# Quantum kinetic theory and (pre-)thermalization

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*based on joint work with*

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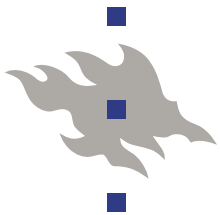

UNIVERSITY OF HELSINKI

CENTRES OF EXCELLENCE
IN RESEARCH

# Part I

# Kinetic theory of "spinless" lattice fermions and bosons

# Spatially homogeneous kinetic theory: a sketch



*Microsystem*

$w_t(k) = \int \mathrm{d}k' \langle a_t(k')^* a_t(k) \rangle$

$\downarrow$

$\partial_\tau W_\tau(k) = \mathcal{C}[W_\tau](k)$

$\downarrow$

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

$\downarrow$

$\sigma[W^{\mathrm{eql}}] = 0$

*Dynamics*: free evolution + $\lambda \times$ perturbation

*Initial state*: translation invariant & "chaotic"

$\downarrow$ (weak coupling)

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

$\downarrow$

$S$ = *kinetic entropy* (H-function)

$\sigma$ = *entropy production* $\geq 0$

$\downarrow$

$\Leftarrow$ $W^{\mathrm{eql}}$ from an *equilibrium state*

(classifies stationary solutions)

## Thermalization in kinetic theory

If the dynamics leads to **spatial homogenization** and **local equilibrium**, expect that after sufficiently large times $t$ "locally" near any point $x$ one has $W_t(x,k) \approx W^{\mathrm{eql}}(k)$ where $W^{\mathrm{eql}}$ comes from some equilibrium state

- Expect allowed $W^{\mathrm{eql}}$ to be determined by the local *conservation laws* of the *microscopic dynamics*
- Each such $W^{\mathrm{eql}}$ must be a stationary solution of the Boltzmann equation
- However, do all solutions to $\sigma[W^{\mathrm{eql}}] = 0$ correspond to unique stationary state?
  (Could many stationary states be mapped into the same $W^{\mathrm{eql}}$?)
- What happens if the kinetic equation has extra conservation laws?
  (Could some observables begin to thermalize slower than the kinetic times, for $t \gg O(\lambda^{-2})$?)

# Bosonic and fermionic (scalar) fields



Consider a gas of $n$ (QM) particles hopping on a lattice $\mathbb{Z}^d$ and with a pair interaction:

$$H^{(n)} = H_0^{(n)} + \lambda V^{(n)}$$

$$H_0^{(n)}\psi_n(x_1,\ldots,x_n) = \sum_{j=1}^{n}\sum_{w\in\mathbb{Z}^d}\alpha(x_j - w)\psi_n(x_1,\ldots,w,\ldots,x_n)$$

$$V^{(n)}\psi_n(x_1,\ldots,x_n) = \tfrac{1}{2}\sum_{i\neq j=1}^{n} V(x_i - x_j)\psi_n(x_1,\ldots,x_n)$$

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$\Rightarrow$ On the Fock space using *creation* and *annihilation operators*

$$H = \sum_{x,y\in\mathbb{Z}^d}\alpha(x-y)a(x)^*a(y) + \tfrac{1}{2}\lambda\sum_{x,y\in\mathbb{Z}^d}V(x-y)a(x)^*a(y)^*a(y)a(x)$$

Fermions:

$$\{a(x),a(y)^*\} = \mathbb{1}_{\{x=y\}}, \quad \{a(x),a(y)\} = 0, \quad \{a(x)^*,a(y)^*\} = 0$$

Bosons:

$$[a(x),a(y)^*] = \mathbb{1}_{\{x=y\}}, \quad [a(x),a(y)] = 0, \quad [a(x)^*,a(y)^*] = 0$$

# Spatially homogeneous kinetic theory: fermions



$$w_t(k) := \int_{\mathbb{T}^d} \mathrm{d}k' \langle \widehat{a}_t(k')^* \widehat{a}_t(k) \rangle = \sum_{y \in \mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}2\pi y \cdot k} \langle a_t(0)^* a_t(y) \rangle$$

$$\downarrow$$

$$W_\tau = \lim_{\lambda \to 0} w_{\lambda^{-2}\tau}\,, \quad \widetilde{W}_\tau := 1 - W_\tau\,, \quad \omega(k) := \widehat{\alpha}(k)$$

$$\mathcal{C}[W](k_0) = \pi \int_{(\mathbb{T}^d)^3} \mathrm{d}k_1 \mathrm{d}k_2 \mathrm{d}k_3\, \delta(k_0 + k_1 - k_2 - k_3) \delta(\omega_0 + \omega_1 - \omega_2 - \omega_3)$$

$$\times \left| \widehat{V}(k_1 - k_2) - \widehat{V}(k_1 - k_3) \right|^2 \left( \widetilde{W}_0 \widetilde{W}_1 W_2 W_3 - W_0 W_1 \widetilde{W}_2 \widetilde{W}_3 \right)$$

$$\downarrow$$

$$S[W] = -\int_{\mathbb{T}^d} \mathrm{d}k \left( W(k) \log W(k) + \widetilde{W}(k) \log \widetilde{W}(k) \right)$$

$$\downarrow$$

$$W^{\mathrm{eql}}(k; \beta, \mu) = \left( \mathrm{e}^{\beta(\omega(k) - \mu)} + 1 \right)^{-1} \qquad \text{(Fermi–Dirac)}$$

# Part II

# Kinetic theory of the Hubbard model (fermions with a spin coupling)

# Hubbard model



- A system of fermions with *two spin-states* $\sigma = \pm 1$ moving on a lattice $x \in \mathbb{Z}^d$, $d \geq 1$:

  $n$-particle Hamiltonian consists of NN-hopping and an on-site interaction of opposite spins

- 1D case ($d = 1$) is *explicitly solvable* [Lieb, Wu, 1968] (Complete eigenbasis can be generated by symmetries and Bethe ansatz [Essler, Korepin, Schoutens, 1991])

- Earlier work focused on statistical properties;

  Time-evolution? Transport properties? (Even in 1D)

Here lowest order transport properties for small coupling:

kinetic theory and the Boltzmann equation for spatially homogeneous states

# Hubbard model: definitions & notations



- $a(x,\sigma) :=$ *fermionic annihilation operators* in the Fock space $(\{a(x,\sigma)^*, a(x',\sigma')\} = \mathbb{1}_{\{(x,\sigma)=(x',\sigma')\}})$
- $a_t(x,\sigma) :=$ time-evolved annihilation operator ($a_0 = a$). Then

$$\partial_t a_t(x,\sigma) = -\mathrm{i}\sum_{y\in\mathbb{Z}^d} \alpha(x-y)a_t(y,\sigma) - \mathrm{i}\lambda a_t(x,-\sigma)^* a_t(x,-\sigma)a_t(x,\sigma)$$

$\alpha : \mathbb{Z}^d \to \mathbb{R} =$ *hopping amplitude* (Hubbard: $\alpha(x) = \mathbb{1}_{\{|x|=1\}}$)
$\omega := \widehat{\alpha} =$ *dispersion relation* ($\omega : \mathbb{T}^d \to \mathbb{R}$)
$\lambda =$ *spin coupling strength*

- The time-evolution is SU(2)-invariant and conserves:
  1. *Total energy* $H :=$ $\sum_{\sigma,x,x'} \alpha(x'-x)a(x',\sigma)^* a(x,\sigma) + \lambda \sum_x a^*(-)a^*(+)a(+)a(-)|_x$
  2. *Total spin* $\Sigma_{\sigma'\sigma} := \sum_x a(x,\sigma')^* a(x,\sigma)$

# Kinetic scaling limit of the Hubbard model



- Consider the *1st reduced density matrix*,

$$\rho_1((x,\sigma),(x',\sigma');t) = \langle a_t(x',\sigma')^* a_t(x,\sigma)\rangle$$

We assume translation invariance $\Rightarrow$
for each $t, x$ there is a $2\times 2$ matrix $w_t(x)$ such that

$$\rho_1((x,\sigma),(x',\sigma');t) = (w_t(x-x'))_{\sigma\sigma'}$$

- Set $W_\tau^\lambda(k) := \widehat{w}_{\tau\lambda^{-2}}(k)$. Then $0 \le W_\tau^\lambda(k) \le 1$ as a matrix
- Kinetic conjecture: There is $W_\tau := \lim_{\lambda\to 0^+} W_\tau^\lambda$

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- Kinetic conjecture: There is $W_\tau := \lim_{\lambda\to 0^+} W_\tau^\lambda$
- Choose a spin-basis such that $R := \langle \Sigma \rangle =$ *expectation of the total spin* is diagonal
  $\Rightarrow$ The analysis of the resulting oscillatory integrals is essentially identical to that in a *two-component dNLS* [Fürst, JL, Mei, Spohn, '13]

# Conjectured Boltzmann equation for the kinetic limit



## Hubbard Boltzmann equation

$$\partial_t W_t(k) = \mathcal{C}_{\mathrm{H}}[W_t](k) - \mathrm{i}\left[H^{\mathrm{eff}}[W_t](k), W_t(k)\right]$$

- $W_t$ is a $2 \times 2$ *Hermitian matrix*
- *Collision energy:* $\underline{\omega} := \omega_0 + \omega_1 - \omega_2 - \omega_3, \quad \omega_i := \omega(k_i)$.

The collision term $\mathcal{C}_{\mathrm{H}}[W]$ is a "non-commutative version" of the fermionic Boltzmann-Nordheim collision operator:

Using $W_j := W(k_j), \quad \tilde{W}_j := 1 - W_j, \quad J[A] := 1 \operatorname{Tr} A - A \in \mathbb{C}^{2\times 2}$,

$$\begin{aligned}\mathcal{C}_{\mathrm{H}}[W](k_0) := \pi \int_{(\mathbb{T}^d)^3} \mathrm{d}k_1 \mathrm{d}k_2 \mathrm{d}k_3 \, \delta(k_0 + k_1 - k_2 - k_3)\delta(\underline{\omega}) \\ \times \Big( \tilde{W}_0 W_2 J[\tilde{W}_1 W_3] + J[W_3 \tilde{W}_1] W_2 \tilde{W}_0 \\ - W_0 \tilde{W}_2 J[W_1 \tilde{W}_3] - J[\tilde{W}_3 W_1] \tilde{W}_2 W_0 \Big)\end{aligned}$$

# The Twist



## Hubbard Boltzmann equation

$$\partial_t W_t(k) = \mathcal{C}_{\mathrm{H}}[W_t](k) - \mathrm{i}\left[H^{\mathrm{eff}}[W_t](k), W_t(k)\right]$$

- *Collision energy:* $\underline{\omega} := \omega_0 + \omega_1 - \omega_2 - \omega_3, \quad \omega_i := \omega(k_i).$
- $(H^{\mathrm{eff}})^\dagger = H^{\mathrm{eff}} \in \mathbb{C}^{2\times 2}$

The second term is of "Vlasov type":
it describes an "effective" rotation of the spin-basis.

$$H^{\mathrm{eff}}[W](k_0) := \mathrm{P.V.} \int_{(\mathbb{T}^d)^3} \mathrm{d}k_1 \mathrm{d}k_2 \mathrm{d}k_3 \delta(k_0 + k_1 - k_2 - k_3) \frac{1}{\underline{\omega}}$$
$$\times \left( \tilde{W}_2 J[W_1 \tilde{W}_3] + W_2 J[\tilde{W}_1 W_3] \right)$$

where the integral is a *principal value integral* around $\underline{\omega} = 0$.

# Hubbard model



The limit in not rigorous, so better to check that the solutions make physical sense...

- Is there always a unique global solution?
- Does it satisfy $0 \leq W_t \leq 1$? (*Fermi constraint*)
- Are *energy* ($\int \mathrm{d}k\, \omega(k) \mathrm{Tr}\, W_t(k)$) and *total spin* ($\int \mathrm{d}k\, W_t(k)$) still conserved?
- Entropy and entropy production? (*H-theorem*)
- Stationary solutions?
- Convergence towards stationary solutions?
- *Also:* ...in which precise mathematical sense?

# Main mathematical result



Assume that

1. the dispersion relation is continuous and symmetric
2. the free evolution is sufficiently dispersive
3. collisions act sufficiently dispersively

in particular,

- one can consider the *Hubbard model with* $d \geq 3$

**Theorem [JL, Mei, Spohn, '15]**

Then for any initial data $W_0 \in L^\infty$ with $0 \leq W_0 \leq 1$, there is a unique global solution to the Hubbard Boltzmann equation which satisfies $0 \leq W_t \leq 1$ for all $t \geq 0$. Total energy and spin are conserved by this solution.

# Hubbard model



- *Entropy*

$$S[W] := -\int \mathrm{d}k \left( \mathrm{Tr}\, W \ln W + \mathrm{Tr}\, \tilde{W} \ln \tilde{W} \right)$$

  satisfies (at least formally) an *H-theorem:* There is an *entropy production function* $\sigma_{\mathrm{S}}[W]$, such that

$$\partial_t S[W_t] = \sigma_{\mathrm{S}}[W_t] \geq 0\,, \qquad \text{for all } t > 0$$

- Candidates for *steady states* by solving $\sigma_{\mathrm{S}}[W] = 0$

# More precisely...



- *Entropy:*

$$S[W] := -\int \mathrm{d}k \left( \mathrm{Tr}\, W \ln W + \mathrm{Tr}\, \tilde{W} \ln \tilde{W} \right)$$

- *H-theorem:* If $(\lambda_a(k), \psi_a(k))_{a=1,2}$ denotes a suitable *spectral decomposition* of $W(k)$, then

$$\partial_t S[W_t] = \sigma[W_t] \geq 0\,, \qquad \text{for all } t > 0$$

$$\sigma[W](k_1) := \frac{\pi}{4} \int \mathrm{d}^4 k\, \delta(k_1 + k_2 - k_3 - k_4) \delta(\underline{\omega}) \sum_{a \in \{1,2\}^4}$$

$$\times \left( \tilde{\lambda}_1 \tilde{\lambda}_2 \lambda_3 \lambda_4 - \lambda_1 \lambda_2 \tilde{\lambda}_3 \tilde{\lambda}_4 \right) \ln \frac{\tilde{\lambda}_1 \tilde{\lambda}_2 \lambda_3 \lambda_4}{\lambda_1 \lambda_2 \tilde{\lambda}_3 \tilde{\lambda}_4}$$

$$\times \left| \langle \psi_1, \psi_3 \rangle \langle \psi_2, \psi_4 \rangle - \langle \psi_1, \psi_4 \rangle \langle \psi_2, \psi_3 \rangle \right|^2$$

where $\psi_i := \psi_{a_i}(k_i)$, $\lambda_i := \lambda_{a_i}(k_i)$ and $\tilde{\lambda} := 1 - \lambda$.

# Steady states



Use a basis such that the total spin is diagonal.

- Then the following are *steady states*:
  1. (*Fermi-Dirac*) There are $\beta > 0$ and $\mu_\pm \in \mathbb{R}$ such that

$$W(k) = \begin{pmatrix} g_+(k) & 0 \\ 0 & g_-(k) \end{pmatrix}$$

     where $g_\pm(k) := (1 + \mathrm{e}^{\beta(\omega(k)-\mu_\pm)})^{-1}$ are standard Fermi-Dirac distributions.
  2. (*empty band*) $W$ diagonal, $W_{--}(k) = 0$, $W_{++}(k)$ is *arbitrary* (or vice versa)
  3. (*full band*) $W$ diagonal, $W_{--}(k) = 1$, $W_{++}(k)$ is *arbitrary* (or vice versa)

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  3. (*full band*) $W$ diagonal, $W_{--}(k) = 1$, $W_{++}(k)$ is *arbitrary* (or vice versa)
- Are there others? For $d \geq 2$ Hubbard, *no*.

  For $d = 1$ Hubbard, yes, many [Fürst, Mendl, Spohn, '12]

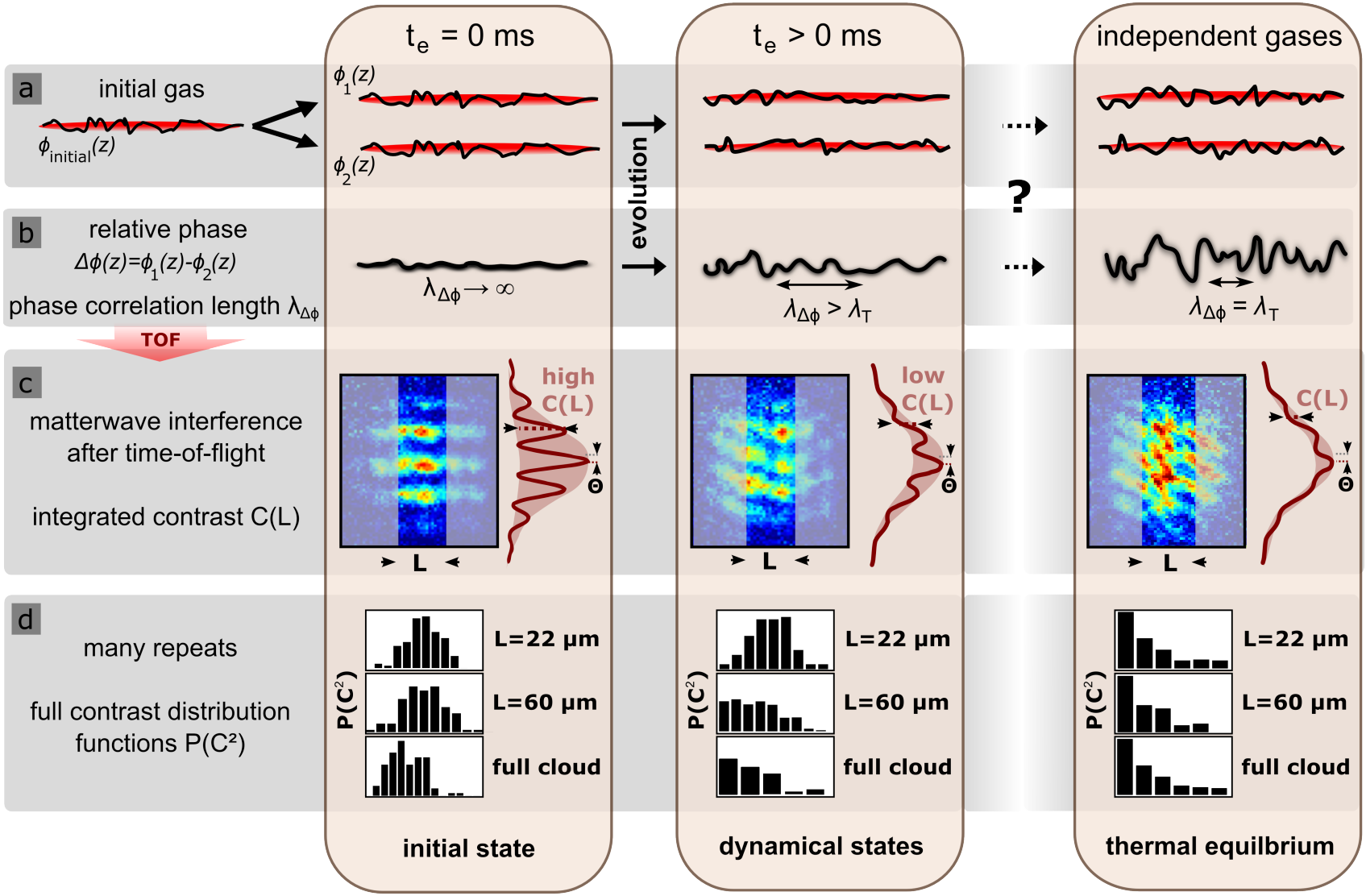
# Part III

# Experiment: 1D Bose condensate with pre-thermalization

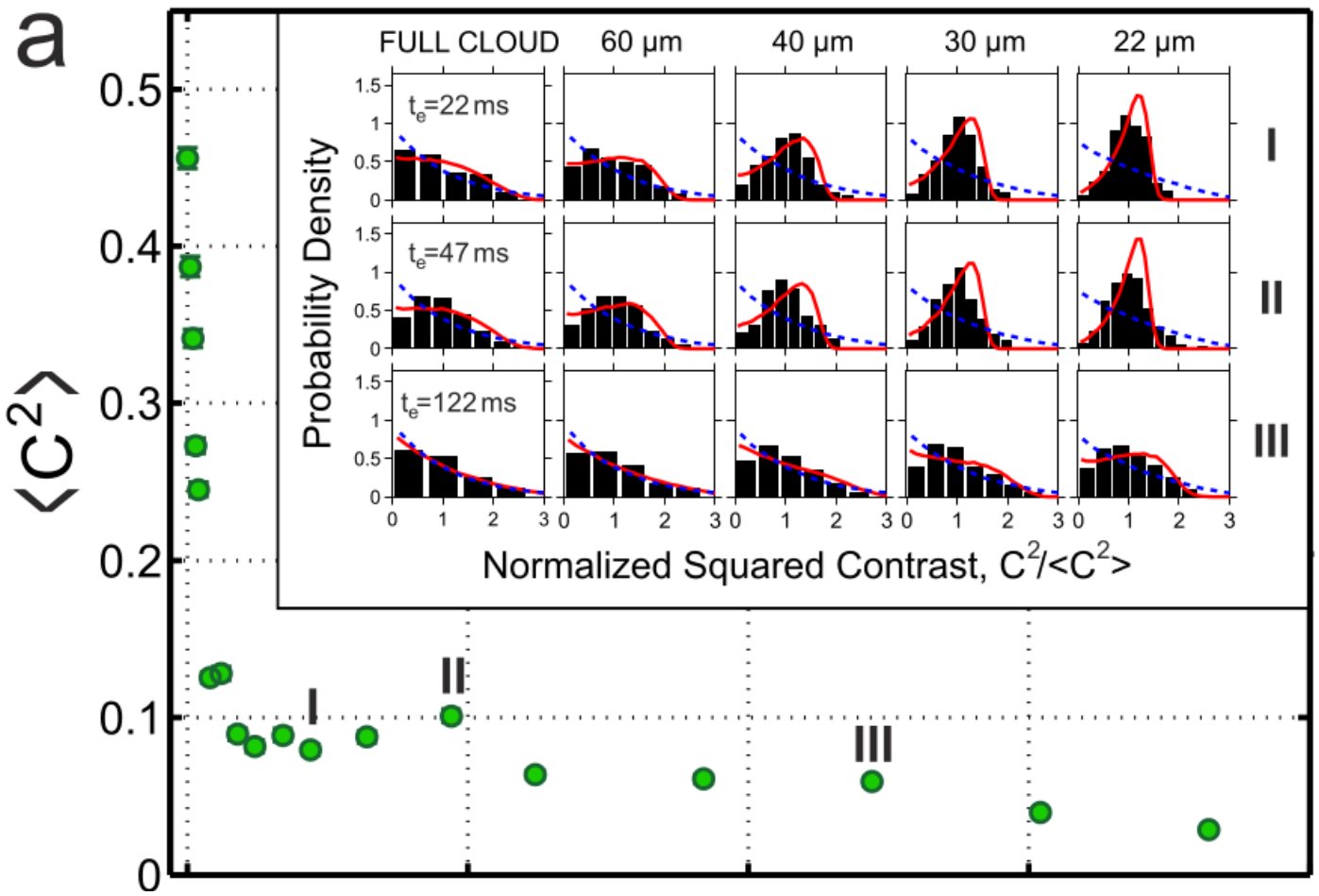
Data and pictures from:

[M. Gring, M. Kuhnert, T. Langen, T. Kitagawa, B. Rauer, M. Schreitl, I. Mazets, D. Adu Smith, E. Demler, and J. Schmiedmayer, *Science*, **337** (2012) 1318–1322]

# Experimental setup: splitting 1D Bose gas ($^{87}$Rb)



# Evolution of $C(L)^2$-distribution




*Black histograms*: Experimental results
*Red solid line*: Best equilibrium fits (with $T_{\mathrm{eff}} < T$)
*Blue dashed line*: Expected equilibrium distribution ($T \approx 80\,\mathrm{nK}$)

# Part IV

# Classical particle chain with pre-thermalization

# 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

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

- 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

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

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

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

# Boltzmann–Peierls equation



This yields, with $W_i = W(k_i, t)$, the kinetic equation

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

- For chosen nearest neighbour interaction, the collision $\delta$-functions have solutions only if $\sum_{j=1}^{3} \sigma_j = -1$

# Boltzmann–Peierls equation



## Kinetic equation (spatially homogeneous initial data)

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

- Stationary solutions are

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

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

# Molecular dynamics simulations (Kenichiro Aoki, 2006) 26


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 $\Delta T \to 0$,

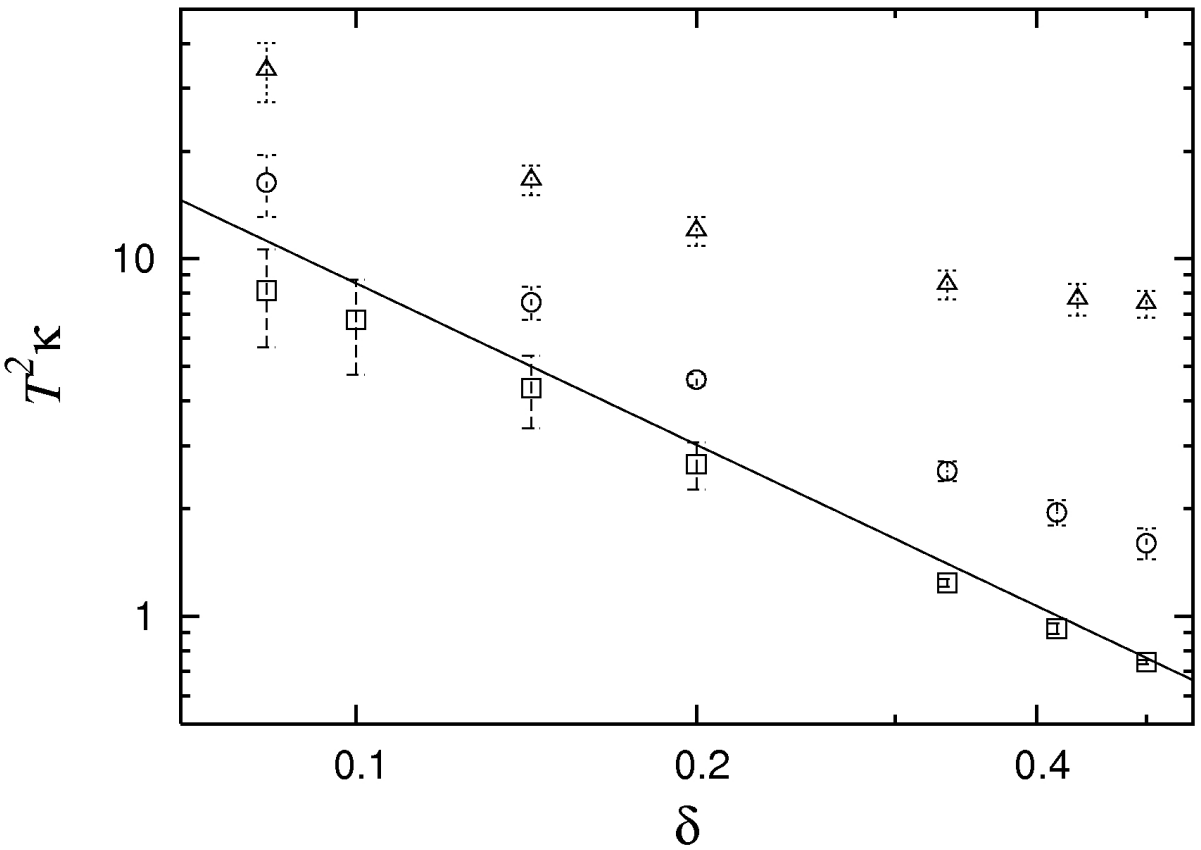
$$-\frac{N}{\Delta T} J \to \kappa(T, N)\,.$$

   Repeat for several $\Delta T$, 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 $T \to 0$, $\delta$ small (*black solid line*)




□ $T = 0.1$
○ $T = 0.4$
△ $T = 4$

# New 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, $\beta$) and fitting numerically to the kinetic formula (two parameters, $\beta', \mu'$) yields

| $\beta$ | 1 | 10 | 100 | 1000 |
|---|---|---|---|---|
| $\beta'$ | 0.912 | 8.98 | 97.1 | 986.4 |
| $\mu'$ | -0.488 | -0.229 | -0.0426 | -0.0120 |

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

Set $N = 64$ (periodic BC), $\delta = \frac{1}{4}$, $\lambda = 1$

Consider two sets of non-equilibrium initial data:

A) Bimodal momentum distribution:

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

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

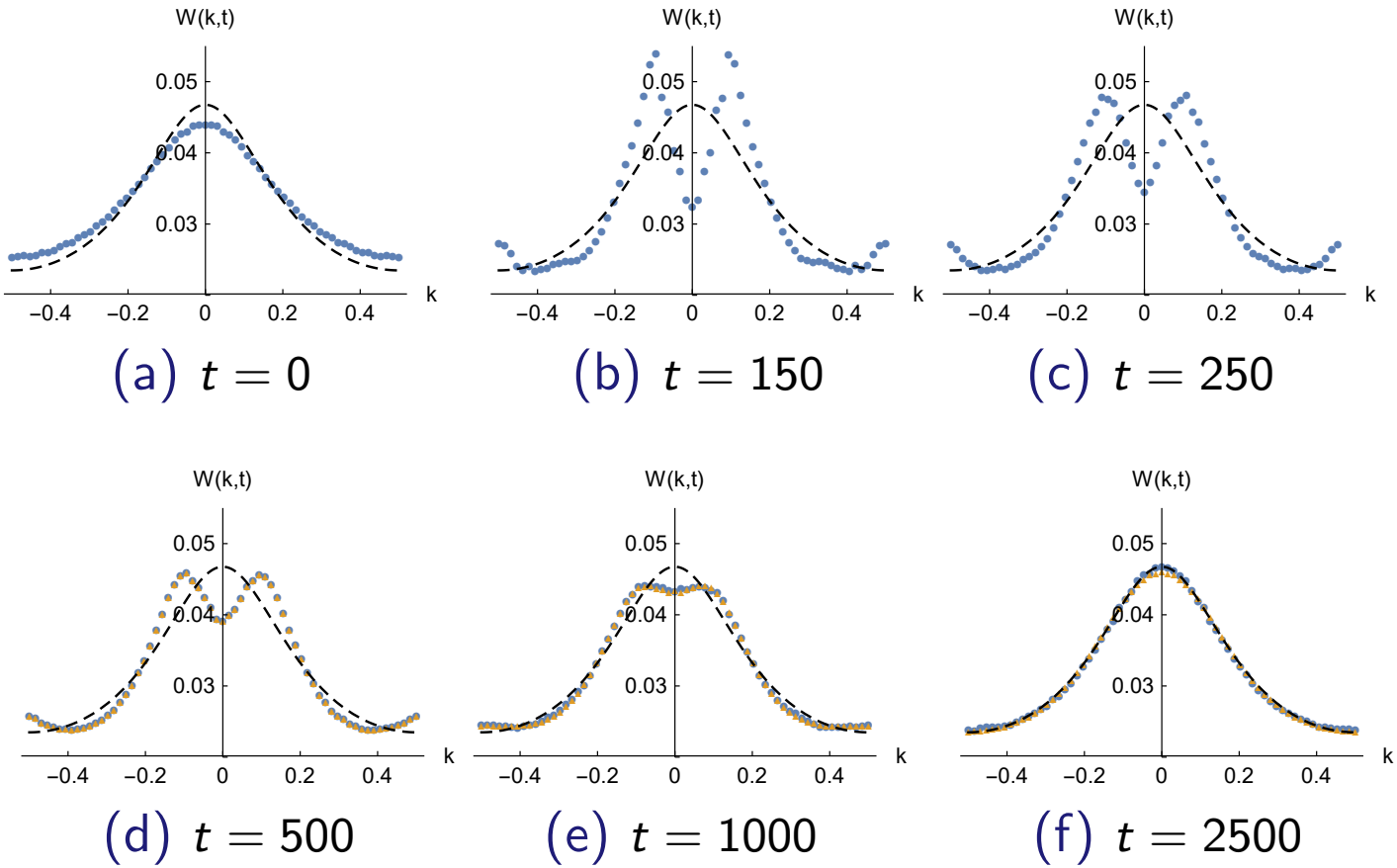
B) Random phase, with given initial Wigner function:

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.d.d. randomly distributed, uniformly on $[0, 2\pi]$

# A) Bimodal initial data

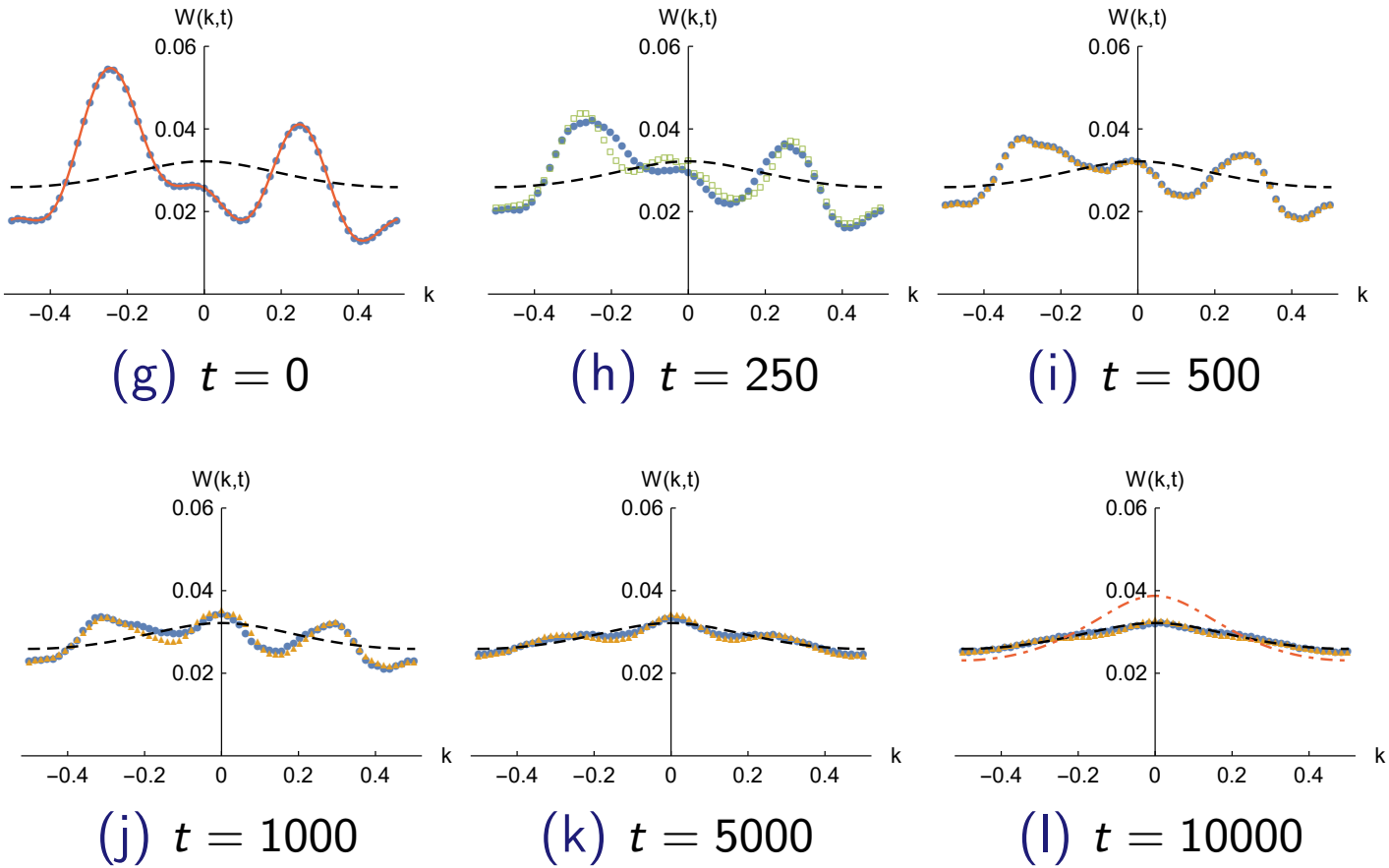



(a) $t = 0$ (b) $t = 150$ (c) $t = 250$

(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




(g) $t = 0$ (h) $t = 250$ (i) $t = 500$

(j) $t = 1000$ (k) $t = 5000$ (l) $t = 10000$

Wigner function from simulations (*blue dots*) vs.
solving the kinetic equation (*yellow triangles*) starting at $t = 500$
(I) Expected equilibrium distribution (*red dot-dashed line*)

# Evolution of entropy

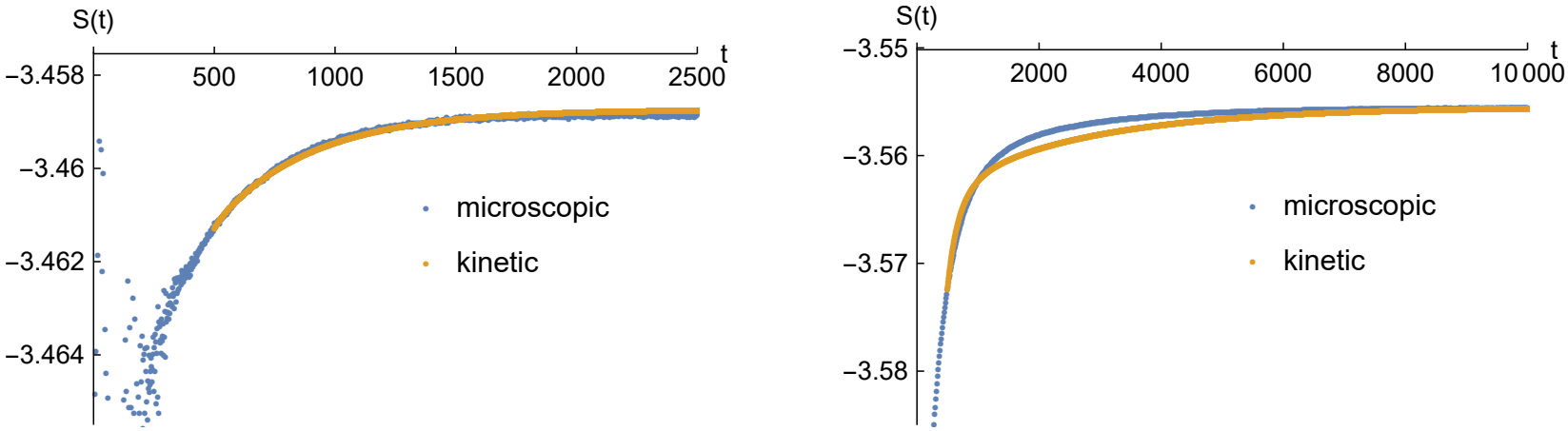
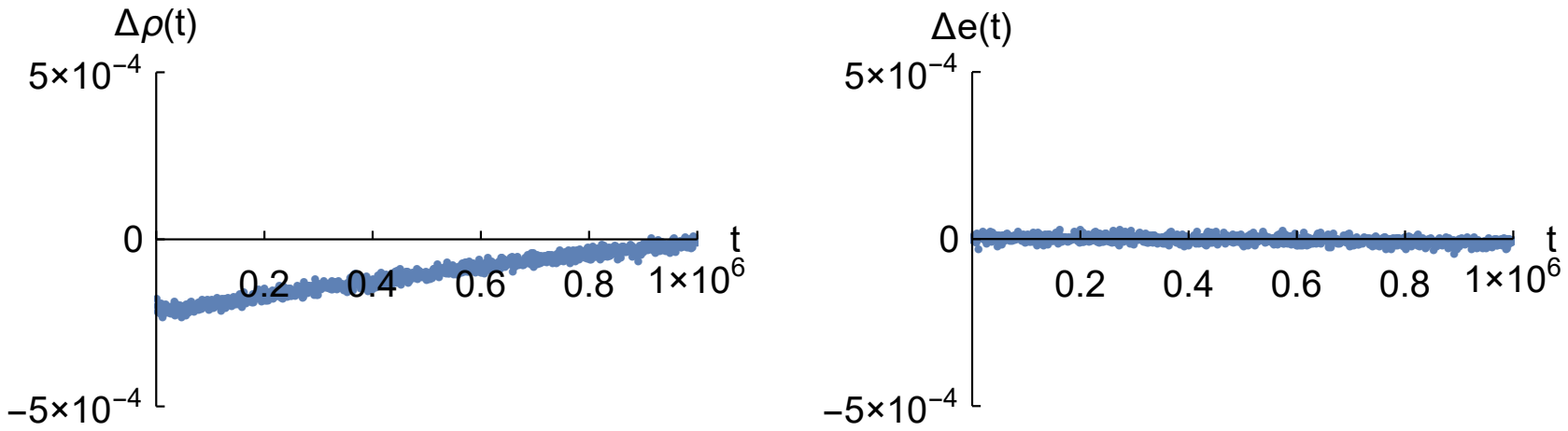



Figure : Time evolution of the entropy based on simulated Wigner functions, superimposing the kinetic solution starting at $t = 500$

# Eventual relaxation towards equilibrium? ($\lambda = 10$)




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

Figure : Time evolution of the density and energy differences using $\lambda = 10$ and longer simulation time $t_{\text{max}} = 10^6$

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? (Kinetic theory of FPU chain: also other dim)

A very much open problem:

Spatially inhomogeneous initial states?

# References

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Thank you for your attention ;

. . . and many happy returns, Herbert!

# Comparison: dNLS



## Discrete nonlinear Schrödinger equation

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

- Here $\psi_t : \mathbb{Z}^d \to \mathbb{C}$, $\lambda > 0$, $\alpha : \mathbb{Z}^d \to \mathbb{R}$.
  Denote $\omega := \widehat{\alpha}$, $\omega : \mathbb{T}^d \to \mathbb{R}$.

Conjectured: For translation invariant states, $\mathbb{E}[\psi_t(x')^*\psi_t(x)] = w_t(x-x')$, and $W_\tau := \lim_{\lambda\to 0} \widehat{w}_{\tau\lambda^{-2}}$ solves a nonlinear Boltzmann-Peierls equation $\partial_\tau W_\tau(k) = \mathcal{C}_{\text{NLS}}[W_\tau](k)$.

Proven: In *thermal equilibrium* ($\widehat{w}_t(k) = T/(\omega(k)-\mu) + O(\lambda)$), the time correlations $\mathbb{E}[\psi_0(0)^*\psi_{\tau\lambda^{-2}}(x)]$ decay in $\tau$ as dictated by the *linearization of the loss term* of $\mathcal{C}_{\text{NLS}}[W]$ around $T/(\omega(k)-\mu)$.

# Definition of the collision integral



2. Set $p_t(x) = \int_{\mathbb{T}^d} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}2\pi x\cdot k} \mathrm{e}^{-\mathrm{i}t\omega(k)}$. We assume that

$$\int_{-\infty}^{\infty} \mathrm{d}t \sum_x |p_t(x)|^3 < \infty\,.$$

- Then for every $k_0 \in \mathbb{T}^d$ the map

$$F \in C((\mathbb{T}^d)^3) \mapsto \lim_{\varepsilon\to 0^+} \int_{(\mathbb{T}^d)^2} \frac{\mathrm{d}k_1 \mathrm{d}k_2}{\pi}\; F(k) \frac{\varepsilon}{\varepsilon^2 + \underline{\omega}^2}\bigg|_{k_3 = k_0 + k_1 - k_2}$$

  defines *bounded positive Radon measure* on $(\mathbb{T}^d)^3$, denoted earlier by $\mathrm{d}^3k\, \delta(k_0 + k_1 - k_2 - k_3)\delta(\underline{\omega})$.
- We use the limit also to extend the collision operator from *continuous* $W$ to $W \in L^\infty$. (If all three assumptions are satisfied, the limit will converge in $L^2$-norm.)

# Assumptions needed for the twist Hamiltonian



3 For $\sigma \in \{-1,1\}^4$ and $k,k' \in (\mathbb{T}^d)^3$ define

$$\Omega(k;\sigma) := \sum_{i=1}^{3} \sigma_i \omega(k_i) + \sigma_4 \omega(k_1+k_2-k_3)$$

$$\Omega_1(k,k';\sigma) := \Omega(k;\sigma)\,, \qquad \Omega_2(k,k';\sigma) := \Omega((k_1,k_2',k_3);\sigma)\,,$$
$$\Omega_3(k,k';\sigma) := \Omega(k';\sigma)\,, \qquad \Omega_4(k,k';\sigma) := \Omega((k_1',k_2,k_3');\sigma)\,.$$

Set for $s \in \mathbb{R}^4$, $\sigma \in \{-1,1\}^4$,

$$\mathcal{G}(s;\sigma) := \int_{(\mathbb{T}^d)^3\times(\mathbb{T}^d)^3} \mathrm{d}^3k'\mathrm{d}^3k\, \mathrm{e}^{\mathrm{i}\sum_{i=1}^4 s_i\Omega_i(k,k';\sigma)}\,.$$

*We assume that* $C_{\mathcal{G}} := \max_\sigma \int_{\mathbb{R}^4} ds|\mathcal{G}(s;\sigma)| < \infty$.

# Definition of the twist Hamiltonian



## Definition of PV-integral

Then for any $W \in L^\infty$ with $0 \leq W_0 \leq 1$, the following limit converges in the $L^2(\mathbb{T}^d, \mathbb{C}^{2\times 2})$-norm:

$$H^{\text{eff}}[W](k_0) = \lim_{\varepsilon \to 0^+} \int_{(\mathbb{T}^d)^3} \mathrm{d}k_1 \mathrm{d}k_2 \mathrm{d}k_3 \delta(k_0 + k_1 - k_2 - k_3) \frac{\mathbb{1}_{\{()}|\underline{\omega}| > \varepsilon)}{\underline{\omega}}$$
$$\times \left( \tilde{W}_2 J[W_1 \tilde{W}_3] + W_2 J[\tilde{W}_1 W_3] \right)$$

- Can also replace $\frac{\mathbb{1}_{\{()}|\underline{\omega}|>\varepsilon)}{\underline{\omega}}$ by $\frac{\underline{\omega}}{\underline{\omega}^2+\varepsilon^2}$

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- Can also replace $\frac{\mathbb{1}_{\{()}|\underline{\omega}|>\varepsilon)}{\underline{\omega}}$ by $\frac{\underline{\omega}}{\underline{\omega}^2+\varepsilon^2}$
- Therefore, even though $0 \leq W_t \leq 1$ the rotations might have singularities!
- Is there a spontaneous generation of SU(2)-vortices?

# Main properties of the solutions



- We first prove that, after regularization of the PV-term, the equation becomes well-posed with $W_t^\varepsilon \in C(\mathbb{T}^d, \mathbb{C}^{2\times 2})$. The solution can then be obtained as an $L^2$-limit.
- Total energy and total spin are conserved
- To prove conservation of the Fermi constraint, $0 \leq W_t \leq 1$, we split the collision operator as in

$$\mathcal{C}[W](k) = \mathcal{G}[W](k) - \mathcal{A}[W](k)W(k) - W(k)\mathcal{A}[W](k)^*$$

and prove that $\mathcal{G}[W](k) \geq 0$ (as a matrix) by using the matrix inequality

$$CJ[BA] + AJ[BC] \geq 0$$

which is valid for any $A, B, C \geq 0$.

# On the derivation of the Hubbard BE



- Before going to the kinetic time-scale $O(\lambda^{-2})$, need to exponentiate the first scale corrections.
  - For times $O(\lambda^{-1})$ the only change is in the dispersion relation: $\omega(k)1 \to \omega^{\lambda}(k) := \omega(k)1 - \lambda R$, where $R := \langle \Sigma \rangle =$ *expectation of the total spin*
  - The correction lifts the spin-degeneracy $\Rightarrow$ we move into a basis where $R$ is diagonal
  - Fortunately, $R \neq R(k,t)$
- In this basis, the "free" semigroup is like that of a two-component dNLS $\Rightarrow$
  The analysis of the resulting oscillatory integrals is essentially identical to that in dNLS
- Therefore, the "term-by-term" limit is given by the Boltzmann equation whose "collision kernel" can be read off from the second order perturbation expansion