SPREADING OF WAVE PACKETS IN ONE DIMENSIONAL DISORDERED CHAINS: DIFFERENT DYNAMICAL REGIMES

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Abstract

We present numerical results for the spatiotemporal evolution of a wave packet in quartic Klein-Gordon (KG) and disordered nonlinear Schrödinger (DNLS) chains, having equivalent linear parts. In the absence of nonlinearity all eigenstates are spatially localized with an upper bound on the localization length (Anderson localization). In the presence of nonlinearity we find three different dynamical behaviors depending on the relation of the nonlinear frequency shift δ (which is proportional to the system's nonlinearity) with the average spacing $\overline{\Delta\lambda}$ of eigenfrequencies and the spectrum width Δ $(\overline{\Delta\lambda} < \Delta)$ of the linear system. The dynamics for small nonlinearities $(\delta < \overline{\Delta\lambda})$ is characterized by localization as a transient, with subsequent subdiffusion (regime I). For intermediate values of the nonlinearity, such that $(\overline{\Delta\lambda} < \delta < \Delta)$ the wave packets exhibit immediate subdiffusion (regime II). In this case, the second moment m_2 and the participation number P increase in time following the power laws $m_2 \sim t^{\alpha}$, $P \sim t^{\alpha/2}$. We find α=1/3. Finally, for even higher nonlinearities ($\delta > \Delta$) a large part of the wave packet is selftrapped, while the rest subdiffuses (regime III). In this case P remains practically constant, while $m_2 \sim t^{\alpha}$.

Models and computational methods

We study [1] two models of one-dimensional lattices:

The quartic Klein – Gordon (KG) model

$$H_K = \sum_{l=1}^{N} \frac{p_l^2}{2} + \frac{\tilde{\varepsilon}_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W}\left(u_{l+1} - u_l\right)^2$$

where u_l and p_l are respectively the generalized coordinates and momenta, l is the lattice site index, W is the disorder strength, E the total energy and typically N=1000.

$\tilde{\varepsilon}_l$ are chosen uniformly from $\left[\frac{1}{2}, \frac{3}{2}\right]$.

The disordered discrete nonlinear Schrödinger (DNLS) equation (see also poster 14)

$$H_D = \sum_{l=1}^{N} \varepsilon_l |\psi_l|^2 + \frac{\beta}{2}|\psi_l|^4 - \left(\psi_{l+1}\psi_l^* + \psi_{l+1}^*\psi_l\right)$$

with complex variables ψ_l. The random on-site energies ε_l are chosen uniformly from $\left[-\frac{W}{2}, \frac{W}{2}\right]$.

Linear case of the KG model (neglecting the term u_l^4)

Ansatz: $u_l = A_l \exp(i\omega t)$

Eigenvalue problem: $\lambda A_l = \varepsilon_l A_l - (A_{l+1} + A_{l-1})$ with $\lambda = W\omega^2 - W - 2,\quad \varepsilon_l = W(\tilde{\varepsilon}_l - 1)$.

Unitary eigenvectors (normal modes - NMs) $A_{\nu,l}$ are ordered according to their **center-of-norm coordinate:** $X_\nu = \sum_{l=1}^{N} l A_{\nu,l}^2$

All eigenstates are localized (Anderson localization) having a localization length which is bounded from above.

Scales

$\omega_\nu^2 \in \left[\frac{1}{2}, \frac{3}{2} + \frac{4}{W}\right]$, **width of the squared frequency spectrum:** $\Delta_K = 1 + \frac{4}{W}$

Localization volume of eigenstate: $p_\nu = \frac{1}{\sum_{l=1}^{N} A_{\nu,l}^4}$

Average spacing of squared eigenfrequencies of NMs within the range of a localization volume:

$$\overline{\Delta\omega^2} \approx \frac{\Delta_K}{p_\nu}.$$

For small values of W we have $\overline{\Delta\omega^2} \sim W^2$.

Nonlinearity induced squared **frequency shift** of a single site oscillator $\delta_l = \frac{3E_l}{2\tilde{\varepsilon}_l} \propto E.$

The relation of the two scales $\overline{\Delta\omega^2} \leq \Delta_K$ with the nonlinear frequency shift δ_l determines the packet evolution.

Distribution characterization

We consider **normalized energy distributions** in normal mode (NM) space $z_\nu \equiv \frac{E_\nu}{\sum_m E_m}$ with $E_\nu = \frac{1}{2}\left(\dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2\right)$, where A_ν is the amplitude of the νth NM.

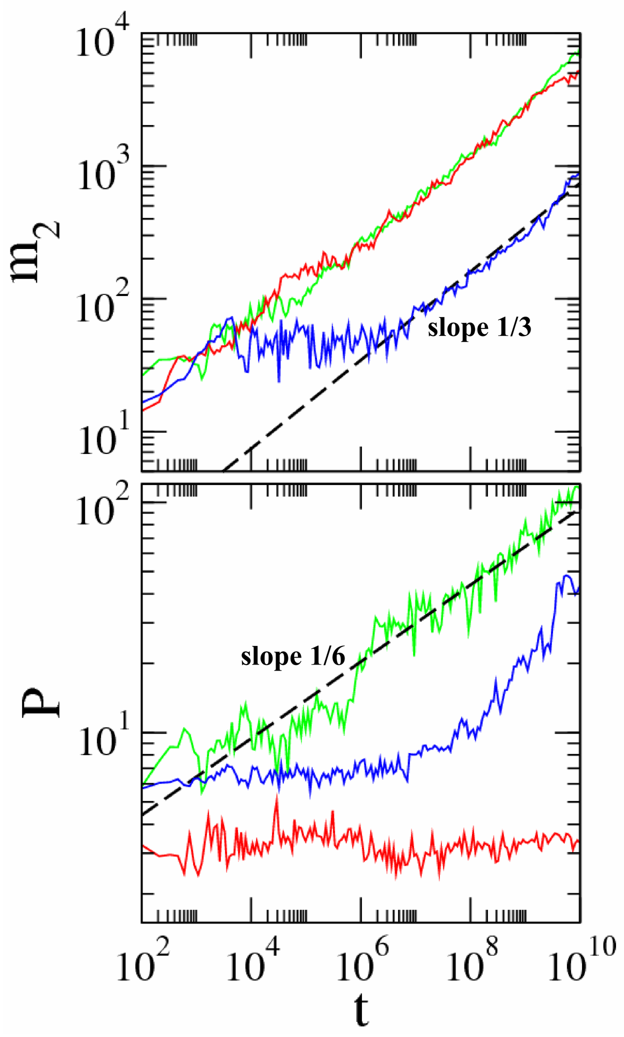
Second moment: $m_2 = \sum_{\nu=1}^{N} \left(\nu - \bar{\nu}\right)^2 z_\nu$, with $\bar{\nu} = \sum_{\nu=1}^{N} \nu z_\nu$ quantifies the wave packet's degree of spreading.

Participation number: $P = \frac{1}{\sum_{\nu=1}^{N} z_\nu^2}$ measures the number of stronger excited modes in z_ν.

Compactness index: $\zeta = \frac{P^2}{m_2}$ measures the sparseness of wave packets.

The KG chain was integrated with the help of a **symplectic integrator** of order O(τ^4) with respect to the integration time step τ, namely the SABA$_2$ integrator with corrector (SABA$_2$C) [2].

Different spreading regimes



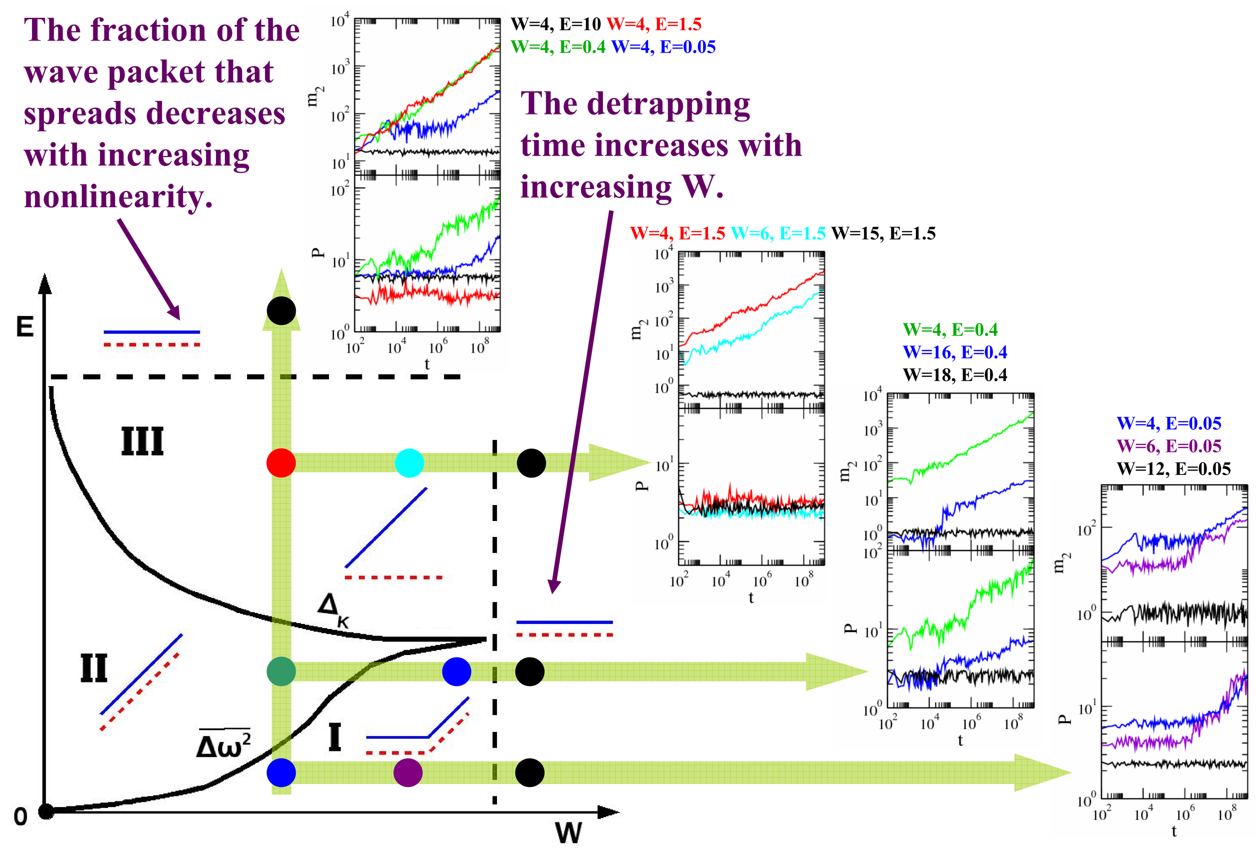
E = 0.05, 0.4, 1.5 - W = 4. Single site excitations

Regime I: Small values of nonlinearity. $\delta_l < \overline{\Delta\omega^2}$
Frequency shift is less than the average spacing of interacting modes. Localization as a transient (like in the linear case), with subsequent subdiffusion.

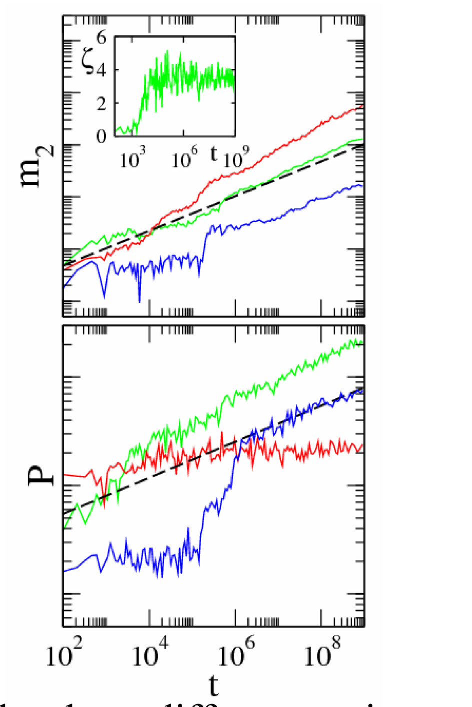
Regime II: Intermediate values of nonlinearity. $\overline{\Delta\omega^2} < \delta_l < \Delta_K$
Resonance overlap may happen immediately. Immediate subdiffusion [3].

Regime III: Big nonlinearities. $\delta_l > \Delta_K$
Frequency shift exceeds the spectrum width. Some frequencies of NMs are tuned out of resonances with the NM spectrum, leading to selftrapping, while a small part of the wave packet subdiffuses [4].

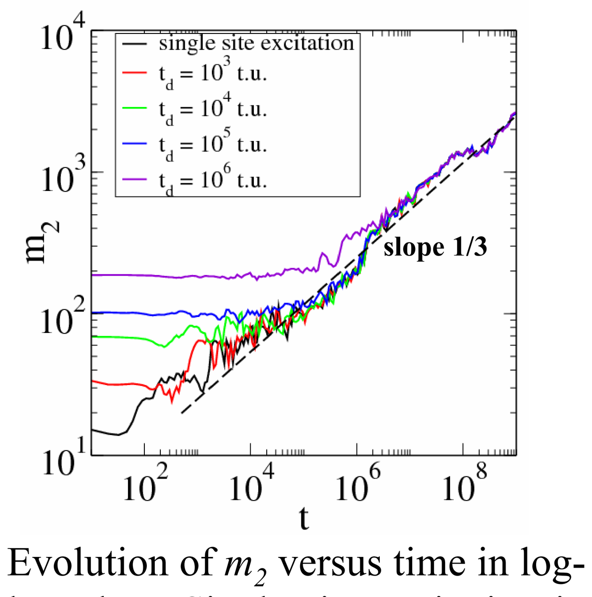
Subdiffusion:
Assuming that the spreading is due to heating of the cold exterior, induced by the chaoticity of the wave packet, we theoretically predict α=1/3 [1].



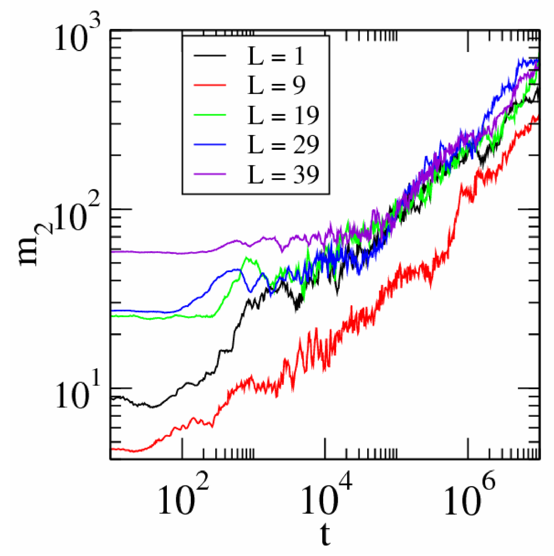
Schematic representation of the three different regimes of spreading for the KG model in the parameter space of disorder strength W and of the nonlinear frequency shift δ at initial time t=0. For each regime the behavior of the second moment m_2 (blue solid curves) and of the participation number P (red dashed curves) are shown schematically. The regions above the horizontal dashed lines (large nonlinearities) and to the right of the vertical dashed lines (large disorder strengths) correspond to parameter values where diffusion is not detected numerically. Numerical examples from the different regions are also presented.



The three different regimes for **single mode excitations** of the KG model. Inset: the compactness index ζ for the regime II case.



Evolution of m_2 versus time in log-log plots. Single site excitation in the intermediate regime II for the KG model corresponds to the black curve. The wave packet after t_d=10^3, 10^4, 10^5, 10^6 time units (t.u.) is registered and **relaunched** as initial distribution.



Nonlocal excitations of the KG chain corresponding to initial homogeneous distributions of energy E=0.4 over L neighboring sites. m_2 versus time in log-log plots for L=1, 9, 19, 29 and 39 sites.

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