# The nonequilibrium, discrete nonlinear Schrödinger equation

**Stefano Lepri**

Istituto dei Sistemi Complessi ISC-CNR Firenze, Italy

istituto dei sistemi complessi

Consiglio Nazionale delle Ricerche

# Outline

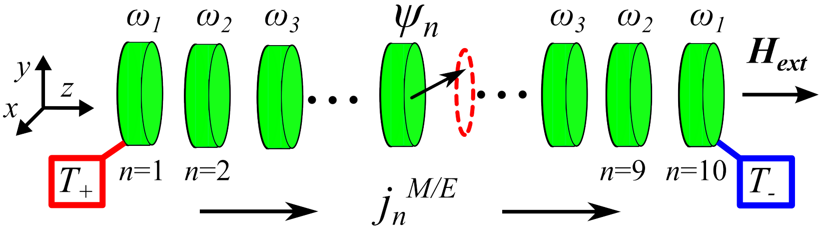
The open, one-dimensional DNLS equation

$$i\dot{\psi}_n = \omega_n \psi_n - \psi_{n+1} - \psi_{n-1} + \nu|\psi_n|^2\psi_n + \dots$$

- "Generic model" in different fields: biomolecules, BEC, nonlinear waveguides
- Nonintegrable many-body problem
- Nonlinear localized solution (discrete breathers)
- Finite-temperature coupled transport
  [S. Iubini, S.L., A. Politi, Phys.Rev E 86, 011108 (2012)]

# A physical system: non-isothermal ferromagnets

Spin-Seebeck effect in an array of magnetic microdisks



# Landau-Lifschiz-Gilbert dynamics

- Dissipative dynamics of the magnetisation vector $\boldsymbol{M}(\boldsymbol{r}, t)$

$$\dot{\boldsymbol{M}} = \gamma \boldsymbol{M} \times \boldsymbol{H}_{\text{eff}} + \frac{\alpha}{M_s} \boldsymbol{M} \times \dot{\boldsymbol{M}},$$

- Effective field $\boldsymbol{H}_{\text{eff}} = \boldsymbol{H}_{\text{exc}} + \boldsymbol{H}_{\text{ext}} + \boldsymbol{H}_{\text{dip}}$.
- Thermal fluctuations: add to $\boldsymbol{H}_{\text{eff}}$ the stochastic term

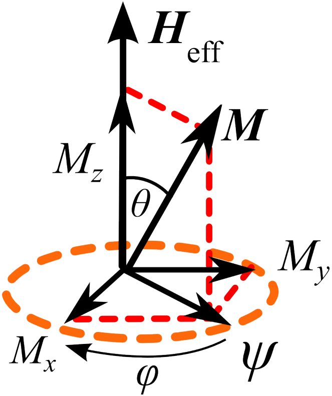
$$\boldsymbol{H}_{\text{th}}(\boldsymbol{r}, t) = \sqrt{DT}(\eta_x, \eta_y, \eta_z),$$

  where $\eta_j(\boldsymbol{r}, t)$, $j = (x, y, z)$, is a Gaussian random process with zero average and

$$\langle \eta_j(\boldsymbol{r}, t) \eta_{j'}(\boldsymbol{r}', t') \rangle = \delta_{jj'} \delta(\boldsymbol{r} - \boldsymbol{r}') \delta(t - t')$$

- Micromagnetic simulations (heavy!)

# From LLG to DNLS



# From LLG to DNLS

Volume-averaged magnetisation of the $n$th disk (macrospin):

$$\boldsymbol{M}^n(t) = \frac{1}{V_n}\int_{V_n} \boldsymbol{M}(\boldsymbol{r}_n, t)\mathrm{d}^3 r_n.$$

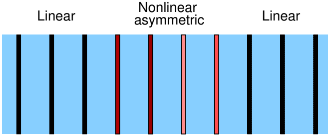
Introduce the complex variables:

$$\psi_n = \frac{M_x^n - iM_y^n}{\sqrt{2M_s(M_s + M_z^n)}}.$$

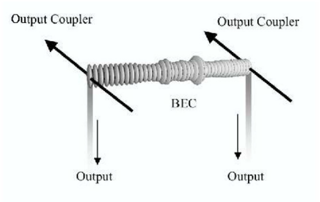
$\longrightarrow$ DNLS equation for $\psi_n$

# Nonequilibrium DNLS: other applications

Nonlinear layered photonic or phononic crystals




Bose-Einstein condensates in optical lattices



# Equilibrium: Grand-canonical thermodynamics

$$i\dot{\psi}_n = -\psi_{n+1} - \psi_{n-1} + \nu|\psi_n|^2\psi_n$$

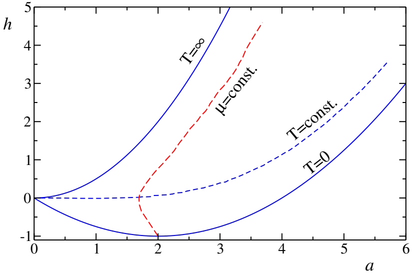
Let $\psi_n = p_n + iq_n$, the isolated systems has 2 integrals of motion

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

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

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 $\nu > 0$) $\psi_n = \sqrt{a}e^{-i\mu t}$

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

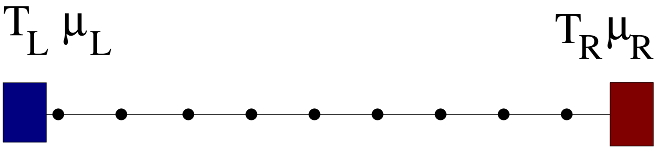
$T = \infty$: random phases (almost uncoupled oscillators)

$$h = \nu a^2$$

[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

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

3. Evolve the Hamiltonian dynamics till the next collision

# Moves for conservative Monte-Carlo heat baths

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

$$\theta_1 \to \theta_1 + \delta\theta \ \ mod(2\pi)$$

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

- *Energy conserving thermostat-* Consider the local energy

$$h_1 = |\psi_1|^4 + 2|\psi_1||\psi_2| \cos(\theta_1 - \theta_2) \quad . \tag{1}$$

  Two steps:

  1. $|\psi_1|$ 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 $|\psi_1|$.

# Langevin heat baths

For interaction with reservoirs $(T_n, \mu_n)$ at each site:

$$i\dot{\psi}_n = (1+i\alpha)\left[\nu|\psi_n|^2\psi_n - \psi_{n+1} - \psi_{n-1}\right] + i\alpha\mu_n\psi_n + \sqrt{\alpha T_n}\,\xi_n(t)$$

- $\xi$ complex Gaussian white noise
- For $T_n = T$, $\mu_n = \mu$ FP equation has the grand-canonical distribution as steady solution with "Hamiltonian"

$$H = \sum_n [-\frac{\nu}{2}|\psi_n|^4 + (\psi_n^*\psi_{n+1} + \psi_n\psi_{n+1}^*)],$$

  $(\psi_n, i\psi_n^*)$ are canonically conjugate variables
- At $T = 0$ the ground state is solution with frequency $\mu$
- Dissipation in coupling, nonlinear

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

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 [Rugh 1997].

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

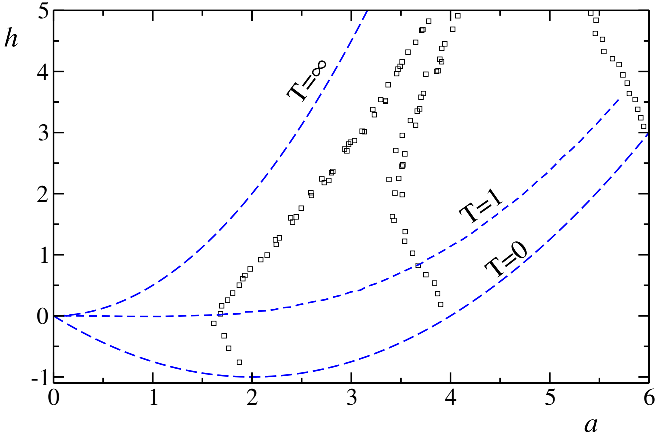
$$\begin{aligned} \vec{\xi} &= \frac{\vec{\nabla} C_1}{\|\vec{\nabla} C_1\|} - \frac{(\vec{\nabla} C_1 \cdot \vec{\nabla} C_2) \vec{\nabla} C_2}{\|\vec{\nabla} C_1\| \|\vec{\nabla} C_2\|^2} \\ W^2 &= \sum_{\substack{j,k=1 \\ j<k}}^{2N} \left[ \frac{\partial C_1}{\partial x_j} \frac{\partial C_2}{\partial x_k} - \frac{\partial C_1}{\partial x_k} \frac{\partial C_2}{\partial x_j} \right]^2 , \end{aligned}$$

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:

$$
\begin{aligned}
j_a &= -L_{aa}\frac{d(\beta\mu)}{dy} + L_{ah}\frac{d\beta}{dy} \\
j_h &= -L_{ha}\frac{d(\beta\mu)}{dy} + L_{hh}\frac{d\beta}{dy}
\end{aligned}
\qquad (2)
$$

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

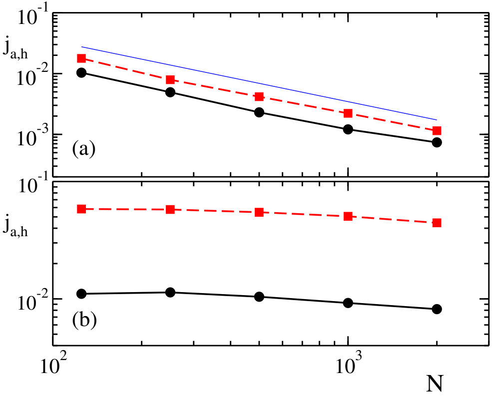
$$ZT = \frac{\sigma S^2 T}{\kappa} = \frac{(L_{ha} - \mu L_{aa})^2}{det L};$$

# Transport properties of DNLS

- High temperatures: diffusive behavior, finite transport coefficients
- Low temperatures: anomalous behavior "phase slips" $|\theta_{n+1} - \theta_n| \approx \pi$ occur with very small rate $\sim e^{-\beta \Delta V}$
- Ultralow temperatures: anomalies due to almost-integrability of the dynamics, ballistic transport
- Negative temperatures: unknown...

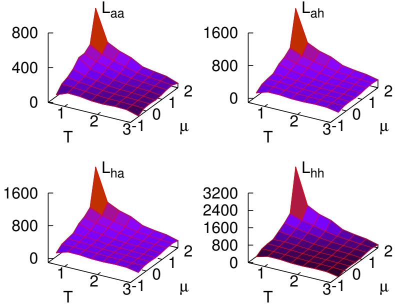
[Mendl and Spohn, 2015]

# Normal transport



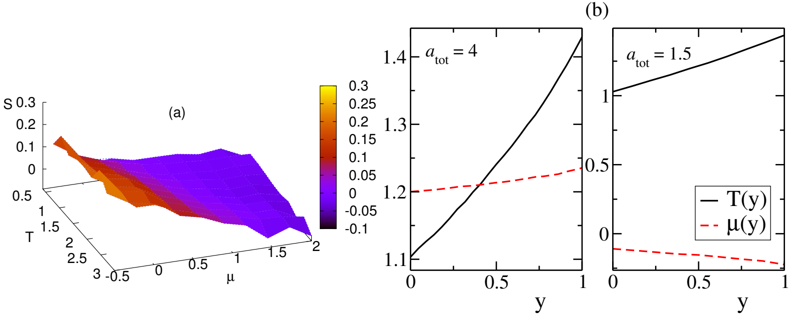

(a) High-temperature regime $T_L = 2$, $T_R = 4$, $\mu = 0$
(b) Low-temperature regime $T_L = 0.3$, $T_R = 0.7$, $\mu = 1.5$

# Linear response: Onsager coefficients




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

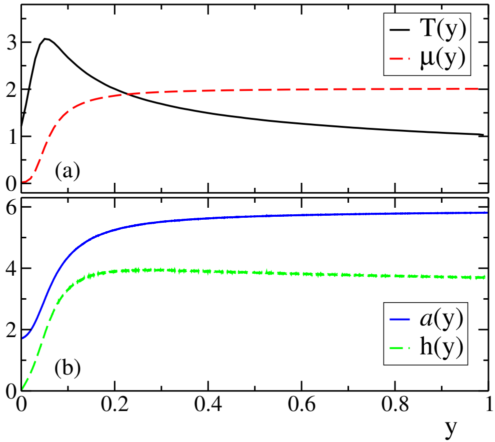
# Linear response: Seebeck coefficient




(a) $S = 0$ for $L_{ha}/L_{aa} = \mu$; (b) $T_L = 1$, $T_R = 1.5$;
norm-conserving thermostats

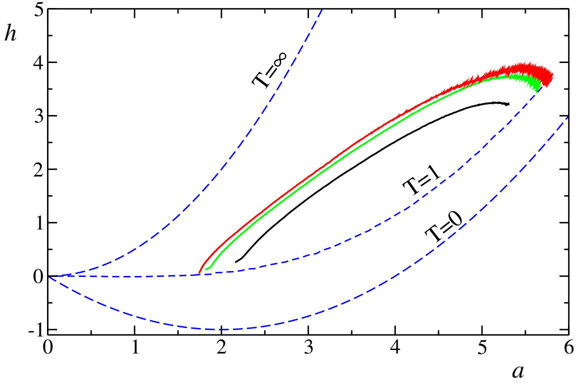
# Nonlinear regimes

Nonmonotonous profiles:




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

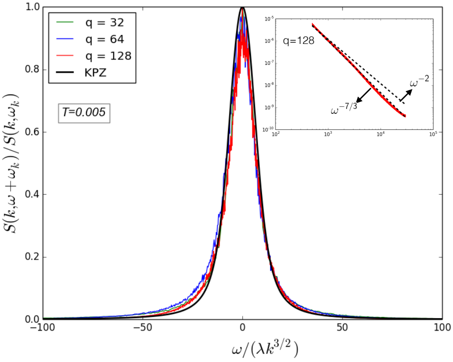
# Nonlinear regimes




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

# Anomalous transport

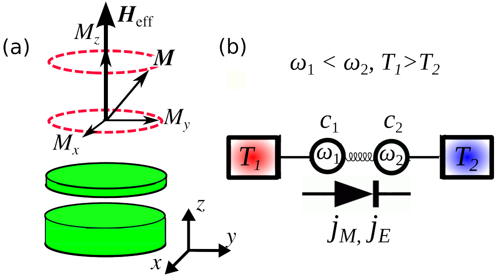
$S(k,\omega)$ structure factor (FT of the correlator of $|\psi_n|^2$)




$$S(k,\omega) \sim f_{KPZ}((\omega - ck)/k^{3/2})$$

[Kulkarni and Lamacraft 2014]

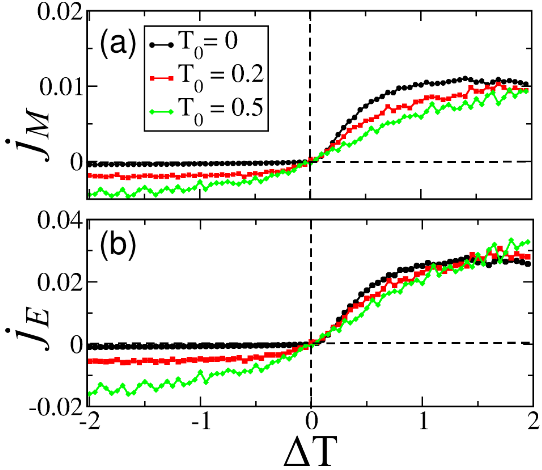
# Thermal rectification



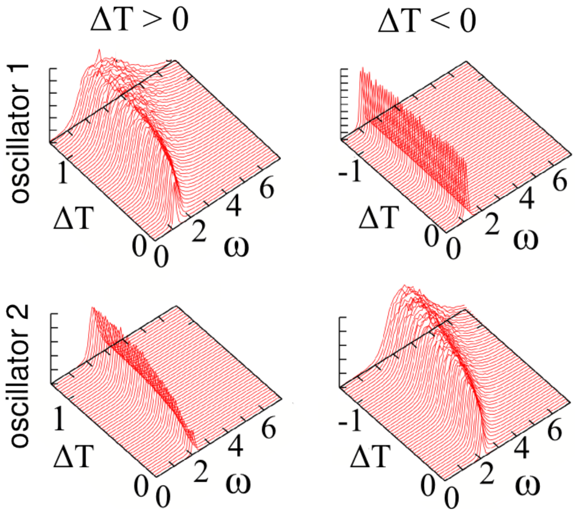

$$
\begin{aligned}
i\dot{\psi}_1 &= (1+i\alpha)(\omega_1\psi_1 + \nu\psi_1|\psi_1|^2 - h\psi_2) + \sqrt{\alpha T_1}\xi_1, \\
i\dot{\psi}_2 &= (1+i\alpha)(\omega_2\psi_2 + \nu\psi_2|\psi_2|^2 - h\psi_1) + \sqrt{\alpha T_2}\xi_2.
\end{aligned}
$$

Can we control the energy and/or magnetization currents?

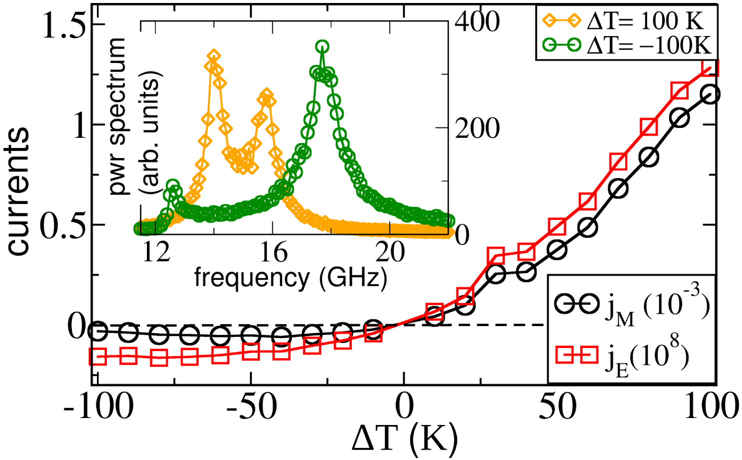
# Thermal rectification: dimer



# Thermal rectification: power spectra

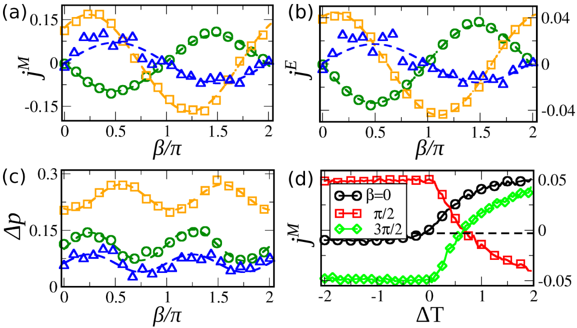


# Micromagnetic simulations



# Dissipative coupling: "Josephson effect" and heat pump

Dimer with coupling $h = C(1 - i\alpha)e^{i\beta}$: for $\beta \neq 0$ no FDT




Green circles, blue triangles $T_1 = T_2 = 0.8$, respectively $(\omega_1^0 = 1, \omega_2^0 = 2)$ and $(\omega_1^0 = 1, \omega_2^0 = 1.2)$. Orange squares: $T_1 = 1.2$ and $T_2 = 0.2$ and $(\omega_1^0 = 1, \omega_2^0 = 2)$.

# Summary

- Nonequilibrium DNLS
- Monte Carlo/Langevin thermostats for DNLS
- Normal transport, except at very low $T$
- Nonmonotonous energy and density profiles
- $S$ changes sign increasing the interaction
- Application to macrospin arrays: Spin-Seebeck thermal rectification

# References


- S. Iubini, S. Lepri, A. Politi
  *Nonequilibrium discrete nonlinear Schroedinger equation*
  Phys. Rev. E 86, 011108 (2012).
- S. Iubini, S. Lepri, R. Livi, A. Politi
  *Off-equilibrium Langevin dynamics of the discrete nonlinear Schrödinger chain*
  J. Stat. Mech. (2013) P08017.
- S. Borlenghi, S. Lepri, L. Bergqvist, A. Delin
  *Thermo-magnonic diode: rectification of energy and magnetization currents*
  Phys. Rev. B 89, 054428 (2014).
- S. Borlenghi, S. Iubini, S. Lepri, et al.
  *Coherent energy transport in classical nonlinear oscillators: An analogy with the Josephson effect*
  Phys. Rev. E 91, 040102(R) (2015)