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# The Nonequilibrium, Discrete Nonlinear Schroedinger Equation

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# The nonequilibrium, discrete nonlinear Schrödinger equation

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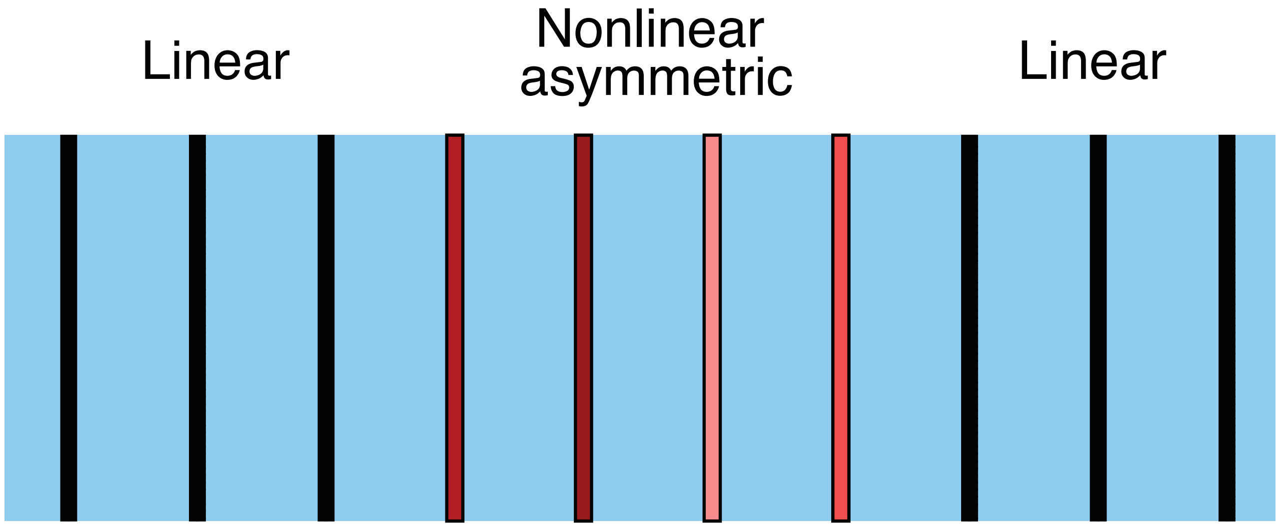
# Outline

The open, one-dimensional DNLS equation

$$i\dot{\phi}_n = V_n\phi_n - \phi_{n+1} - \phi_{n-1} + \alpha_n|\phi_n|^2\phi_n + \dots$$

- Part I : Finite-temperature coupled transport
  [S. Iubini, S.L., A. Politi, Phys.Rev E 86, 011108 (2012)]
- Part II : Short driven chains, nonreciprocal transmission
  [S.L., G. Casati, Phys. Rev. Lett. 106, 164101 (2011)]

# DNLS for layered photonic or phononic crystal




For linear propagation perpendicular to the layers:

$$\cos k(d_1 + d_2) = \cos(\frac{\omega d_1}{c_1}) \cos(\frac{\omega d_2}{c_2}) - \frac{1}{2}(\frac{c_1}{c_2} + \frac{c_2}{c_1}) \sin(\frac{\omega d_1}{c_1}) \sin(\frac{\omega d_2}{c_2})$$

# DNLS for layered nonlinear media

- Thin layers $d_1 \ll d_2$: "Kronig-Penney model"
- Approximate dispersion for high-frequency bands: $\omega(k) = \omega_0 \pm 2C \cos kd$ (single band approx.)
- Defective layers
- Kerr nonlinearity
- Rescale units, band center at $\omega = 0$

Altogether:

$$i\dot{\phi}_n = V_n\phi_n - \phi_{n+1} - \phi_{n-1} + \alpha_n|\phi_n|^2\phi_n$$

Conservation of energy and norm, no harmonics.
[A. Kosevich, JETP (2001)]

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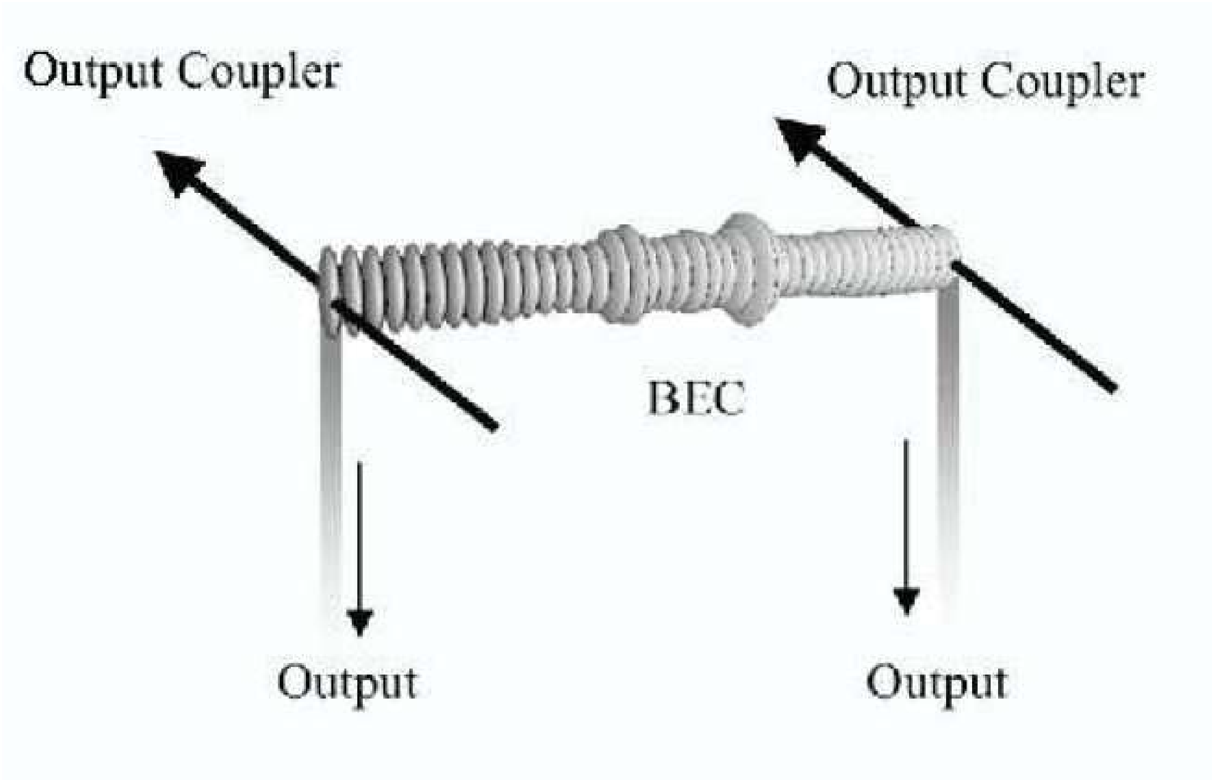
# DNLS for BEC in optical lattices




Tight-binding + semiclassical approximations → DNLS eq.
[Franzosi, Livi, Oppo, Politi, Nonlinearity (2011)]

Part I

# Finite-temperature transport

# Equilibrium: Grand-canonical thermodynamics

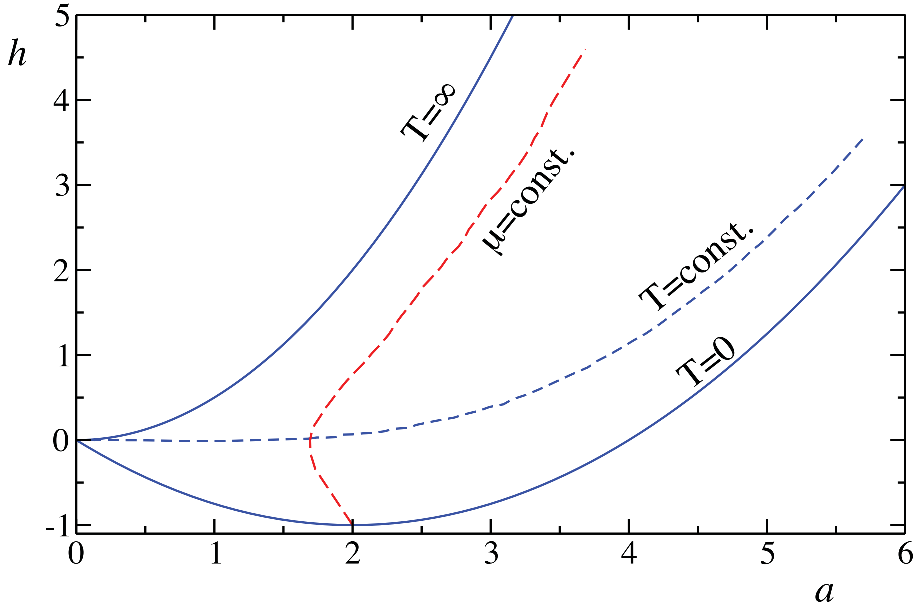
Let $\phi_n = p_n + iq_n$, the isolated systems has 2 integrals of motion ($V_n = 0$, $\alpha_n = \alpha$).

$$H = \frac{\alpha}{4}\sum_{i=1}^{N}\left(p_i^2 + q_i^2\right)^2 + \sum_{i=1}^{N-1}\left(p_i p_{i+1} + q_i q_{i+1}\right)$$

$$A = \sum_{i=1}^{N}(p_i^2 + q_i^2) \quad .$$

Statistical weight: $\exp[-\beta\,(H - \mu A)]$.
Equilibrium states: identified by $(\mu, T)$ or by the densities $h = H/N$, $a = A/N$.

# Phase diagram




$T = 0$: Ground state (for $\alpha > 0$) $\phi_n = \sqrt{a} e^{-i\mu t}$

$$h = -2a + \frac{\alpha}{2} a^2$$

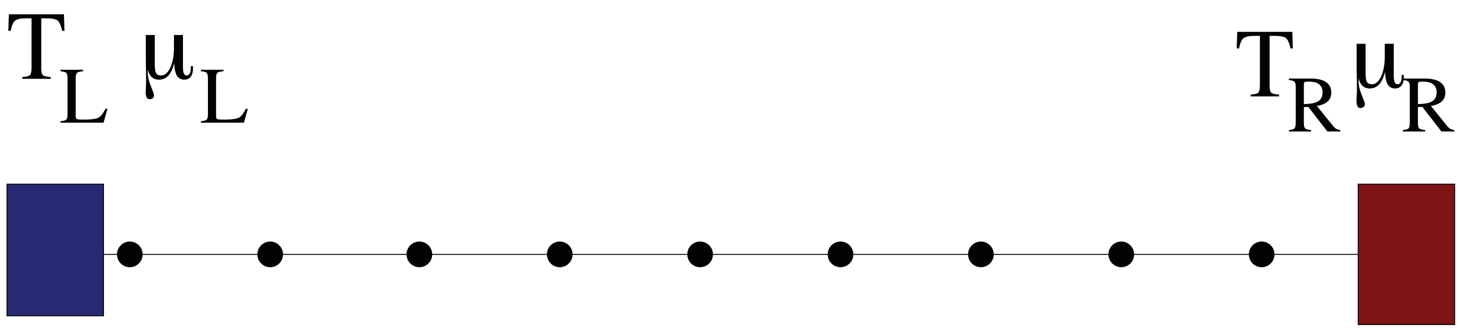
$T = \infty$: random phases (almost uncoupled oscillators)

$$h = \alpha a^2$$

[Rasmussen et al, PRL 2001]

# The usual game ...

Put DNLS chain in contact with two thermostats at the edges:




Not trivial! for instance: "naive" Langevin will not work!
Dissipation must preserve the ground state.

# Monte-Carlo heat baths

1. At random time intervals (distributed in $[t_{min}, t_{max}]$), let

$$p_1 \to p_1 + \delta p; \quad q_1 \to q_1 + \delta q$$

$\delta p$ and $\delta q$ are i.i.d. random variables uniformly distributed in $[-R, R]$.

2. If $(\Delta H - \mu_L \Delta A) < 0$ accept the move, otherwise accept with probability

$$\exp\left\{-T_L^{-1}(\Delta H - \mu_L \Delta A)\right\}$$

3. Evolve the Hamiltonian dynamics till the next collision

# Moves for conservative Monte-Carlo heat baths

- *Norm conserving thermostat-* Random change of the phase:

$$\theta_1 \rightarrow \theta_1 + \delta\theta \quad mod(2\pi)$$

$\delta\theta$ i.i.d., uniform in $[0, 2\pi]$. The total norm $A$ is conserved.

- *Energy conserving thermostat-* Consider the local energy

$$h_1 = |\phi_1|^4 + 2|\phi_1||\phi_2| \cos(\theta_1 - \theta_2) \quad . \tag{1}$$

Two steps:

1. $|\phi_1|$ is randomly perturbed. As a result, both the local amplitude and the local energy change.
2. Then, by inverting, Eq. (1), a value of $\theta_1$ that restores the initial energy is seeked. If no such solution exists, choose a new perturbation for $|\phi_1|$.

# Microscopic expressions for $T$ and $\mu$

For nonseparable Hamiltonians kinetic temperature is not simply $\langle p^2 \rangle$!

$$\frac{1}{T} = \frac{\partial \mathcal{S}}{\partial H}, \frac{\mu}{T} = -\frac{\partial \mathcal{S}}{\partial A},$$

where $\mathcal{S}$ is the thermodynamic entropy.

[Franzosi, PRE 2011] For a system with two conserved quantities $C_1$, $C_2$

$$\frac{\partial \mathcal{S}}{\partial C_1} = \left\langle \frac{W\|\vec{\xi}\|}{\vec{\nabla} C_1 \cdot \vec{\xi}} \vec{\nabla} \cdot \left( \frac{\vec{\xi}}{\|\vec{\xi}\| W} \right) \right\rangle_{mic}$$

where

$$\vec{\xi} = \frac{\vec{\nabla} C_1}{\|\vec{\nabla} C_1\|} - \frac{(\vec{\nabla} C_1 \cdot \vec{\nabla} C_2)\vec{\nabla} C_2}{\|\vec{\nabla} C_1\| \|\vec{\nabla} C_2\|^2}$$

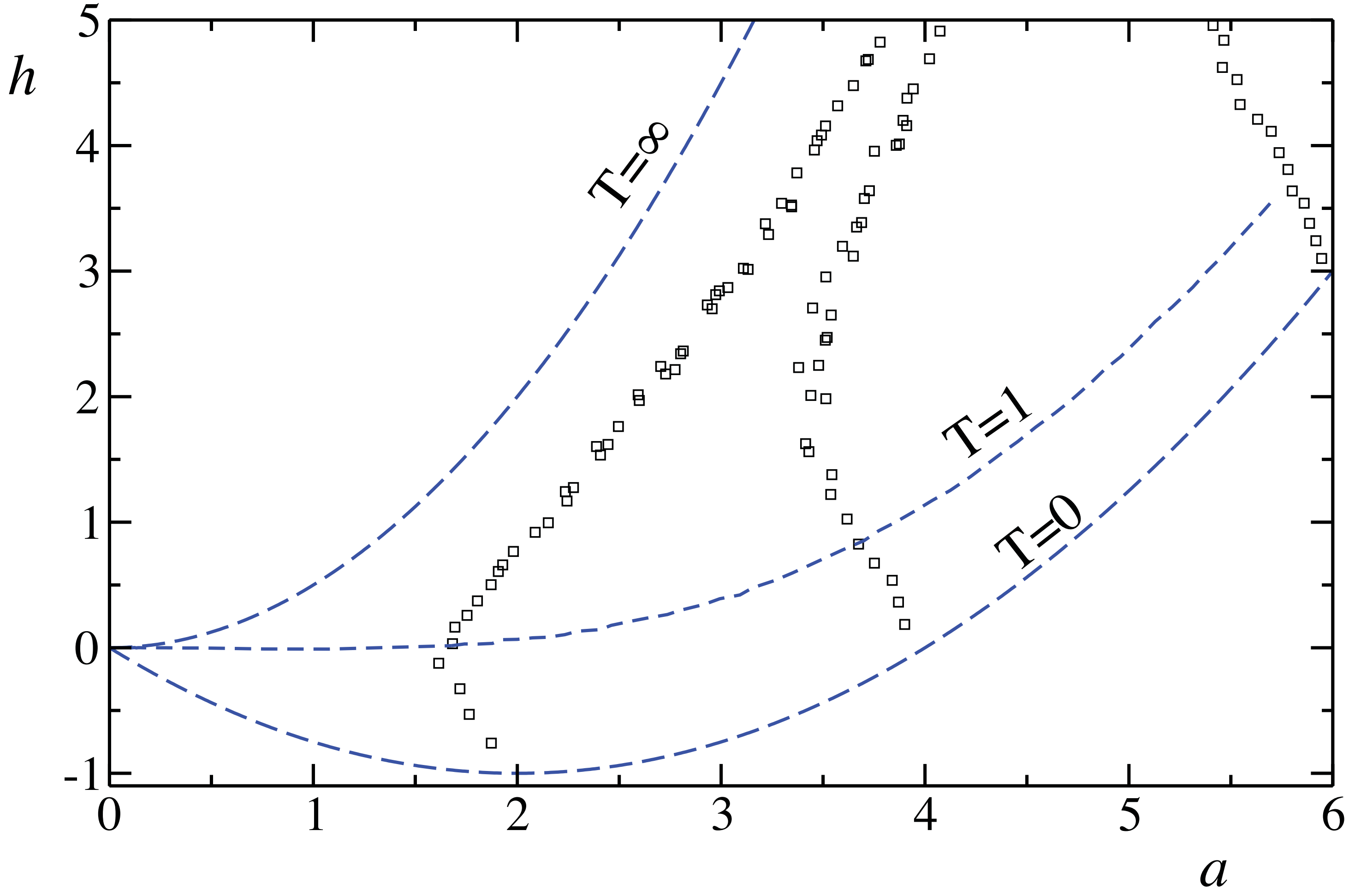
$$W^2 = \sum_{\substack{j,k=1 \\ j<k}}^{2N} \left[ \frac{\partial C_1}{\partial x_j} \frac{\partial C_2}{\partial x_k} - \frac{\partial C_1}{\partial x_k} \frac{\partial C_2}{\partial x_j} \right]^2 ,$$

and $x_{2j} = q_j$, $x_{2j+1} = p_j$.

# Microscopic expressions for $T$ and $\mu$

- Setting $C_1 = H$ and $C_2 = A$: expression for $T$
- Setting $C_1 = A$ and $C_2 = H$: expression for $\mu$
- Both expressions are (ugly and) nonlocal (involve several neighbouring $p_n$ and $q_n$)
- In practice: time-average expressions on short subchains around site $n$ to obtain local values $T_n$ and $\mu_n$.
- Check in equilibrium conditions $T_L = T_R$, $\mu_L = \mu_R$

# Equilibration




Computation of the isochemicals $\mu = 0$, $\mu = 1$ and $\mu = 2$

# Microscopic Currents

The expressions for the local energy- and particle-fluxes are derived in the usual way from the continuity equations for norm and energy densities, respectively

$$j_a(n) = 2\left(p_{n+1}q_n - p_n q_{n+1}\right)$$
$$j_h(n) = -\left(\dot{p}_n p_{n-1} + \dot{q}_n q_{n-1}\right)$$

Steady state : $(\overline{j_a(n)} = j_a$ and $\overline{j_h(n)} = j_h)$. Moreover it is also checked that $j_a$ and $j_h$ are respectively equal to the average energy and norm exchanged per unit time with the reservoirs.

# Linear irreversible thermodynamics

For small applied gradients:

$$j_a = -L_{aa}\frac{d(\beta\mu)}{dy} + L_{ah}\frac{d\beta}{dy} \qquad (2)$$

$$j_h = -L_{ha}\frac{d(\beta\mu)}{dy} + L_{hh}\frac{d\beta}{dy}$$

where we have introduced the continuous variable $y = i/N$,
$\mathbf{L}$ is the symmetric, positive definite, $2 \times 2$ Onsager matrix.
$\det\mathbf{L} = L_{aa}L_{hh} - L_{ha}^2 > 0$.
In energy-density representation the thermodynamic forces are $\nabla(-\beta\mu)$ and $\nabla\mu$.

# Thermodiffusion

The particle ($\sigma$) and thermal ($\kappa$) conductivities

$$\sigma = \beta L_{aa}; \quad \kappa = \beta^2 \frac{\det \mathbf{L}}{L_{aa}} .$$

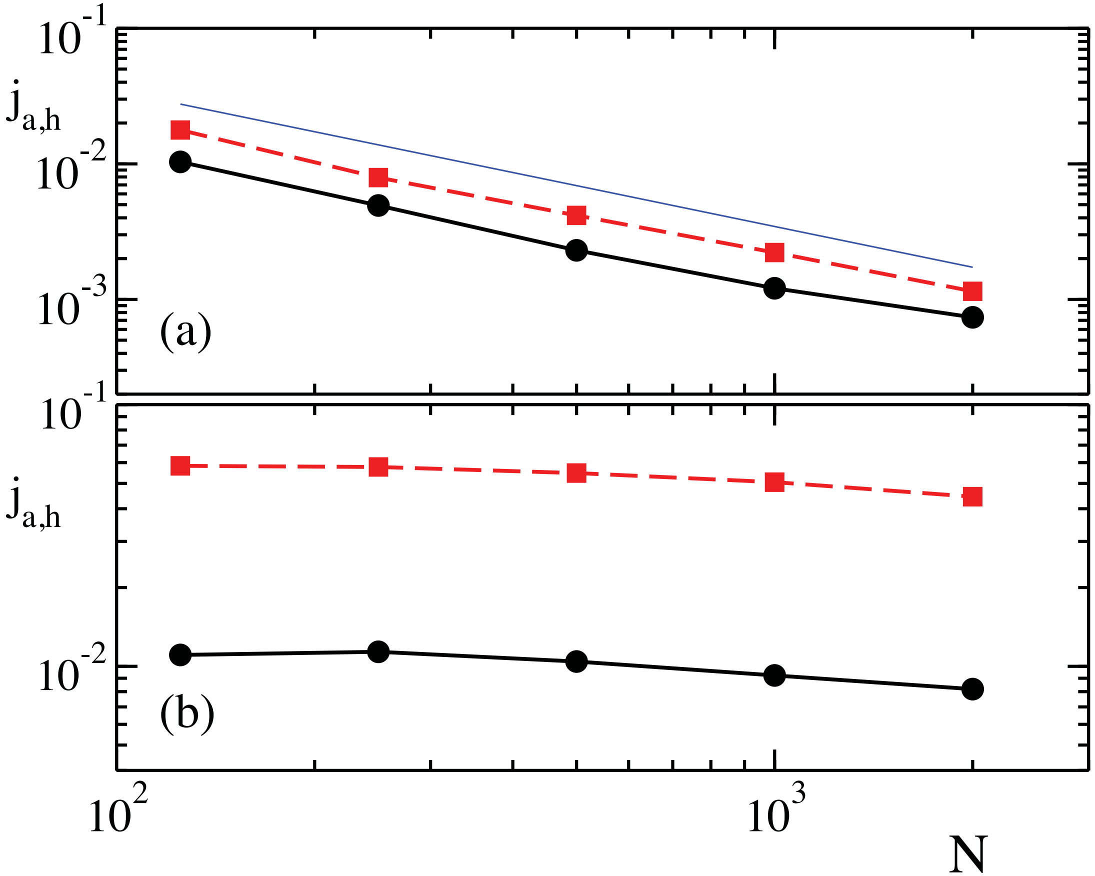
"Seebeck coefficient" ($j_a = 0$)

$$S = \beta \left( \frac{L_{ha}}{L_{aa}} - \mu \right) ,$$

Figure of merit

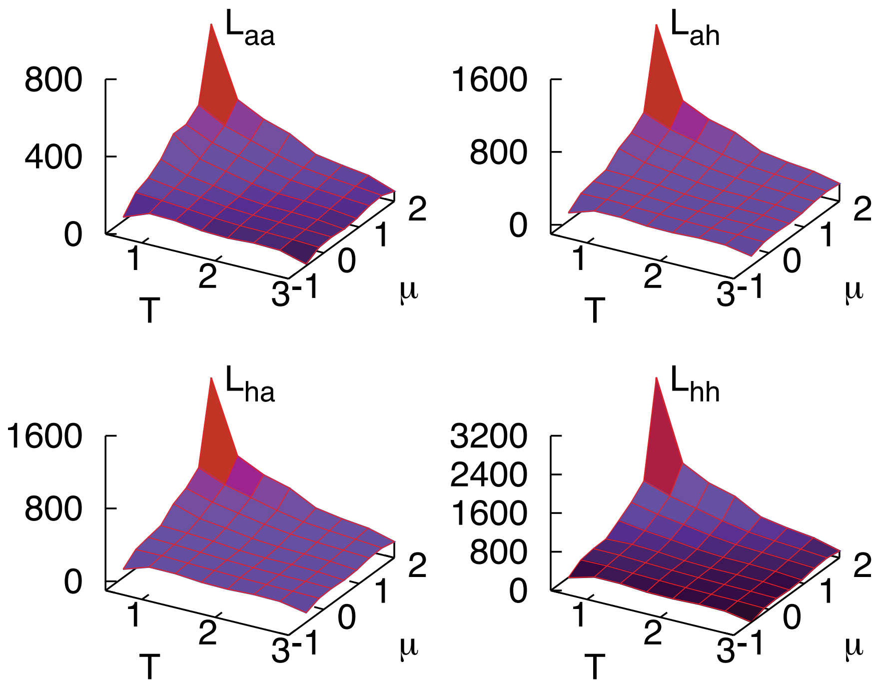
$$ZT = \frac{\sigma S^2 T}{\kappa} = \frac{(L_{ha} - \mu L_{aa})^2}{detL};$$

# Transport

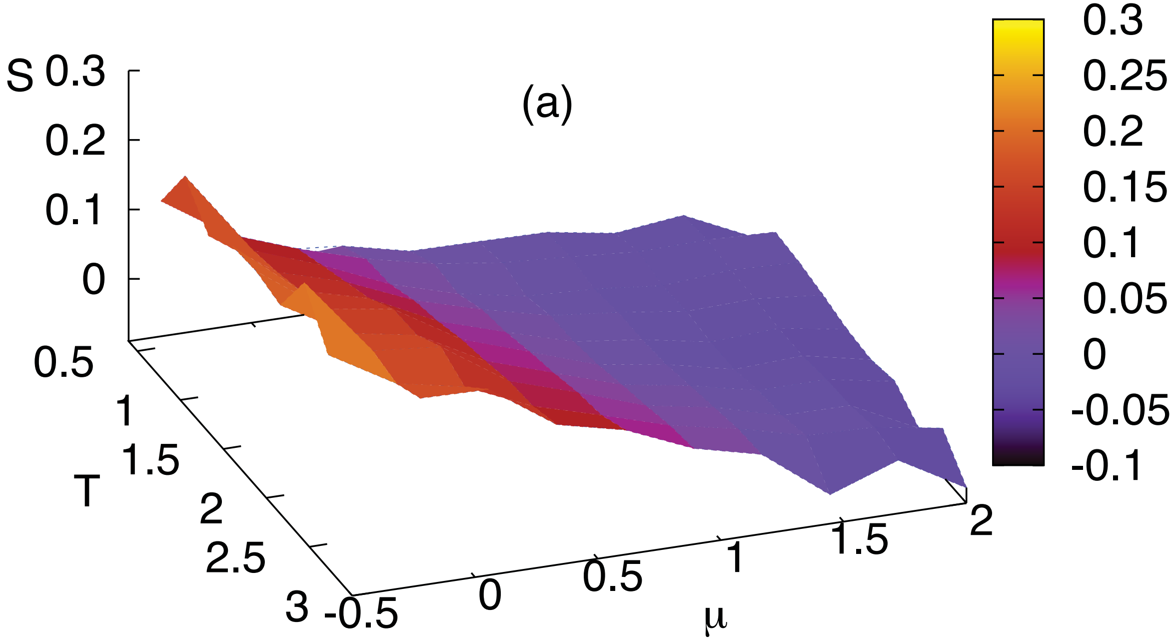



(a) High-temperature regime $T_L = 2$, $T_R = 4$, $\mu = 0$
(b) Low-temperature regime $T_L = 0.3$, $T_R = 0.7$, $\mu = 1.5$

# Linear response: Onsager coefficients

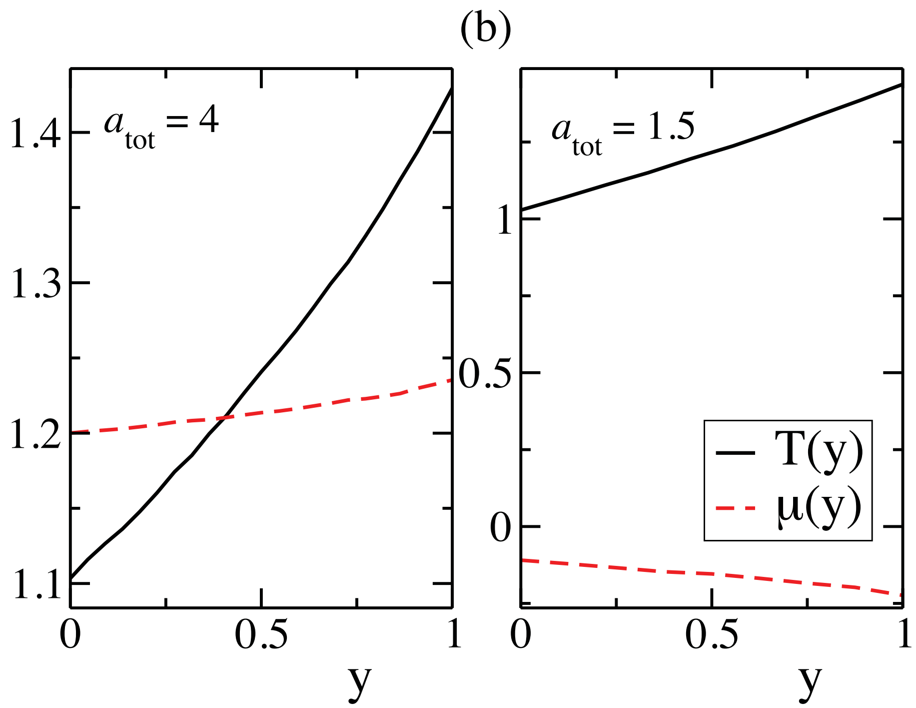



$$N = 500;\ \Delta T = 0.1,\ \Delta\mu = 0.05$$




$$S = 0 \text{ for } L_{ha}/L_{aa} = \mu$$

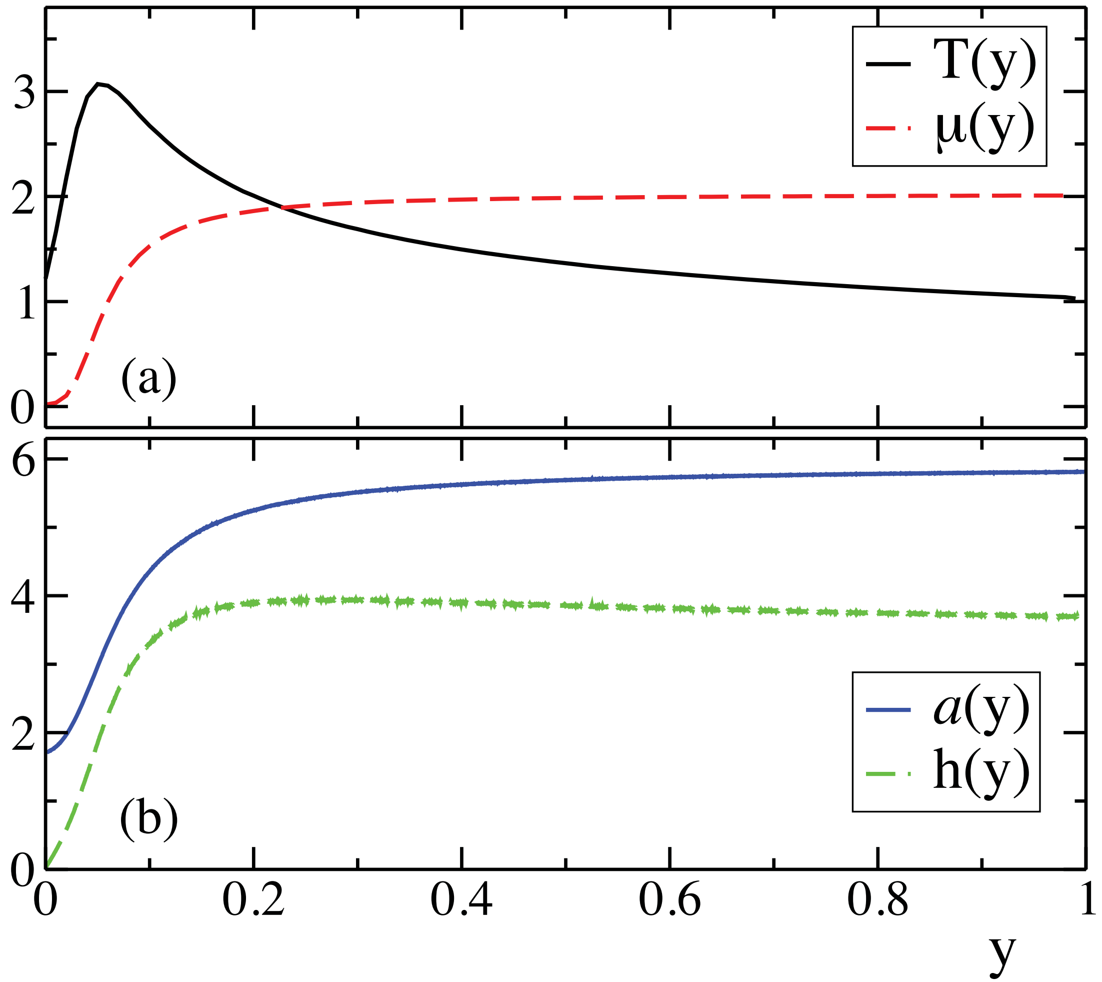
# Linear response




$T_L = 1$, $T_R = 1.5$; norm-conserving thermostats

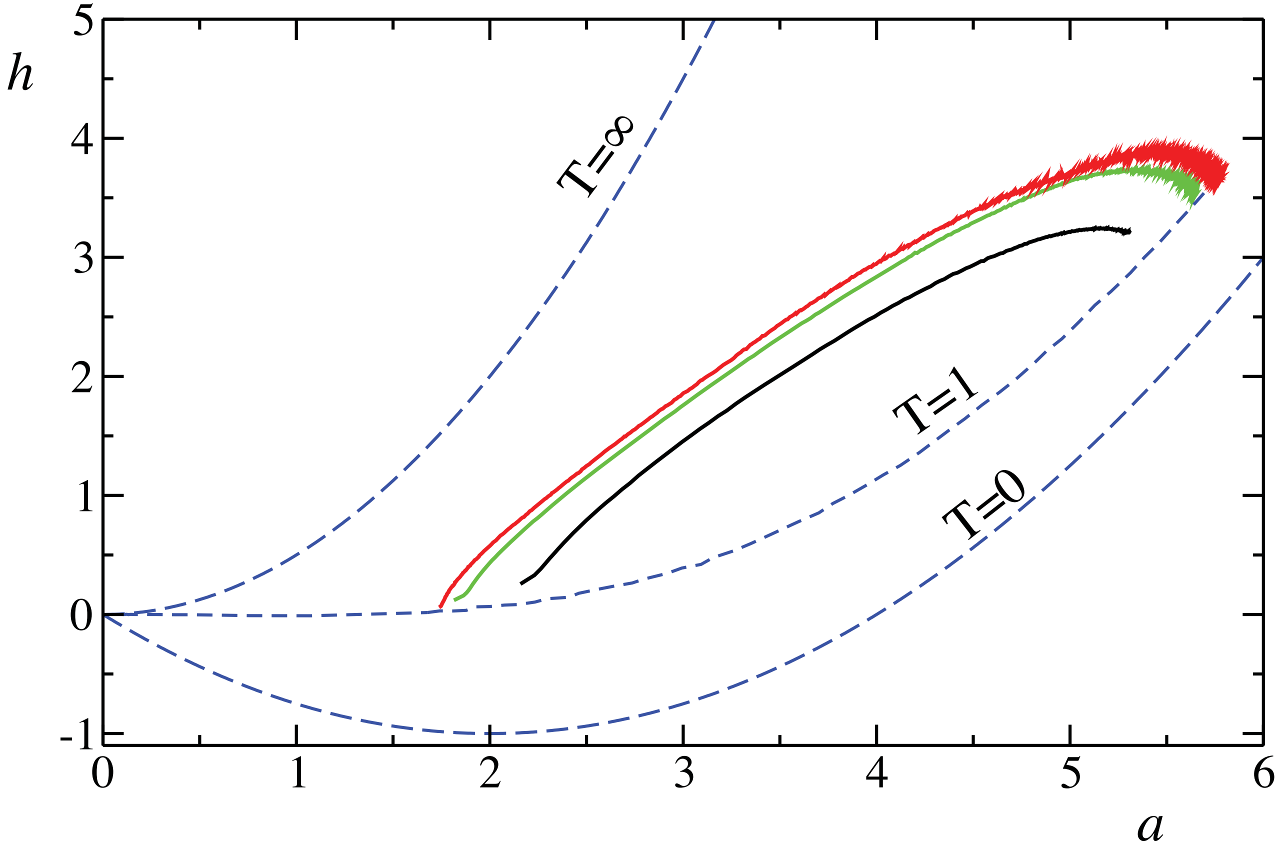
# Nonlinear regimes

Nonmonotonous profiles:




$N = 3200$ sites and $T_L = T_R = 1,\ \mu_L = 0,\ \mu_R = 2$

# Nonlinear regimes




$N = 200, 800, 3200$, $(a(y), h(y))$ "pushed" away from the $T = 1$ isothermal.

# Profile reconstruction

1. Rewrite constitutive equations as

$$\begin{pmatrix} j_a \\ j_h \end{pmatrix} = \mathbf{A}(\mu, T) \frac{d}{dy} \begin{pmatrix} \mu \\ T \end{pmatrix}$$

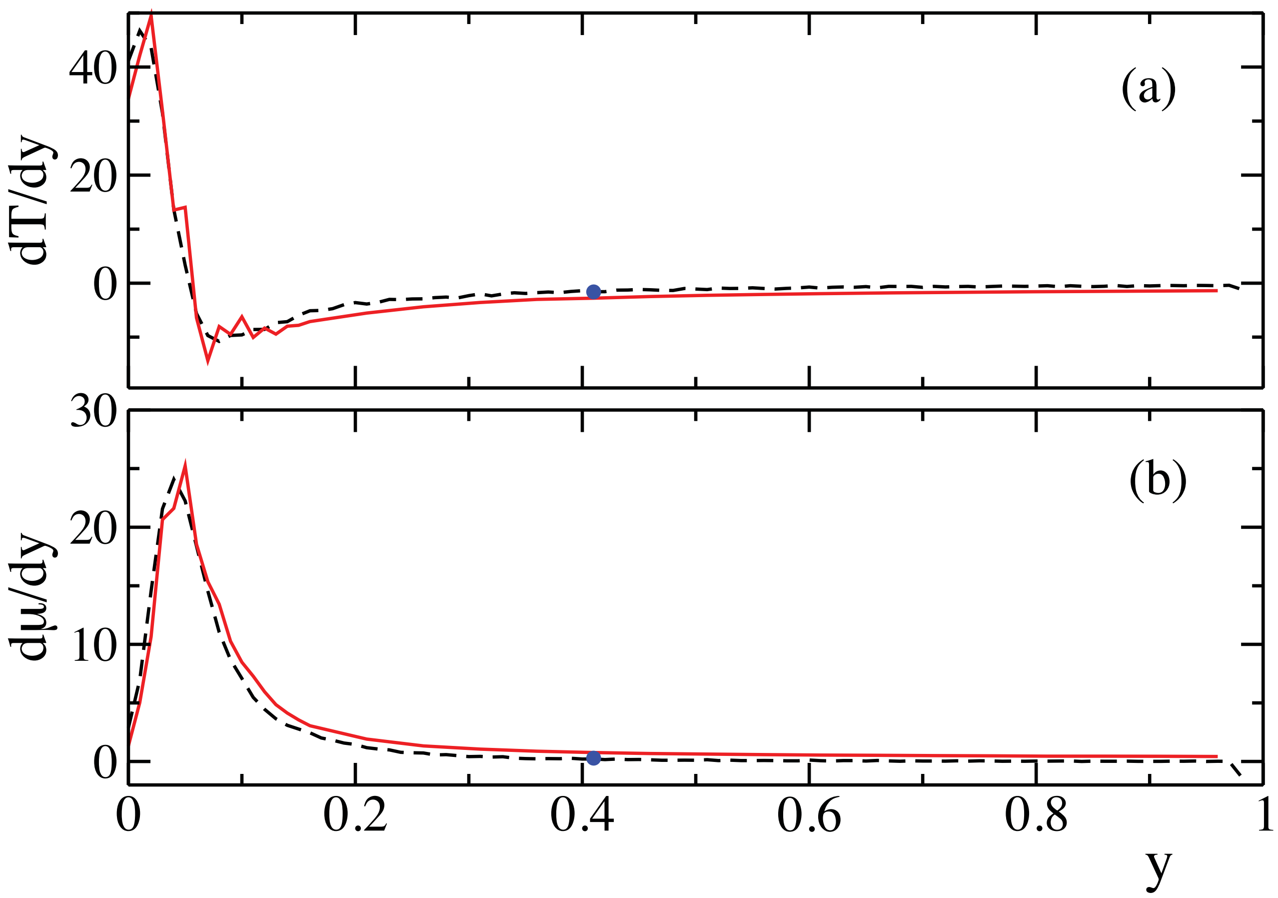
   $\mathbf{A}$ is expressed in terms of $\mathbf{L}$, $T$ and $\mu$ (e.g. $A_{11} = -L_{aa}/T$).

2. If $\mathbf{A}^{-1}$ exists

$$\frac{d}{dy} \begin{pmatrix} \mu \\ T \end{pmatrix} = \mathbf{A}^{-1}(\mu, T) \begin{pmatrix} j_a \\ j_h \end{pmatrix}$$

3. Compute $\mathbf{A}$ in the linear response regime
4. Integrate the two "nonautonomous" linear differential equations with the numerical values $(j_a, j_h)$ to reconstruct the profile.

# Profile reconstruction




$N = 250$, $N = 1000$ (dot)

Part II

# Driven DNLS: Nonreciprocal transmission

# A DNLS chain embedded in a linear lattice

$$i\dot{\phi}_n = V_n\phi_n - \phi_{n+1} - \phi_{n-1} + \alpha_n|\phi_n|^2\phi_n$$

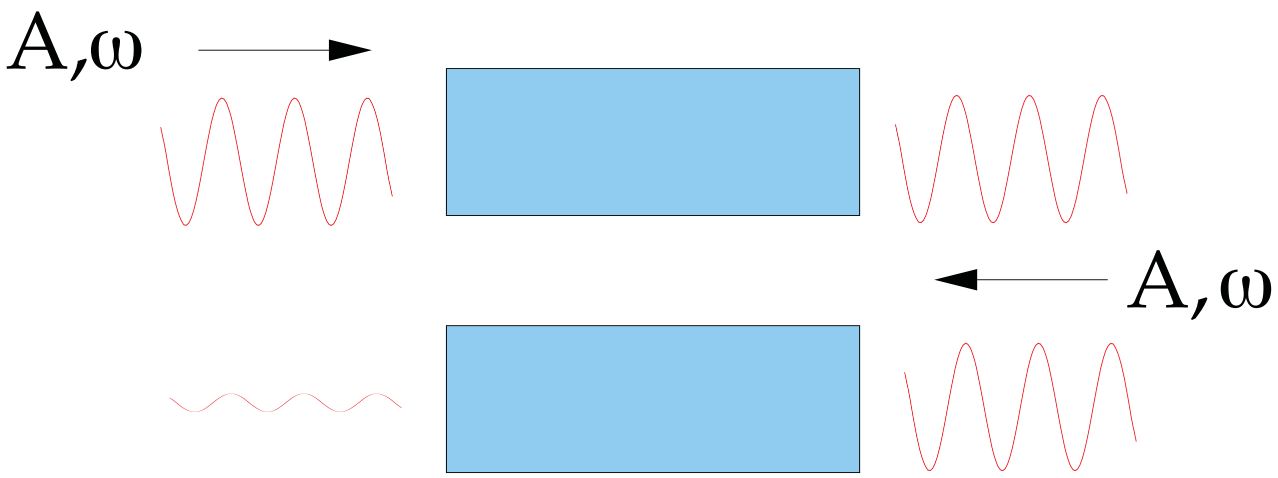
Infinite lattice , $V_n, \alpha_n \neq 0$ only for $1 \leq n \leq N$
Integrate out the $\phi_n$ for $n \leq 0$ and $n > N$:

$$\phi_0(t) = F_0(t) - i\int_0^t G(t-s)\phi_1(s)ds$$

$$\phi_{N+1}(t) = F_{N+1}(t) - i\int_0^t G(t-s)\phi_N(s)ds$$

Memory term $G(t) = J_1(2t)/t$.
From Hamiltonian problem to *driven, dissipative*

# Motivation: the (ideal) “wave diode”

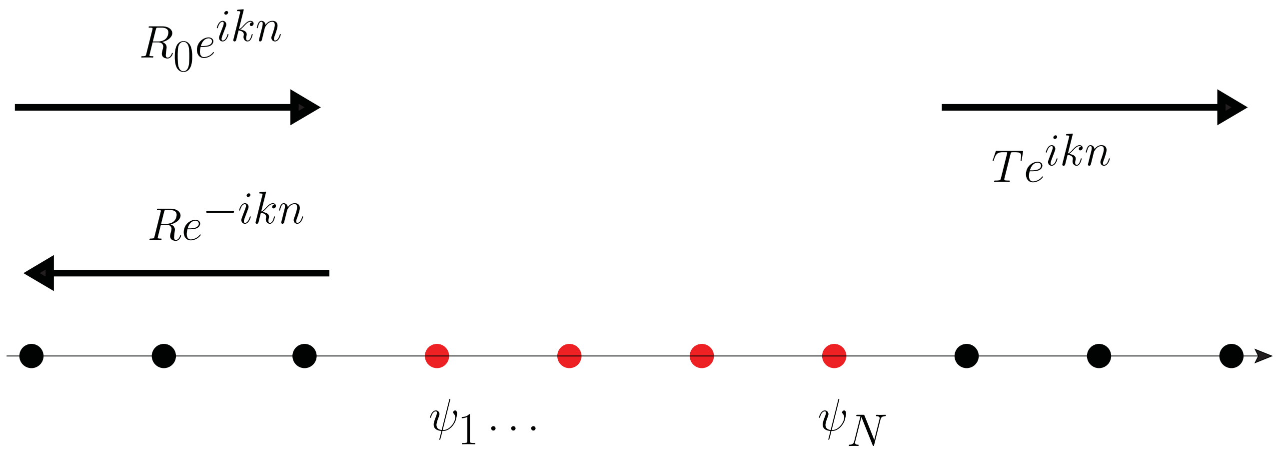



To violate the *reciprocity theorem* (without breaking time-reversal) both asymmetry *and* nonlinearity are necessary !

# Transmission problem

Stationary DNLS, $\phi_n = \psi_n e^{-i\omega t}$, $V_n \neq 0$ and $\alpha_n \neq$ for $1 \leq n \leq N$

$$\omega\psi_n = V_n\psi_n - \psi_{n+1} - \psi_{n-1} + \alpha_n|\psi_n|^2\psi_n$$




$$\omega = -2\cos k, \qquad 0 \leq k \leq \pi$$

# Transmission problem

Look for complex solutions such that:

$$\psi_n = \begin{cases} R_0 e^{ikn} + R e^{-ikn} & n \leq 1 \\ T e^{ikn} & n \geq N \end{cases}$$

- $\psi_n$ complex, current $J = 2|T|^2 \sin k$
- Non-mirror symmetric couplings: $V_n \neq V_{N-n+1}$ and/or $\alpha_n \neq \alpha_{N-n+1}$
- Convention: $k < 0$ is for $(V_n, \alpha_n) \longrightarrow (V_{N-n+1}, \alpha_{N-n+1})$ ("flipped sample")
- For $\alpha_n = 0$: reciprocity for any $V_n$

# Reduction to nonlinear map

Let $u_n = \psi_n$ and $v_n = \psi_{n+1}$. Back iterating from $u_N = T\exp(ikN)$, $v_N = T\exp(ik(N+1))$

$$u_{n-1} = -v_n + (V_n - \omega + \alpha_n |u_n|^2) u_n, \quad v_{n-1} = u_n$$

Map is area preserving.
For given $T$ and $k$

$$R_0 = \frac{\exp(-ik)u_0 - v_0}{\exp(-ik) - \exp(ik)}, \quad R = \frac{\exp(ik)u_0 - v_0}{\exp(ik) - \exp(-ik)}$$

Transmission coefficient

$$t(k, |T|^2) = \frac{|T|^2}{|R_0|^2}$$

# The simplest case: the dimer $N = 2$

For $k > 0$:

$$t = \left| \frac{e^{ik} - e^{-ik}}{1 + (\nu - e^{ik})(e^{ik} - \delta)} \right|^2$$

$$\delta = V_2 - \omega + \alpha_2 T^2, \quad \nu = V_1 - \omega + \alpha_1 T^2 [1 - 2\delta \cos k + \delta^2].$$

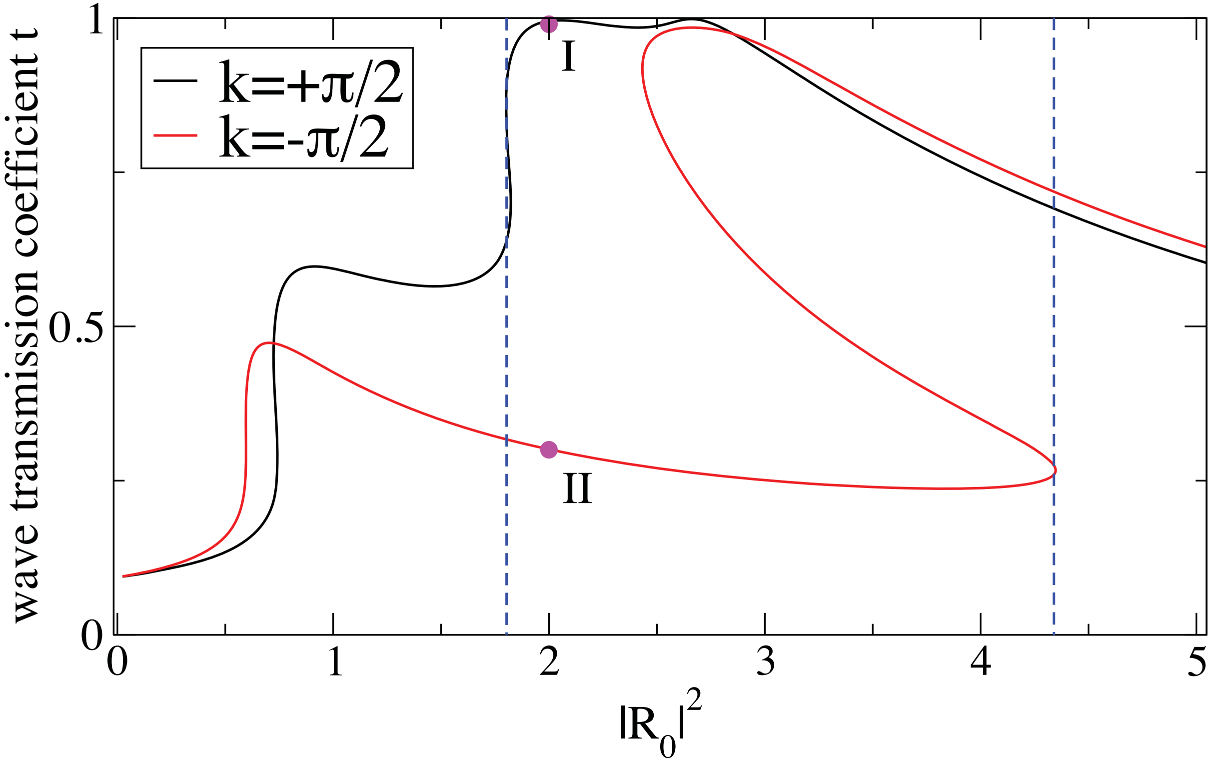
For $k < 0$: exchange the subscripts $1$ and $2$

Symmetric case ($V_{1,2} = V_0, \alpha_{1,2} = \alpha$): two nonlinear resonances

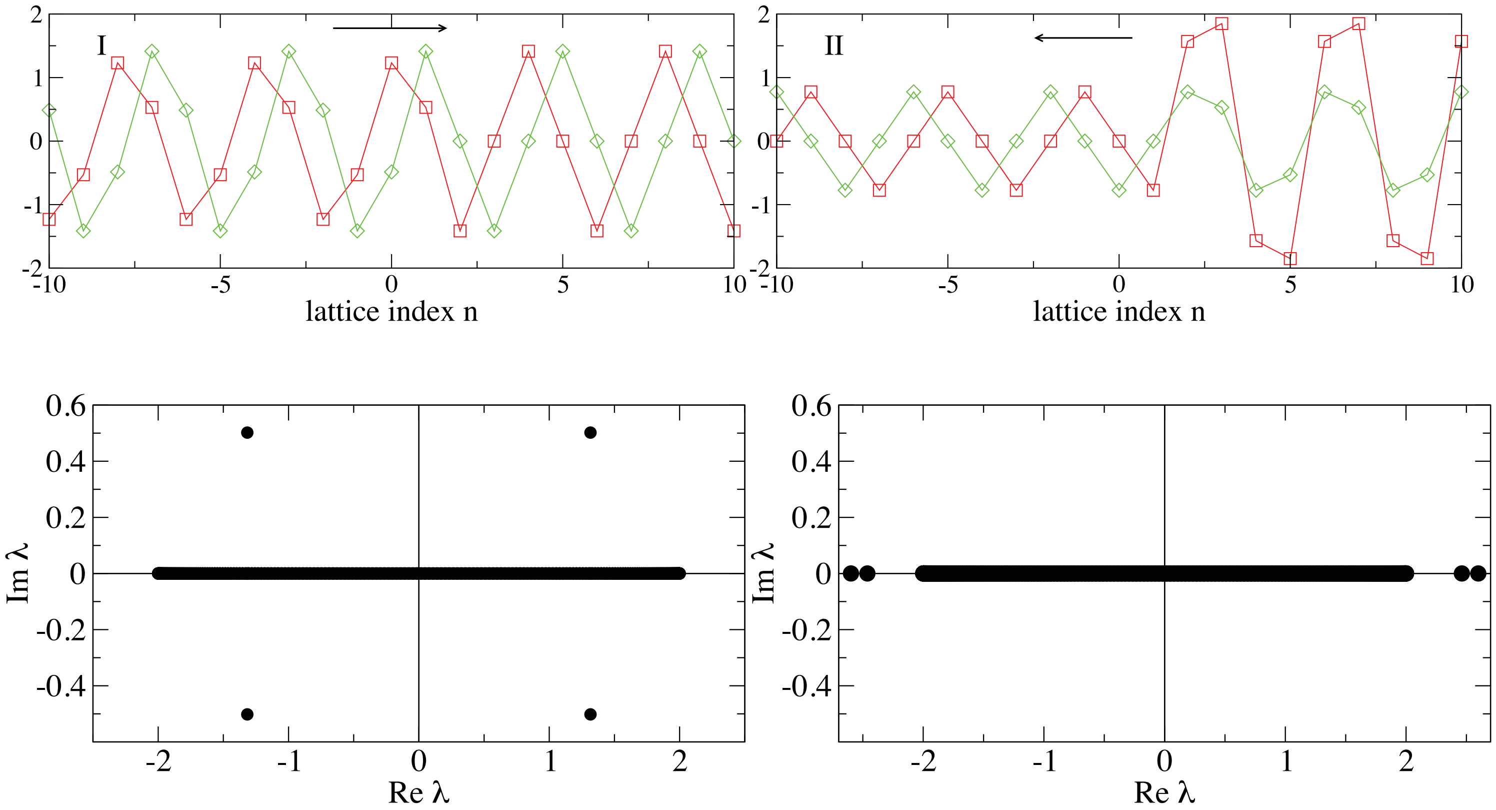
$$V_0 + \alpha T^2 = 0 \qquad (V_0 < 0)$$

$$V_0 + \alpha T^2 = \omega \qquad (V_0 < \omega)$$

# The dimer $N = 2$: transmission curves

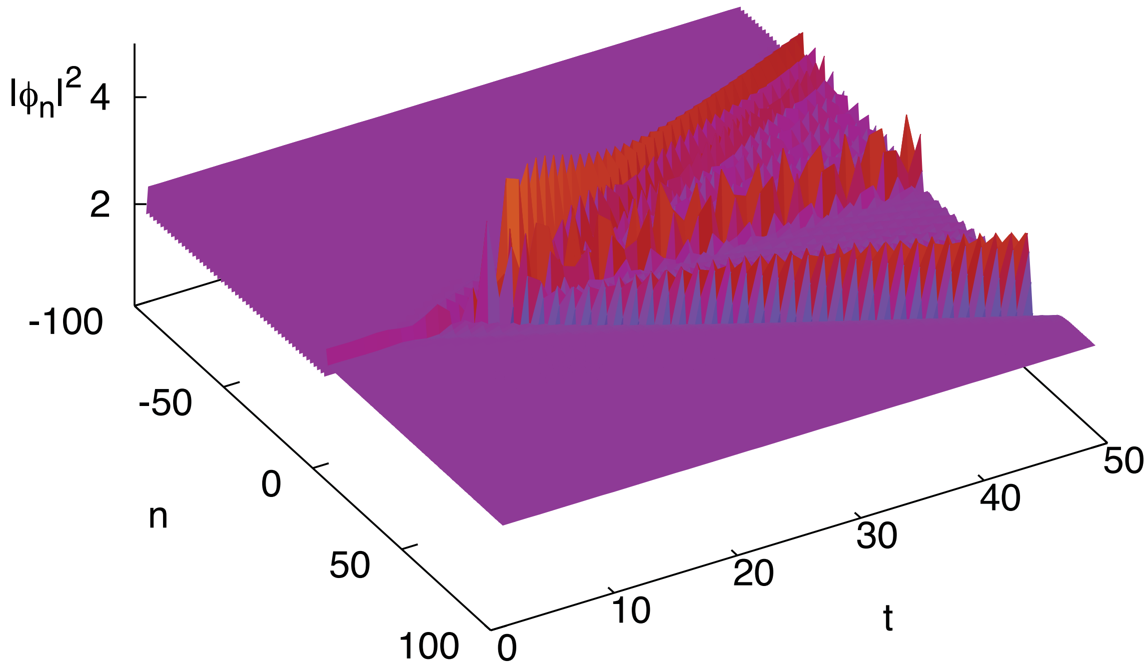



$k = \pi/2$, $\alpha_n = 1$, $V_{1,2} = V_0(1 \pm \varepsilon)$ $V_0 = -2.5$ $\varepsilon = 0.05$.



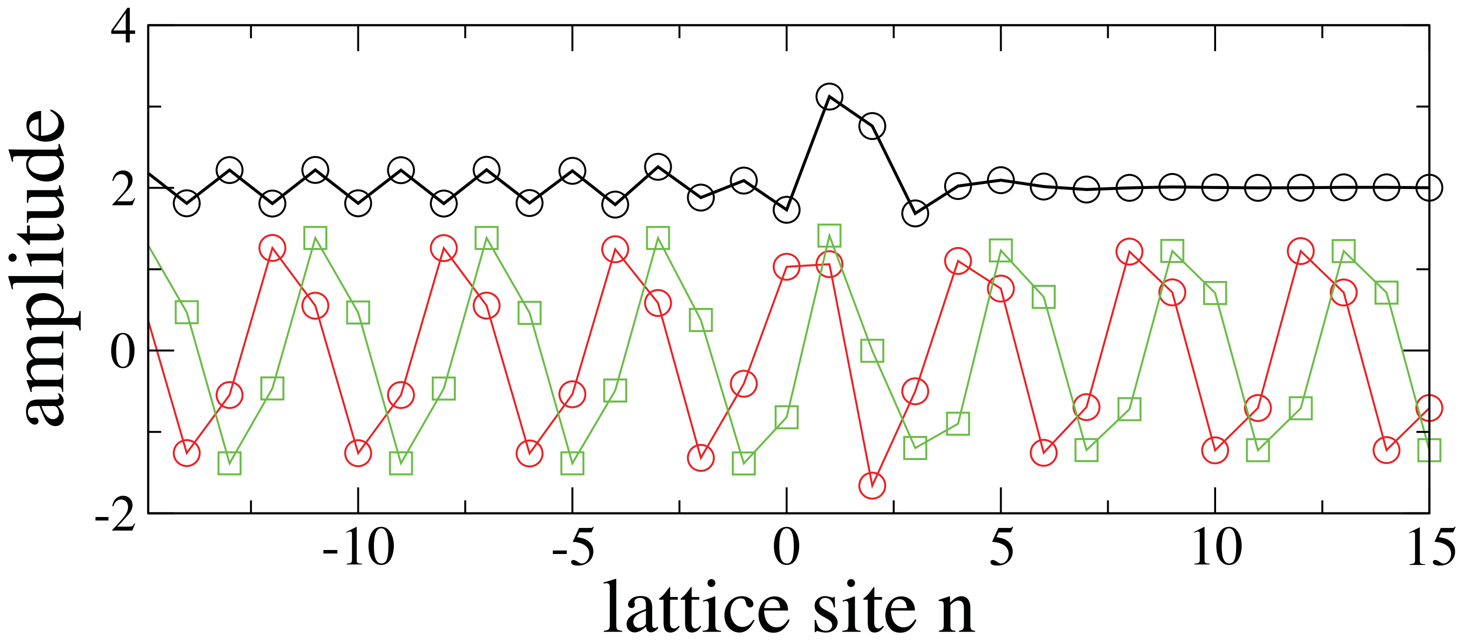

$|R_0|^2 = 2$ $t_I = 0.99$ and $t_{II} = 0.30$

# Oscillatory instability




Radiation and birth of localized mode (with frequency outside of the phonon band) on a plane-wave background.

# Quasiperiodic solution



# Wavepacket transmission

Numerical simulation on a finite lattice $|n| < M$

$$i\dot{\phi}_n = V_n\phi_n - \phi_{n+1} - \phi_{n-1} + \alpha_n|\phi_n|^2\phi_n$$

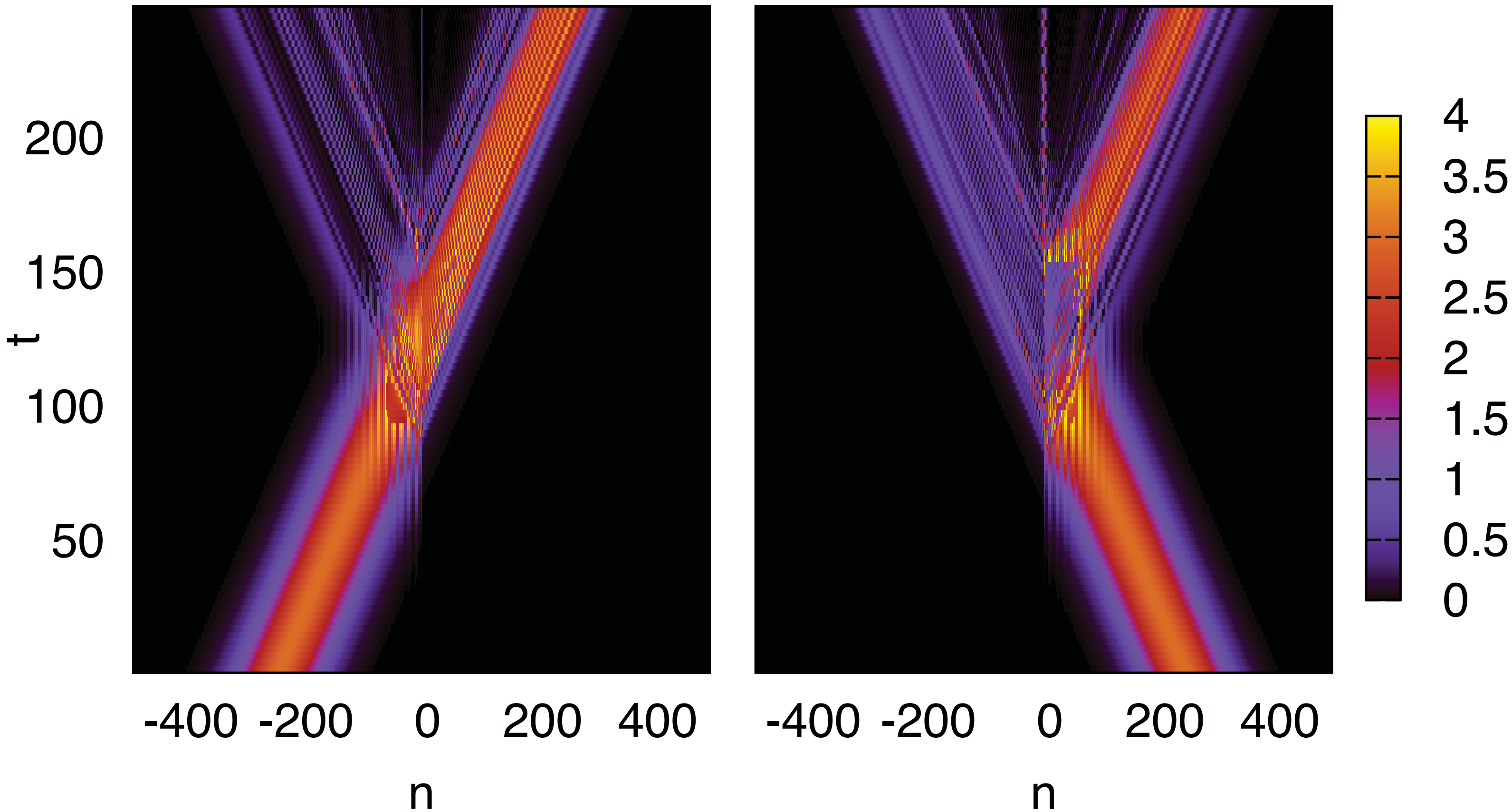
Initial condition: Gaussian

$$\phi_n(0) \; = \; I \exp\left[-\frac{(n-n_0)^2}{w^2} + ik_0 n\right]$$

Transmission coefficient (for $n_0 < 0$)

$$t_p = \frac{\sum_{n>N} |\phi_n(t_{fin})|^2}{\sum_{n<0} |\phi_n(0)|^2}$$

# Wavepacket transmission



# Summary

1. Steady coupled transport
    - Monte Carlo thermostats
    - Normal transport, except at very low $T$
    - Nonmonotonous energy and density profiles
    - $S$ changes sign increasing the interaction
2. Driven chains: nonreciprocal transmission
    - Simple modeling of "wave diode"
    - Nonlinear resonances and multistability
    - Oscillatory instabilities
    - Nonreciprocal wavepacket trasmission