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)

\[ i \frac{d}{dt} \psi_j = -\frac{1}{2m} \Delta \psi_j + g |\psi_j|^2 \psi_j \]

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

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!
Polar coordinates: \( \psi_j = \sqrt{\rho_j} \ e^{i\phi_j} \)

- **density** \( \rho_j = |\psi_j|^2 \)
- **phase difference** \( r_j = \varphi_{j+1} - \varphi_j \) (almost conserved at low \( T \))
- **energy** \( e_j = \frac{1}{2m} |\psi_{j+1} - \psi_j|^2 + \frac{1}{2} g |\psi_j|^4 \)
Polar coordinates: \( \psi_j = \sqrt{\rho_j} \, e^{i\varphi_j} \)

**Density** \( \rho_j = |\psi_j|^2 \)

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

**Energy** \( e_j = \frac{1}{2m} |\psi_{j+1} - \psi_j|^2 + \frac{1}{2} g |\psi_j|^4 \)

Example: density conservation law

\[
\frac{d}{dt} \rho_j(t) + J_{\rho,j+1}(t) - J_{\rho,j}(t) = 0
\]

\[
\to \sum_{j=0}^{N-1} \rho_j(t) = \text{const}!
\]

**Corresponding density current**

\[
J_{\rho,j} = \frac{1}{2m} i(\psi_{j-1} \partial \psi^*_{j-1} - \psi^*_{j-1} \partial \psi_{j-1})
\]
At macroscopic scale: hyperbolic conservation law

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

with \( j \) the density current.
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 \( \leadsto \) Langevin equation

$$\partial_t \rho + \partial_x \left( j'(\bar{\rho}) \rho + \frac{1}{2} j''(\bar{\rho}) \rho^2 - D \partial_x \rho + B \xi \right) = 0$$

\( D \): diffusion constant, \( \xi(x, t) \): space-time white noise
Nonlinear fluctuating hydrodynamics (scalar case)

Langevin equation (noisy Burgers equation, cf KPZ equation)

\[ \partial_t \rho + \partial_x \left( j'(\bar{\rho}) \rho + \frac{1}{2} j''(\bar{\rho}) \rho^2 - D \partial_x \rho + B \xi \right) = 0 \]

Mathematical solution theory: Martin Hairer, Fields Medal 2014
Langevin equation (noisy Burgers equation, cf KPZ equation)

\[ \partial_t \rho + \partial_x \left( j'(\bar{\rho}) \rho + \frac{1}{2} j''(\bar{\rho}) \rho^2 - D \partial_x \rho + B \xi \right) = 0 \]

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

\[ S(x, t) = \chi(\lambda |t|)^{-2/3} f_{\text{KPZ}}((\lambda |t|)^{-2/3}(x - ct)) \]
Generalization to several fields

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

\[
\partial_t \mathbf{\tilde{u}} + \partial_x \left( A \mathbf{\tilde{u}} + \frac{1}{2} \langle \mathbf{\tilde{u}}, \mathbf{\tilde{H}} \mathbf{\tilde{u}} \rangle - \partial_x \mathbf{\tilde{D}} \mathbf{\tilde{u}} + \mathbf{\tilde{B}} \mathbf{\tilde{\xi}}(x, t) \right) = 0
\]

Hessians: \( H_{\alpha'\alpha} = \partial_{\gamma} \partial_{\gamma'} j_{\alpha}, \quad j_{\alpha} = \langle J_{\alpha} \rangle \)

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

\[
\partial_t \vec{u} + \partial_x (A \vec{u} + \frac{1}{2} \langle \vec{u}, \vec{H} \vec{u} \rangle - \partial_x \vec{D} \vec{u} + \vec{B} \vec{\xi}(x, t)) = 0
\]

Hessians: \( H_{\gamma\gamma'}^{\alpha} = \partial_{u_\gamma} \partial_{u_{\gamma'}} j_\alpha, \quad j_\alpha = \langle J_\alpha \rangle \)

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

Diagonalization:

\[
\vec{\phi} = R \vec{u}, \quad RAR^{-1} = \text{diag}(-c, 0, c), \quad RCR^T = I \quad \leadsto
\]

\[
\partial_t \phi_\alpha + \partial_x \left( c_\alpha \phi_\alpha + \frac{1}{2} \langle \vec{\phi}, G^\alpha \vec{\phi} \rangle - \partial_x D \phi_\alpha + B \vec{\xi}(x, t) \right) = 0
\]
Low temperature Hamiltonian

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

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

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

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

Low temperature approximation: regard angles \( \varphi_j \) as variables in \( \mathbb{R} \) and replace

\[
-\frac{1}{m} \cos(\varphi_{j+1} - \varphi_j) \rightarrow U(\varphi_{j+1} - \varphi_j) \quad \text{with}
\]

\[
U(x) = -\frac{1}{m} \cos(x) \quad \text{for} \quad |x| \leq \pi , \quad U(x) = \infty \quad \text{for} \quad |x| > \pi
\]
polar coordinates: $\psi_j = \sqrt{\rho_j} e^{i\varphi_j}$,
phase difference: $r_j = \varphi_{j+1} - \varphi_j$ (almost conserved at low $T$)

Canonical ensemble:

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

Averages denoted by $\langle \cdot \rangle$
polar coordinates: $\psi_j = \sqrt{\rho_j} \, \text{e}^{i\varphi_j}$,
phase difference: $r_j = \varphi_{j+1} - \varphi_j$ (almost conserved at low $T$)

Canonical ensemble:

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

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

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

$\beta = 15$

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

$\beta = 15$

Figure: Central heat mode $S_{00}(j, t)$, at $\beta = 15$
Simulation results
\( \beta = 200 \) (traces of integrability)

Figure: \( S_{11}(j, t) \) (top) and \( S_{00}(j, t) \) (bottom) at \( \beta = 200 \)
Split Hamiltonian into kinetic and nonlinear part, $H = T + U$:

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

Flow over time $t$:

$$
\Phi^T_t : \hat{\psi}_k \mapsto e^{-i \frac{1}{m} (1 - \cos(2\pi k/N)) t} \hat{\psi}_k,
\Phi^U_t : \psi_j \mapsto e^{-i g |\psi_j|^2 t} \psi_j
$$

Generalization of Strang splitting: Runge-Kutta-Nyström method $\text{SRKN}^b_6$ by Blanes and Moan 2002 for a time step $h$:

$$
\Psi_h = \Phi^U_{b_{s+1}h} \circ \Phi^T_{a_sh} \circ \cdots \circ \Phi^U_{b_2h} \circ \Phi^T_{a_1h} \circ \Phi^U_{b_1h}
$$
Numerical implementation
Evaluating the partition function

\[ Z_N(\mu, \nu, \beta) = \int e^{-\beta(H - \mu \sum_j \rho_j - \nu \sum_j r_j)} \prod_{j=0}^{N-1} d\rho_j dr_j \]

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

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

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

\[ K_1(x, y) = 2\pi I_0(\beta \frac{1}{m} \sqrt{xy}) e^{-\frac{1}{2m}(x+y)}, \quad K_0(y) = e^{\beta \frac{1}{2} \mu^2 / g} e^{-\frac{1}{2}g(y - \frac{\mu}{g})^2} \]

Then

\[
\lim_{N \to \infty} \frac{1}{N} \log Z_N(\mu, 0, \beta) = \log(\lambda_{\text{max}}(K))
\]
Use a Nyström-type discretization for the kernel: given a Gauss quadrature rule

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

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 $\lambda_1$. Then

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

$\Rightarrow$ exponential convergence with respect to the number of quadrature points
Integrable Ablowitz-Ladik model

\[ i \frac{d}{dt} \psi_j = -\frac{1}{2m} \Delta \psi_j + \frac{1}{2} g |\psi_j|^2 (\psi_{j+1} + \psi_{j-1}) \]

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

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


