)$ for any $\theta \in \mathbb{R}$
  $\Rightarrow$ also ψ_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 ℓ_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, $W_t(x, k) = W_t(k)$ $=$ *Wigner function* (as defined in earlier works)

Higher order Wigner functions

$$\psi_t(x,+1) = \psi_t(x) \quad \text{and} \quad \psi_t(x,-1) = \psi_t(x)^*$$

IF ℓ_p-clustering is preserved by the time-evolution, should study

Order-n "Wigner functions": $x \in \mathbb{Z}^d$, $k \in (\mathbb{T}^d)^{n-1}$, $\sigma \in \{\pm 1\}^n$

$$F_t^{(n)}(x,k,\sigma) = \sum_{y \in (\mathbb{Z}^d)^{n-1}} \mathrm{e}^{-\mathrm{i}2\pi k\cdot y} \kappa[\psi_t(x,\sigma_1), \psi_t(x+y_1,\sigma_2), \ldots, \psi_t(x+y_{n-1},\sigma_n)]$$

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 $\omega(k) = \widehat{\alpha}(k)$ and $\rho_t(x) = \mathbb{E}[|\psi_t(x)|^2] = \int dk\, W_t(x,k)$,

$$\begin{aligned}\partial_t W_t(x,k) = &-\mathrm{i} \sum_z \alpha(z) \mathrm{e}^{\mathrm{i}2\pi k\cdot z} \left(W_t(x,k) - W_t(x-z,k)\right) \\ &-\mathrm{i}2\lambda \sum_z \left(\rho_t(x+z) - \rho_t(x)\right) \int \mathrm{d}k'\, \mathrm{e}^{\mathrm{i}2\pi z\cdot(k'-k)} W_t(x,k') \\ &-\mathrm{i}\lambda \int \mathrm{d}k_1' \mathrm{d}k_2' \left(F_t^{(4)}(x, k_1', k_2', k - k_1' - k_2') - F_t^{(4)}(x, k_1', k_2', k)\right)\end{aligned}$$

With $\omega(k) = \widehat{\alpha}(k)$ and $\rho_t(x) = \mathbb{E}[|\psi_t(x)|^2] = \int dk\, W_t(x, k)$,

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

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

$$-\mathrm{i}\lambda \int \mathrm{d}k_1' \mathrm{d}k_2' \left(F_t^{(4)}(x, k_1', k_2', k - k_1' - k_2') - F_t^{(4)}(x, k_1', k_2', k) \right)$$

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

$$+ \lambda^2 \mathcal{C}_{\mathrm{NL}}[W_t(x, \cdot)](k)$$

- $O(\lambda)$ 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

[C.B. Mendl, J. Lu, and JL,
Phys. Rev. E **94** (2016) 062104 (9 pp)]

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 $L \gg 1$

FPU-type chains

We consider a chain of classical particles with nearest neighbour interactions, *dynamics* defined by

The Hamiltonian

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

- $\lambda \geq 0$ 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

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

- The parameter $0 < \delta \leq \frac{1}{2}$ controls the *pinning onsite potential*
- This model is expected to have (diffusive) *normal heat conduction* for $\lambda, \delta > 0$

Normal modes

From a solution $(q_i(t), p_i(t))$ define

Phonon fields

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

$$\Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\widehat{a}_t(k,\sigma) = -\mathrm{i}\sigma\omega(k)\widehat{a}_t(k,\sigma)$$

$$-\mathrm{i}\sigma\lambda \sum_{\sigma'\in\{\pm1\}^3} \int_{(\Lambda^*)^3} \mathrm{d}^3 k' \delta_\Lambda\Big(k - \sum_{j=1}^3 k'_j\Big) \prod_{\ell=0}^3 \frac{1}{\sqrt{2\omega(k'_\ell)}} \prod_{j=1}^3 \widehat{a}_t(k'_j, \sigma'_j)$$

- Here $k \in \Lambda^* := \{-\frac{1}{2}+\frac{1}{N}, \dots, \frac{1}{2}-\frac{1}{N}, \frac{1}{2}\}$ for a finite periodic chain of length N $(= |\Lambda^*|)$

Wigner function

Assume a spatially homogeneous state and consider the corresponding *Wigner function*

$$w_t(k;L) := \int_{\Lambda^*} \mathrm{d}k' \langle \widehat{a}_t(k')^* \widehat{a}_t(k) \rangle = \sum_{y\in\Lambda} \mathrm{e}^{-\mathrm{i}2\pi y\cdot k} \langle a_t(0)^* a_t(y) \rangle$$

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* ($t = \lambda^{-2}\tau = O(\lambda^{-2})$)

Boltzmann–Peierls equation

In addition, the limiting Wigner functions should satisfy the following *phonon Boltzmann equation*

$$\frac{\partial}{\partial t} W(k_0,t) = 12\pi\lambda^2 \sum_{\sigma\in\{\pm1\}^3} \int_{\mathbb{T}^3} \mathrm{d}^3 k \prod_{\ell=0}^{3} \frac{1}{2\omega_\ell}$$
$$\times \delta(k_0 + \sum_{j=1}^{3} \sigma_j k_j)\, \delta\Big(\omega_0 + \sum_{j=1}^{3} \sigma_j \omega_j\Big)$$
$$\times \big[W_1 W_2 W_3 + W_0(\sigma_1 W_2 W_3 + \sigma_2 W_1 W_3 + \sigma_3 W_1 W_2)\big]$$

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

Boltzmann–Peierls equation

Kinetic equation (spatially homogeneous initial data)

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

- Stationary solutions are

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

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

Spatially homogeneous kinetic theory

Microsystem	*Dynamics*: free evolution $+\ \lambda \times$ perturbation
$w_t(k) = \int \mathrm{d}k' \langle a_t(k')^* a_t(k) \rangle$	*Initial state*: translation invariant & "chaotic"
$\downarrow$	$\downarrow$ (weak coupling)
$\partial_\tau W_\tau(k) = \mathcal{C}[W_\tau](k)$	*Boltzmann equation* for $W_\tau = \lim_{\lambda\to 0} w_{\lambda^{-2}\tau}$
$\downarrow$	$\downarrow$
$\partial_\tau S[W_\tau] = \sigma[W_\tau]$	S = *kinetic entropy* (H-function) σ = *entropy production* ≥ 0
$\downarrow$	$\downarrow$
$\sigma[W^{\mathrm{eql}}] = 0$	$\Leftarrow$ W^{eql} from an *equilibrium state* (classifies stationary solutions)

Numerical simulations (Christian Mendl)

- To compare in more detail to kinetic theory, we consider several stochastic, periodic and *translation invariant* initial data: Then

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

- Computing the covariance from simulated equilibrium states (one parameter, β) and fitting numerically to the kinetic formula (two parameters, β', μ') yields

β	1	10	100	1000
β'	0.912	8.98	97.1	986.4
μ'	-0.488	-0.229	-0.0426	-0.0120

- As expected, $\beta' \approx \beta$ and $\mu' \approx 0$ for large β

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" β_0 and sample positions q_j from the corresponding equilibrium distribution and the momenta p_j from the bimodal distribution

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

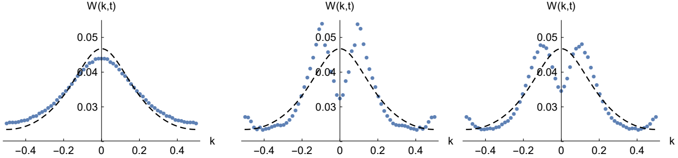
B) Random phase, with given initial Wigner function ($\lambda = \frac{1}{2}, 10$):

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

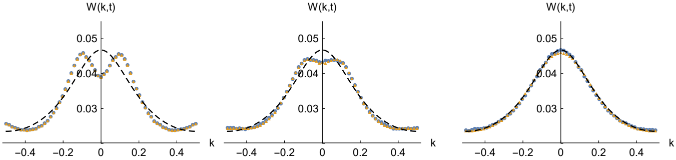
$$a(k) = \sqrt{N W_0(k)}\,\mathrm{e}^{\mathrm{i}\varphi(k)}$$

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

A) Bimodal initial data



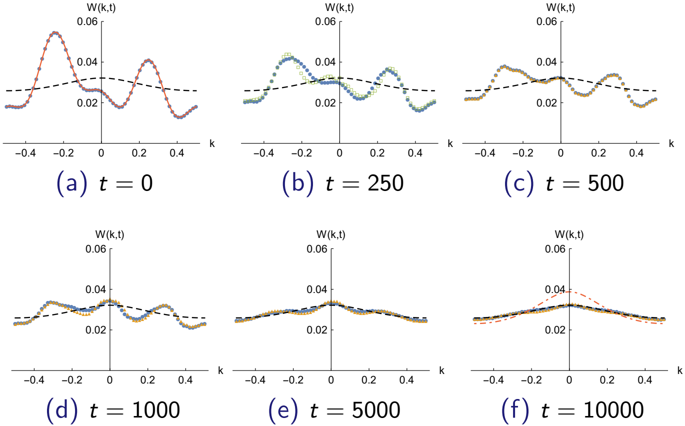
(a) $t = 0$ (b) $t = 150$ (c) $t = 250$



(d) $t = 500$ (e) $t = 1000$ (f) $t = 2500$

Wigner function from simulations (*blue dots*) vs.
solving the kinetic equation (*yellow triangles*) starting at $t = 500$.
(*black dashed line*) Kinetic equilibrium profile fitted to (f)

B) Random phase initial data ($\lambda = \frac{1}{2}$)

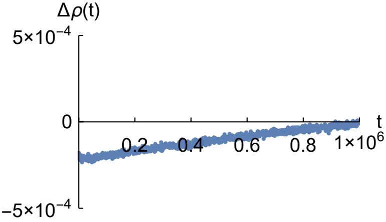


(a) $t = 0$ (b) $t = 250$ (c) $t = 500$

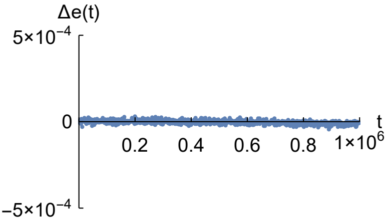
(d) $t = 1000$ (e) $t = 5000$ (f) $t = 10000$

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? ($\lambda = 10$)



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



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

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

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 [JL, M. Marcozzi and A. Nota, *arXiv:1601.08163*]

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

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

Then with $\partial_\lambda^J := \prod_{i\in J}\partial_{\lambda_i}$, $y^J = \prod_{i\in J} y_i$,

$$\kappa[\psi_t(x)_J] = \partial_\lambda^J g_t(0)\,, \quad \mathbb{E}[\psi_t(x)^J] = \partial_\lambda^J g_{\mathrm{mom},t}(0)$$

Define

$$G_{\mathrm{w}}(\psi_t,\lambda) = \frac{\mathrm{e}^{\lambda\cdot\psi_t}}{\mathbb{E}[\mathrm{e}^{\lambda\cdot\psi_t}]}$$

$$\Rightarrow \quad \partial_t\kappa[\psi_t(x)_J] = \partial_\lambda^J\partial_t g_t(\lambda)\big|_{\lambda=0} = \partial_\lambda^J\mathbb{E}[\lambda\cdot\partial_t\psi_t\, G_{\mathrm{w}}(\psi_t,\lambda)]\big|_{\lambda=0}$$

$$= \sum_{\ell\in J}\mathbb{E}[\partial_t\psi_t(x_\ell)\,\partial_\lambda^{J\setminus\ell}G_{\mathrm{w}}(\psi_t,0)]$$

$\partial_\lambda^J G_{\mathrm{w}}(\psi_t,0) = {:}\psi_t(x)^J{:}$ 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*,

  $$G_{\rm w}(y, \lambda) = \exp[\lambda \cdot (y - \langle y \rangle) - \lambda \cdot C\lambda/2] \,.$$

  $\Rightarrow$ Wick polynomials are *Hermite polynomials*

- The resulting orthogonality properties are used in the Wiener chaos expansion and Malliavin calculus

Truncated moments-to-cumulants formula

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

- ${:}y^J{:}$ are μ-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_ℓ, $\ell = 1, \ldots, L$. Then with $I = J' \cup \left(\cup_{\ell=1}^{L} J_\ell \right)$

$$\mathbb{E}\left[y^{J'} \prod_{\ell=1}^{L} {:}y^{J_\ell}{:} \right] = \sum_{\pi \in \mathcal{P}(I)} \prod_{A \in \pi} \left(\kappa[y_A] \mathbb{1}_{\{A \not\subset J_\ell, \forall \ell\}} \right) .$$

Suppose that the evolution equation of the random variables $y_j(t)$ can be written in a form

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

Then the cumulants satisfy

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

where the *truncated moments-to-cumulants formula* implies

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

$\Rightarrow$ evolution hierarchy for cumulants

The discrete NLS equation on the lattice $\mathbb{Z}^d$ deals with functions $\psi : \mathbb{R} \times \mathbb{Z}^d \to \mathbb{C}$ which satisfy

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

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

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

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

- This splitting was called *"pair truncation"* in [JL, Spohn] (Part I)

Molecular dynamics simulations (Kenichiro Aoki, 2006)

1. Simulate a chain of N particles with two heat baths (Nosé-Hoover) at ends, waiting until a *steady state* reached
2. Measure temperature and current profiles:

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

3. Fourier's Law predicts that when $\Delta T \to 0$,

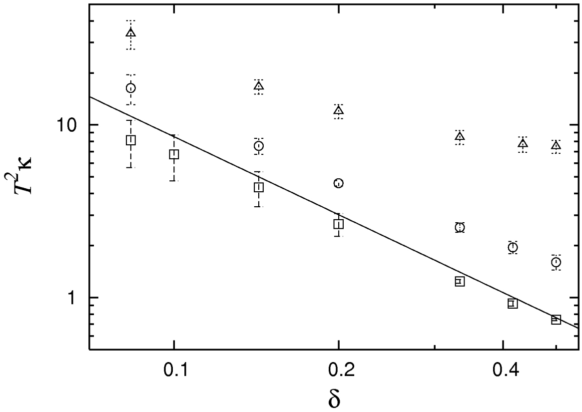
$$-\frac{N}{\Delta T} J \to \kappa(T, N)\,.$$

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

4. Increase N to estimate $\kappa(T) = \lim_{N\to\infty} \kappa(T,N)$.

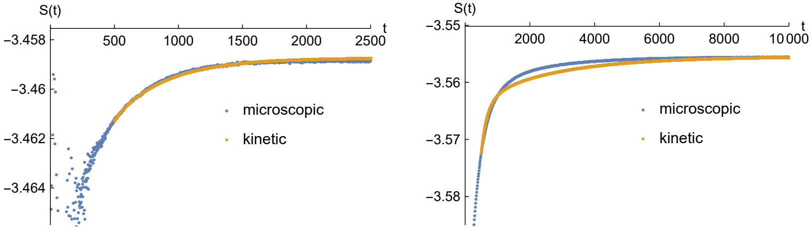
Comparison to kinetic prediction

Simulations yield good agreement with the kinetic prediction of $T^2\kappa(T) \approx 0.28\,\delta^{-3/2}$ for $T \to 0$, δ small (*black solid line*)



□ $T = 0.1$
○ $T = 0.4$
△ $T = 4$

Evolution of entropy



(a) Bimodal initial data (b) Random phase initial data

- Time evolution of entropy $S(t) = \int \mathrm{d}k \, \log W(k,t)$

(blue dots) W = Wigner function measured from simulations

(orange dots) W = solution to the kinetic equation, initial data from $t = 500$ simulation results