Spreading mechanism of wave packets in one dimensional disordered Klein-Gordon chains

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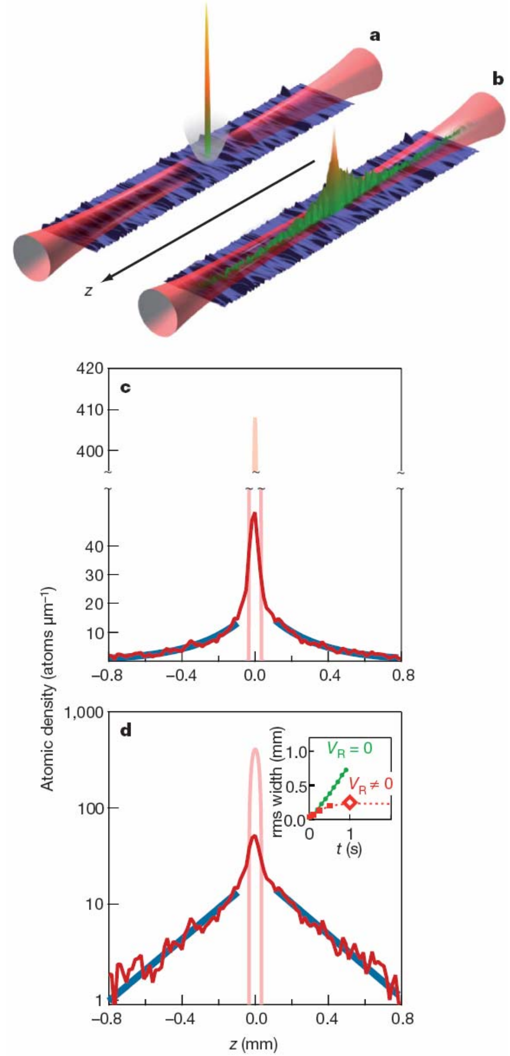
Outline

- The quartic Klein-Gordon (KG) disordered lattice
- Computational methods
- Three different dynamical behaviors
- Numerical results
- Similarities with the disordered nonlinear Schrödinger equation (DNLS)
- Conclusions

Interplay of disorder and nonlinearity

Waves in disordered media – Anderson localization

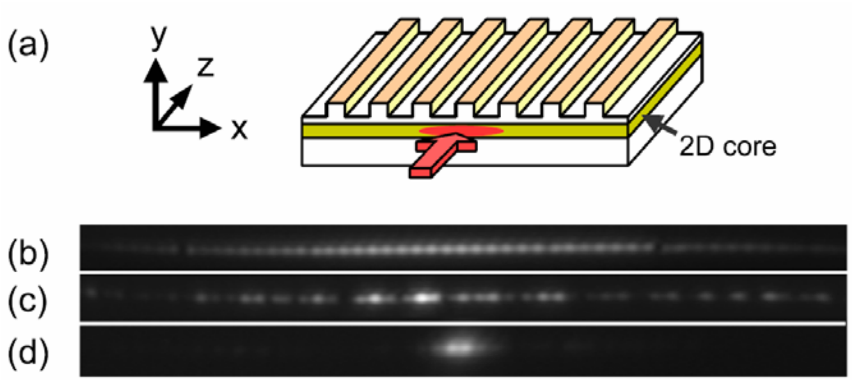
(Anderson Phys. Rev. 1958). Experiments on BEC (Billy et al. Nature 2008)



Waves in nonlinear disordered media – localization or delocalization?

Theoretical and/or numerical studies (Shepelyansky PRL 1993, Molina Phys. Rev. B 1998, Pikovsky & Shepelyansky PRL 2008, Kopidakis et al. PRL 2008)

Experiments: propagation of light in disordered 1d waveguide lattices (Lahini et al. PRL 2008)



The Klein – Gordon (KG) model

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

with **fixed boundary conditions** $u_0=p_0=u_{N+1}=p_{N+1}=0$. Usually N=1000.

Parameters: **W** and the **total energy E**. $\tilde{\varepsilon}_l$ **chosen uniformly from** $\left[\frac{1}{2},\frac{3}{2}\right]$.

Linear case (neglecting the term $u_l^4/4$)

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: $\overline{\Delta\omega^2} = \frac{\Delta_K}{\overline{p_\nu}}$

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

$$z_\nu \equiv \frac{E_\nu}{\sum_m E_m} \quad \text{with} \quad E_\nu = \frac{1}{2}\left(\dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2\right)$$

, where A_ν is the amplitude of the νth NM.

Second moment: $$m_2 = \sum_{\nu=1}^{N} \left(\nu - \bar{\nu}\right)^2 z_\nu \quad \text{with} \quad \bar{\nu} = \sum_{\nu=1}^{N} \nu z_\nu$$

Participation number: $$P = \frac{1}{\sum_{\nu=1}^{N} z_\nu^2}$$

measures the number of stronger excited modes in z_ν. Single mode $P=1$, Equipartition of energy $P=N$.

Integration scheme

We use a symplectic integration scheme developed for Hamiltonians of the form

$$H=A+\varepsilon B$$

where A, B are both integrable and ε a parameter. Formally the solution of the Hamilton equations of motion for such a system can be written as:

$$\frac{d\vec{X}}{ds} = \left\{H, \vec{X}\right\} = L_H \vec{X} \Rightarrow \boxed{\vec{X}^f = \sum_{n \geq 0} \frac{s^n}{n!} L_H^n \vec{X}^i = e^{sL_H} \vec{X}^i}$$

where $\vec{X}$ is the full coordinate vector and L_H the Poisson operator:

$$L_H f = \sum_{j=1}^{3} \left\{ \frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right\}$$

Symplectic Integrator $SABA_2C$

The operator e^{sL_H} can be approximated by the symplectic integrator (Laskar & Robutel, Cel. Mech. Dyn. Astr., 2001):

$$SABA_2 = e^{c_1 s L_A}\ e^{d_1 s L_{\varepsilon B}}\ e^{c_2 s L_A}\ e^{d_1 s L_{\varepsilon B}}\ e^{c_1 s L_A}$$

with $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6},\ c_2 = \frac{\sqrt{3}}{3},\ d_1 = \frac{1}{2}.$

The integrator has only small positive steps and its error is of order $O(s^4\varepsilon + s^2\varepsilon^2)$.

In the case where A is quadratic in the momenta and B depends only on the positions the method can be improved by introducing a corrector C, having a small negative step:

$$C = e^{-s^3 \varepsilon^2 \frac{c}{2} L_{\{\{A,B\},B\}}}$$

with $c = \frac{2-\sqrt{3}}{24}.$

Thus the full integrator scheme becomes: $SABAC_2 = C\ (SABA_2)\ C$ and its error is of order $O(s^4\varepsilon + s^4\varepsilon^2)$.

Symplectic Integrator SABA$_2$C

We apply the SABAC$_2$ integrator scheme to the KG Hamiltonian by using the splitting:

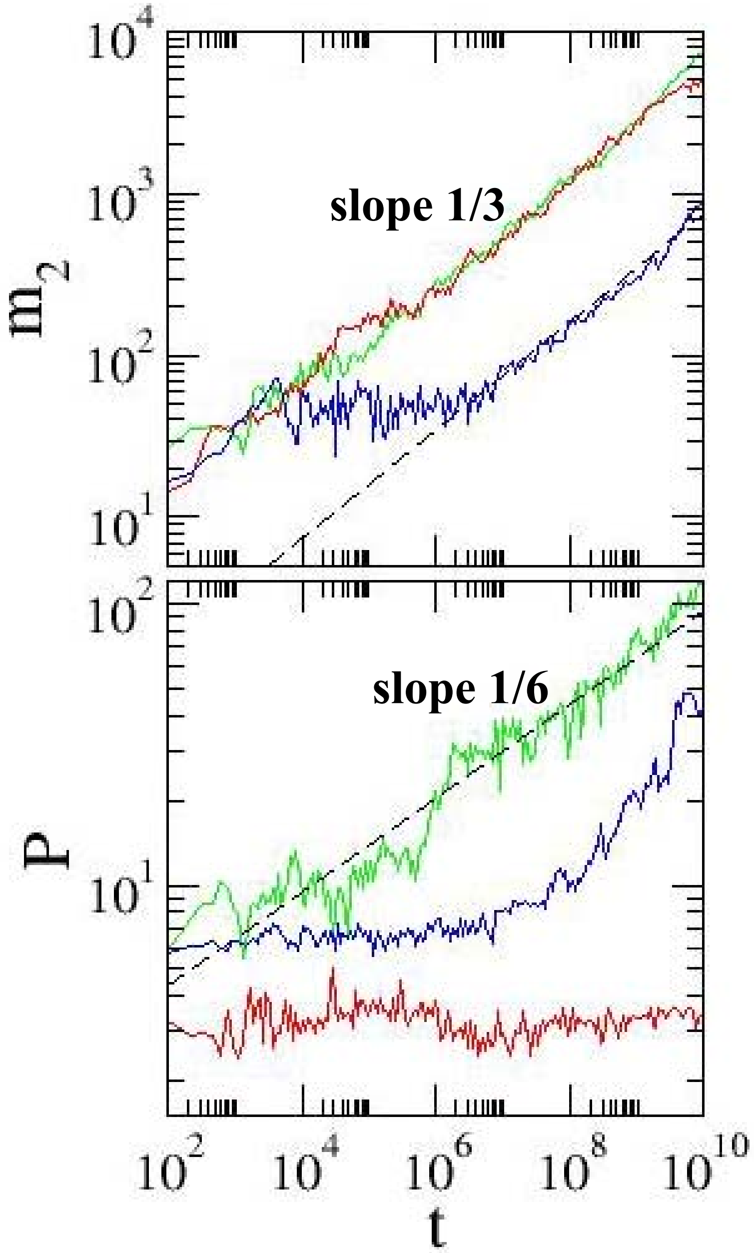
$$A = \sum_{l=1}^{N} \frac{p_l^2}{2}$$

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

$$\varepsilon = 1$$

with a corrector term which corresponds to the Hamiltonian function:

$$\left\{ \left\{ A, B \right\}, B \right\} = \sum_{l=1}^{N} \left[u_l (\tilde{\varepsilon}_l + u_l^2) - \frac{1}{W} (u_{l-1} + u_{l+1} - 2u_l) \right]^2 .$$



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. $\Delta\omega^2 < \delta_l < \Delta_K$ resonance overlap may happen immediately. Immediate subdiffusion (Molina Phys. Rev. B 1998, Pikovsky & Shepelyansky PRL 2008).

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 (Kopidakis et al. PRL 2008).

Subdiffusion: $m_2 \sim t^a, \quad P \sim t^{a/2}$

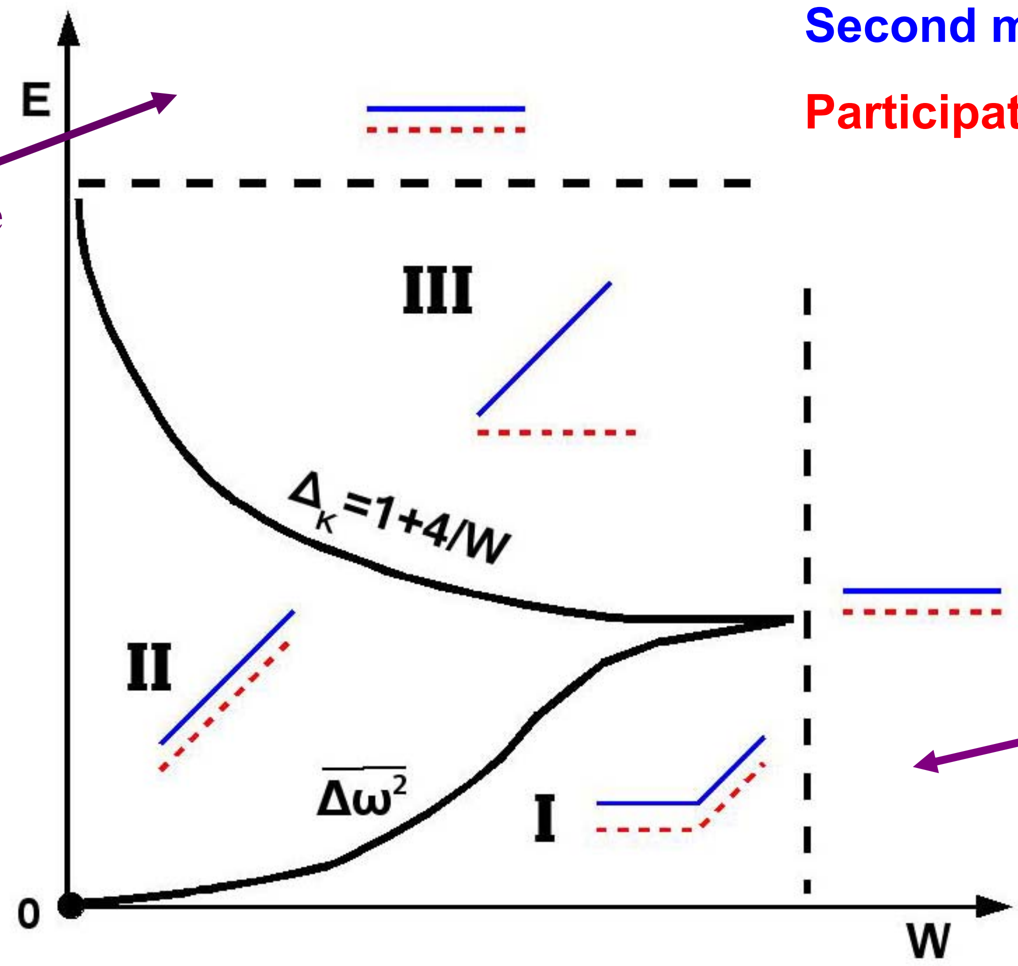
Assuming that the spreading is due to heating of the cold exterior, induced by the chaoticity of the wave packet, we theoretically predict α=1/3.

Different spreading regimes

Second moment m_2

Participation number P

The fraction of the wave packet that spreads decreases with increasing nonlinearity.



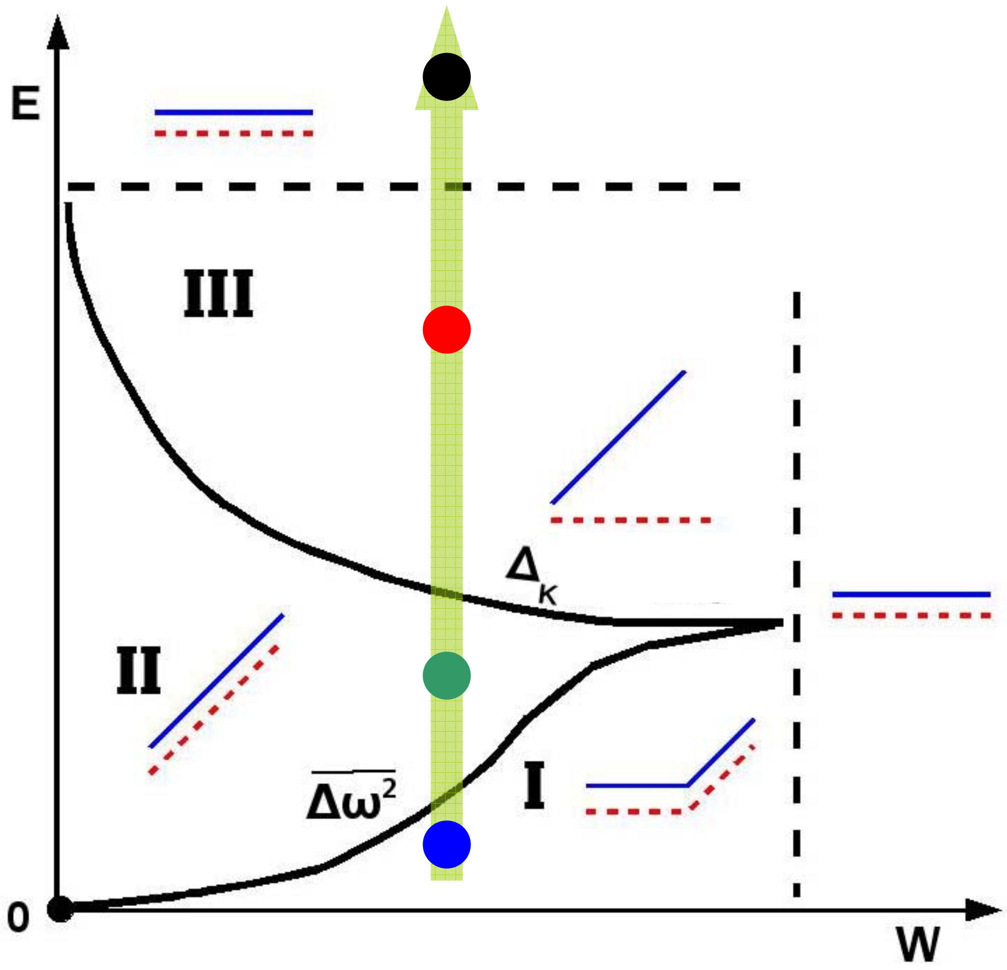
The detrapping time increases with increasing W.

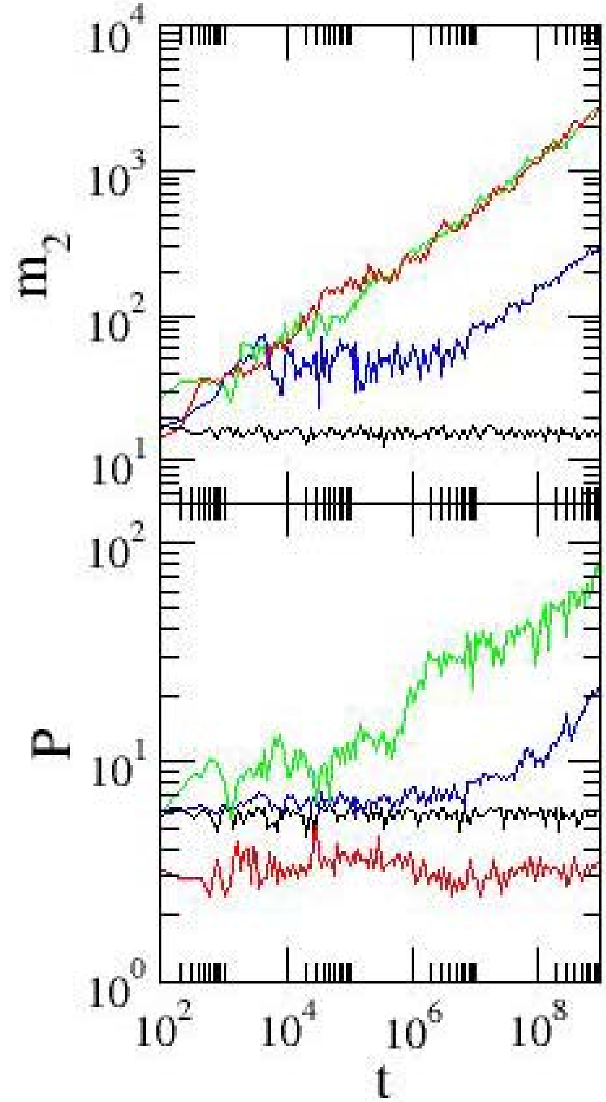
W=4, E=10

W=4, E=1.5

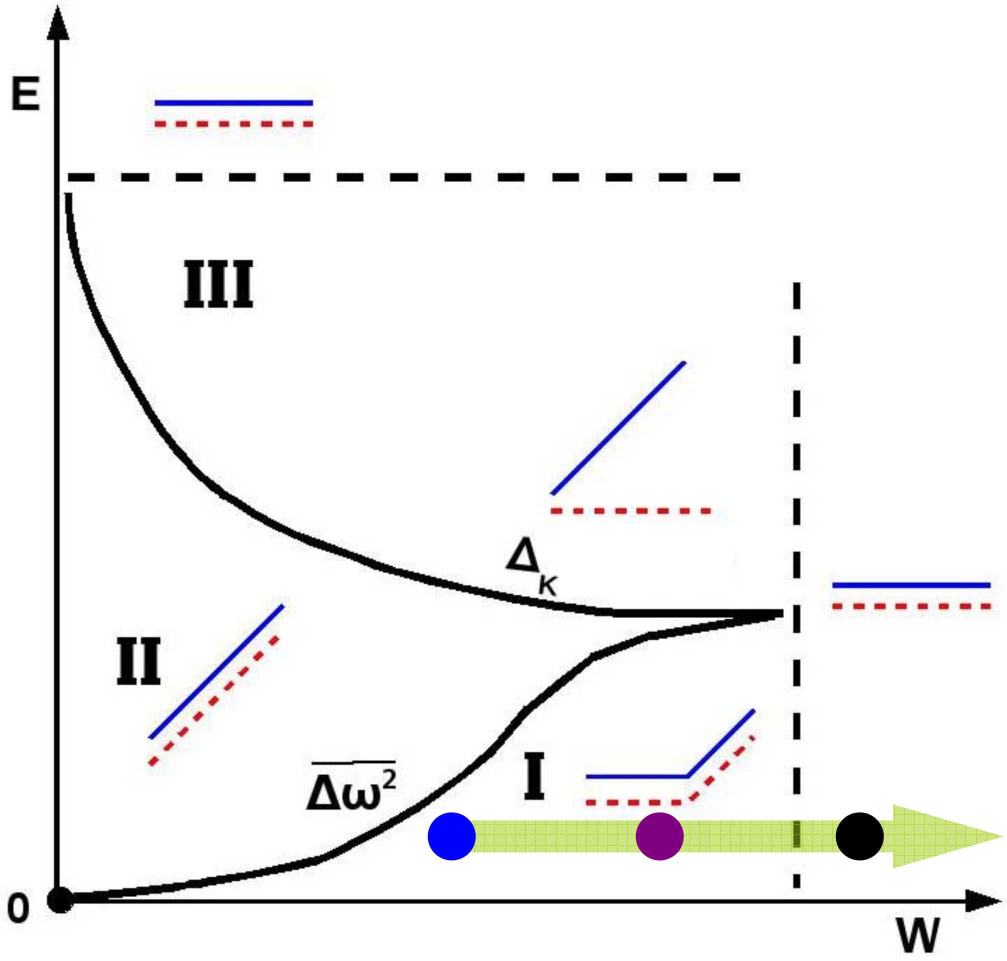
W=4, E=0.4

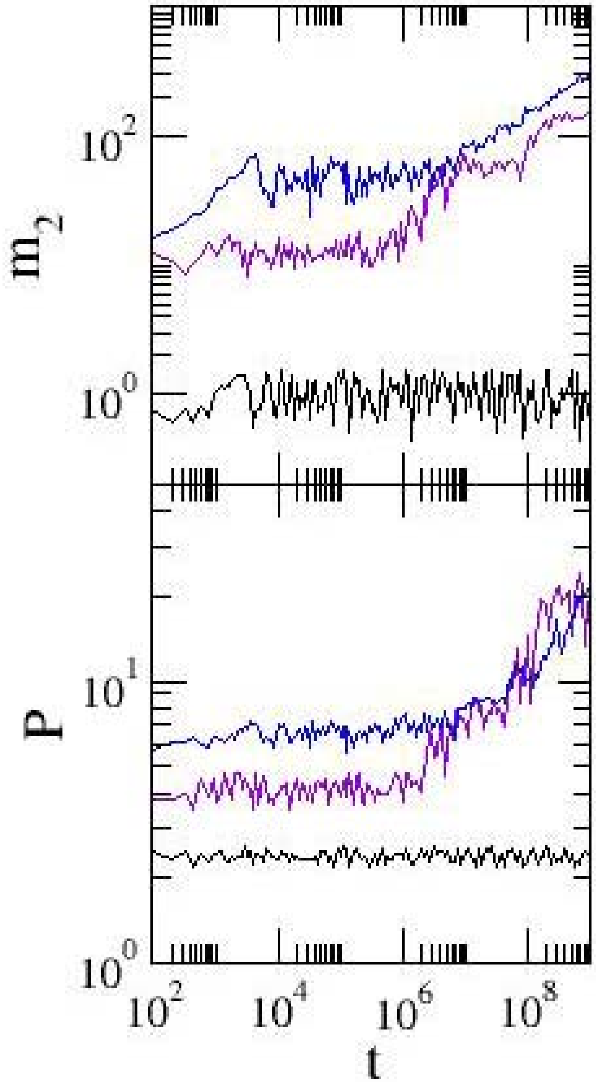
W=4, E=0.05



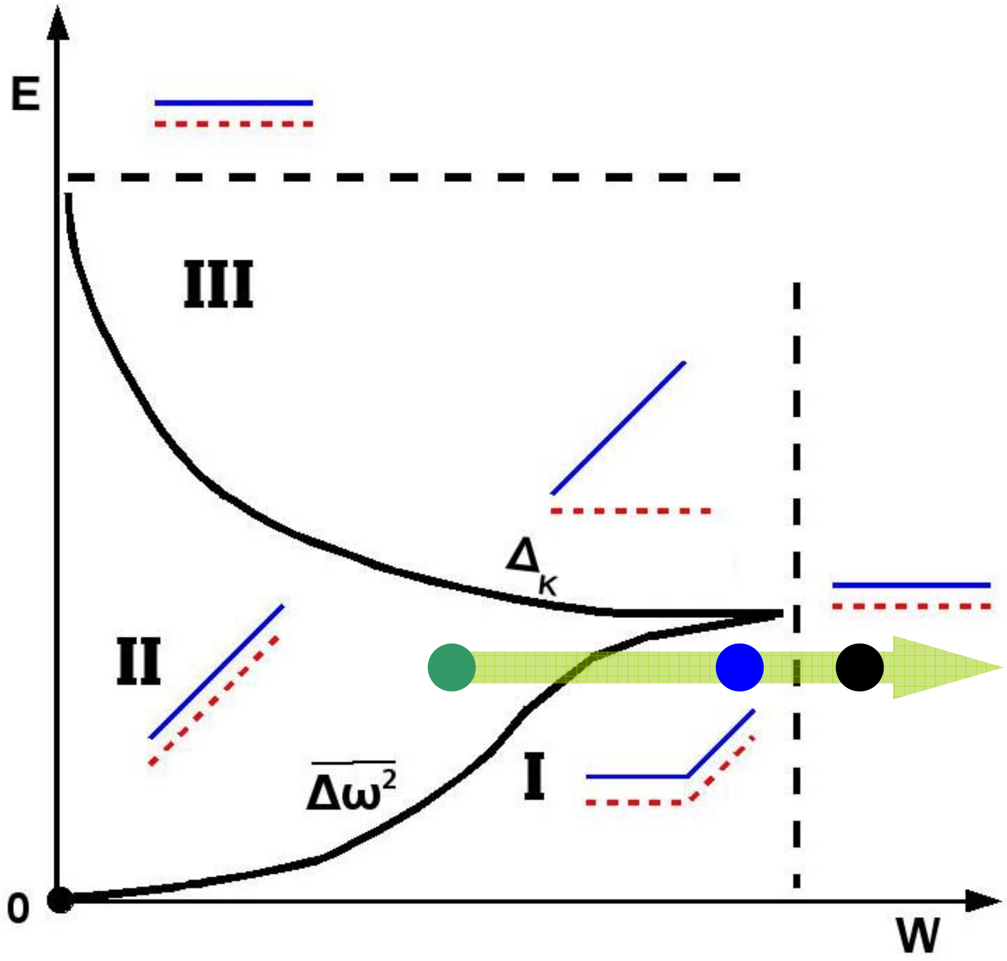


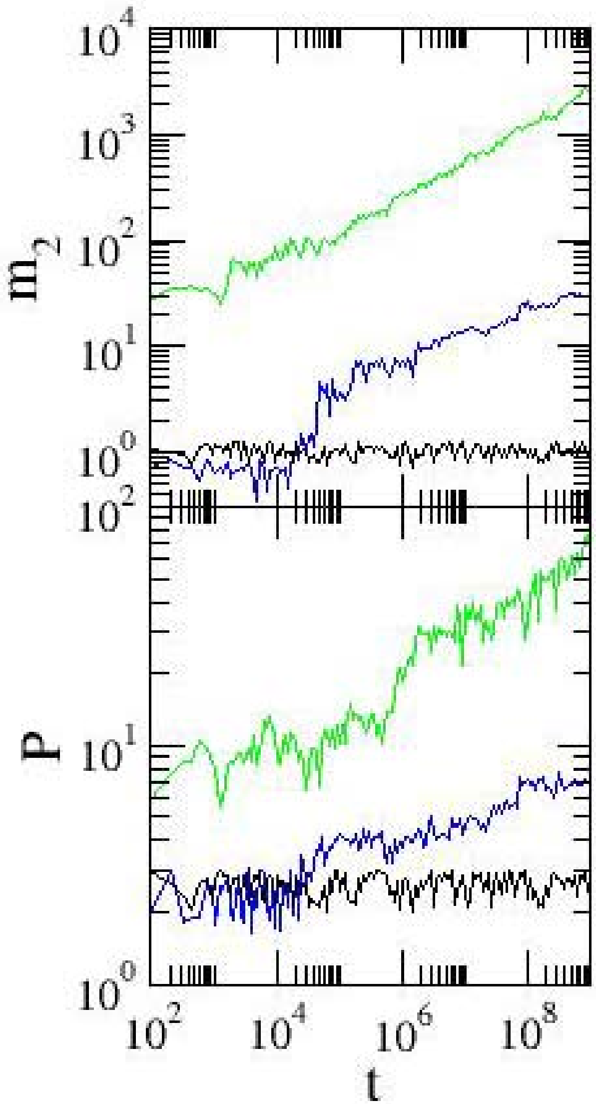
W=4, E=0.05 W=6, E=0.05 W=12, E=0.05



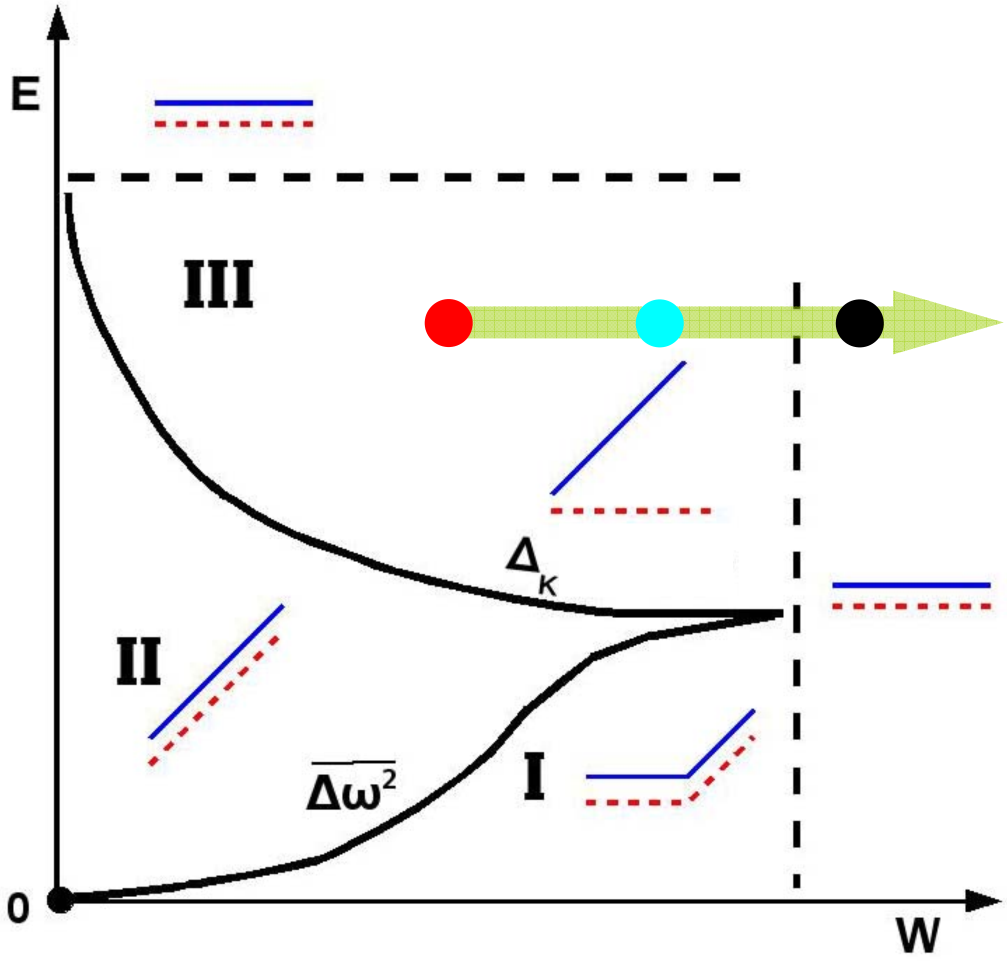


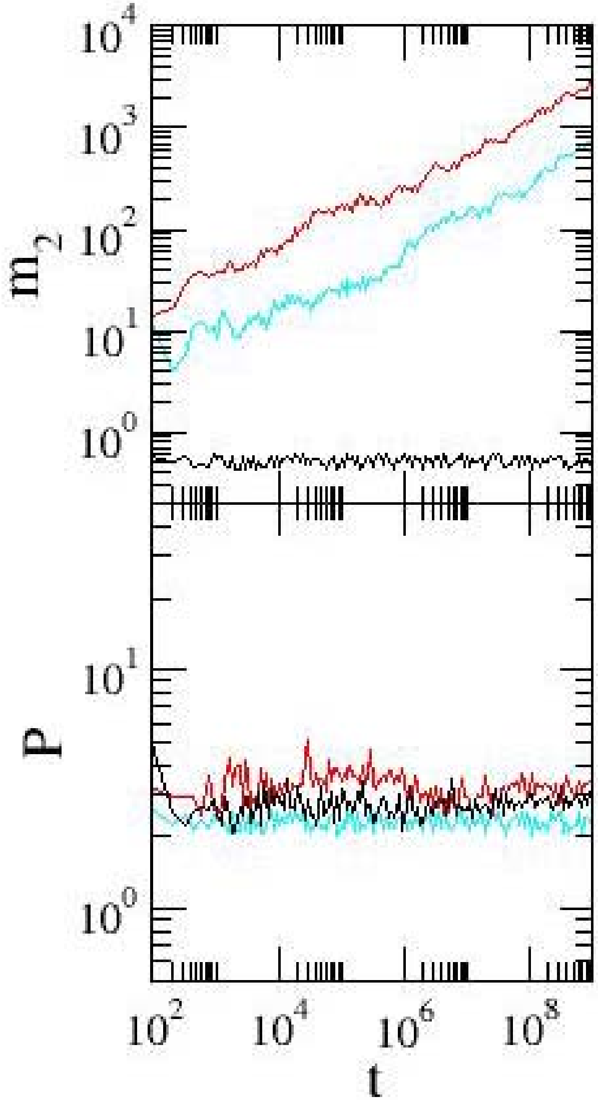
W=4, E=0.4 W=16, E=0.4 W=18, E=0.4





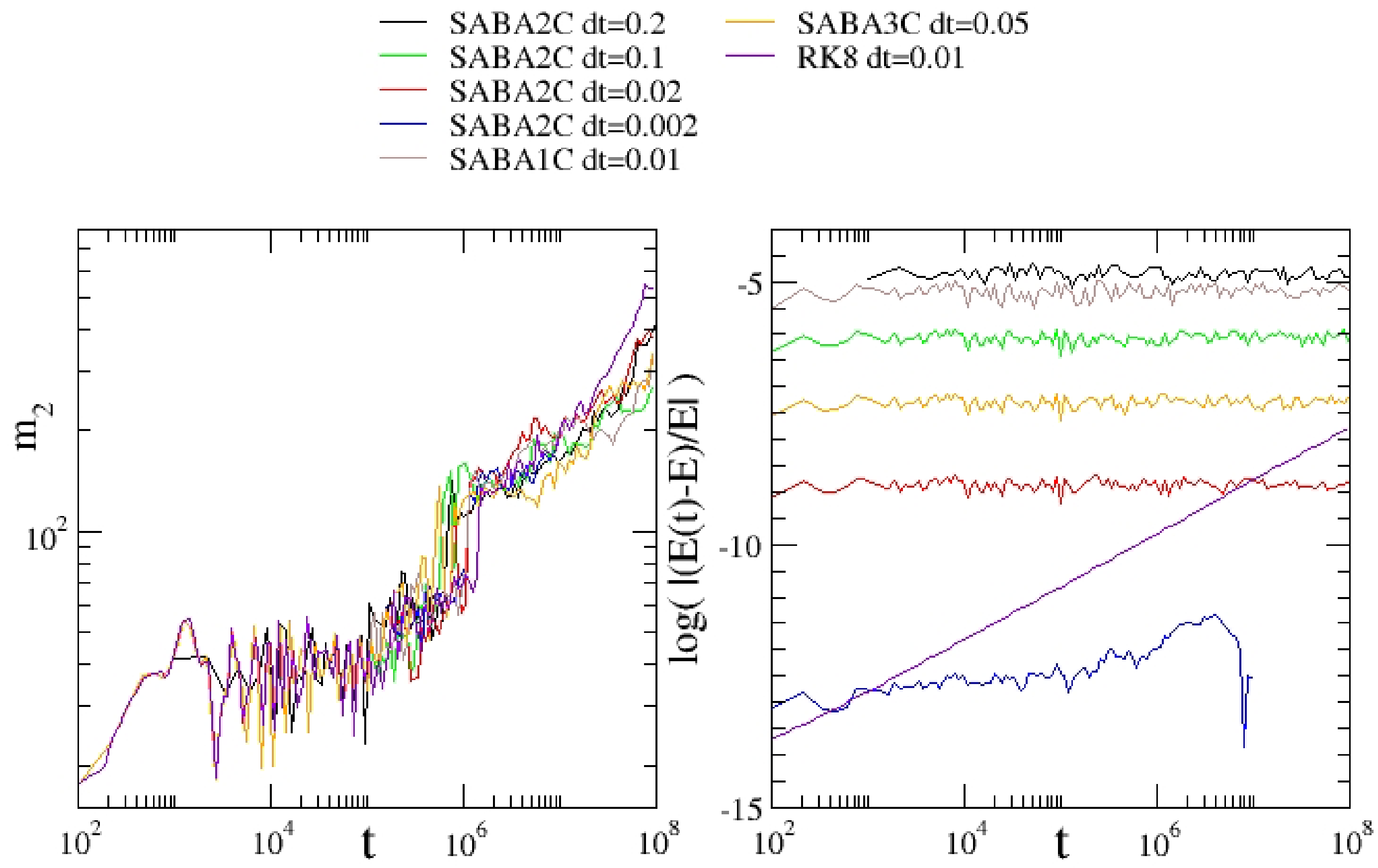
W=4, E=1.5 W=6, E=1.5 W=15, E=1.5





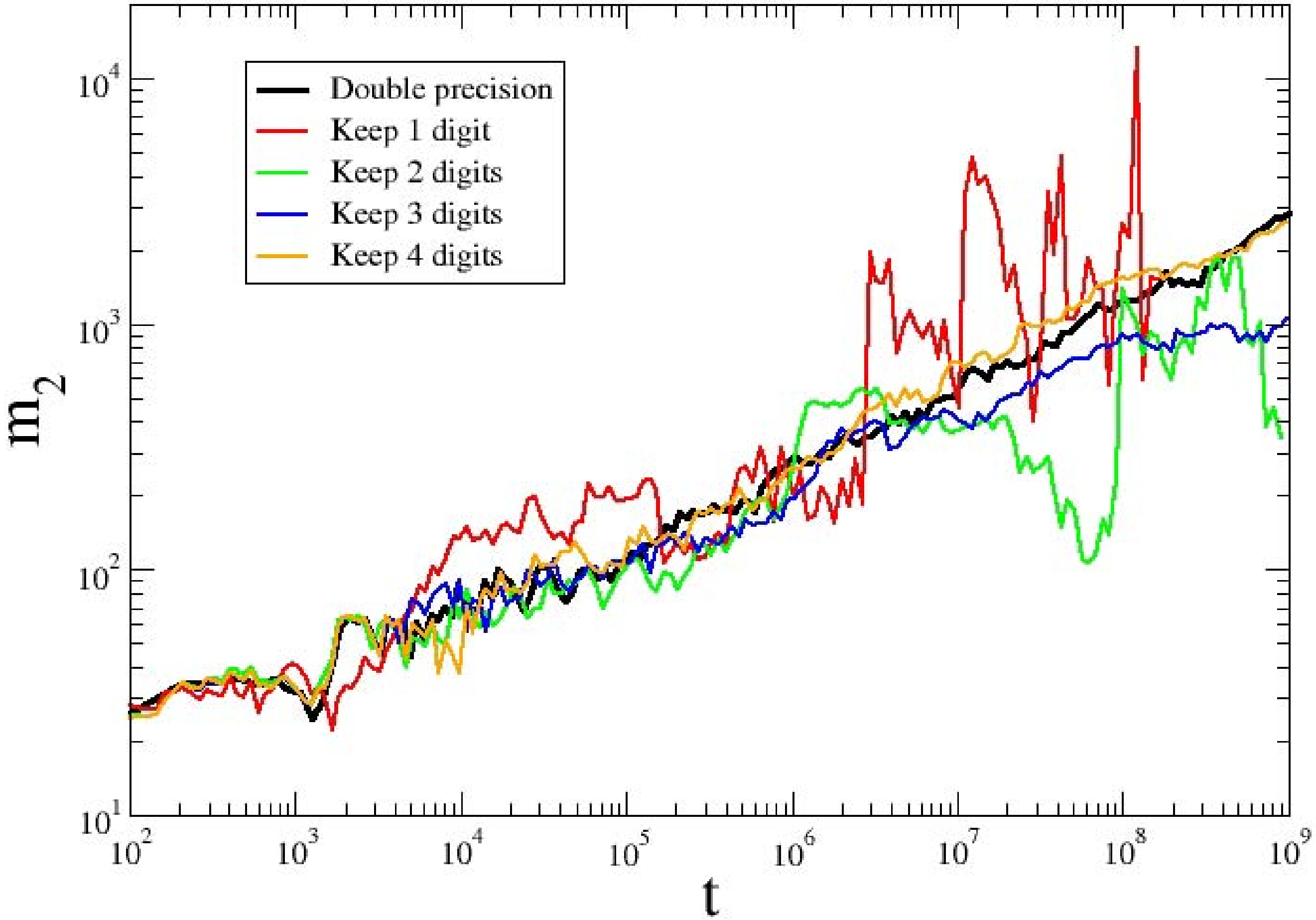
Accuracy

Regime I. Different integration schemes.



Accuracy

Regime II. Roundoff every 1 t. u.

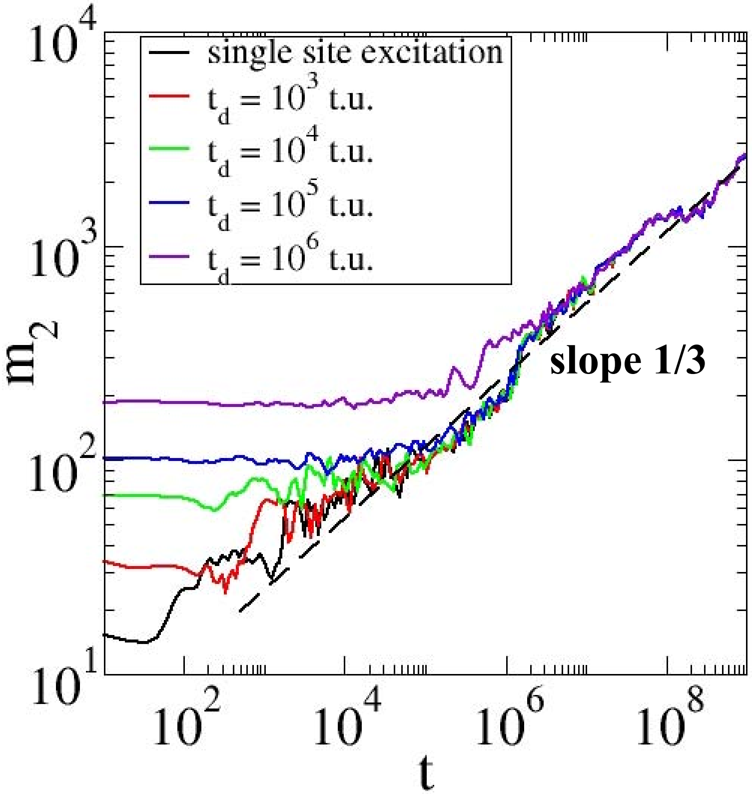


Relation of regimes I and II

We start a single site excitation in the intermediate regime II, measure the distribution at some time t_d, and relaunch the distribution as an initial condition at time t=0.

$$m_2(t) = M(t + t_d)^{1/3}$$

Detrapping time $\tau_d \approx t_d$



Detrapping

Nonlocal excitations of the KG chain corresponding to initial homogeneous distributions of energy E=0.4 (regime II of single site excitation) over L neighboring sites.

Assuming that $m_2 \sim t^{1/3}$ and that spreading is due to some diffusion process we conclude for the diffusion rate *D* that

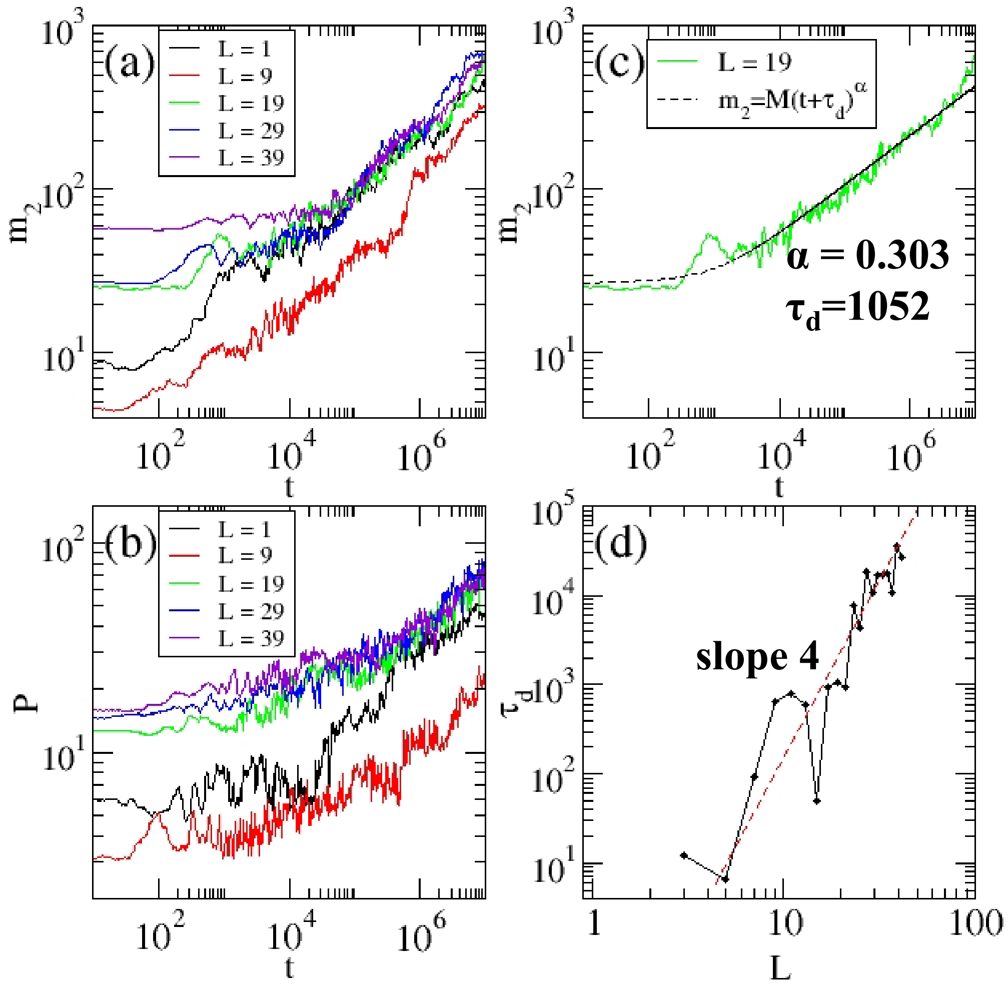
$$D=\tau_d^{-1} \sim n^4$$

where *n* is the average energy density of the excited NMs, i.e.

$$L \sim n^{-1}.$$

Thus we expect:

$$\boxed{\tau_d \sim L^4}$$



The discrete nonlinear Schrödinger (DNLS) equation

We also consider the system:

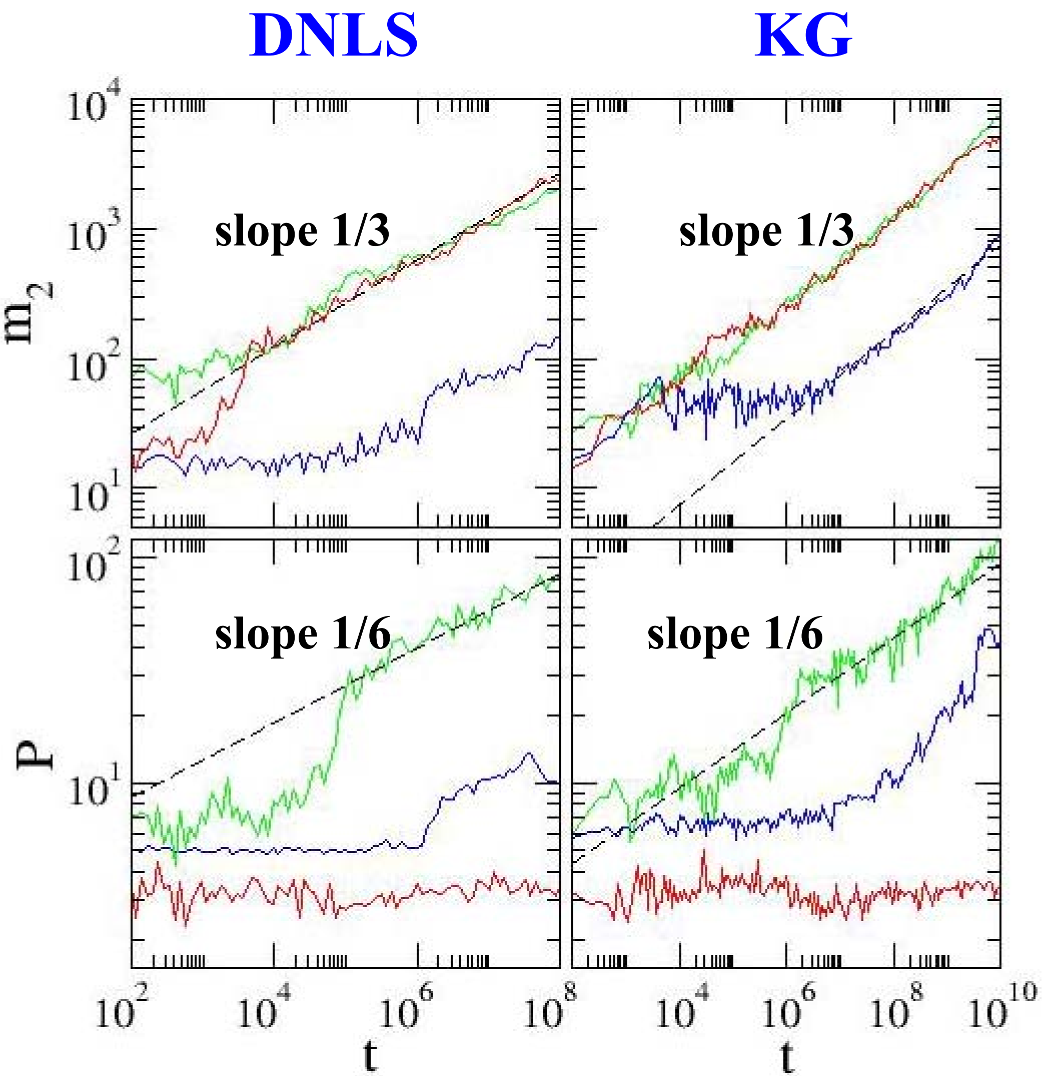
$$H_D = \sum_{l=1}^{N} \varepsilon_l |\psi_l|^2 + \frac{\beta}{2}|\psi_l|^4 - (\psi_{l+1}\psi_l^* + \psi_{l+1}^*\psi_l)^2$$

where ε_l chosen uniformly from $\left[-\frac{W}{2}, \frac{W}{2}\right]$ and β is the nonlinear parameter.

The parameters of the KG and the DNLS models was chosen so that the linear parts of both Hamiltonians would correspond to the same eigenvalue problem.

Conserved quantities: The energy and the norm of the wave packet.

Similar behavior of DNLS



Single site excitations

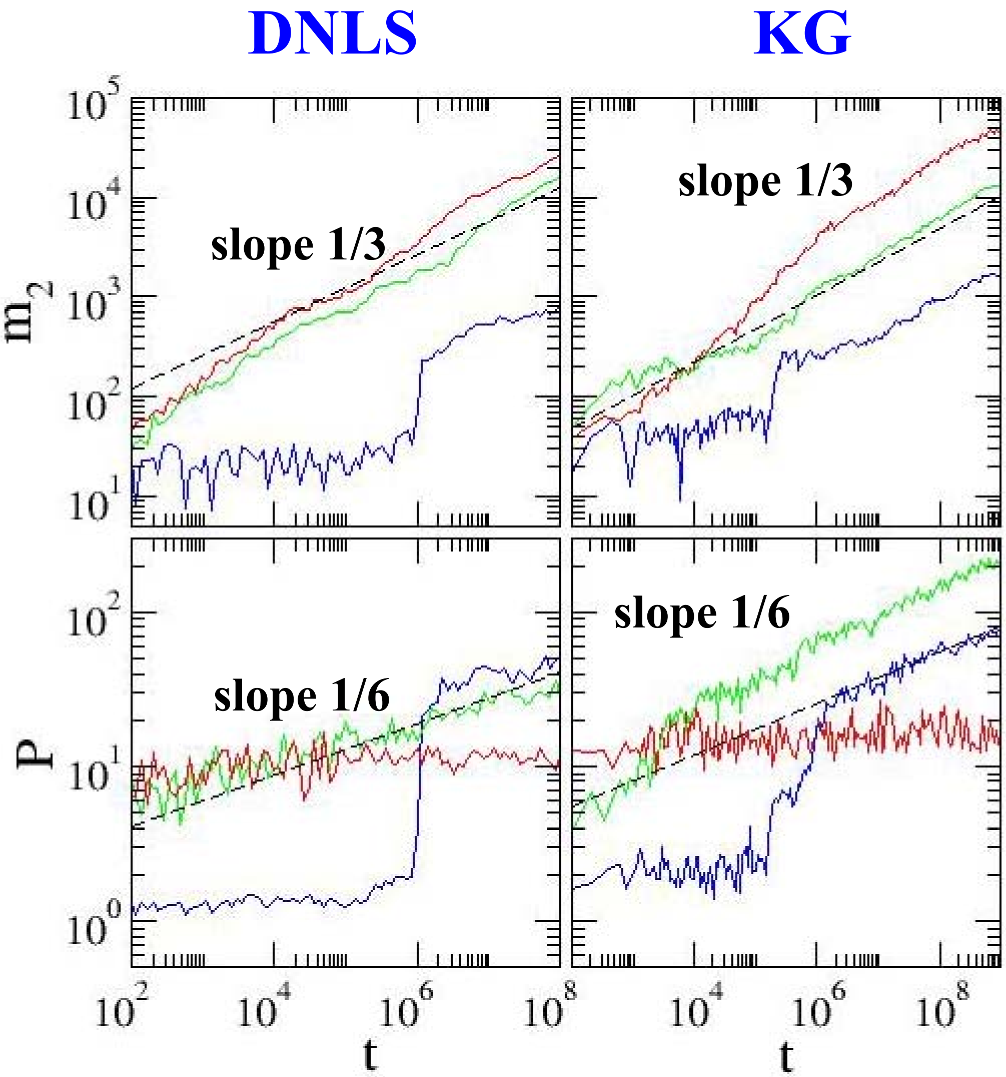
Regimes I, II, III

In regime II we averaged the measured exponent α over 20 realizations:

α=0.33±0.05 (KG)

α=0.33±0.02 (DLNS)

Similar behavior of DNLS



Single mode excitations

Regimes I, II, III

Evolution of the second moment

We use the DNLS model for theoretical considerations.

Equations of motion in normal mode space:

$$i\dot{\varphi}_\mu = \lambda_\mu \varphi_\mu + \beta \sum_{\nu_1,\nu_2,\nu_3} I_{\nu,\nu_1,\nu_2,\nu_3} \varphi^*_{\nu_1} \varphi_{\nu_2} \varphi_{\nu_3}$$

with the overlap integral: $I_{\nu,\nu_1,\nu_2,\nu_3} = \sum_l A_{\nu,l} A_{\nu_1,l} A_{\nu_2,l} A_{\nu_3,l}.$

Assume that at some time t the wave packet contains $1/n >> \overline{P_\nu}$ **modes and each mode on average has a norm** $|\varphi_\nu|^2 \sim n << 1.$
Then for the second moment we have: $m_2 = Dt \sim 1/n^2.$

The heating of an exterior mode φ_μ should evolve as:

$$i\dot{\varphi}_\mu \sim \lambda_\mu \varphi_\mu + F\beta n^{3/2} f(t) \quad \text{where} \quad \langle f(t) f(t') \rangle = \delta(t - t')$$

with *F* being the fraction of resonant modes inside the packet, and φ_μ being a mode at the cold exterior. Then

$$|\varphi_\mu|^2 \sim F^2 \beta^2 n^3 t.$$

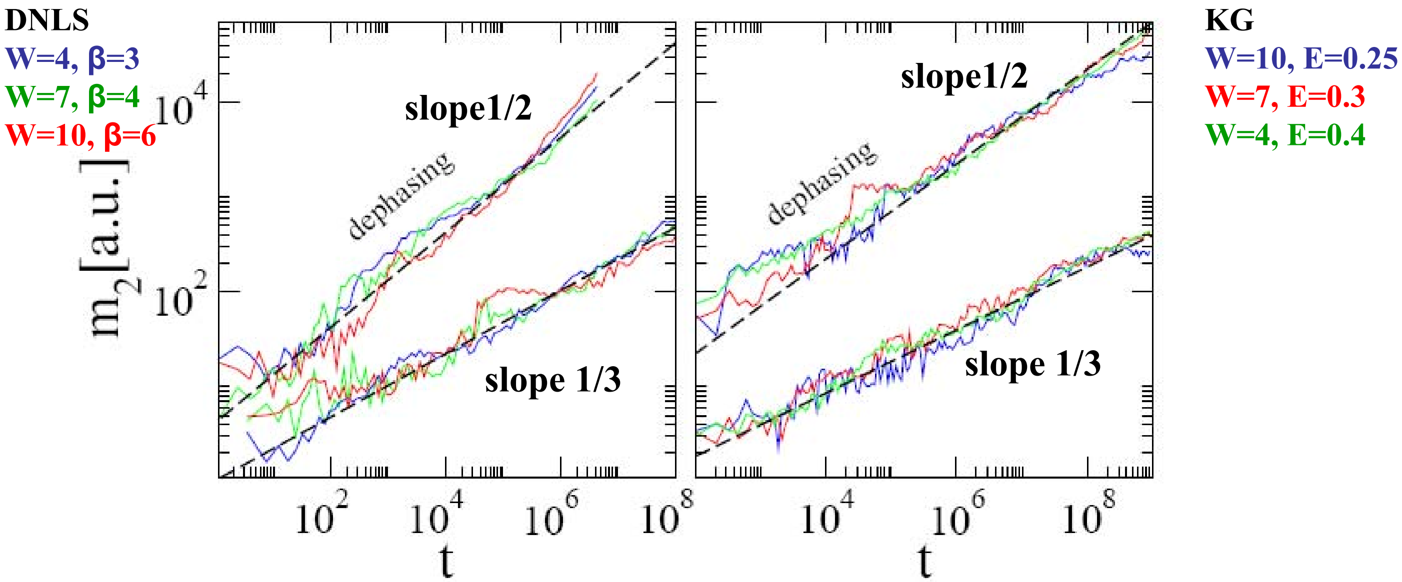
Dephasing

Let us assume that all modes in the packet are chaotic, i.e. *F=1*.

The momentary diffusion rate of packet equals the inverse time the exterior mode needs to heat up to the packet level:

$$D \sim \frac{1}{T} \sim \beta^2 n^2 \Rightarrow m_2 \sim t^{1/2}$$

We test this prediction by additionally dephasing the normal modes:



Evolution of the second moment

Thus not all modes in the wave packet evolve chaotically.

We numerically estimated the probability *F* for a mode, which is excited to a norm n (the average norm density in the packet), to be resonant with at least one other mode and found:

$$F \sim \beta n$$

So we get:

$$D \sim \frac{1}{T} \sim \beta^4 n^4 \Rightarrow m_2 \sim t^{1/3}$$

Conclusions

- **Chart of different dynamical behaviors:**
  - ✓ **Weak nonlinearity: Anderson localization on finite times. After some detrapping time the wave packet delocalizes (Regime I)**
  - ✓ **Intermediate nonlinearity: wave packet delocalizes without transients (Regime II)**
  - ✓ **Strong nonlinearity: partial localization due to selftrapping, but a (small) part of the wave packet delocalizes (Regime III)**
- **Subdiffusive spreading induced by the chaoticity of the wave packet**
- **Second moment of wave packet ~ t^{α} with $\alpha=1/3$**
- **Spreading is universal due to nonintegrability and the exponent α does not depend on strength of nonlinearity and disorder**
- **Conjecture: Anderson localization is eventually destroyed by the slightest amount of nonlinearity?**

S. Flach, D.O. Krimer, Ch. Skokos, 2009, PRL, 102, 024101
Ch. Skokos, D.O. Krimer, S. Komineas, S. Flach, 2009, PRE, 79, 056211