Low temperature dynamics of the one-dimensional discrete nonlinear Schrödinger equation
(joint work with Herbert Spohn)

Christian B. Mendl

Stanford University, USA

February 23, 2016

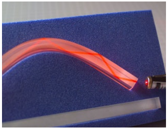
KITP, UC Santa Barbara "New approaches to non-equilibrium and random systems"

Discrete nonlinear Schrödinger equation (DNLS)

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\psi_j = -\frac{1}{2m}\Delta\psi_j + g\,|\psi_j|^2\,\psi_j$$

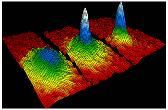
$$H = \sum_{j=0}^{N-1} \frac{1}{2m}|\psi_{j+1} - \psi_j|^2 + \frac{1}{2}\,g\,|\psi_j|^4$$

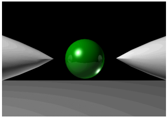
with $j \in \mathbb{Z}$; here: defocusing case $g > 0$.



Applications:

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





Discrete (lattice) NLS is non-integrable!

Conservation laws

Polar coordinates: $\psi_j = \sqrt{\rho_j}\, \mathrm{e}^{\mathrm{i}\varphi_j}$

density $\rho_j = |\psi_j|^2$

phase difference $r_j = \varphi_{j+1} - \varphi_j$ (almost conserved at low T)

energy $e_j = \frac{1}{2m}|\psi_{j+1} - \psi_j|^2 + \frac{1}{2}\, g\, |\psi_j|^4$

Conservation laws

Polar coordinates: $\psi_j = \sqrt{\rho_j}\,\mathrm{e}^{\mathrm{i}\varphi_j}$

$$\begin{aligned} \text{density} \quad & \rho_j = |\psi_j|^2 \\ \text{phase difference} \quad & r_j = \varphi_{j+1} - \varphi_j \quad \text{(almost conserved at low } T\text{)} \\ \text{energy} \quad & e_j = \tfrac{1}{2m}|\psi_{j+1} - \psi_j|^2 + \tfrac{1}{2}\,g\,|\psi_j|^4 \end{aligned}$$

Example: density conservation law

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

$$\rightsquigarrow \sum_{j=0}^{N-1} \rho_j(t) = \mathrm{const!}$$

Corresponding density current

$$\mathcal{J}_{\rho,j} = \tfrac{1}{2m}\mathrm{i}\big(\psi_{j-1}\,\partial\psi^*_{j-1} - \psi^*_{j-1}\,\partial\psi_{j-1}\big)$$

Nonlinear fluctuating hydrodynamics (scalar case)

At macroscopic scale: hyperbolic conservation law

$$\partial_t \varrho(x,t) + \partial_x j(\varrho(x,t)) = 0$$

with j the density current.

Nonlinear fluctuating hydrodynamics (scalar case)

At macroscopic scale: hyperbolic conservation law

$$\partial_t \varrho(x,t) + \partial_x j(\varrho(x,t)) = 0$$

with j the density current.
Fluctuations relative to background: $\varrho(x,t) = \bar{\rho} + \rho(x,t)$,
add dissipation and noise $\rightsquigarrow$ Langevin equation

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

D: diffusion constant, $\xi(x,t)$: space-time white noise

Nonlinear fluctuating hydrodynamics (scalar case)

Langevin equation (noisy Burgers equation, cf KPZ equation)

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

Mathematical solution theory: Martin Hairer, Fields Medal 2014

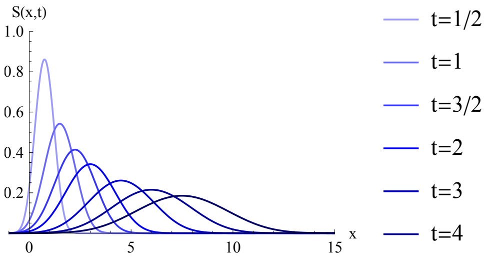
Nonlinear fluctuating hydrodynamics (scalar case)

Langevin equation (noisy Burgers equation, cf KPZ equation)

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

Mathematical solution theory: Martin Hairer, Fields Medal 2014
Want to obtain correlator $S(x,t) = \langle \rho(x,t); \rho(0,0) \rangle$
Long-time limit

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



Generalization to several fields

$\vec{u} = \vec{u}(x,t)$: deviation of the conserved fields from background

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

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

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

Generalization to several fields

$\vec{u} = \vec{u}(x,t)$: deviation of the conserved fields from background

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

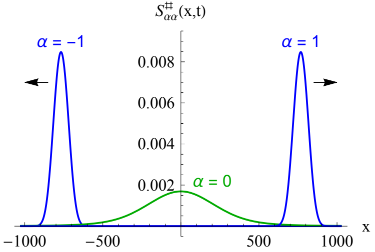
Hessians: $H^{\alpha}_{\gamma\gamma'} = \partial_{u_\gamma}\partial_{u_{\gamma'}} \mathrm{j}_\alpha, \quad \mathrm{j}_\alpha = \langle \mathcal{J}_\alpha \rangle$

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

Diagonalization:

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

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



Low temperature Hamiltonian

polar coordinates: $\psi_j = \sqrt{\rho_j}\, \mathrm{e}^{\mathrm{i}\varphi_j}$,
phase difference: $r_j = \varphi_{j+1} - \varphi_j$ (almost conserved at low T)

Exact Hamiltonian in polar coordinates (angles φ_j and $\rho_j \geq 0$):

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

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

Low temperature approximation: regard angles φ_j as variables in $\mathbb{R}$ and replace

$$-\tfrac{1}{m}\cos(\varphi_{j+1} - \varphi_j) \to U(\varphi_{j+1} - \varphi_j) \quad \text{with}$$

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

Thermodynamic current averages for DNLS

polar coordinates: $\psi_j = \sqrt{\rho_j}\,\mathrm{e}^{\mathrm{i}\varphi_j}$,
phase difference: $r_j = \varphi_{j+1} - \varphi_j$ (almost conserved at low T)

Canonical ensemble:

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

Averages denoted by $\langle\cdot\rangle$

Thermodynamic current averages for DNLS

polar coordinates: $\psi_j = \sqrt{\rho_j}\, \mathrm{e}^{\mathrm{i}\varphi_j}$,
phase difference: $r_j = \varphi_{j+1} - \varphi_j$ (almost conserved at low T)

Canonical ensemble:

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

Averages denoted by $\langle \cdot \rangle$
Field variables ρ_j, r_j, e_j, corresponding current averages:

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

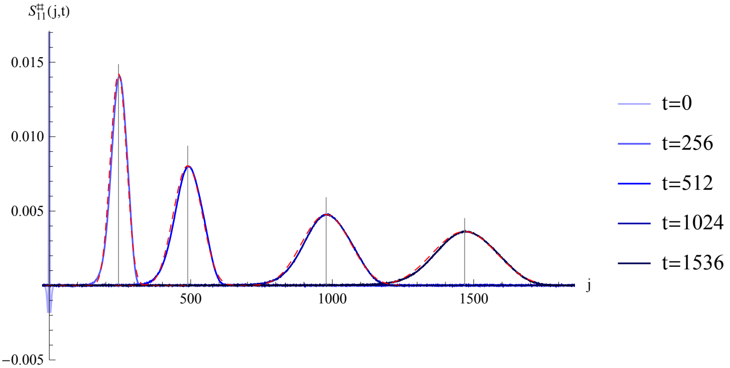
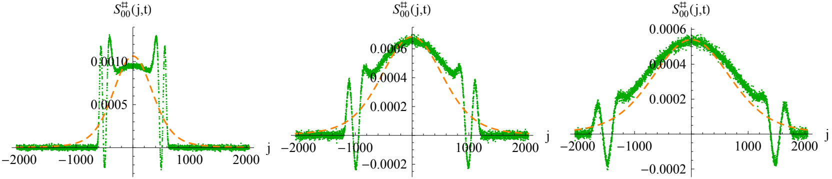


Figure: Equilibrium two-point correlations $S_{11}^{\sharp}(j,t)$, showing the right-moving sound peak at different time points; equilibrium inverse temperature $\beta = 15$

Simulation results

$\beta = 15$



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

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

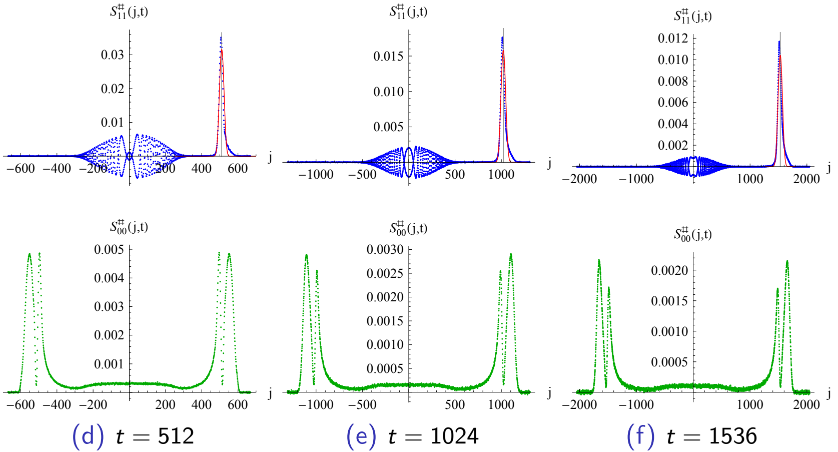


Figure: $S^{\sharp}_{11}(j,t)$ (top) and $S^{\sharp}_{00}(j,t)$ (bottom) at $\beta = 200$

Split Hamiltonian into kinetic and nonlinear part, $H = T + U$:

$$T = \sum_{j=0}^{N-1} \frac{1}{2m} |\psi_{j+1} - \psi_j|^2 , \qquad U = \sum_{j=0}^{N-1} \frac{1}{2}\, g\, |\psi_j|^4 .$$

Flow over time t:

$$\Phi_t^T : \; \hat{\psi}_k \mapsto \mathrm{e}^{-\mathrm{i}\,(1-\cos(2\pi k/N))\, t/m}\, \hat{\psi}_k ,$$
$$\Phi_t^U : \; \psi_j \mapsto \mathrm{e}^{-\mathrm{i}\, g\, |\psi_j|^2\, t}\, \psi_j$$

Generalization of Strang splitting: Runge-Kutta-Nyström method SRKN_6^b by Blanes and Moan 2002 for a time step h:

$$\Psi_h = \Phi^U_{b_{s+1}h} \circ \Phi^T_{a_s h} \circ \cdots \circ \Phi^U_{b_2 h} \circ \Phi^T_{a_1 h} \circ \Phi^U_{b_1 h}$$

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

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

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

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

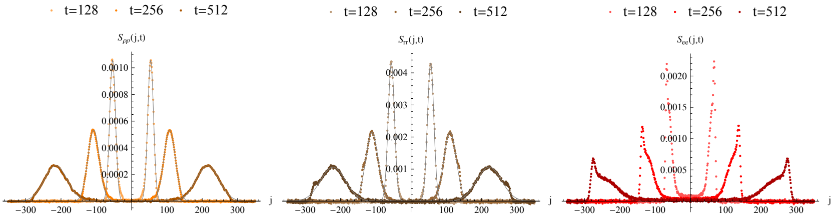
$$\log(\lambda_{\max}(K)) \approx \beta\, \frac{1}{2} \frac{\mu^2}{g} + \log \lambda_1\,.$$

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

Integrable Ablowitz-Ladik model

$$i \frac{\mathrm{d}}{\mathrm{d}t}\psi_j = -\frac{1}{2m}\Delta\psi_j + \frac{1}{2}\, g\, |\psi_j|^2 \left(\psi_{j+1} + \psi_{j-1}\right)$$

Expecting ballistic (linear in time) spreading of the correlation functions due to integrability



(a) density $S^{\mathrm{al}}_{\rho\rho}(j,t)$ (b) stretch $S^{\mathrm{al}}_{rr}(j,t)$ (c) energy $S^{\mathrm{al}}_{ee}(j,t)$

Figure: Equilibrium time-correlations of the Ablowitz-Ladik model at inverse temperature $\beta = 15$

References

- Blanes, S. and Moan, P. C. (2002). "Practical symplectic partitioned Runge-Kutta and Runge-Kutta-Nyström methods". In: *J. Comput. Appl. Math.* 142, pp. 313–330.
- Kulkarni, M. and Lamacraft, A. (2013). "Finite-temperature dynamical structure factor of the one-dimensional Bose gas: From the Gross-Pitaevskii equation to the Kardar-Parisi-Zhang universality class of dynamical critical phenomena". In: *Phys. Rev. A* 88, 021603(R).
- Kulkarni, M. et al. (2015). "Fluctuating hydrodynamics for a discrete Gross-Pitaevskii equation: mapping to Kardar-Parisi-Zhang universality class". In: *arXiv:1502.06661*.
- Mendl, C. B. and Spohn, H. (2013). "Dynamic correlators of FPU chains and nonlinear fluctuating hydrodynamics". In: *Phys. Rev. Lett.* 111, p. 230601.
- – (2015). "Low temperature dynamics of the one-dimensional discrete nonlinear Schrödinger equation". In: *J. Stat. Mech.* 2015, P08028.
- Rasmussen, K. O. et al. (2000). "Statistical mechanics of a discrete nonlinear system". In: *Phys. Rev. Lett.* 84, pp. 3740–3743.
- Spohn, H. (2014). "Nonlinear fluctuating hydrodynamics for anharmonic chains". In: *J. Stat. Phys.* 154, pp. 1191–1227.