# EQUILIBRIUM AND NON-EQUILIBRIUM DESCRIPTION OF NEGATIVE TEMPERATURE STATES IN A ONE-DIMENSIONAL LATTICE USING A WAVE KINETIC APPROACH

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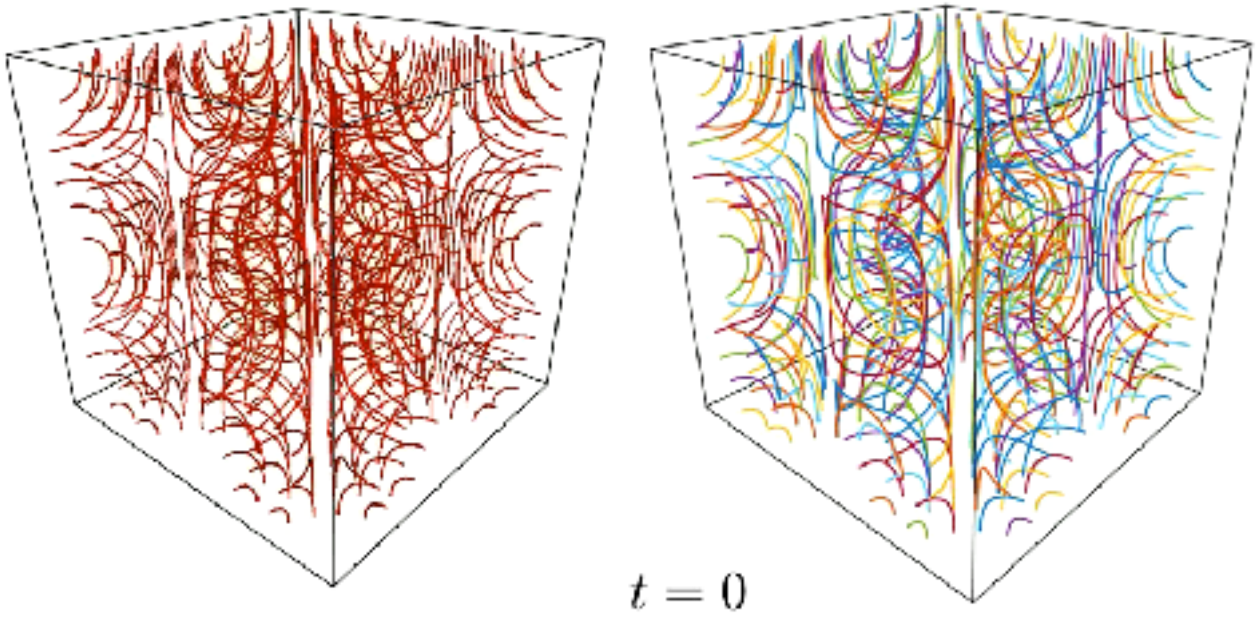
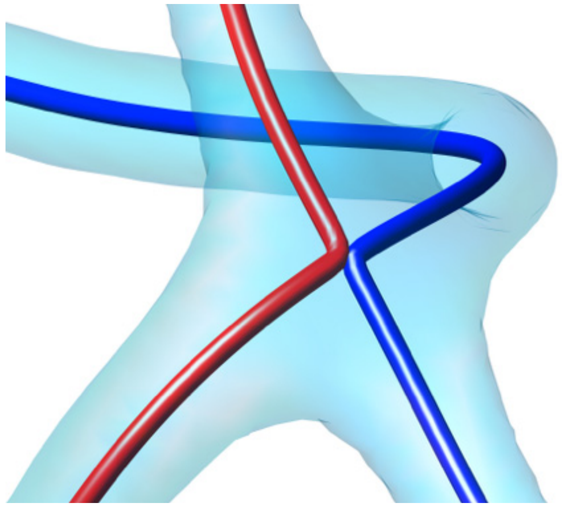
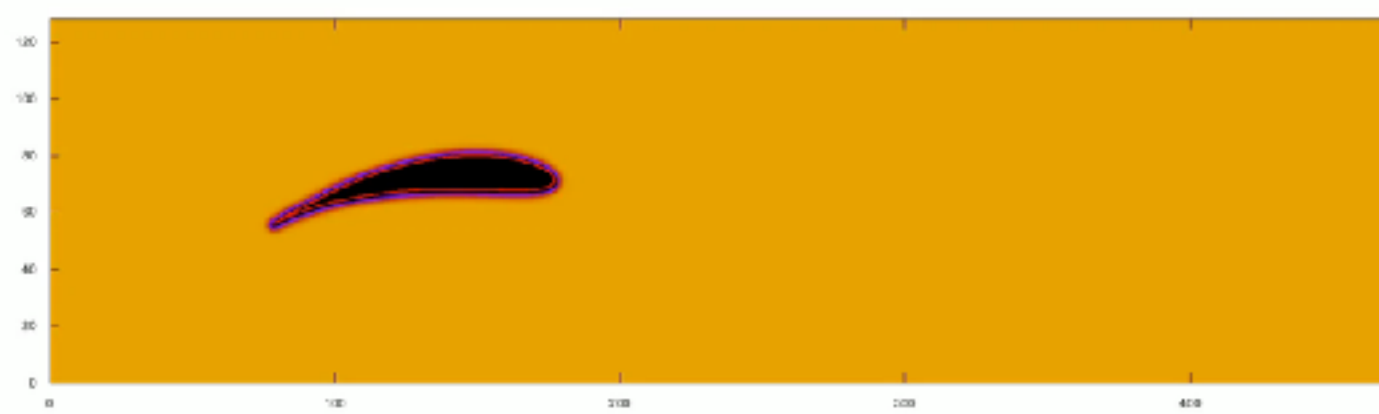
# MY RESEARCH INTERESTS

- Wave turbulence and hydrodynamics turbulence in quantum fluids
- Thermalisation, transport, and extreme events in nonlinear systems
- Vortex dynamics in two- and three-dimensional quantum fluids
- Topological aspects of quantum fluid vortices
- Interaction between quantum fluids and external obstacles or active impurities







Onorato, Dematteis, DP, Pezzi, Ballarin, and Rondoni

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# EQUILIBRIUM AND NON-EQUILIBRIUM DESCRIPTION OF NEGATIVE TEMPERATURE STATES IN A ONE-DIMENSIONAL LATTICE USING A WAVE KINETIC APPROACH

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- Negative temperature states
- Discrete nonlinear Schroedinger model (DNLS)
- Wave interaction and turbulence theory
- Our results and conclusions

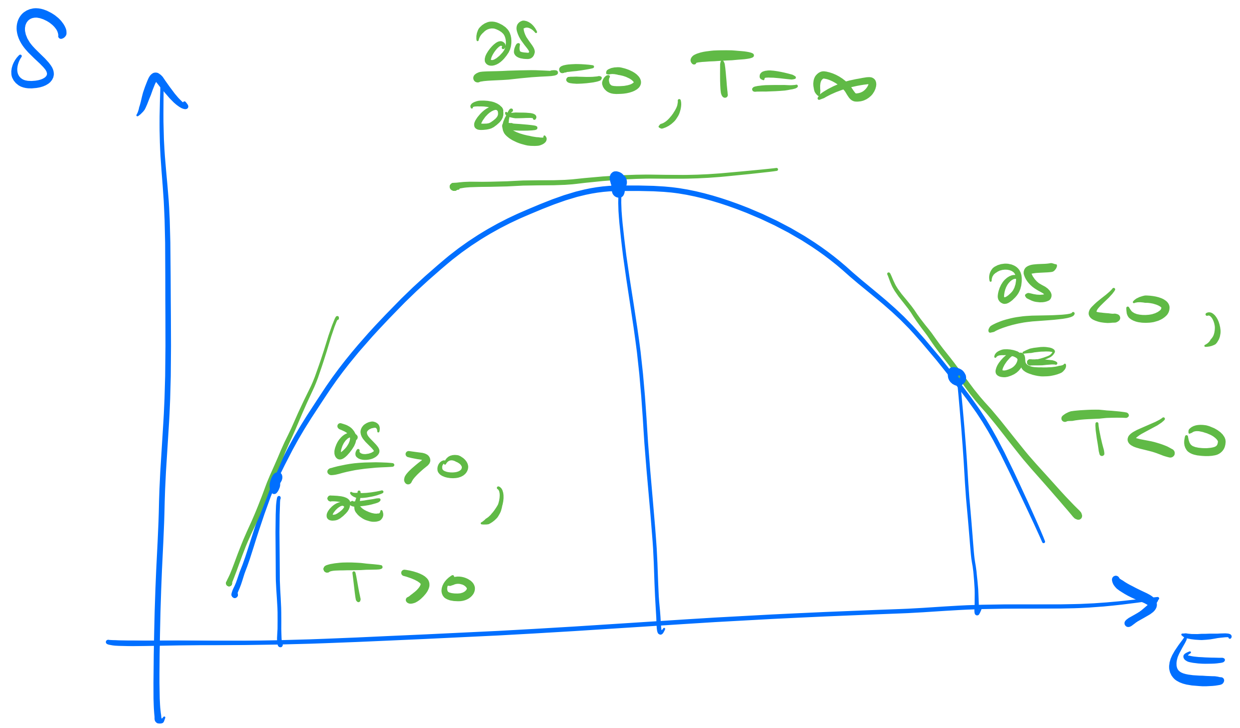
# HOW WE DEFINE TEMPERATURE?

- In a non-interactive (ideal) gas, the temperature is proportional to the macroscopic average of the kinetic energies of the gas components
- Formally, temperature is only defined at equilibrium, that is for a classical gas when the Maxwell-Boltzmann distribution is reached
- At equilibrium, the energy per particle is $E_p = n\frac{1}{2}k_b T$
- In statistical mechanics temperature is more generally defined as

$$\frac{1}{T} = \frac{\partial S}{\partial E} \quad \Longrightarrow \quad T = \frac{1}{\frac{\partial S}{\partial E}}$$

# HOW WE DEFINE TEMPERATURE?

- Usually, entropy is a monotonic growing function vs. energy and higher energies corresponds to higher temperatures
- Some peculiar systems shows entropy decreasing after reaching a global maximum

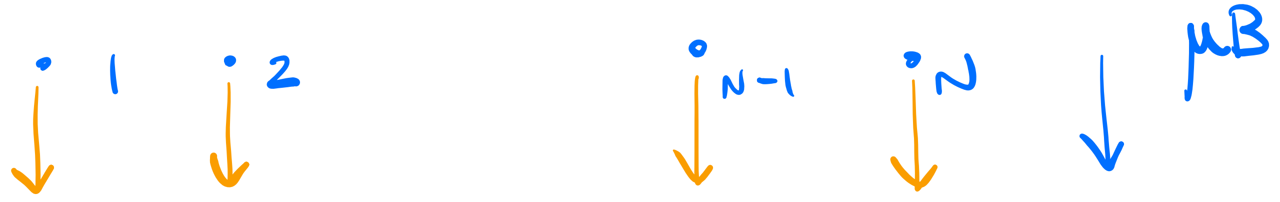


$$\frac{1}{T} = \frac{\partial S}{\partial E}$$

- Negative temperature states are thus "hotter states" as temperature first grows to infinity before becoming negative

# SYSTEMS POSSESSING NEGATIVE TEMPERATURES

Non-interacting spin chain, $E = (N_+ - N_-)\,\mu B$



$N_+ = 0, N\_ = N$

$S = \ln(\Omega = 1) = 0, E = E_{\min}$

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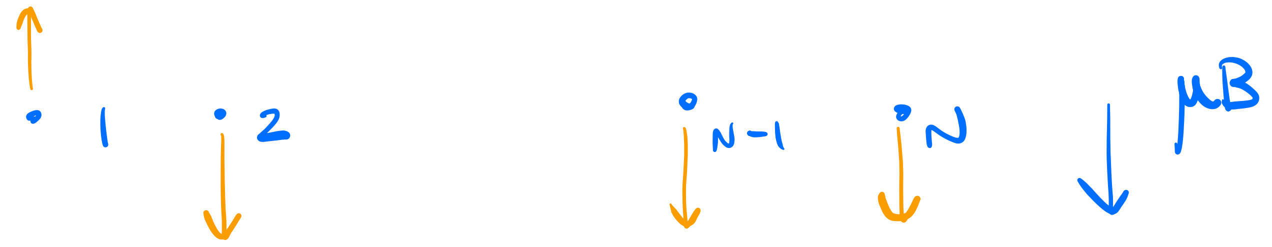

$N_+ = 1, N\_ = N - 1$

$S = \ln(\Omega = N), E > E_{\min}$

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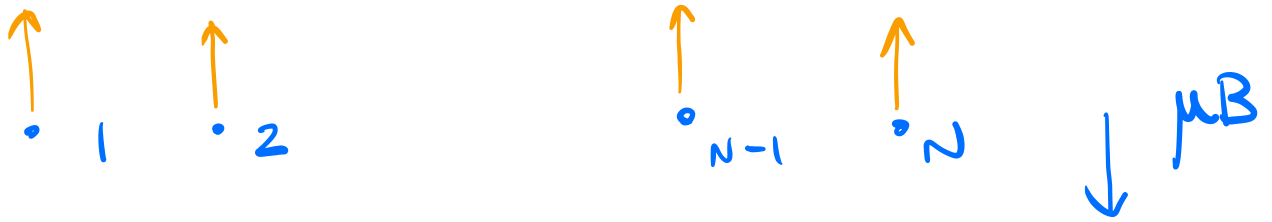


$N_+ = N, N\_0$

$S = \ln(\Omega = 1) = 0, E = E_{\max}$

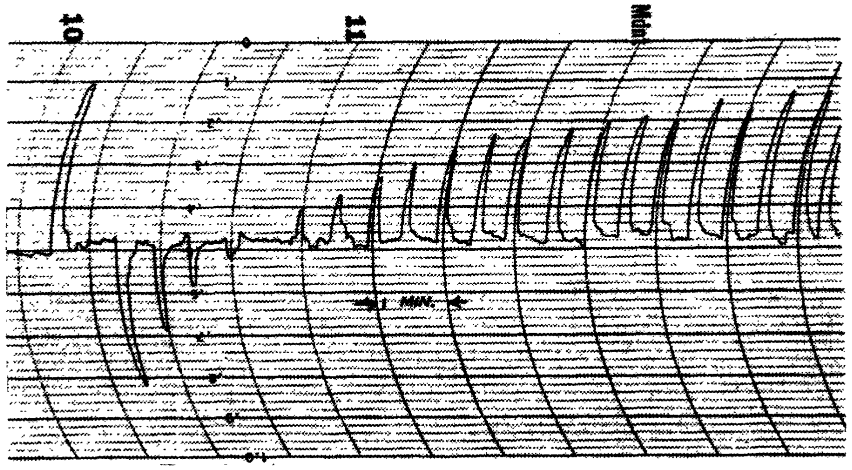


FIG. 1. A typical record of the reversed nuclear magnetization. On the left is a deflection characteristic of the normal state at equilibrium magnetization ($T \approx 300°$K), followed by the reversed deflection ($T \approx -350°$K), decaying ($T \to -\infty$) through zero deflection ($T = \infty$) to the initial equilibrium state.

**A Nuclear Spin System at Negative Temperature**

E. M. PURCELL AND R. V. POUND

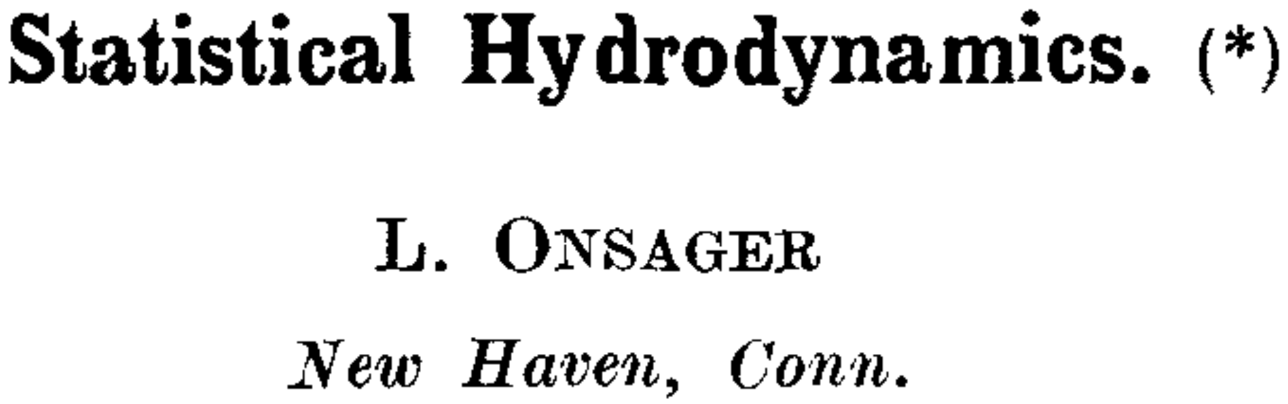
*Department of Physics, Harvard University, Cambridge, Massachusetts*

November 1, 1950

[Purcell & Pound, Physical Review 81, 1951]

# SYSTEMS POSSESSING NEGATIVE TEMPERATURES

## Confined point vortex model

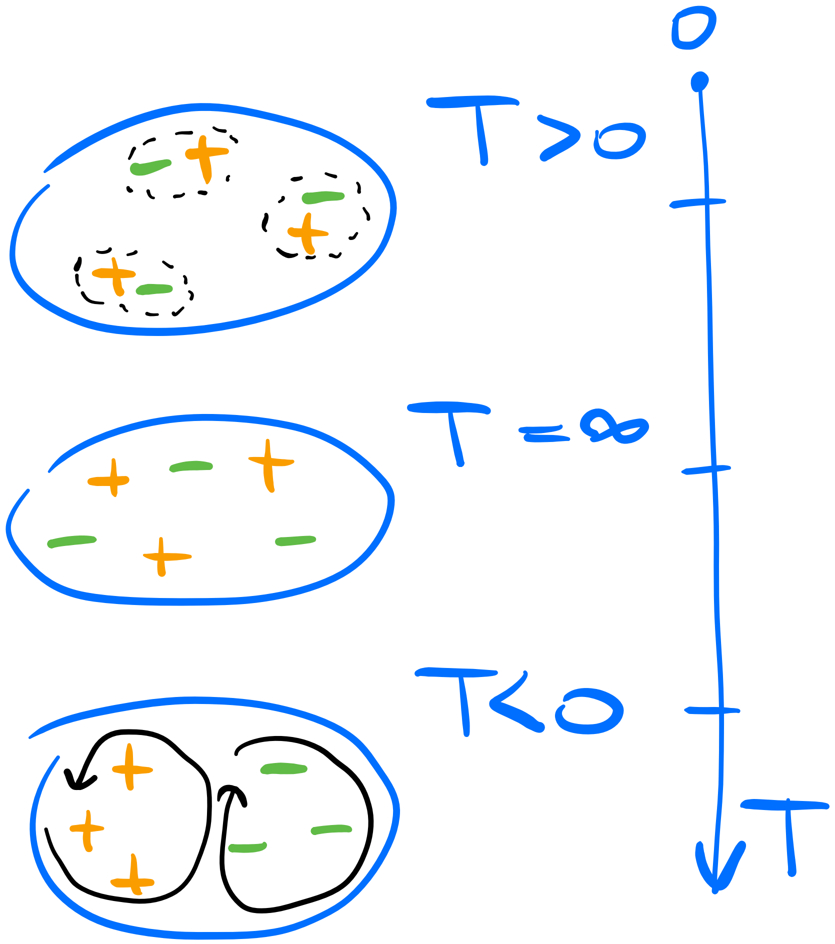


**Statistical Hydrodynamics.** (*)

L. ONSAGER

*New Haven, Conn.*

[Onsager, Il Nuovo Cimento 6, 1949]



### Evolution of large-scale flow from turbulence in a two-dimensional superfluid

**Shaun P. Johnstone[1]*, Andrew J. Groszek[1]†, Philip T. Starkey[1], Christopher J. Billington[1,2], Tapio P. Simula[1]‡, Kristian Helmerson[1,3]***

[Johnstone et al., Science 364, 2019]

### Giant vortex clusters in a two-dimensional quantum fluid

**Guillaume Gauthier[1]*, Matthew T. Reeves[2]*, Xiaoquan Yu[3], Ashton S. Bradley[3], Mark A. Baker[1], Thomas A. Bell[1], Halina Rubinsztein-Dunlop[1], Matthew J. Davis[2], Tyler W. Neely[1]†**

[Gauthier et al., Science 364, 2019]

# THE DISCRETE NONLINEAR SCHROEDINGER EQUATION

The discrete nonlinear Schroedinger (DNLS) equation reads

$$i\frac{d\psi_m}{dt} + \left(\psi_{m+1} + \psi_{m-1} - 2\psi_m\right) + \nu\,|\psi_m|^2\psi_m = 0\,, \quad m = 1,\ldots,M$$

- $\psi_m$ is the complex amplitude of the oscillator at site $m$
- two conserved quantities

$$H = \sum_{m=1}^{M}\left(|\psi_{m+1} - \psi_m|^2 - \frac{1}{2}\nu\,|\psi|^4\right)\,, \quad \text{energy}$$

$$N = \sum_{m=1}^{M}|\psi|^2, \quad \text{wave-action}$$

- (local) discretisation of the continuous one-dimensional NLS model $i\partial_t\psi + \nabla^2\psi + \nu\,|\psi|^2\psi = 0$, but it is not an integrable model

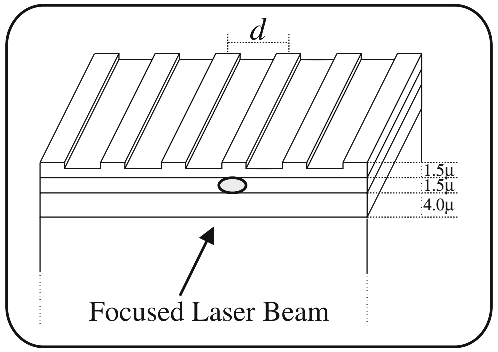
# THE DISCRETE NONLINEAR SCHROEDINGER EQUATION

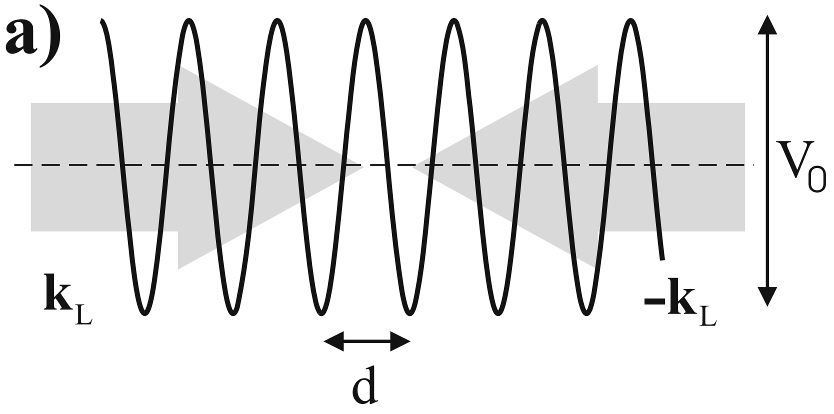
The discrete nonlinear Schroedinger (DNLS) equation reads

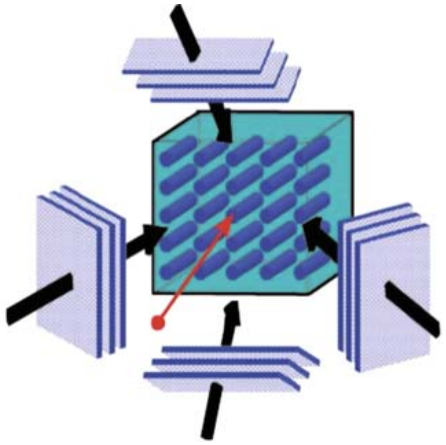
$$i\frac{d\psi_m}{dt} + \left(\psi_{m+1} + \psi_{m-1} - 2\psi_m\right) + \nu\,|\psi_m|^2\psi_m = 0\,, \quad m = 1,\ldots,M$$

DNLS is a very good model, in the limit of tight-binding approximation, for

- lossless optical wave guide arrays
- Bose-Einstein condensates in optical traps







DNLS is also a qualitatively good model to describe some phenomena observed in photo refractive crystals

[Kevrekidis The Discrete Nonlinear Schroedinger Equation, 2009]

# THE DISCRETE NONLINEAR SCHROEDINGER EQUATION

Assuming periodic boundary conditions, and introducing discrete Fourier direct and inverse transforms

$$\psi_m = \sum_{m=1}^{M} \hat{\psi}_k e^{i2\pi km/M} \quad \text{and} \quad \hat{\psi}_k = \frac{1}{M}\sum_{m=1}^{M} \psi_m e^{-i2\pi km/M}$$

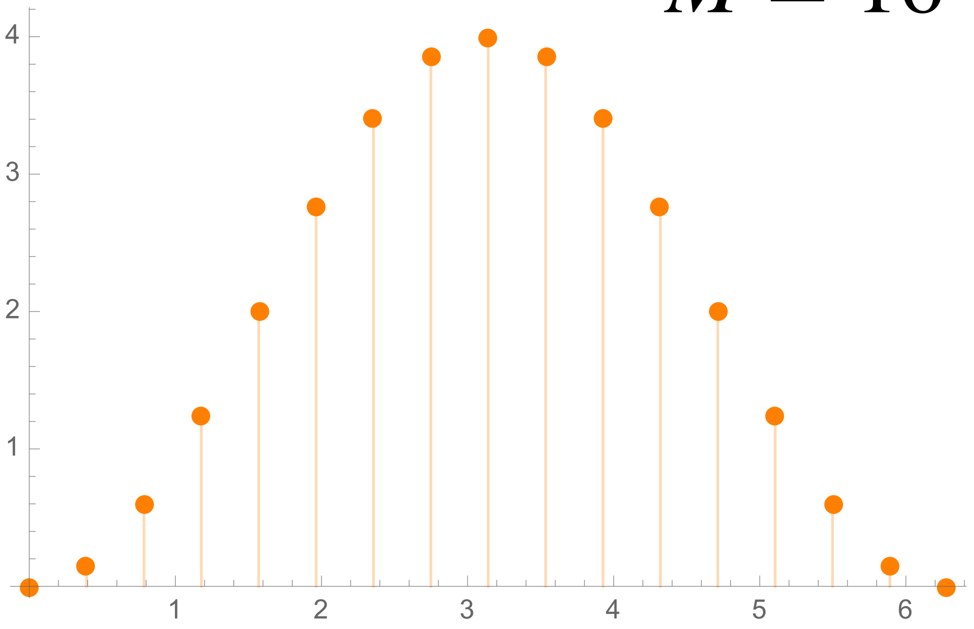
the DNLS becomes in Fourier space

$$i\frac{d\hat{\psi}_{k_1}}{dt} = \omega_{k_1}\hat{\psi}_{k_1} - \nu \sum_{k_2,k_3,k_4} \hat{\psi}^*_{k_2}\psi_{k_3}\psi_{k_4}\delta^{34}_{12}$$

where the dispersion relation is

$$\omega_k = 4\sin^2(\pi k/M)$$

$M = 16$



and the Kronecker's $\delta^{34}_{12} = \delta_{k_1+k_2,k_3+k_4}$ accounts for the Umklapp scattering processes, that is $k_1 + k_2, k_3 + k_4 \mod M$

# THE WAVE INTERACTION/TURBULENCE APPROACH

Wave turbulence (WT) theory is a statistical mechanics approach to weakly dispersive wave systems (waves in optics, plasma, ocean, Bose-Einstein condensates)

[Nazarenko, Wave Turbulence, 2011]

The (large time) efficient energy transfer in the system goes only trough exact resonant n-wave interaction processes satisfying

$$\boxed{\begin{aligned} k_1 \pm k_2 \pm \dots k_n = 0 \\ \omega_1 \pm \omega_2 \pm \dots \omega_n = 0 \end{aligned}}$$

(resonant manifold)

# WT IN DNLS (ACTION-ANGLE VARIABLES)

$$i\frac{d\hat{\psi}_{k_1}}{dt} = \omega_{k_1}\hat{\psi}_{k_1} - \nu \sum_{k_2,k_3,k_4} \hat{\psi}^*_{k_2}\psi_{k_3}\psi_{k_4}\delta^{34}_{12}$$

Writing $\hat{\psi}_k = \sqrt{I_k}e^{-i\theta_k}$ in action-angle variables

$$\frac{dI_{k_1}}{dt} = -2\nu \sum_{k_2,k_3,k_4} \sqrt{I_{k_1}I_{k_2}I_{k_3}I_{k_4}}\sin\left(\Delta\theta^{34}_{12}\right)\delta^{34}_{12}$$

$$\frac{d\theta_{k_1}}{dt} = \omega_{k_1} - \nu \sum_{k_2,k_3,k_4} \sqrt{\frac{I_{k_2}I_{k_3}I_{k_4}}{I_{k_1}}}\cos\left(\Delta\theta^{34}_{12}\right)\delta^{34}_{12}$$

where $\Delta\theta_{12} = \theta_1 + \theta_2 - \theta_3 - \theta_4$

# WT IN DNLS ($M \to \infty$ AND KINETIC EQUATION)

- Statistical approach, averaging over realisations having phases uniformly distributed $\theta_k \in [0,2\pi)$
- Consider weakly nonlinear limit, that is $|\nu| \ll 1$
- First non zero moment is the wave-action density $n_k(t) \propto \langle I_k \rangle$
- Take the thermodynamic (large box) limit $M \to \infty$ and I
- At a large time-scale $\tau$

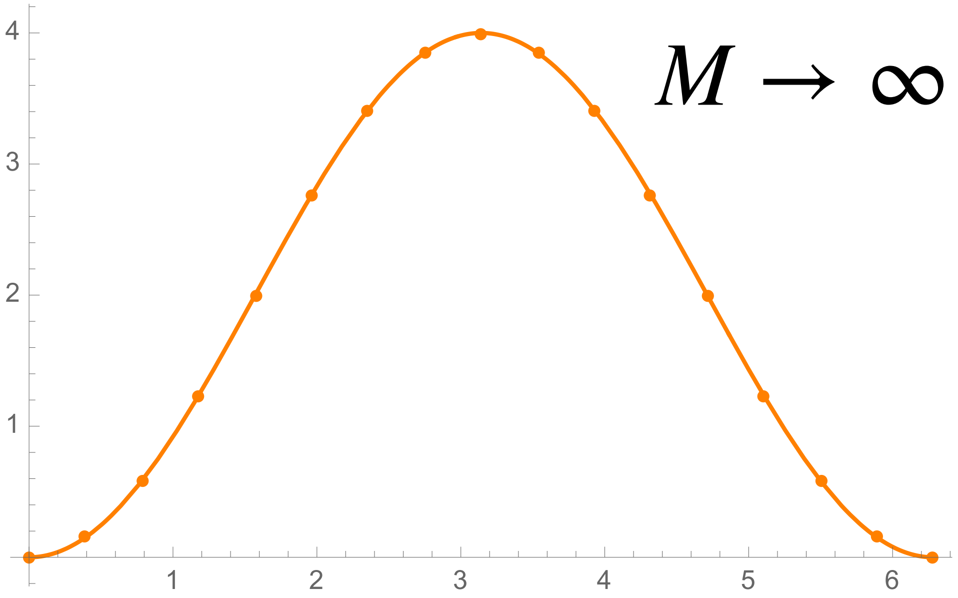
$$\frac{dn_{k_1}}{d\tau} = 4\pi\nu^2 \int_0^{2\pi} n_{k_1}n_{k_2}n_{k_3}n_{k_4}\left(\frac{1}{n_{k_1}} + \frac{1}{n_{k_2}} - \frac{1}{n_{k_3}} - \frac{1}{n_{k_4}}\right)$$

$$\delta\left(\Delta\omega_{12}^{34}\right)\delta_{12}^{34}\, dk_2 dk_3 dk_4\,,$$

where $\Delta\omega_{12} = \omega_1 + \omega_2 - \omega_3 - \omega_4$,
$k \in [0,2\pi]$ and $\omega_k = 4\sin^2(k/2)$

[Onorato & Dematteis, JPC 4, 2020]

$M = 16$ and $M \to \infty$



# WT IN DNLS ($M \to \infty$ AND KINETIC EQUATION)

- 4-wave interactions
- resonant manifold given by

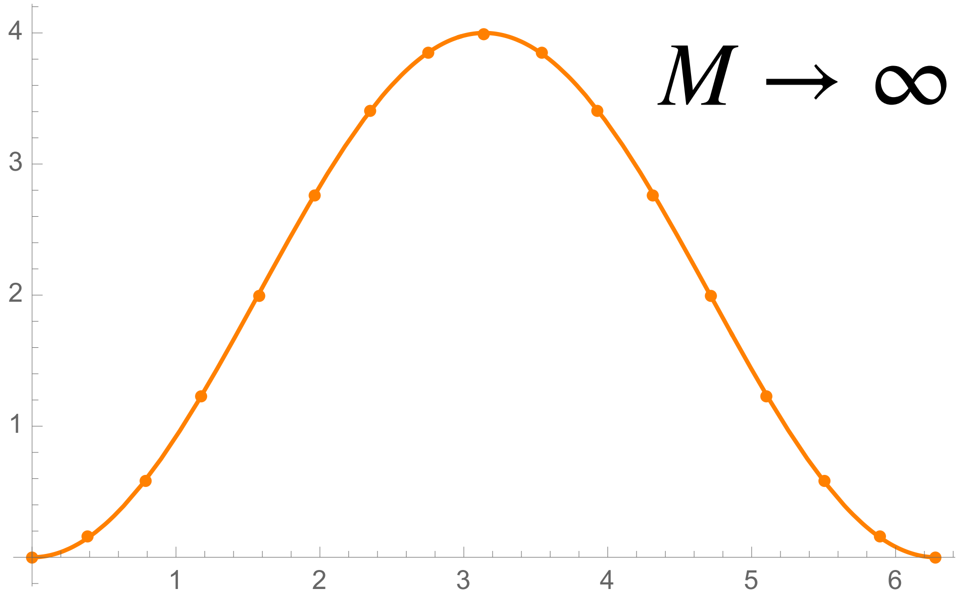
$$\boxed{\begin{aligned} &k_1 + k_2 - k_3 - k_4 = 0 \mod 2\pi \\ &\omega_1 + \omega_2 - \omega_3 - \omega_4 = 0 \end{aligned}}$$

$$\frac{dn_{k_1}}{d\tau} = 4\pi\nu^2 \int_0^{2\pi} n_{k_1} n_{k_2} n_{k_3} n_{k_4} \left( \frac{1}{n_{k_1}} + \frac{1}{n_{k_2}} - \frac{1}{n_{k_3}} - \frac{1}{n_{k_4}} \right) \delta\left(\Delta\omega_{12}^{34}\right) \delta_{12}^{34}\, dk_2 dk_3 dk_4\,,$$

where $\Delta\omega_{12} = \omega_1 + \omega_2 - \omega_3 - \omega_4$,
$k \in [0,2\pi]$ and $\omega_k = 4\sin^2(k/2)$

[Onorato & Dematteis, JPC 4, 2020]

$M = 16$ and
$M \to \infty$



# WT IN DNLS (TAKING THE THERMODYNAMIC LIMIT)

$$\frac{dn_{k_1}}{d\tau} = 4\pi\nu^2 \int_0^{2\pi} n_{k_1} n_{k_2} n_{k_3} n_{k_4} \left( \frac{1}{n_{k_1}} + \frac{1}{n_{k_2}} - \frac{1}{n_{k_3}} - \frac{1}{n_{k_4}} \right)$$

$$\delta\left(\Delta\omega_{12}^{34}\right) \delta_{12}^{34}\, dk_2 dk_3 dk_4$$

- Two invariants

$$E = \int_0^{2\pi} \omega_k\, n_k\, dk \quad \text{and} \quad N = \int_0^{2\pi} n_k\, dk$$

- KE is time-irreversible as, given the entropy $S(t) = \int_0^{2\pi} \ln n_k(t)\, dk$, an H-theorem $dS/dt \geq 0$ holds

- The equilibrium is the Rayleigh-Jeans distribution $(T, \mu)$

$$n_k^{(RJ)} = \frac{T}{\omega_k - \mu} = \frac{1}{\beta\omega_k - \gamma} \quad \text{with} \quad \beta = 1/T, \gamma = \mu/T$$

# RJ AND NEGATIVE TEMPERATURE STATES

$$n_k^{(RJ)} = \frac{T}{\omega_k - \mu} = \frac{1}{\beta\omega_k - \gamma} \quad \text{with} \quad \beta = 1/T, \gamma = \mu/T$$

- Play with $T$ and $\mu$ to have negative temperatures, $T < 0$, but still a positive-defined distribution
- energy density distribution $e_k = \omega_k n_k$

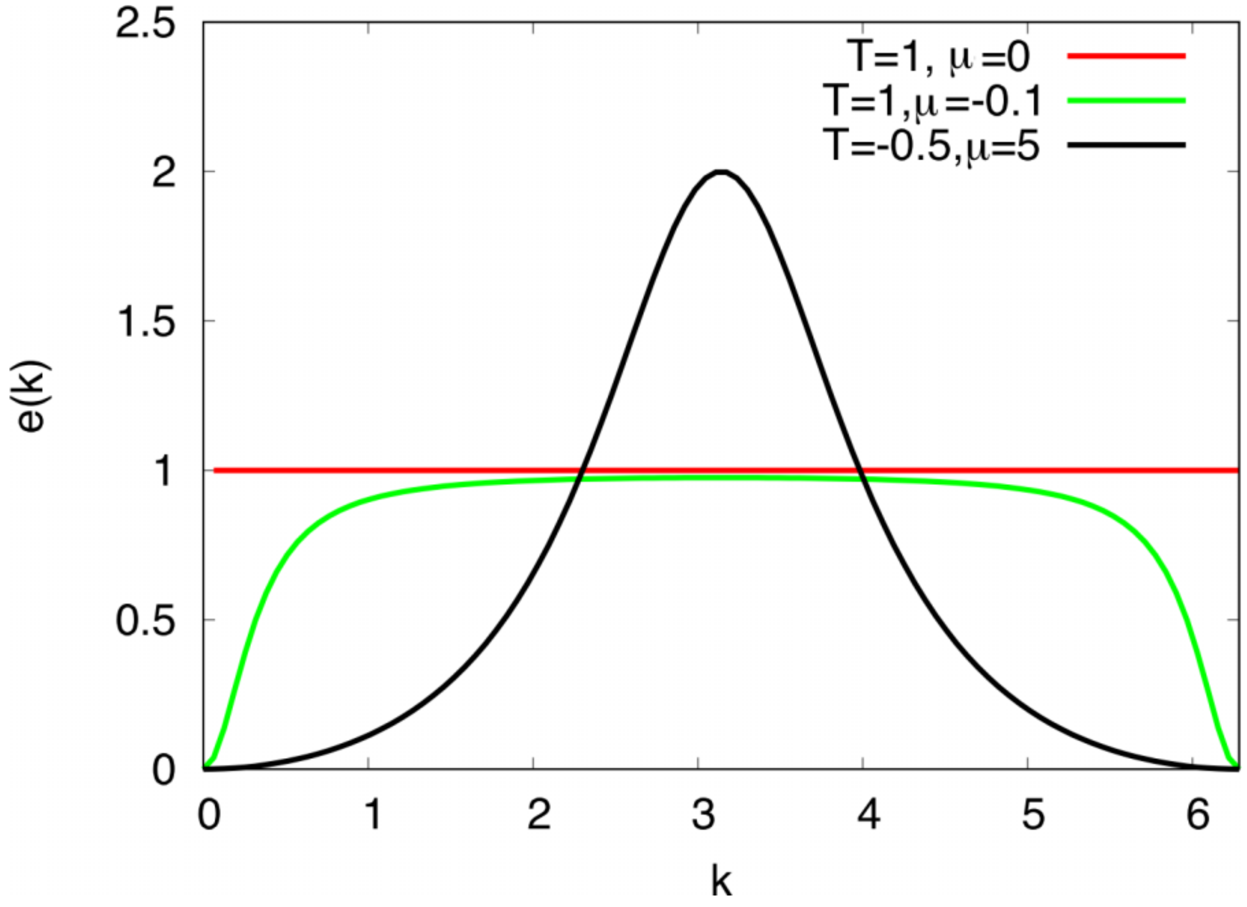


FIG. 1. Spectral energy density $e(k) = \omega(k)n(k)$ for different temperatures and chemical potentials. The red horizontal line is the typical equipartition of energy and corresponds to $T = 1$ and $\mu = 0$; the green line corresponds to $T = 1$ and $\mu = -0.1$ and the black line (sharply peaked around $k = \pi$) corresponds to negative temperatures, i.e., $T = -0.5$ and $\mu = 5$. All these curves are exact stationary solutions of the WK equation.

# LINKING INTENSIVE AND EXTENSIVE QUANTITIES

$$E = \int_0^{2\pi} \omega_k n_k \, dk, \quad N = \int_0^{2\pi} n_k \, dk \quad \text{and} \quad S(t) = \int_0^{2\pi} \ln n_k(t) \, dk$$

Given the RJ distribution $n_k^{(RJ)} = \dfrac{1}{\beta\omega_k - \gamma}$, one can obtain

$$\beta(E,N) = \frac{4\pi(E-2N)}{E(E-4N)}$$

$$\gamma(E,N) = \frac{2\pi E}{N(E-4N)}$$

$$S(E,N) = 2\pi \ln\left[\frac{E(4N-E)}{8\pi N}\right]$$

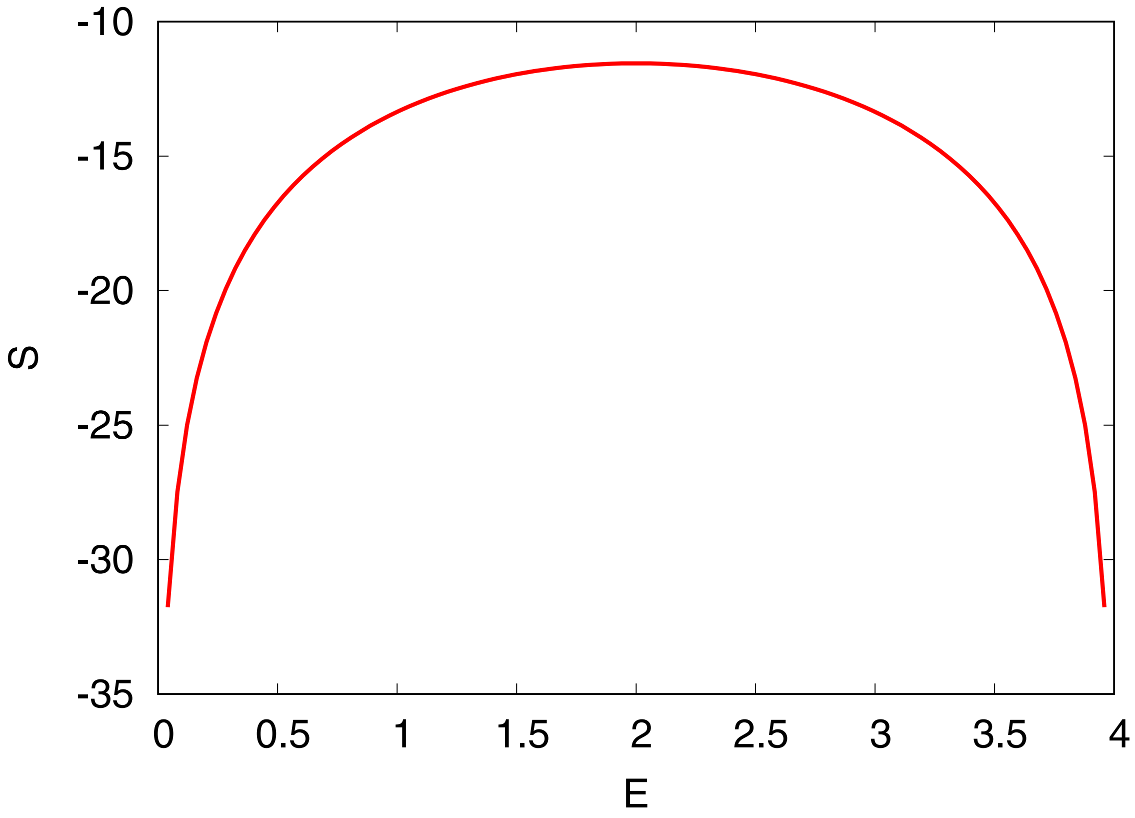


FIG. 3. The entropy, $S$, as a function of the energy, $E$, for $N = 1$. The derivative of $S$ is the inverse of the temperature. For $E > 2N{=}2$ the derivative is negative, implying a negative temperature. Note that entropy is defined for $0 < E < 4N$.

# LINKING INTENSIVE AND EXTENSIVE QUANTITIES

$$E = \int_0^{2\pi} \omega_k n_k \, dk, \quad N = \int_0^{2\pi} n_k \, dk \quad \text{and} \quad S(t) = \int_0^{2\pi} \ln n_k(t) \, dk$$

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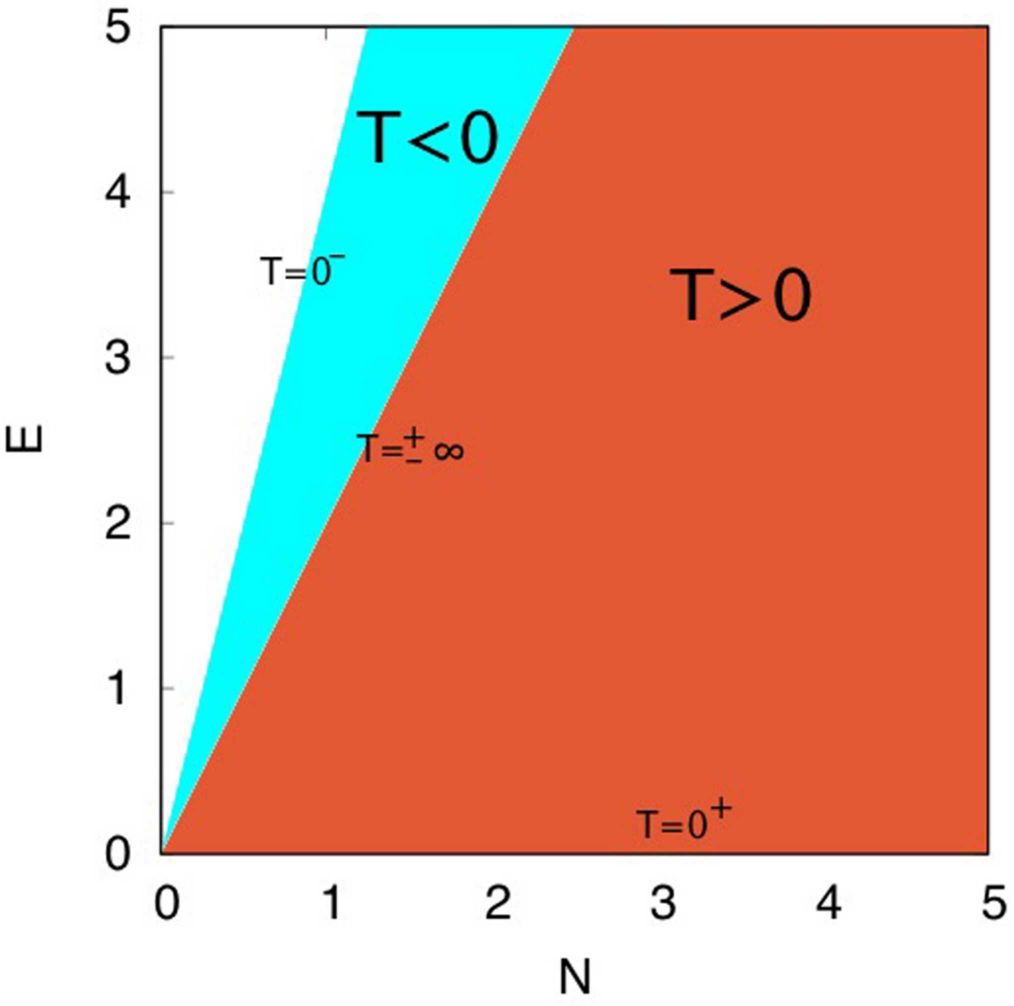


# DIRECT NUMERICAL SIMULATIONS OF THE DNLS MODEL

$$i\frac{d\psi_m}{dt} + \left(\psi_{m+1} + \psi_{m-1} - 2\psi_m\right) + \nu\,|\psi_m|^2\psi_m = 0\,, \quad m = 1,\ldots,M$$

- Can we obtain negative temperature states?
- Are the predictions of the wave kinetic equation accurate?

# DIRECT NUMERICAL SIMULATIONS OF THE DNLS MODEL

$$i\frac{d\psi_m}{dt} + \left(\psi_{m+1} + \psi_{m-1} - 2\psi_m\right) + \nu\,|\,\psi_m\,|^2\psi_m = 0\,, \quad m = 1,\ldots,M$$

- Solve DNLS using a standard forth-order RK algorithm that preserves (sufficiently well) the conserved quantities for large time-scales
- Average over 1,000 realisations initialised with the same spectral density but phases randomly distributed $\theta_k \in [0,2\pi)$

# NUMERICAL RESULTS: RJ EQUILIBRIUM

## initial wave-action distribution

$$n_k = B + A \exp\left\{ \frac{-[(k-k_0)\Delta k]^2}{2\sigma^2} \right\}$$

with $\sigma = 0.9$, $A = 2$, $B = 0$, $\Delta k = 2\pi/M$, $M = 512$, and $k_0 = M/2$. With this choice $E = \sum \omega_k n_k \Delta k = 18.80$ and $N = \sum n_k \Delta k = 5.63$; therefore $2N < E < 4N$ which corresponds to $T = -0.74$ and $\mu = 4.16$, i.e., negative temperatures. One thousand realizations of the same spectrum (deterministic amplitudes) with different random phases have been considered and the results are obtained by averaging over the ensemble. The nonlinear parameter $\nu$ was set to 0.03. In

$$e_k = \langle \omega_k n_k \rangle$$

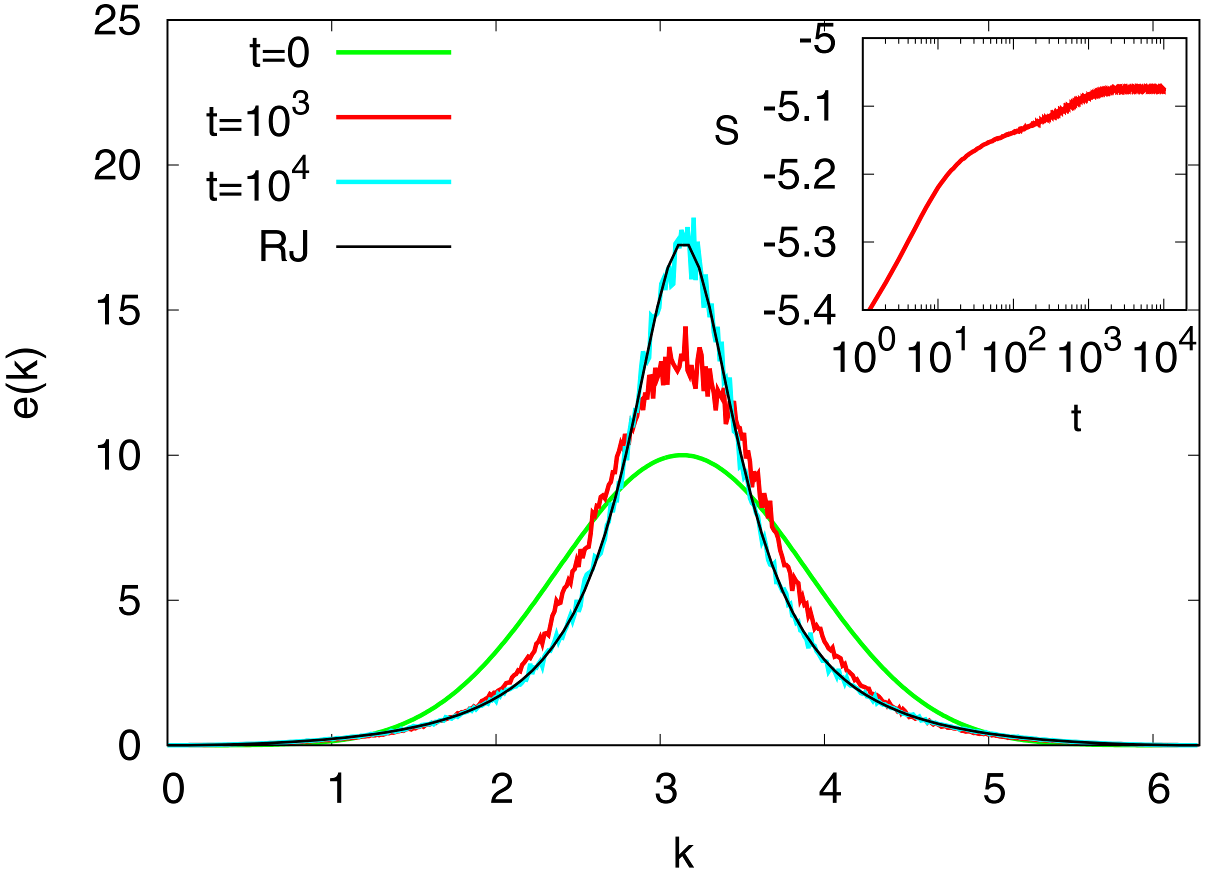
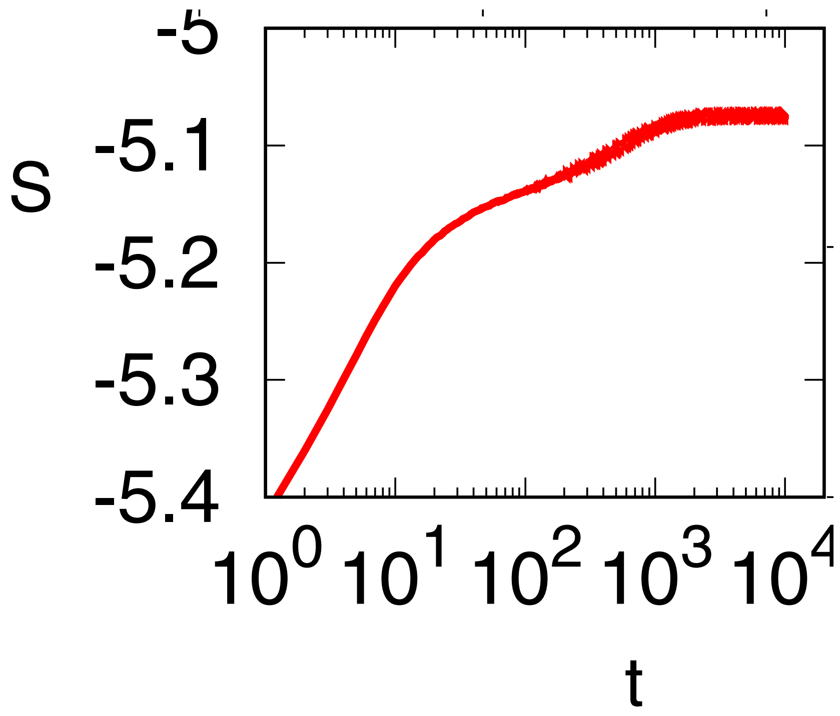


FIG. 4. Energy density as a function of wave number for a simulation of the DNLS equation characterized by the initial condition in (30) that corresponds to $T = -0.74$ and $\mu = 4.16$. Note that, because of the conservation of energy and number of particles, temperature and chemical potential do not change in time [44,45].



$$S(t) = \left\langle \int_0^{2\pi} \ln n_k(t)\, dk \right\rangle$$

# NUMERICAL RESULTS: FLUCTUATIONS

The WT theory also allows to derive higher order moments of the angle-action variables, for example the second moment $\Lambda_k \propto \langle I_k^2 \rangle$

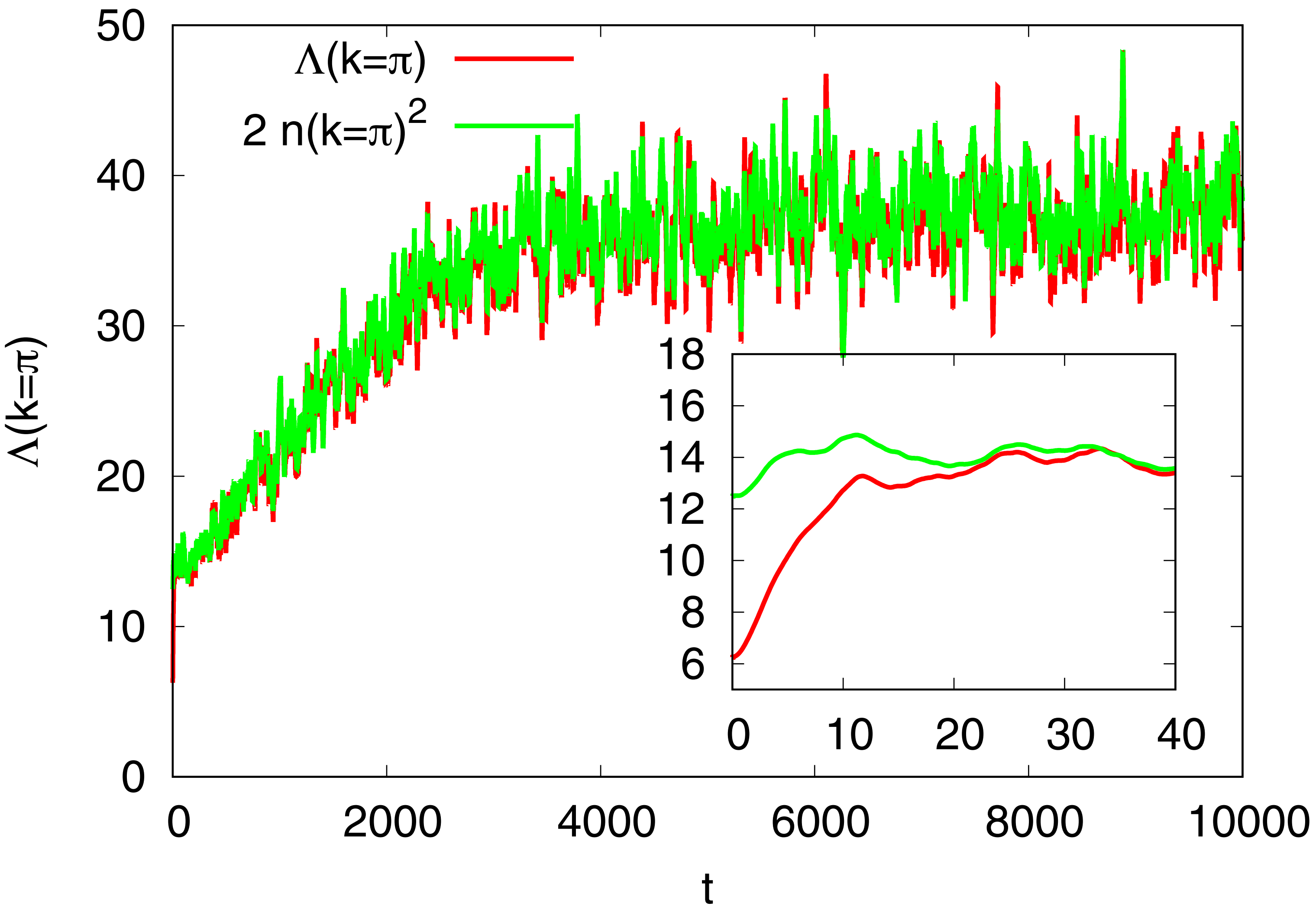
$$\frac{d\Lambda_{k_1}}{d\tau} = 4n_{k_1}\xi_{k_1} - 2\gamma_{k_1}\Lambda_{k_1} \quad \text{with}$$

$$\xi_{k_1} = 4\pi\nu^2 \int_0^{2\pi} n_{k_2}n_{k_3}n_{k_4}\delta\left(\Delta\omega_{12}^{34}\right)\delta_{12}^{34}dk_2dk_3dk_4$$

$$\gamma_{k_1} = -4\pi\nu^2 \int_0^{2\pi} (n_{k_3}n_{k_4} - n_{k_2}n_{k_3} - n_{k_2}n_{k_4})\delta\left(\Delta\omega_{12}^{34}\right)\delta_{12}^{34}dk_2dk_3dk_4$$

One can check that if $\Lambda_k(t) = 2\,n_k^2(t)$, then the top equation is always satisfied provided that $n_k(t)$ follows the KE described before. One can then test this relation!

# NUMERICAL RESULTS: FLUCTUATIONS



- We tested it for the mode $k = \pi$ in the negative temperature regime
- The higher-order moment $\langle I_k \rangle$ starts to follow the kinetic theory at very short time-scale

One can check that if $\Lambda_k(t) = 2\,n_k^2(t)$, then the top equation is always satisfied provided that $n_k(t)$ follows the KE described before. One can then test this relation!

# NUMERICAL RESULTS: FLUCTUATIONS

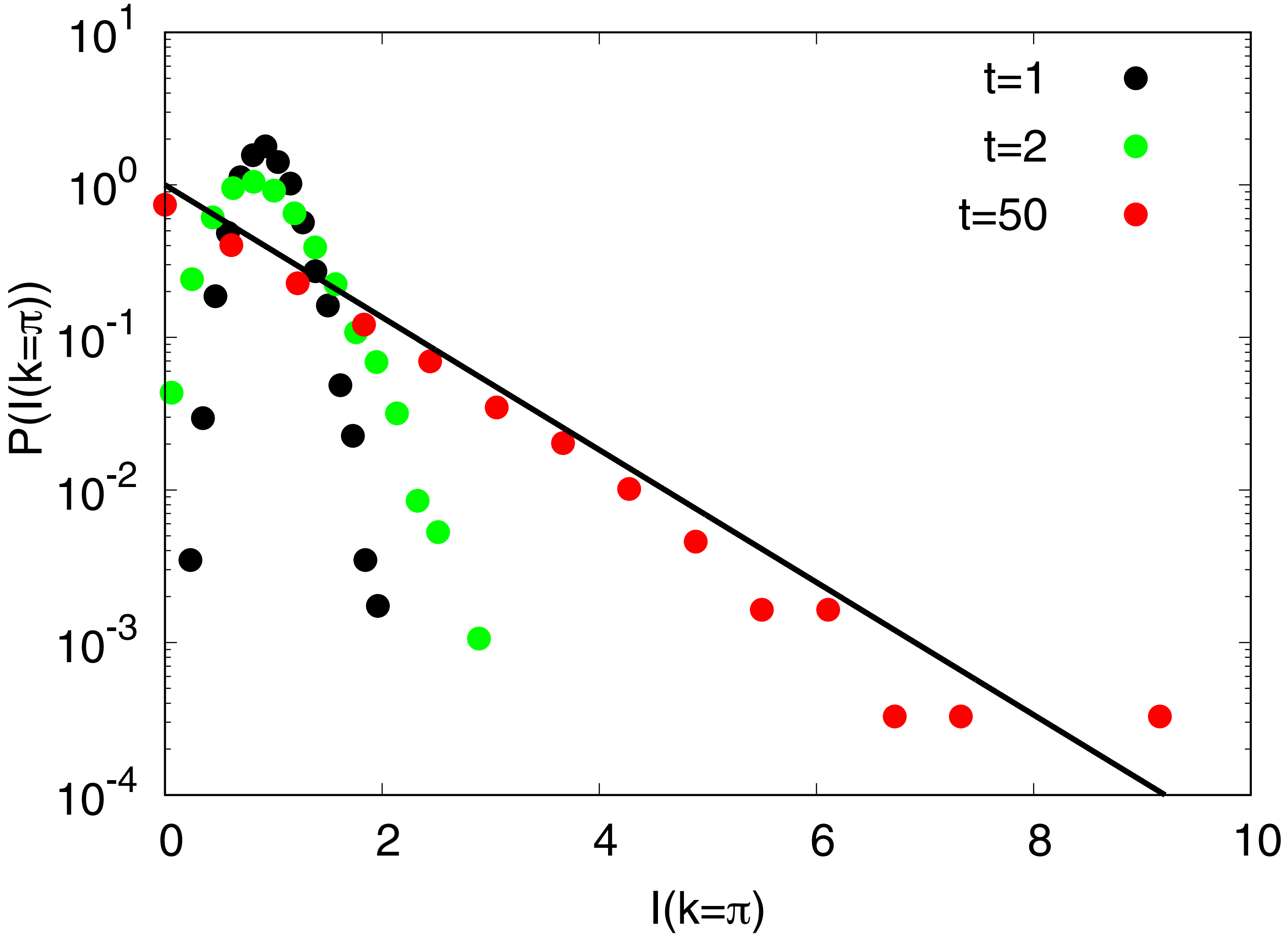


FIG. 6. Probability density function of $I(k = \pi)$ for different times. The dark line corresponds to the exponential distribution derived in Refs. [15,41,46].

- We tested it for the mode $k = \pi$ in the negative temperature regime
- The pdf starts to follow the kinetic theory (Rayleigh distributed according to an exponential) at very short time-scale

Another way of testing how quickly the microscopic dynamics approaches the kinetic dynamics is to measure the probability density function of the fluctuations

# CONCLUSIONS

$$i\frac{d\psi_m}{dt} + \left(\psi_{m+1} + \psi_{m-1} - 2\psi_m\right) + \nu\,|\psi_m|^2\psi_m = 0\,, \quad m = 1,\ldots,M$$

- Negative temperatures are possible in DNLS due to the (i) upper bound of the dispersion relation and (ii) the fact that the system conserves two quantities
- Relations between intensive and extensive quantities can be found in a closed form for DNLS
- Negative temperature states are not so exotic, as their dynamics is very well described (in the weakly nonlinear limit) by WT kinetic theory as well as standard positive temperature states
- Our conclusions are likely to be valid to any other dispersive wave system characterised by 4-wave interactions where the dispersion relation is bounded from above

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# THANKS FOR YOUR ATTENTION!

**Joint work with: M. Onorato, G. Dematteis, A. Pezzi, M. Ballarin, and L. Rondoni**

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# CONCLUSIONS

$$i\frac{d\psi_m}{dt} + \left(\psi_{m+1} + \psi_{m-1} - 2\psi_m\right) + \nu\,|\psi_m|^2\psi_m = 0\,, \quad m = 1,\ldots,M$$

- Any experimental realisation?

## Negative Absolute Temperature for Motional Degrees of Freedom

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the Bose-Hubbard Hamiltonian (*12*)

$$H = -J\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + V\sum_i \mathrm{r}_i^2 \hat{n}_i \quad (2)$$

[Braun et al., Science 339, 2013]