(Nonlinear) Fluctuating Hydrodynamics and Physics on Mesoscopic Scales

joint work with Herbert Spohn
Part 1

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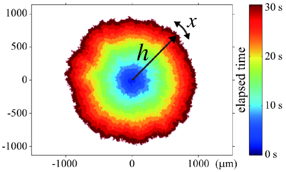


First Berlin – Leipzig Workshop on Fluctuating Hydrodynamics

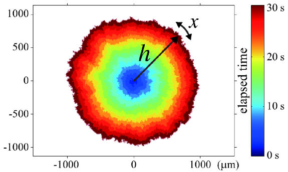
Overview

Nonlinear fluctuating hydrodynamics perspective of Hamiltonian systems

Multiple scales:

- microscopic:
  Fermi-Pasta-Ulam (FPU)-type anharmonic chains

- mesoscopic:
  KPZ partial differential equation



- macroscopic:
  fluid dynamics (hyperbolic conservation laws)

Fermi-Pasta-Ulam (FPU)-type anharmonic chains

Particles with positions q_i and momenta p_i
Hamiltonian:

$$H = \sum_i \frac{1}{2m_i} p_i^2 + V(q_{i+1} - q_i)$$

Interaction potential depends only on difference $q_{i+1} - q_i \rightsquigarrow$ momentum conservation

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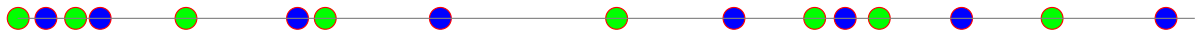
Equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t} r_i = \frac{1}{m_{i+1}} p_{i+1} - \frac{1}{m_i} p_i$$
$$\frac{\mathrm{d}}{\mathrm{d}t} p_i = V'(r_i) - V'(r_{i-1})$$

with the *stretch* $r_i = q_{i+1} - q_i$



FPU-type anharmonic chains: Conserved fields

Conserved fields:

$$\vec{u}(i) = \begin{pmatrix} r_i \\ p_i \\ e_i \end{pmatrix} \quad \begin{matrix} \text{stretch} \\ \text{momentum} \\ \text{energy} \end{matrix}$$

with stretch $r_i = q_{i+1} - q_i$ and energy $e_i = \frac{1}{2m_i} p_i^2 + V(r_i)$

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Microscopic currents

$$\vec{\mathcal{J}}(i) = \begin{pmatrix} -\frac{1}{m_i} p_i \\ -V'(r_{i-1}) \\ -\frac{1}{m_i} p_i V'(r_{i-1}) \end{pmatrix}$$

$\rightsquigarrow$ microscopic conservation law

$$\frac{\mathrm{d}}{\mathrm{d}t} \vec{u}(i,t) + \vec{\mathcal{J}}(i+1,t) - \vec{\mathcal{J}}(i,t) = 0$$

Connecting anharmonic chains ↔ stochastic PDE

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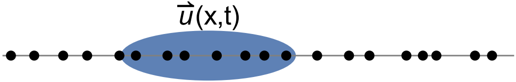
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathfrak{u}(i,t) + \mathcal{J}(i+1,t) - \mathcal{J}(i,t) = 0$$

↓ (local) thermal Gibbs equilibrium $\frac{1}{Z}\,\mathrm{e}^{-\beta(e_i + P r_i)}\mathrm{d}p_i\mathrm{d}r_i$



2. Euler equation

$$\partial_t u(x,t) + \partial_x \mathrm{j}(u(x,t)) = 0$$

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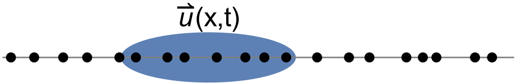

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$$\partial_t u(x,t) + \partial_x \mathsf{j}(u(x,t)) = 0$$

3. Expand current to *second* order in u, add dissipation plus noise ⇝ Langevin (stochastic Burgers) equation

$$\partial_t u(x,t) + \partial_x\Big(\underbrace{\mathsf{j}'(\bar{u})}_{\text{velocity } c}\; u + \underbrace{\tfrac{1}{2}\mathsf{j}''(\bar{u})u^2}_{\text{nonlinear current}} - \underbrace{D\partial_x u}_{\text{dissipation}} + \underbrace{\xi}_{\text{noise}} \Big) = 0$$

Connecting anharmonic chains $\leftrightarrow$ stochastic PDE

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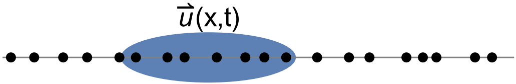

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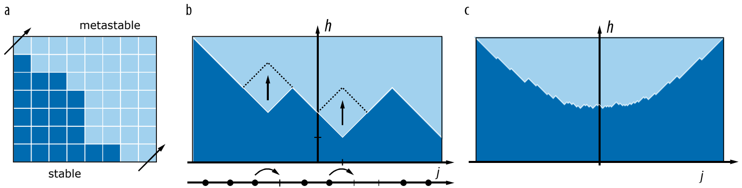
$\rightsquigarrow$ KPZ equation with $u(x,t) = \partial_x h(x,t)$

Spohn J. Stat. Phys. (2014), Mendl and Spohn PRL (2013)

Kardar-Parisi-Zhang (KPZ) and 1D surface growth

Kardar Parisi Zhang (1986)

$$\partial_t h(x,t) = \underbrace{\tfrac{1}{2}\lambda(\partial_x h)^2}_{\text{tilt-dependent growth}} + \underbrace{D\partial_x^2 h}_{\text{dissipation}} + \underbrace{\xi}_{\text{noise}}$$



(a) single-step model, TASEP; cf. Johansson 2000

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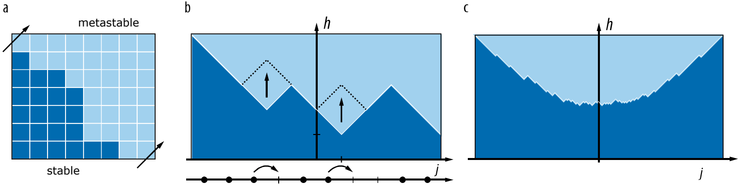

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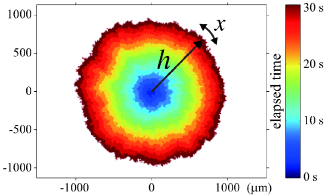
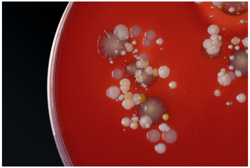


(b) Growing interfaces of liquid-crystal turbulence (Takeuchi et al. 2010)



(c) Bacteria growth (APS Physics, Yunker et al. 2013)

Experimental evidence for KPZ universality

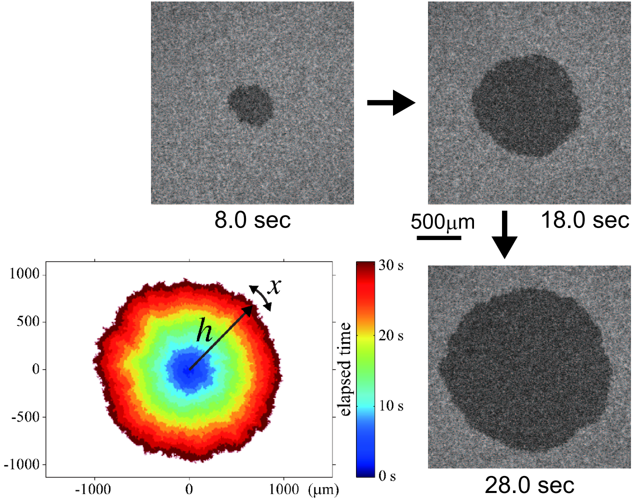


Figure: Growing cluster in a nematic liquid crystal (Takeuchi and Sano 2010)

KPZ prediction for space-time correlations (scalar case)

Langevin (noisy Burgers) equation

$$\partial_t u + \partial_x \big(\underbrace{\mathrm{j}'(\bar{u})}_{c} u + \tfrac{1}{2}\mathrm{j}''(\bar{u}) u^2 - D\partial_x u + \xi \big) = 0$$

Want to obtain correlator $S(x,t) = \langle u(x,t); u(0,0) \rangle$

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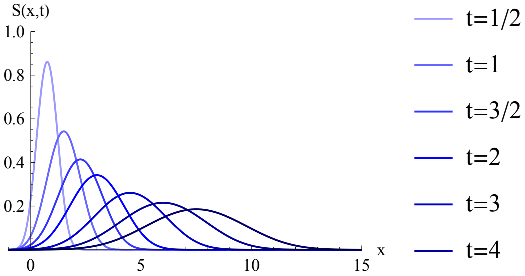
Want to obtain correlator $S(x,t) = \langle u(x,t); u(0,0) \rangle$
Long-time limit

$$S(x,t) \simeq \chi(\lambda|t|)^{-2/3} f_{\mathrm{KPZ}}\big((\lambda|t|)^{-2/3}(x - ct)\big)$$



Halpin-Healy and Takeuchi 2015

Generalization to several fields

Langevin equation for several fields:

$$\partial_t \vec{u} + \partial_x \left(A\vec{u} + \tfrac{1}{2}\langle \vec{u}, \vec{H}\vec{u}\rangle - \partial_x \tilde{D}\vec{u} + \vec{\xi} \right) = 0$$

with

$$A_{\alpha\beta} = \partial_{u_\beta} \mathrm{j}_\alpha, \quad \text{Hessians: } H^{\alpha}_{\beta\beta'} = \partial_{u_\beta}\partial_{u_{\beta'}} \mathrm{j}_\alpha, \quad \mathrm{j}_\alpha = \langle \mathcal{J}_\alpha \rangle$$

$$\text{Initial correlations:} \quad \langle u_\alpha(x,0); u_{\alpha'}(x',0)\rangle = C_{\alpha\alpha'}\,\delta(x-x')$$

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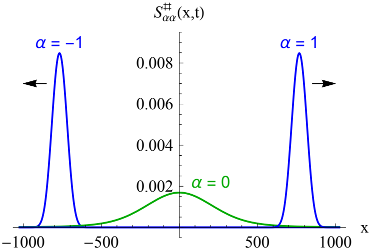
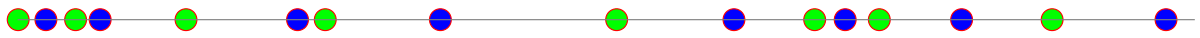
Diagonalize A: $\vec{\phi} = R\vec{u}, \quad RAR^{-1} = \mathrm{diag}(-c, 0, c), \quad RCR^{\mathrm{T}} = \mathbb{1} \quad \rightsquigarrow$

$$\partial_t \phi_\alpha + \partial_x \big(c_\alpha \phi_\alpha + \tfrac{1}{2}\langle \vec{\phi}, G^\alpha \vec{\phi}\rangle - \partial_x D\phi_\alpha + B\vec{\xi} \big) = 0$$



Spohn J. Stat. Phys. (2014), Mendl and Spohn PRL (2013)

Application to hard-point chains



$$H = \sum_i \frac{1}{2m_i} p_i^2 + V(r_i), \quad \text{stretch } r_i = q_{i+1} - q_i$$

Canonical ensemble $\rightsquigarrow$ local thermal Gibbs equilibrium factorizes:

$$Z^{-1}\, \mathrm{e}^{-\beta(e_i + P r_i)} \mathrm{d}p_i \mathrm{d}r_i$$

$\vec{u} = (\ell, v, \mathfrak{e})$ with $\ell = \langle r_i \rangle_{P,\beta}, \mathfrak{e} = \langle e_i \rangle_{P,\beta}$, one-to-one map $(\ell, \mathfrak{e}) \leftrightarrow (P, \beta)$

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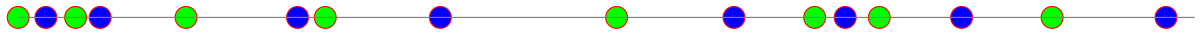
Coupling matrices: $G^\alpha = \frac{1}{2} \sum_{\alpha'=1}^{3} R_{\alpha\alpha'} (R^{-1})^{\mathrm{T}} H^{\alpha'} R^{-1}$

$$G^1 = \frac{c_{\bar{m}}}{2\sqrt{6}} \begin{pmatrix} -2 & -1 & 2 \\ -1 & 0 & -1 \\ 2 & -1 & 2 \end{pmatrix}, \quad G^0 = \frac{c_{\bar{m}}}{\sqrt{6}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Mendl and Spohn PRE (2014), https://github.com/cmendl/fluct-hydro-chains

Numerical simulation results for hard-point chains

Average over 10^7 realizations



KPZ prediction for correlations of field variables:

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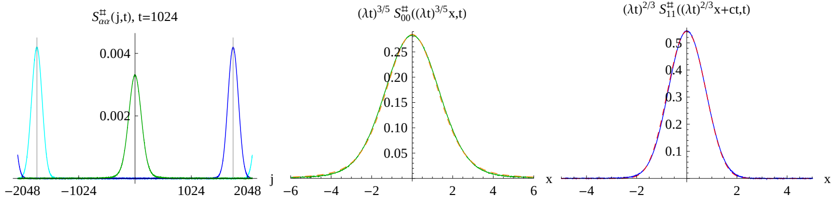


(a) overview (b) heat peak (c) sound peak

↑

Mendl and Spohn: PRL (2013), PRE (2014)

Nonlinear fluctuating hydrodynamics for the discrete nonlinear Schrödinger equation (DNLS)

Discrete nonlinear Schrödinger equation (DNLS)

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\psi_i = -\frac{1}{2m}(\psi_{i+1} - 2\psi_i + \psi_{i-1}) + g\,|\psi_i|^2\,\psi_i$$

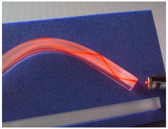
$$H = \sum_{i=0}^{N-1} \frac{1}{2m}|\psi_{i+1} - \psi_i|^2 + \frac{1}{2}\,g\,|\psi_i|^4$$

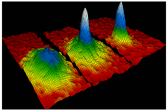
with $i \in \mathbb{Z}$; here: defocusing case $g > 0$

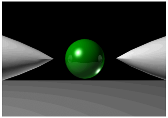
cf. Gross-Pitaevskii equation

Applications:

- nonlinear optical wave guides
- Bose-Einstein condensates
- electronic transport







Discrete (lattice) NLS is non-integrable!

Relation to quantum liquids

$$\mathbb{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\psi_i = -\frac{1}{2m}(\psi_{i+1} - 2\psi_i + \psi_{i-1}) + g\,|\psi_i|^2\,\psi_i$$

- Bose-Hubbard model in the limit of large density and weak coupling $U/t \ll 1$

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- Bose-Hubbard model in the limit of large density and weak coupling $U/t \ll 1$
- goal: dynamical correlations, e.g., density-density $\langle\rho_i(t);\rho_0(0)\rangle$ with $\rho_i(t) = |\psi_i(t)|^2$ (cf. Green-Kubo)

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- goal: dynamical correlations, e.g., density-density $\langle \rho_i(t); \rho_0(0) \rangle$ with $\rho_i(t) = |\psi_i(t)|^2$ (cf. Green-Kubo)
- relation to "second sound" in a Fermi gas:

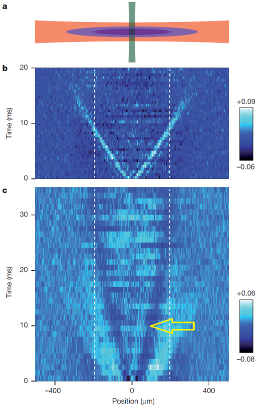

Figure: Sidorenkov et al. Nature (2013)

Conservation laws and currents

Polar coordinates: $\psi_i = \sqrt{\rho_i}\, \mathrm{e}^{\mathrm{i}\varphi_i}$

density	$\rho_i = \|\psi_i\|^2$
phase difference	$r_i = \varphi_{i+1} - \varphi_i$ (almost conserved at low T)
energy	$e_i = \frac{1}{2m}\|\psi_{i+1} - \psi_i\|^2 + \frac{1}{2}\, g\, \|\psi_i\|^4$

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$$
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\end{aligned}
$$

Example: local density conservation law

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\rho_i(t) + \mathcal{J}_{\rho,i+1}(t) - \mathcal{J}_{\rho,i}(t) = 0,$$

corresponding density current

$$\mathcal{J}_{\rho,i} = \tfrac{1}{2m}\mathbb{i}\left(\psi_{i-1}\,\partial\psi^*_{i-1} - \psi^*_{i-1}\,\partial\psi_{i-1}\right)$$

High temperatures: vanishing currents, diffusive transport

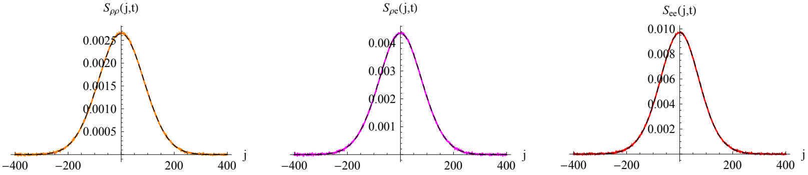
Canonical ensemble:

$$Z_N(\mu,\beta)^{-1}\,\mathrm{e}^{-\beta(H-\mu\mathrm{N})}\prod_{i=-N/2}^{N/2-1}\mathrm{d}\psi_i\mathrm{d}\psi_i^*$$

Density and energy currents are of the form $\mathbb{i}(z-z^*)$ $\rightsquigarrow$

$$\langle\mathcal{J}_{\rho,i}\rangle=0\,,\quad\langle\mathcal{J}_{e,i}\rangle=0$$

$\rightsquigarrow$ based on linear fluctuating hydrodynamics, one expects *diffusive* spreading of time-correlations (cf. kernel of heat equation)



(a) $\langle\rho_i(t);\rho_0(0)\rangle$ (b) $\langle\rho_i(t);e_0(0)\rangle$ (c) $\langle e_i(t);e_0(0)\rangle$

Figure: Equilibrium time-correlations at $\beta=1$ and $t=1536$

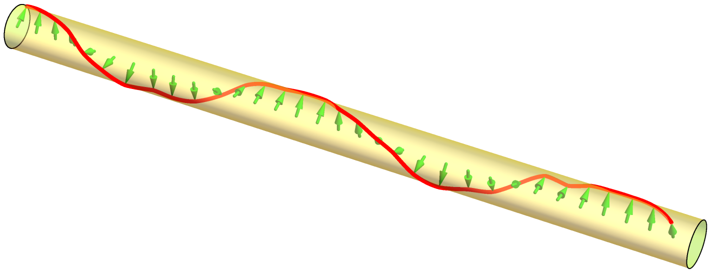
Low temperature analysis

polar coordinates: $\psi_i = \sqrt{\rho_i}\, \mathrm{e}^{\mathrm{i}\varphi_i}$,
phase difference: $r_i = \varphi_{i+1} - \varphi_i$ (almost conserved at low T)

Exact Hamiltonian in polar coordinates (angles φ_i and $\rho_i \geq 0$):

$$H = \sum_{j=0}^{N-1} \left(-\tfrac{1}{m}\sqrt{\rho_{i+1}\,\rho_i}\, \cos(\varphi_{i+1} - \varphi_i) + \tfrac{1}{m}\rho_i + \tfrac{1}{2}\, g\, \rho_i^2\right)$$

Umklapp: $|\varphi_{i+1}(t) - \varphi_i(t)| = \pi$



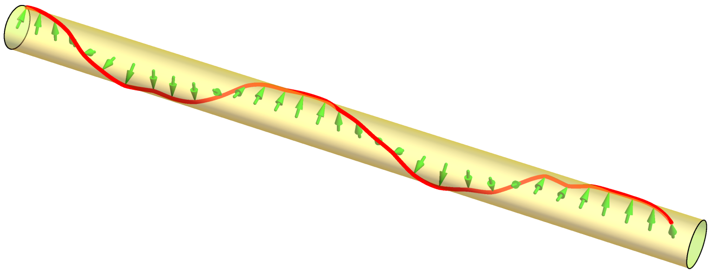
Low temperature analysis

Umklapp: $|\varphi_{i+1}(t) - \varphi_i(t)| = \pi$

Low temperature analysis: regard angles φ_i as variables in $\mathbb{R}$ and suppress Umklapp processes, i.e., replace

$$-\frac{1}{m}\cos(\varphi_{i+1} - \varphi_i) \to U(\varphi_{i+1} - \varphi_i) \quad \text{with}$$

$$U(x) = -\frac{1}{m}\cos(x) \;\; \text{for} \;\; |x| \leq \pi\,, \qquad U(x) = \infty \;\; \text{for} \;\; |x| > \pi$$



Low temperature analysis: average currents

polar coordinates: $\psi_i = \sqrt{\rho_i}\,\mathrm{e}^{\mathbb{i}\varphi_i}$,
phase difference: $r_i = \varphi_{i+1} - \varphi_i$

Canonical ensemble:

$$Z_N(\mu,\nu,\beta)^{-1}\,\mathrm{e}^{-\beta\left(H-\mu\sum_i \rho_i - \nu\sum_i r_i\right)}\prod_{j=0}^{N-1}\mathrm{d}\rho_i\,\mathrm{d}r_i$$

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Field variables ρ_i, r_i, e_i, corresponding average currents:

$$\vec{\mathrm{j}} = \langle \vec{\mathcal{J}}_i \rangle = \langle (\mathcal{J}_{\rho,i}, \mathcal{J}_{r,i}, \mathcal{J}_{e,i}) \rangle = (\nu, \mu, \mu\, \nu)$$

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phase difference: $r_i = \varphi_{i+1} - \varphi_i$

Canonical ensemble:

$$Z_N(\mu,\nu,\beta)^{-1}\,\mathrm{e}^{-\beta\left(H-\mu\sum_i \rho_i-\nu\sum_i r_i\right)}\prod_{j=0}^{N-1}\mathrm{d}\rho_i\,\mathrm{d}r_i$$

Field variables ρ_i, r_i, e_i, corresponding average currents:

$$\vec{\mathrm{j}} = \langle\vec{\mathcal{J}}_i\rangle = \langle(\mathcal{J}_{\rho,i},\mathcal{J}_{r,i},\mathcal{J}_{e,i})\rangle = (\nu,\mu,\mu\,\nu)$$

(Omitting r_i and setting $\nu = 0$ reverts back to zero average currents, as for high temperatures)

Simulation results for the DNLS

inverse temperature $\beta = 15$

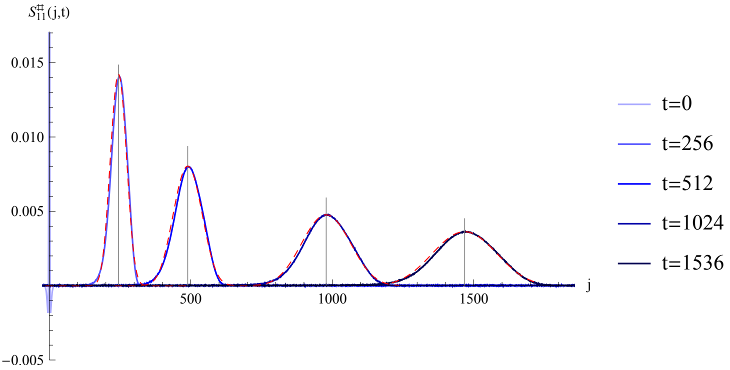
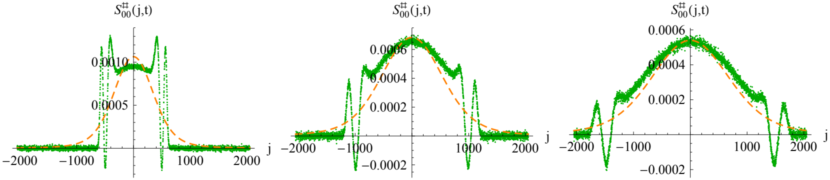


Figure: Equilibrium two-point correlations $S_{11}^{\sharp}(j,t)$, showing the right-moving sound peak at different time points

Simulation results for the DNLS
inverse temperature $\beta = 15$



(a) $t = 512$ (b) $t = 1024$ (c) $t = 1536$

Figure: Central heat mode $S^{\sharp}_{00}(j, t)$, at $\beta = 15$

$$Z_N(\mu,\nu,\beta) = \int \mathrm{e}^{-\beta\left(H-\mu\sum_i \rho_i - \nu\sum_i r_i\right)} \prod_{j=0}^{N-1} \mathrm{d}\rho_i \mathrm{d}r_i$$

For $\nu = 0$, first evaluate angular integrals r_i on $[-\pi,\pi]$ (Rasmussen et al. 2000) $\rightsquigarrow$

$$Z_N(\mu,0,\beta) = \int \prod_{j=0}^{N-1} K(\rho_{i+1},\rho_i)\,\mathrm{d}\rho_i$$

with *transfer operator* or kernel $K(x,y) = K_1(x,y)K_0(y)$ and

$$K_1(x,y) = 2\pi I_0\left(\beta\tfrac{1}{m}\sqrt{x\,y}\right)\mathrm{e}^{-\beta\frac{1}{2m}(x+y)}\,, \quad K_0(y) = \mathrm{e}^{\beta\frac{1}{2}\mu^2/g}\,\mathrm{e}^{-\beta\frac{1}{2}g\left(y-\frac{\mu}{g}\right)^2}$$

Then

$$\lim_{N\to\infty}\frac{1}{N}\log Z_N(\mu,0,\beta) = \log(\lambda_{\max}(K))$$

Use a Nyström-type discretization for the kernel: given a Gauss quadrature rule

$$\int_0^\infty f(\rho)\, \mathrm{e}^{-\beta \frac{1}{2} g \left(\rho - \frac{\mu}{g}\right)^2} \mathrm{d}\rho \approx \sum_{i=1}^{n} w_i\, f(x_i)\,,$$

construct the symmetric matrix

$$\left(K_1(x_i, x_{i'})\, \sqrt{w_i\, w_{i'}}\right)_{i,i'=1}^{n}$$

and calculate its largest eigenvalue, denoted λ_1. Then

$$\log(\lambda_{\max}(K)) \approx \beta\, \frac{1}{2} \frac{\mu^2}{g} + \log \lambda_1\,.$$

$\rightsquigarrow$ exponential convergence with respect to number of quadrature points

cf. Bornemann 2010: "On the numerical evaluation of Fredholm determinants"

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