Localized Dynamical Structures in infinite nonlinear networks and open problems

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Dynamical Optimization in PDE and Geometry
Applications to Hamilton-Jacobi
Ergodic Optimization, Weak KAM Bordeaux 12-21 décembre 2011

Warning: This is not a course of Mathematics but a course of Physics
Many aspects (but not all) need to be proved in the mathematical sense.

Course I- Discrete Breathers (DBs) in Periodic Networks

Existence proofs of DBs and Multi(sites)breathers
Linear Stability
Numerical calculations of DBs

Course II- Playing with Discrete Breathers

Spontaneous Manifestation of DBs
Spreading of a wave packet
Interaction of DBs with phonons (elastic and inelastic)
Energy Transportation:Mobility of DBs, Energy transport by phase torsion (Multibreathers)
Targeted Transfer….. Biochemistry

Course III- Random Nonlinear Networks

DBs in systems with discrete phonon spectrum (random etc…)
Open problem: Spreading of a wave packet in random nonlinear networks with discrete linear spectrum

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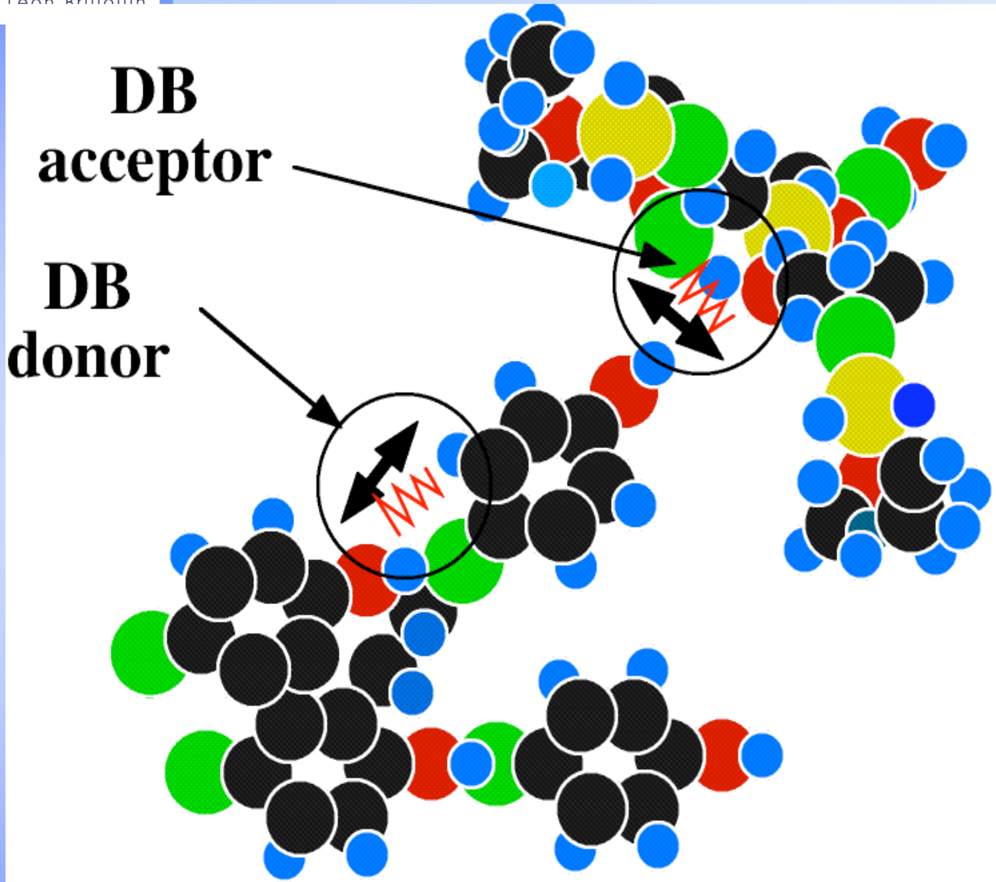
DBs: Discrete Breathers (Time periodic solutions) interest in physics: energy (or charge) trapping



Spontaneous Energy trapping by Discrete Breathers (DB) in complex extended dynamical systems

DBs are spatially localized time-periodic solutions (avoid resonances with linear spectrum)

DBs families behave as Single Anharmonic Oscillators (their frequency depends on the amplitude): Energy versus Action H(I)

Course I: Discrete Breathers in Periodic Networks

Pioneering Discovery:
Sievers and Takeno 1988 (ILM)
Campbell and Peyrard 1990 (Discrete Breathers-DBs)

Generic Nonlinear Excitations (not restricted to special Integrable Models)

1- Existence proofs of DBs and Multi(sites)breathers
2-Linear Stability

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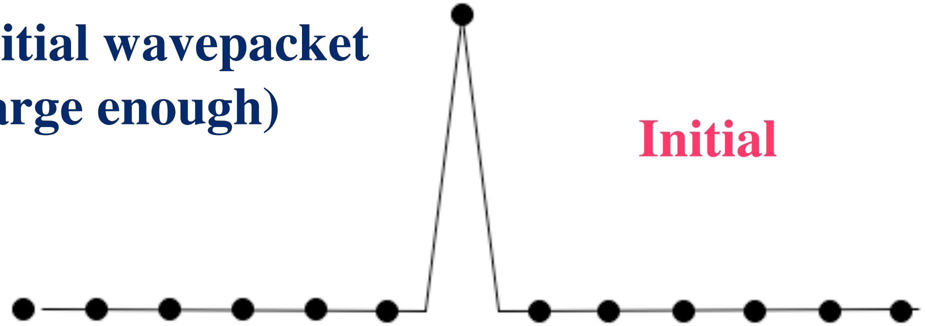
Spontaneous Formation of a DISCRETE BREATHER

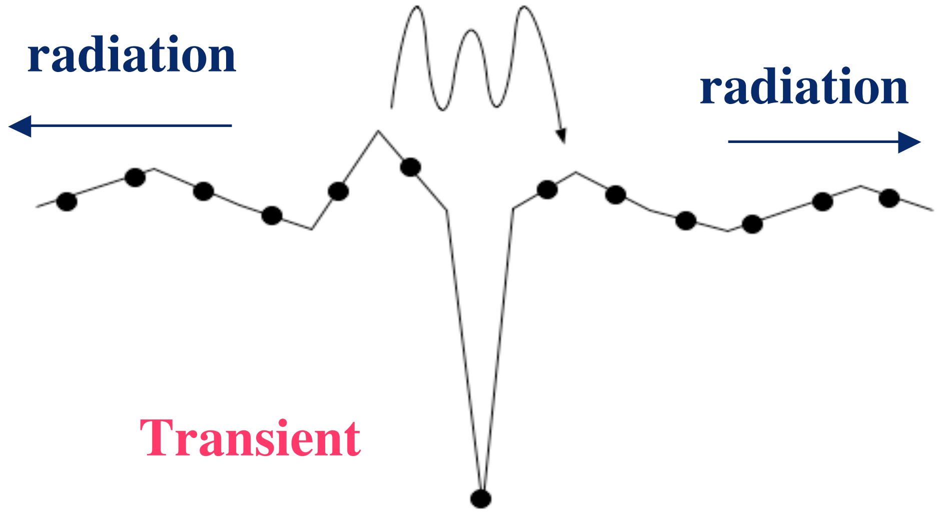
Sievers and Takeno 1988

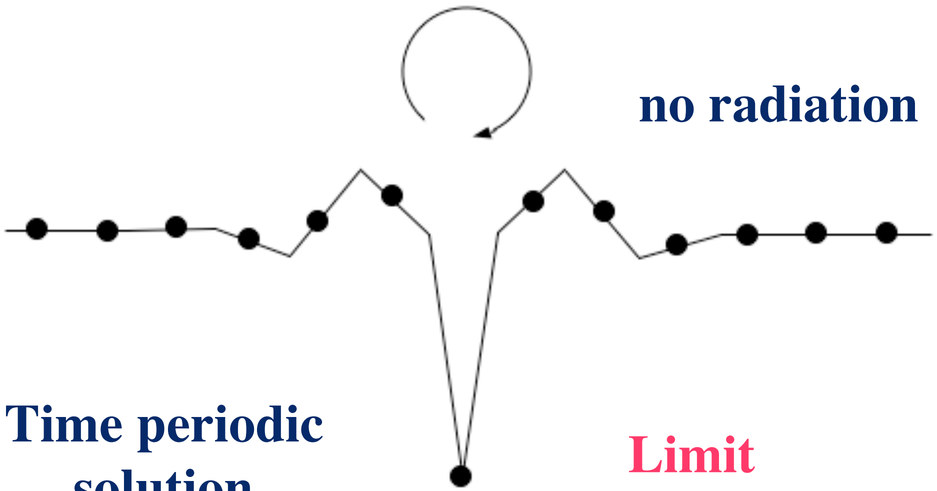
Initial wavepacket (large enough)



Sievers and Takeno (1988): from a initial localized wavepacket

Chaotic or « quasiperiodic » transient





Time periodic solution

A large part of the initial energy remains localized as a DB, the rest spreads to zero at infinity

The second moment diverges but the participation number does not

Part of the energy does not spread at infinity
The limit state is a DISCRETE BREATHER

Discrete Breathers-DBs are spatially localized TIME-PERIODIC solutions
They may spontaneously manifest in various situations

DBs are generic Nonlinear Excitations (not restricted to special Integrable Models)

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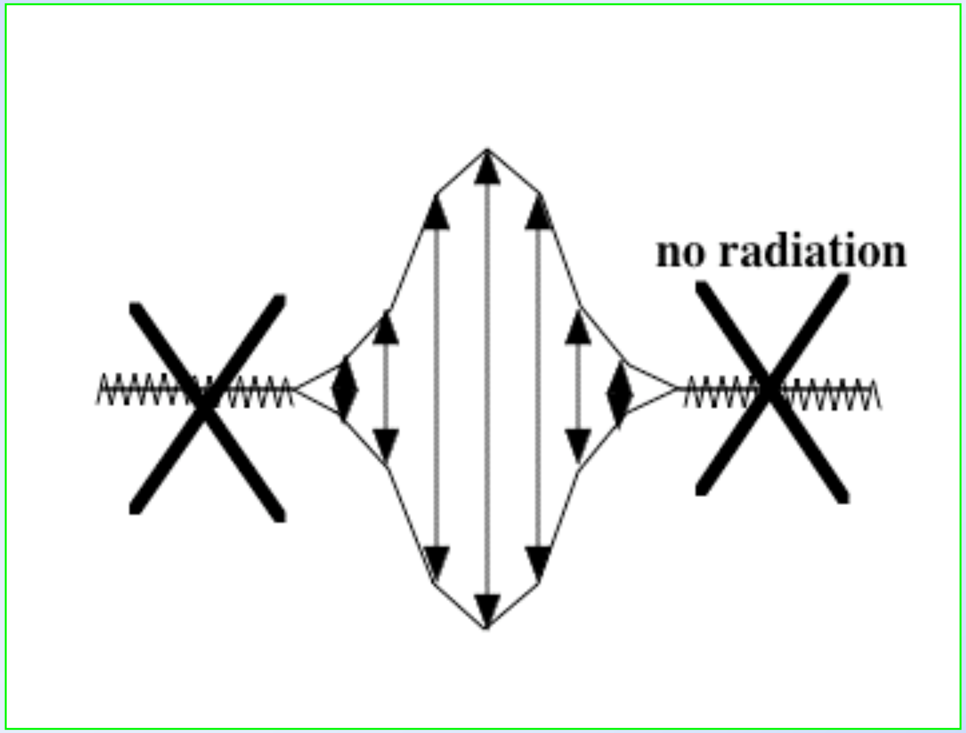
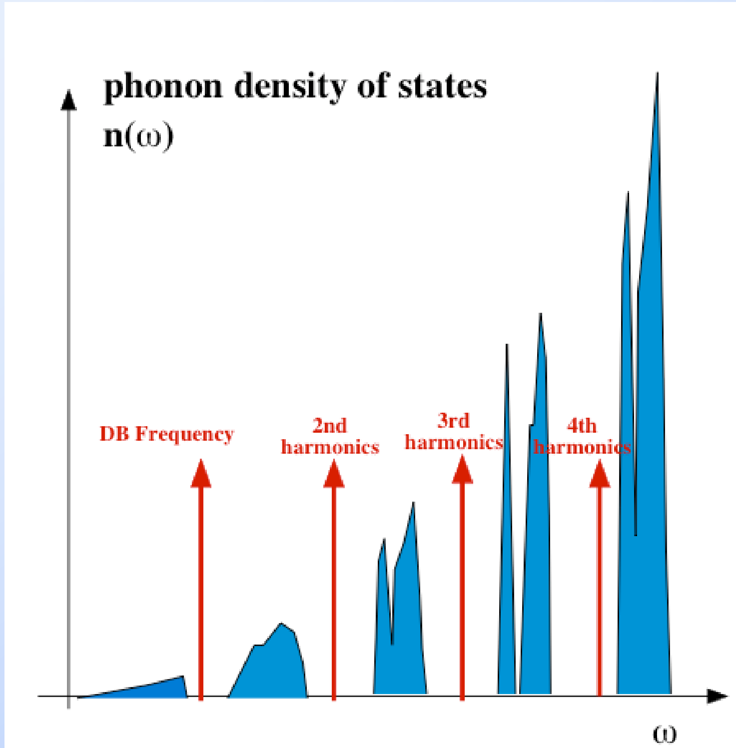
1-Existence Proofs of DBs:

General Principles

Anharmonicity: the frequency depends on the amplitude
Discreteness: The frequency (and harmonics) escape the linear continuous spectrum





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Typical Models with DBs on networks in d dimensions

Klein-Gordon

$$H=\sum_{\mathbf{n}}\left(\frac{p_{\mathbf{n}}^2}{2}+V(u_{\mathbf{n}})\right)+\sum_{<\mathbf{m},\mathbf{n}>}W(u_{\mathbf{m}}-u_{\mathbf{n}})$$

FPU

$$H=\sum_{n}\left(\frac{p_{\mathbf{n}}^2}{2}+W(u_{n+1}-u_{n})\right)$$

DNLS models

$$H=\sum_{\mathbf{n}}\left(\epsilon_0|\psi_{\mathbf{n}}|^2+\frac{\chi}{2}|\psi_{\mathbf{n}}|^2\right)+C\sum_{<\mathbf{m},\mathbf{n}>}(\psi_{\mathbf{m}}|\psi_{\mathbf{n}}^{\star}+\psi_{\mathbf{n}}|\psi_{\mathbf{m}}^{\star})$$

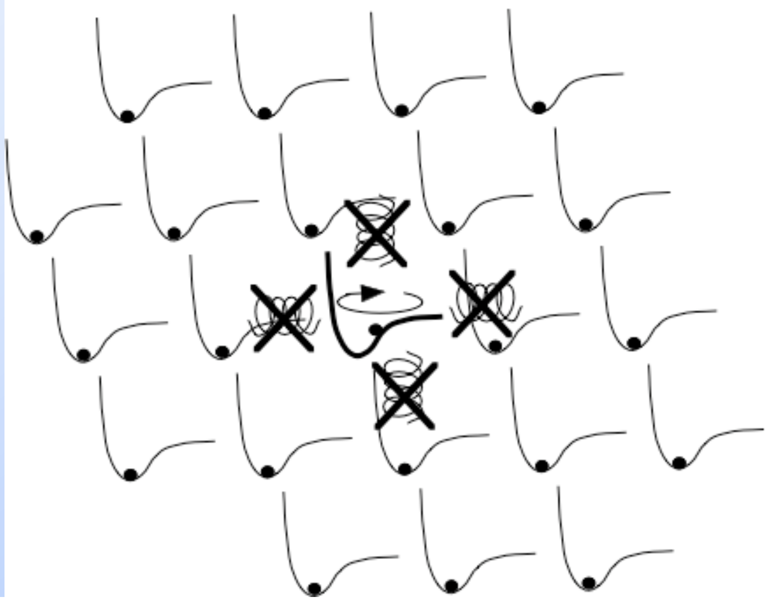
1-Existence Proofs of DBs by the Principle of Anticontinuity

(MacKay SA 1994) An array of weakly coupled nonlinear oscillators (any dimension not necessarily spatially periodic)

$$\mathcal{H} = \sum_i \left(\frac{1}{2}p_i^2 + V(u_i)\right) + C \sum_{\langle i,j\rangle} W(u_i - u_j)$$

At C=0, the anharmonic oscillators oscillate independantly periodicallywith theit own period

Anticontinuous limit: the system is a collection of uncoupled anharmonic oscillators *C=0*.



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At C=0, time periodic solutions which are time reversible can be Described by a discrete coding sequence e.g.

- $\sigma_i = 0$ oscillator i is at rest
- $\sigma_i = 1$ oscillator i moves at frequency Ω in phase (phase 0)
- $\sigma_i = -1$ oscillator i moves at frequency Ω in antiphase (phase π)

Coding sequence at C=0

Single DB: σ_i=0 for all i except for one value of i

Multisite DBs σ_i=0, 1 or -1

Theorem: Continuation at C≠0 in the space of time reversible solutions of the solutions at C=0 by the Implicit Function Theorem

Implicit function theorem (Wikipedia):

Let X, Y, Z be Banach Spaces. Let the mapping $f: X{\times}Y \to Z$ be continuously Frechet Differentiable. If $(x_0,y_0) \in X{\times}Y$, $f(x_0,y_0) = 0$, and $y \to D\, f(x_0,y_0)\,.\,(0,y)$ is a Banach space isomorphism from Y onto Z, then there exist neighbourhoods U of x_0 and V of y_0 and a Frechet differentiable function $g : U \to V$ such that $f(x,g(x)) = 0$ and $f(x,y) = 0$

if and only if $y = g(x)$, for all $(x,y) \in U{\times}V$.

Definition. $SL_{T,1}$ is the space of bounded infinite sequences $z = (z_n)_{n \in \mathbb{Z}}$ of pairs $z_n = (x_n, p_n)$ of continuously differentiable functions of period T with the symmetry properties

$$x_n(-t) = x_n(t)$$
$$p_n(-t) = -p_n(t). \tag{2.8}$$

We measure the size of the oscillation on site n by the norm

$$|z_n| = \sup\{|x_n(t)|, |p_n(t)|, |\dot{x}_n(t)|, |\dot{p}_n(t)| : t \in \mathbb{R}\}. \tag{2.9}$$

We measure the size of $z \in SL_{T,1}$ by

$$|z| = \sup\{|z_n| : n \in \mathbb{Z}\}. \tag{2.10}$$

With this norm, $SL_{T,1}$ becomes a Banach space (a complete normed vector space).

The operator $F : SL_{T,1} \times \mathbb{R} \to SM_{T,0}$ is defined by

$$F(z, \alpha) = w \tag{2.10d}$$

where, denoting $z = (x_n, p_n)_{n \in \mathbb{Z}}$, $w = (u_n, v_n)_{n \in \mathbb{Z}}$, we have

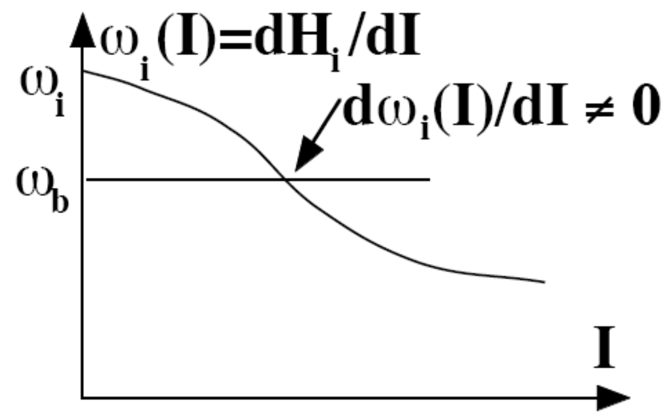
$$u_n(t) = \partial H / \partial x_n + \dot{p}_n(t)$$
$$v_n(t) = \partial H / \partial p_n - \dot{x}_n(t)$$

Conditions for implicit function theorem hold at the anticontinuous limit ($\omega = 2\pi/T$) if

$$n\,\omega \neq \omega_0 \text{ for all } n$$
$$d\,\Omega/d\,I \neq 0 \text{ at } \Omega(I) = \omega$$

Action-angle representation

The frequency of a single anharmonic oscillator $\Omega(I)$ depends on its action I



- The frequency of the DB has no harmonics $n\omega_b$ (n integer) in the linearized phonon spectrum $\{\bar{\omega}_j\}$

This theorem hold close to an anticontinuous limit

Example of model without anticontinuous limit:

$$H_{FPU} = \sum_i \frac{1}{2} p_i^2 + W\left(u_{i+1} - u_i\right)$$

2-Existence Proofs of hard DBs by variational Methods for Hamiltonian with the form

$H = \Sigma_i \mathbf{p}_i^2 / 2m + V(\{\mathbf{u}_i\})$ *Aubry Kopidakis Kadelburg 2001*

V is a convex function. Works for « Hard DBs » in -Translationally Invariant systems -at any dimension- with or without acoustic Phonons

(Hold for ß-FPU) $u_i(t) = a_i + g_i(\omega t + \alpha)$

$$\mathcal{V}(\{\mathbf{u_i}\}) = \sum_{\mathbf{i}} \mathbf{V}(\mathbf{u_i}) + \mathbf{C} \sum_{\langle \mathbf{i,j} \rangle} \mathbf{W}(\mathbf{u_i} - \mathbf{u_j})$$

DB= Invariant 2π periodic loops

$$\int_0^{2\pi} \mathbf{g_i}(\phi) \mathbf{d}\phi = \mathbf{0}$$

$$\mathbf{J}(\{\mathbf{g_i}(\phi)\}) = \frac{\mathbf{1}}{\mathbf{2}\pi} \sum_{\mathbf{i}} \int_0^{2\pi} \left(\frac{\mathbf{d g_i}(\phi)}{\mathbf{d}\phi}\right)^2 \mathbf{d}\phi$$

$$\mathbf{E}(\{\mathbf{g_i}(\phi)\}) = \frac{\mathbf{1}}{\mathbf{2}\pi} \min_{\{\mathbf{a_i}\}} \int_0^{2\pi} \mathcal{V}(\{\mathbf{a_i} + \mathbf{g_i}(\phi)\}) \mathbf{d}\phi$$

Extrema of E at constant J with respect to a_i and 2π–periodic g_i yields solutions. Lagrange multiplier is the square frequency.

Theorem: If on can find a 2π–periodic$_i$ (trying) function g such that J≠0 and

$$\frac{1}{2}\Omega_c^2 \mathbf{J}(\{\mathbf{g_i}(\phi)\}) < \mathbf{E}(\{\mathbf{g_i}(\phi)\})$$

Then (hard) DB exists

Example of application: DBs in FPU chain

$$H_{FPU} = \sum_i \frac{1}{2} p_i^2 + W(u_{i+1} - u_i) \tag{5}$$

where the coupling potential $W(x)$ vanishes at its minimum at $x = 0$. It is assumed to be a smooth function, which can be expanded for small x as

$$W(x) \approx \frac{W''(0)}{2} x^2 + \frac{W'''(0)}{6} x^3 + \frac{W''''(0)}{24} x^4 + \cdots \tag{6}$$

Trying loops $\tilde{g}_i(\phi) = \lambda_i \cos\phi$

with

$$\lambda_i = \kappa\alpha(-1)^{|i|}(1-\alpha)^{i-1} \quad \text{for} \quad i \geq 1$$
$$\lambda_i = \kappa\alpha(-1)^{|i|}(1-\alpha)^{-i} \quad \text{for} \quad i \leq 0$$

$0<\alpha<1$

For $\varkappa$ small

$$\tilde{E} \approx \frac{1}{2}\Omega_c^2 J \left(1 + \frac{1}{4}\left(\frac{\kappa^2}{2\Omega_c^4}(W''''(0)W''(0) - 2W'''^2(0)) - 1\right)\alpha^2 + \dots\right).$$

When $$\frac{1}{2} W''''(0) W''(0) < (W'''(0))^2$$

Proof for the existence of DBs near Band edge
« James Condition »

3-Existence Proofs of DBs near band edge by central manifold theorem

(G. James 2001-2003)

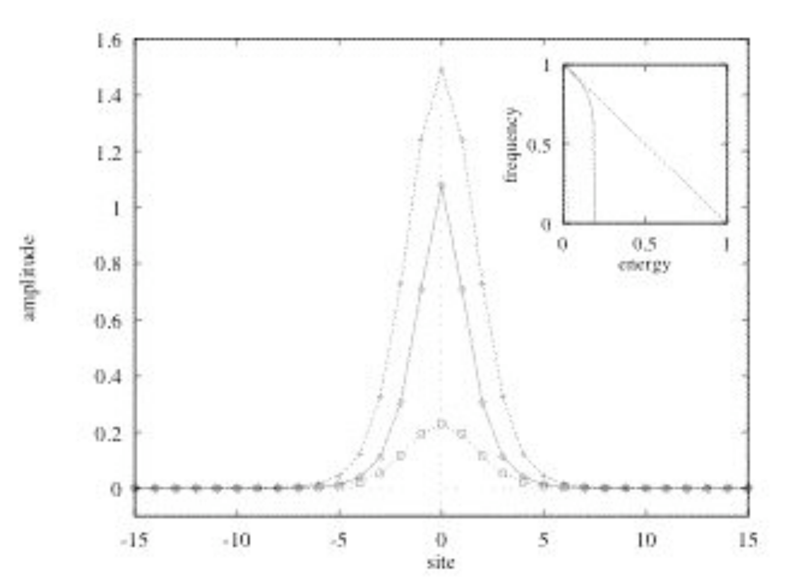
Numerical calculations of DBs

can be easily done by following by continuation (by small steps and a Newton scheme), the trivial DBs from the anticontinuous limit C=0

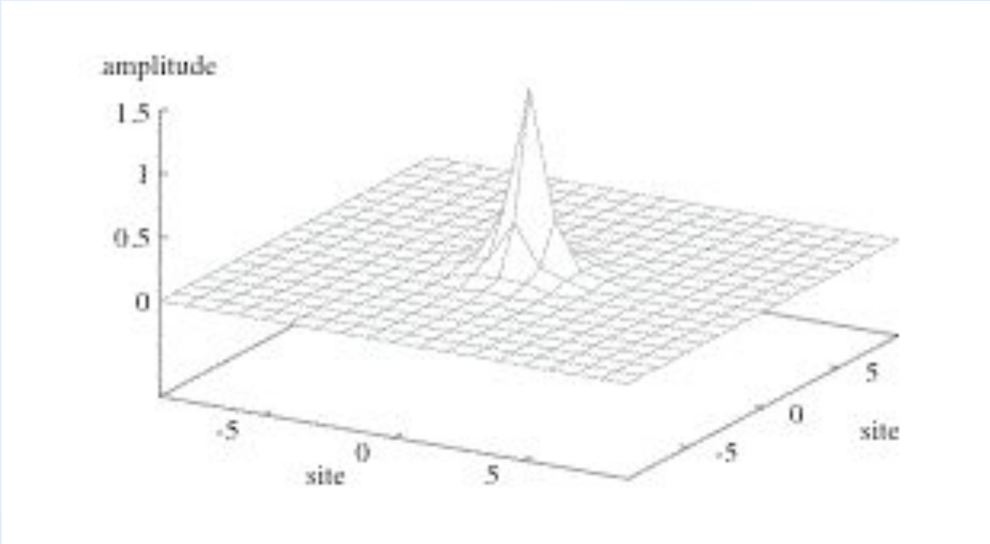
One discovers various bifurcations simple or pitchfok for DBs away from the anticontinuous limit.

Some similarity with the standard map (related with the Frenkel Kontorowa model

Discrete Breathers can be numerically calculated with a high accuracy:



DB profiles in a 1d chain of harmonically coupled Cubic, Morse and Lenard-Jones potentials



DB profile in 2d (cubic potential)

$$H = \sum_i \left(\dot{u}_i^2/2 + V(u_i) + C/2(u_{i+1} - u_i)^2 \right)$$

2-Linear Stability of DBs:

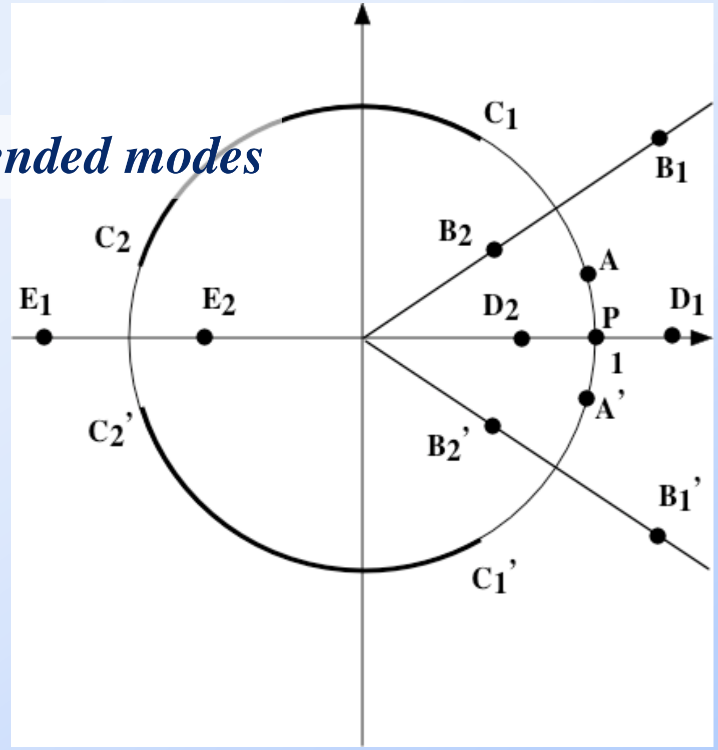
The Hill equation:
Linear with time periodic coefficients period T

$$\ddot{\epsilon}_i + \sum_j \frac{\partial^2 \mathcal{V}}{\partial u_i \partial u_j} \epsilon_j = 0$$

Linear symplectic Floquet operator

$$\begin{pmatrix} \{\epsilon_i(T)\} \\ \{\dot{\epsilon}_i(T)\} \end{pmatrix} = \mathbf{F} \begin{pmatrix} \{\epsilon_i(0)\} \\ \{\dot{\epsilon}_i(0)\} \end{pmatrix}$$

Extended modes



Floquet spectrum

Internal modes and continuum

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DBs are linearly stable when all the eigenvalues of the Floquet operator are on the unit circle

Near the anticontinuous limit, single DBs are linearly stable while multi DBs may be either linearly stable or unstable.

For multi DBs, there is always a choice of the sign of the σ_i of the coding sequence $\{\sigma_i\}$ such that the multi DBs is linearly stable near the anticontinuous limit

There is always a Floquet eigenvalue 1 corresponding to the eigenvector obtained by phase derivation $u_i(t) = g_i(\omega_b t+\alpha)$ with respect to phase α. $\varepsilon_i(t) = g_i'(\omega_b t+\alpha)$ is solution of

$$\ddot{\epsilon}_i + \sum_j \frac{\partial^2 \mathcal{V}}{\partial u_i \partial u_j} \epsilon_j = 0$$

This eigenvalue 1 generally is twice degenerate with a single eigenvector

DBs can be continued versus ω_b by the implicit function theorem when this condition is fulfilled.
It is always continuable in some neighbourhood of the anticontinuous limit.

DBs can be generally continued as a function of ω_b (or the action, amplitude etc…) $u_i(t, \omega_b) = g_i(\omega_b t+\alpha,\omega_b)$

$du_i(t, \omega_b)/ d\, \omega_b = t\, g_i'(\omega_b t+\alpha,\omega_b) + \partial g_i(\omega_b t+\alpha,\omega_b) / \partial \omega_b$ fulfills the Hill equation

$$\ddot{\epsilon}_i + \sum_j \frac{\partial^2 \mathcal{V}}{\partial u_i \partial u_j} \epsilon_j = 0$$

But is not an eigenvector with eigenvalue 1 because it grows linearly with time and thus is not bound.

This marginal mode is called growth mode

Bifurcation when $\partial g_i(\omega_b t+\alpha,\omega_b) / \partial \omega_b$ is not defined (∞)

Band Analysis of DBs

Introduce the eigenvalue problem of the self-adjoint operator

$$\ddot{\epsilon}_i + \sum_j \frac{\partial^2 \mathcal{V}}{\partial u_i \partial u_j} \epsilon_j = E\epsilon_i$$

Since $u_i(t)$ is time-periodic with period T, Bloch-Floquet theorem holds and the eigen solutions fulfills:

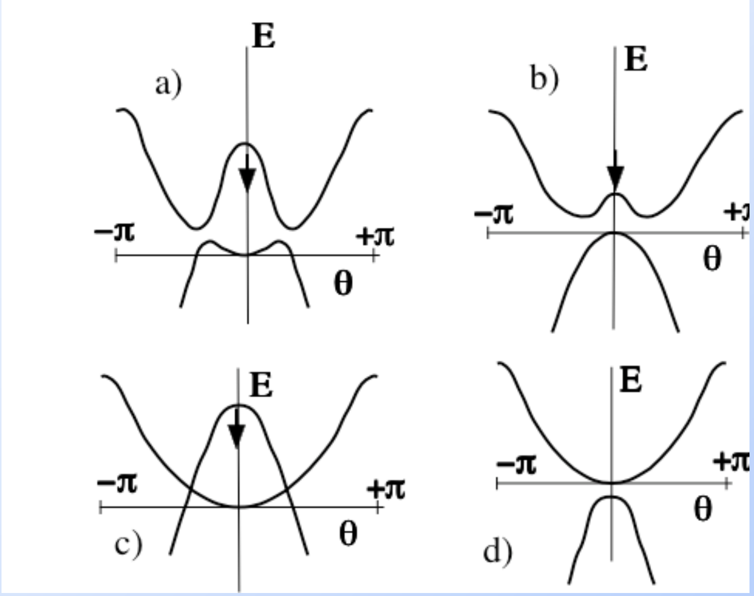
$$\epsilon_i(t) = e^{i\theta\frac{t}{T}}\chi_i(t) \qquad \chi_i(t+T) = \chi_i(t)$$

Bands ν

$$E_\nu(\theta) = E_\nu(-\theta) \qquad E_\nu(\theta) = E_\nu(\theta + 2\pi)$$

Equations $E_\nu(\theta) = 0$ yield the arguments of the Floquet eigenvalues on the unit circle

Instability at θ=0



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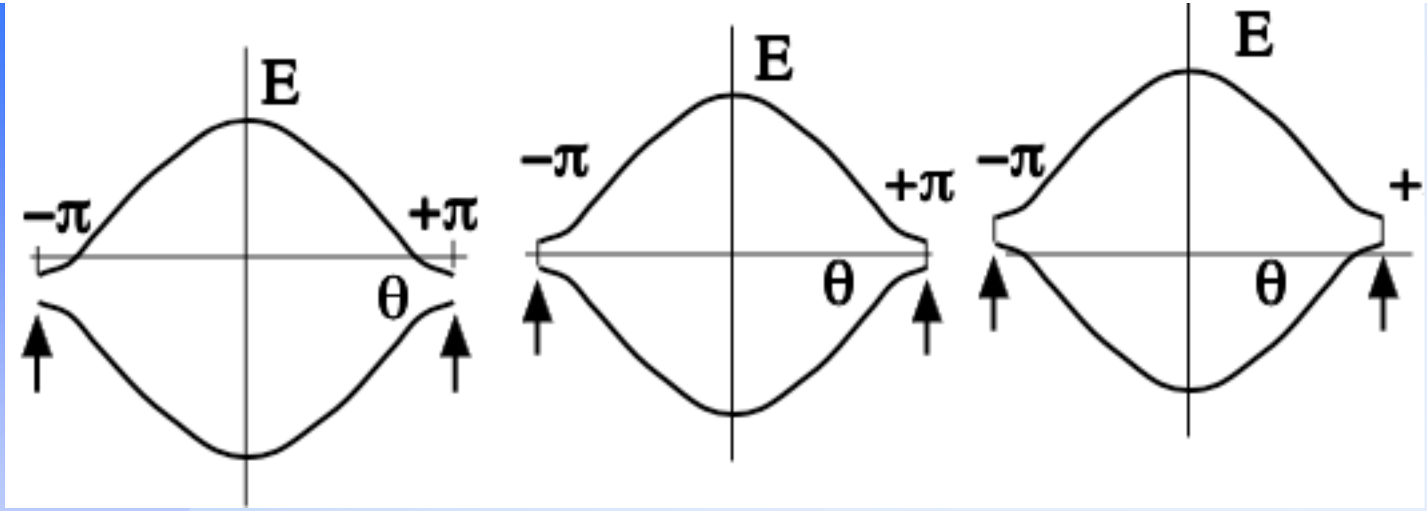
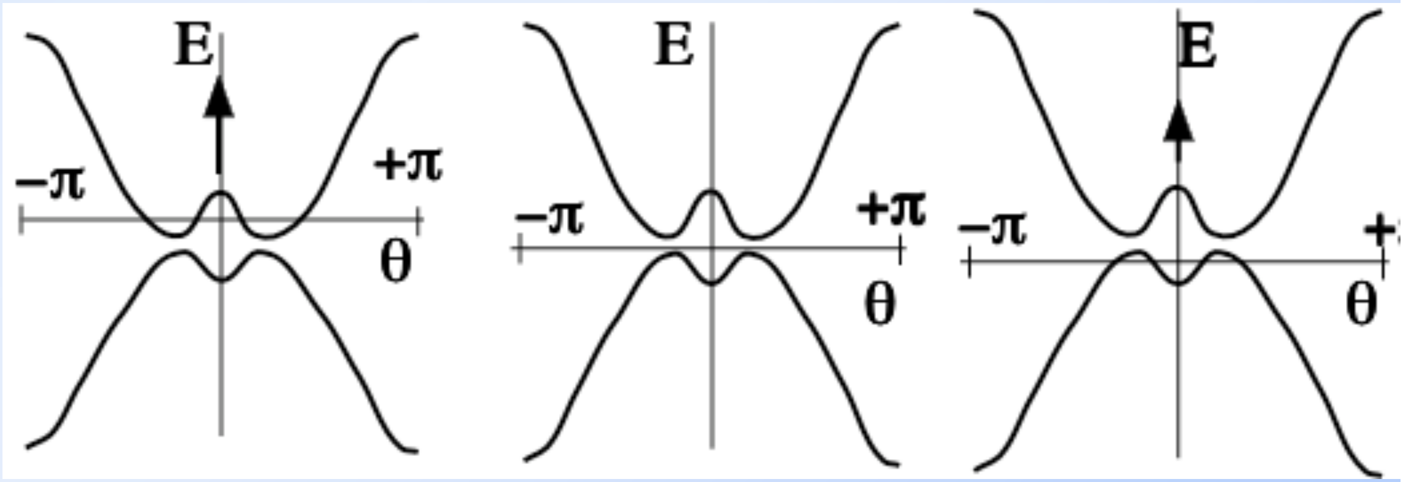


Instability at θ=π

Krein Instability



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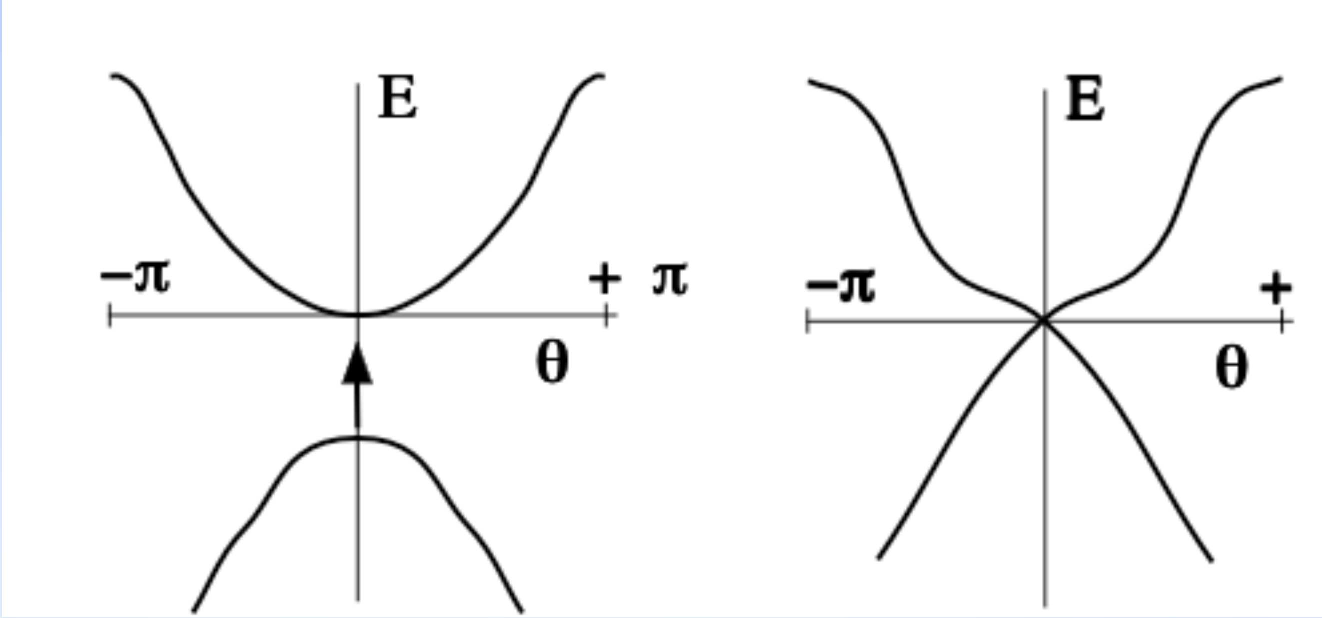
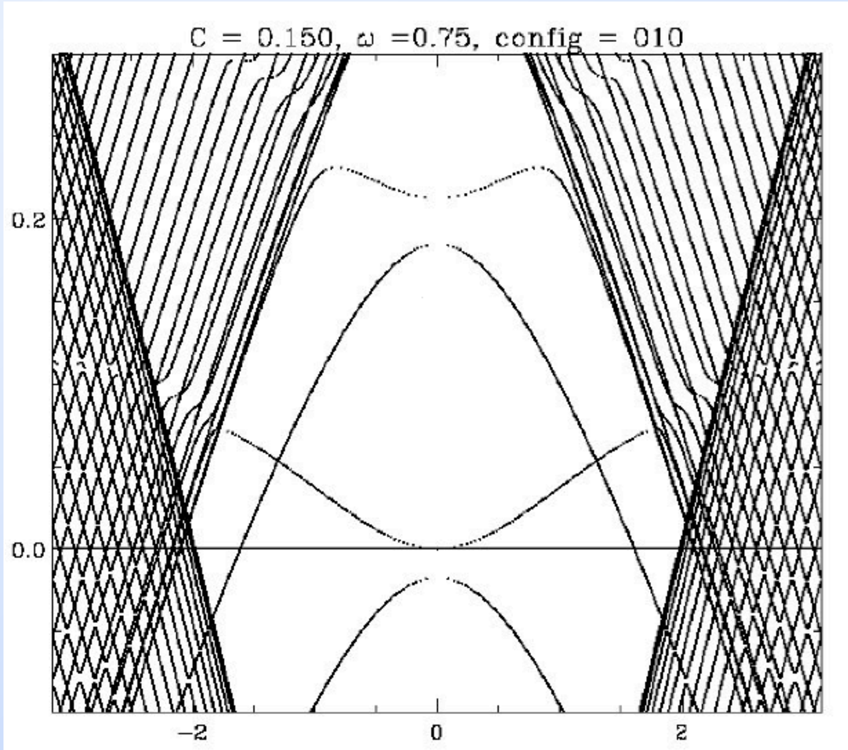
DB Bifurcation



Example of Band Structure
(KG chain with Morse potential)



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Course II- Playing with Discrete Breathers

Spontaneous Manifestation of DBs

Spreading of a wave packet

Interaction of DBs with phonons (elastic and inelastic)

Energy Transportation:Mobility of DBs, Energy transport by phase torsion (Multibreathers)

Targeted Transfer….. Biochemistry

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1- Spontaneous Manifestation of DBs

1- At thermal equilibrium ?

2-Out of thermal equilibrium:

1-by a local injection of a big packet of energy

Takeno and Sievers

2- by modulational instability

M. Peyrard

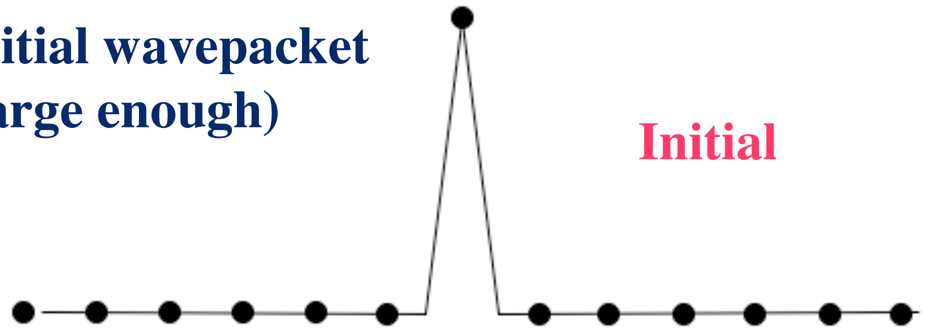
3- by fast quenching

Aubry and Tsironis

Spontaneous Formation of a DB from an initial wave packet

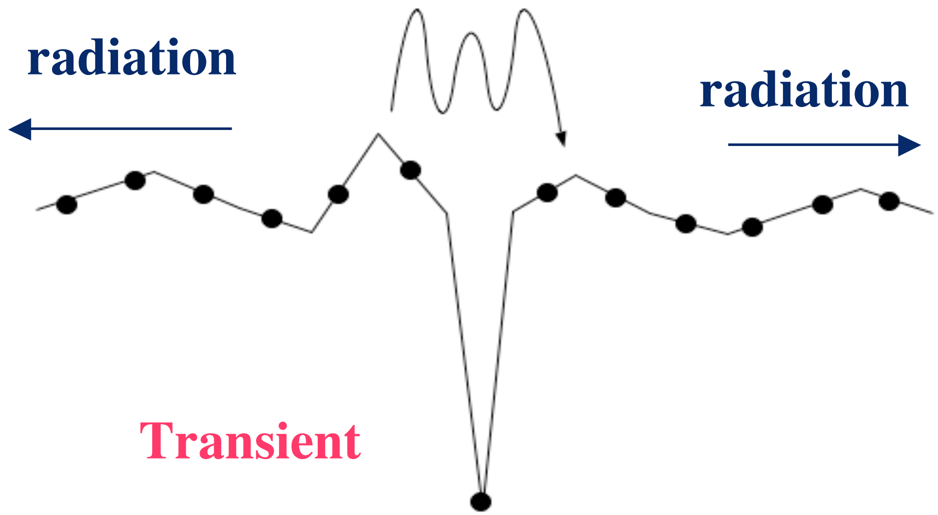
Sievers and Takeno 1988

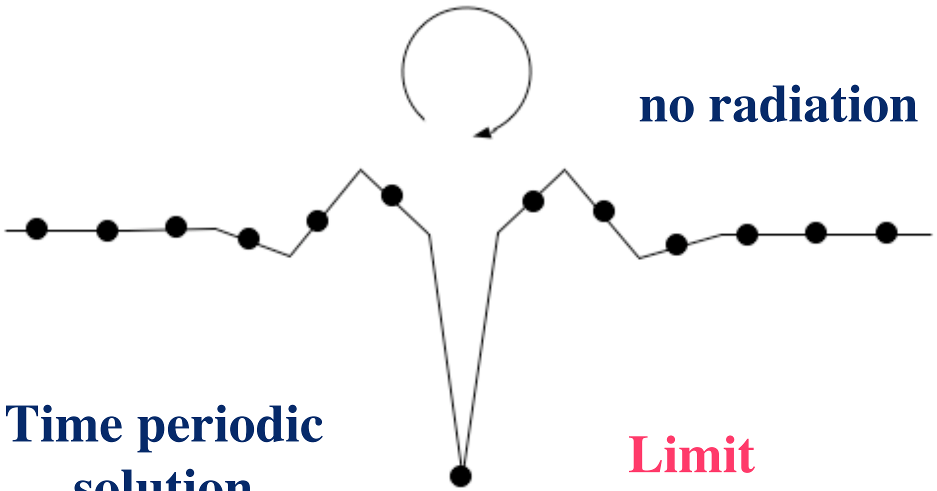
Initial wavepacket
(large enough)



Sievers and Takeno (1988):
from a initial localized wavepacket

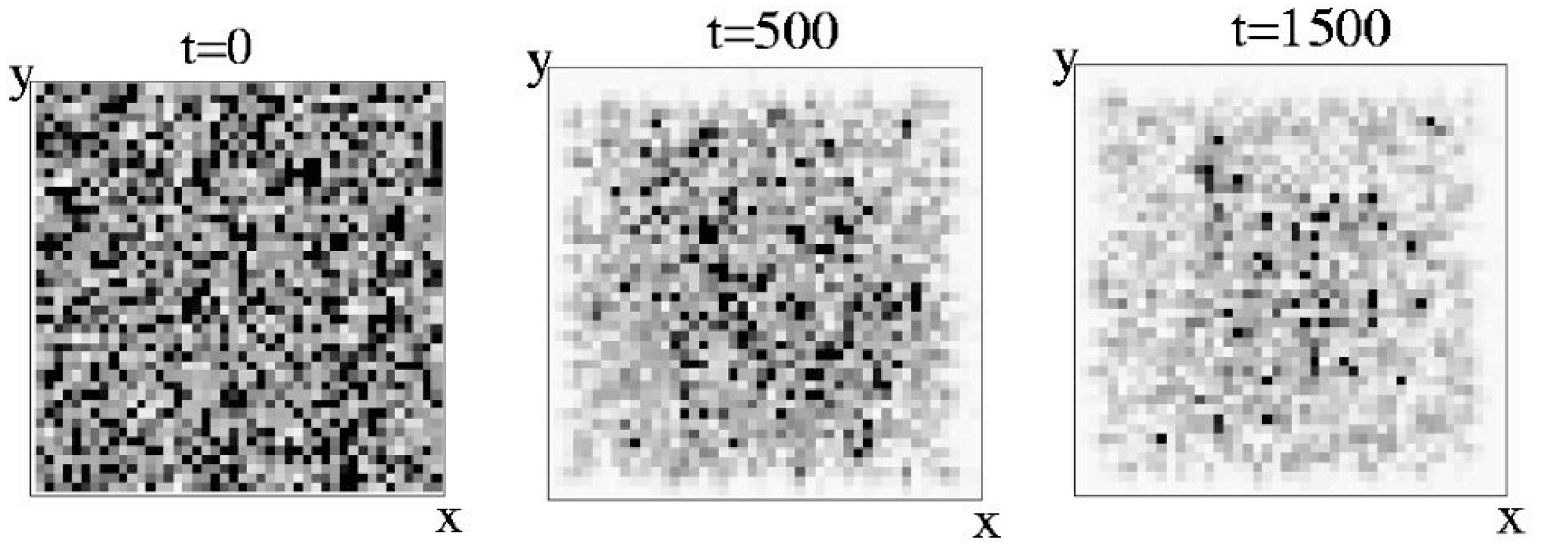
Chaotic or « quasiperiodic » transient



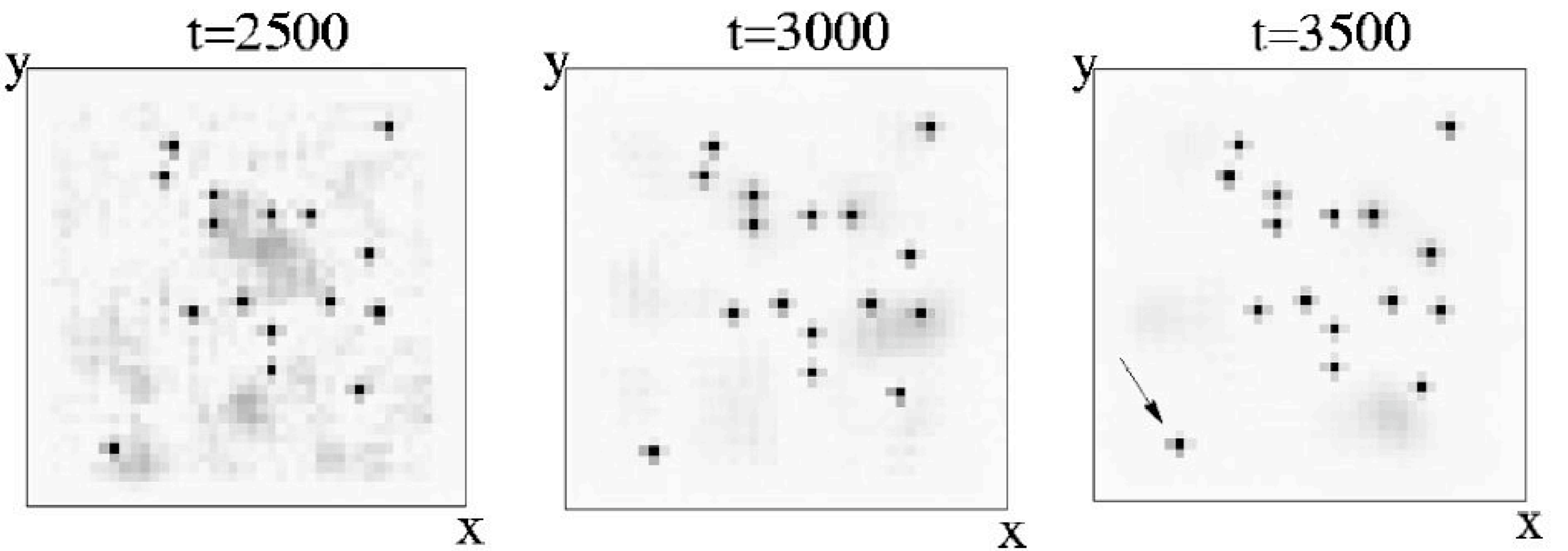


A large part of the initial energy remains localized as a DB, the rest spreads to zero at infinity

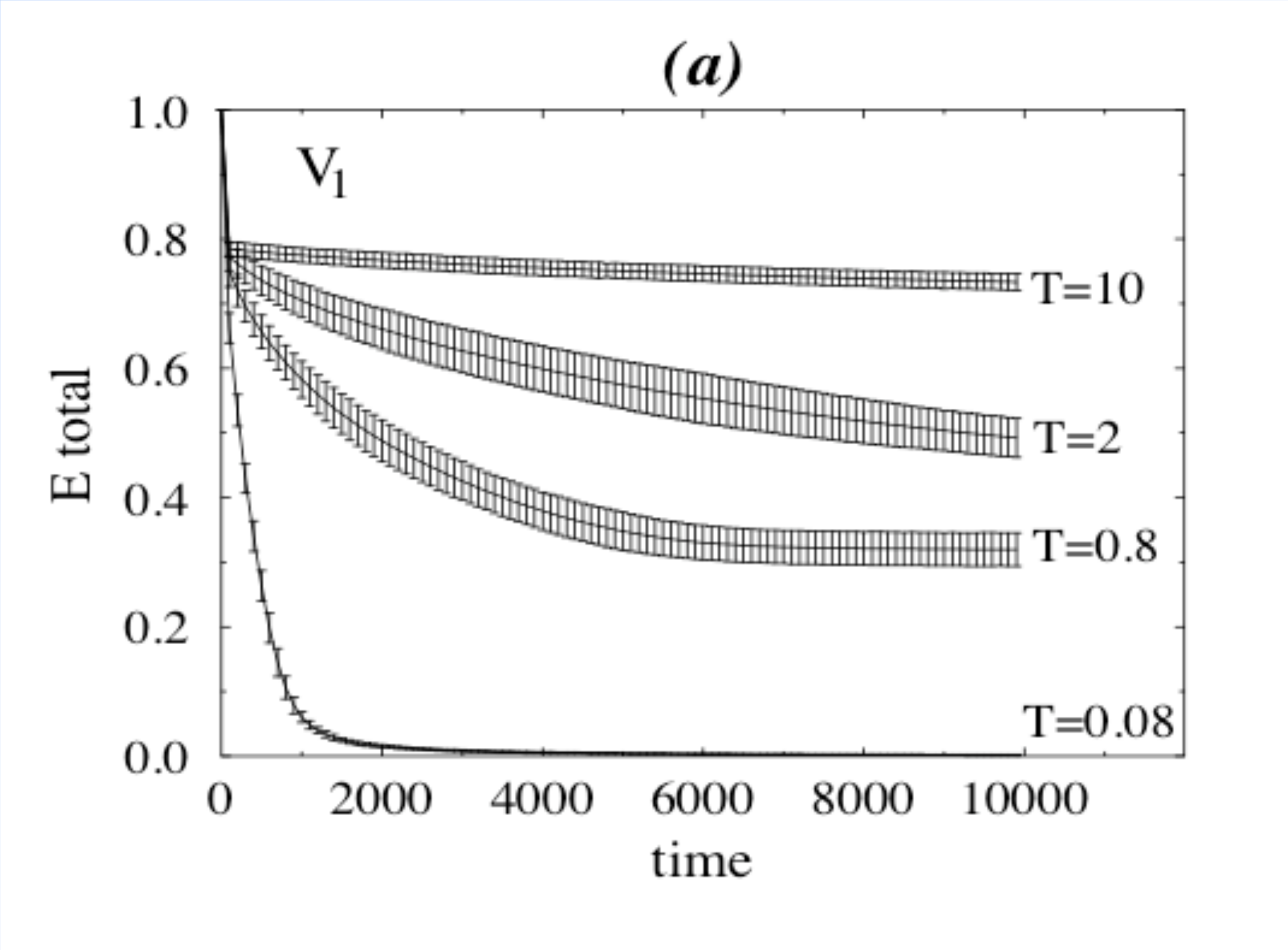
The second moment diverges but the participation number does not



DBs generation by fast quenching of a 2d KG quartic model



Tsironis SA PRL 1996



Anomalous slow relaxation of the energy observed as $t^{-\alpha}$ where $\alpha(T)$ depends on the initial temperature T

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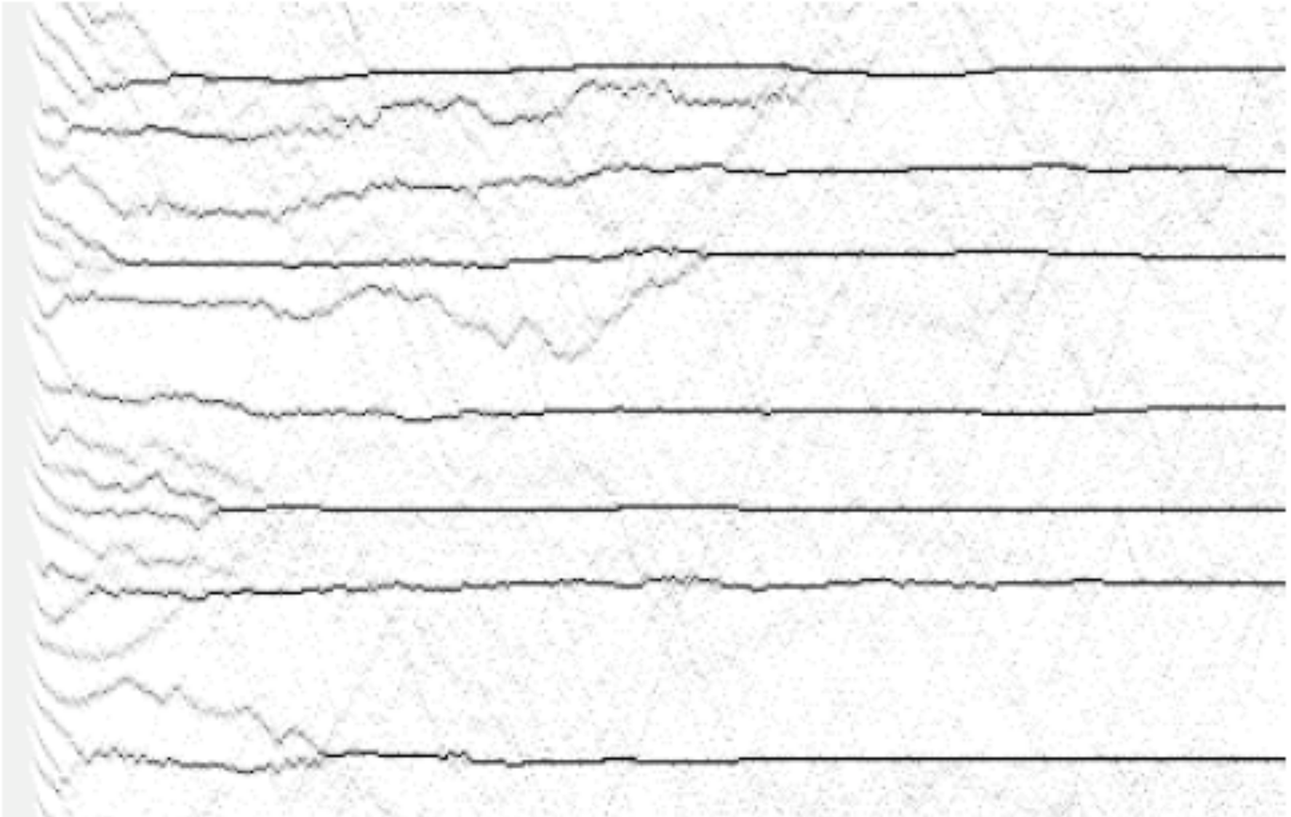
DBs creation from modulational instability



$$\ddot{u}_n = K(u_{n+1} + u_{n-1} - 2u_n) - \omega_0^2 u_n + \alpha u_n^2 + \beta u_n^3.$$

From a small amplitude plane wave $u_n(0) = a\,(-1)^n$ **at q= π**

I. Daumont, T. Dauxois & M. Peyrard 1997

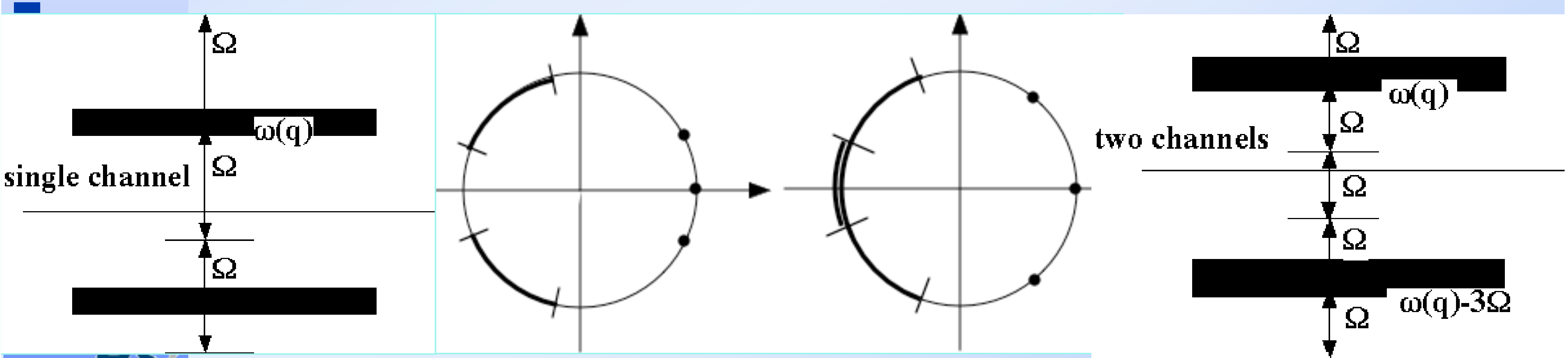
2-DBs interacting with small amplitude travelling waves

(phonon with frequency ω(q))

1-linear interaction (the Hill equation)

$$\ddot{\epsilon}_i + V''(u_i(t))\epsilon_i - C(\epsilon_{i+1} + \epsilon_{i-1} - 2\epsilon_i) = 0$$

One channel **Two-channels**



Generation of harmonics ±ω(q) + nΩ

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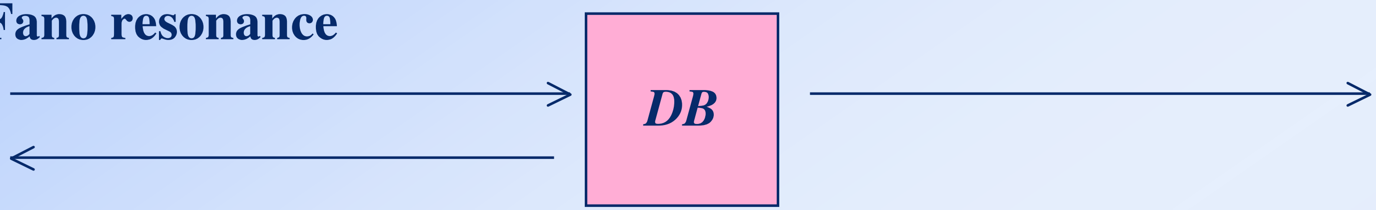
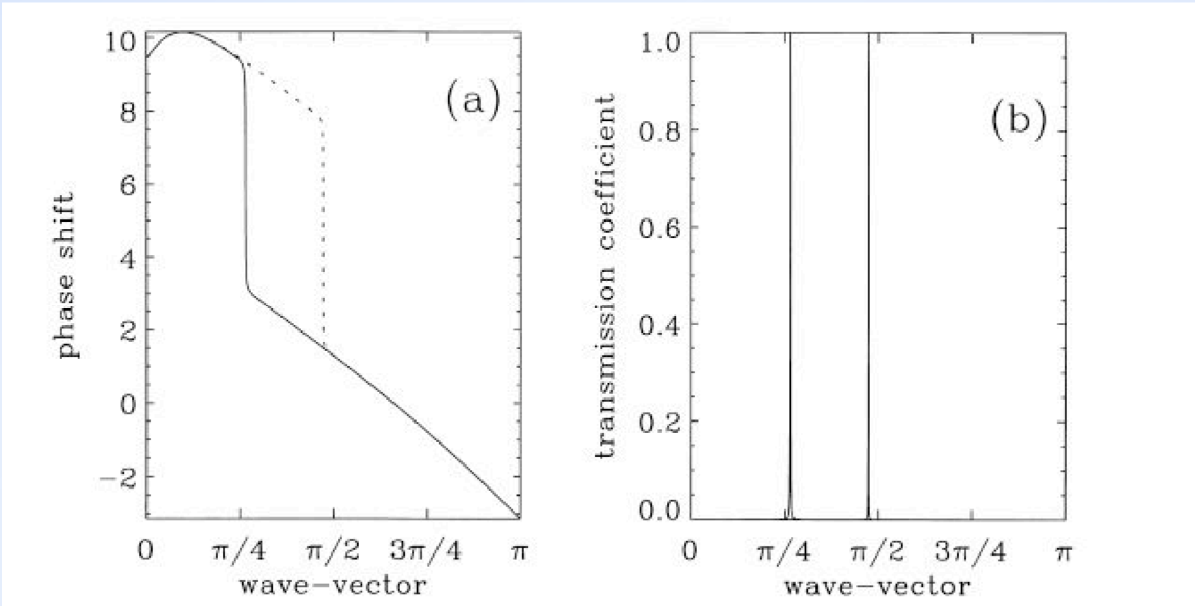
One-channel: Elastic phonon scattering on a single impurity

Fano resonance



Phase shifts (Levinson theorem): Transmission coefficient

$$\mathbf{T}(\mathbf{q}) = \sin^2(\delta_+(\mathbf{q}) - \delta_-(\mathbf{q}))$$



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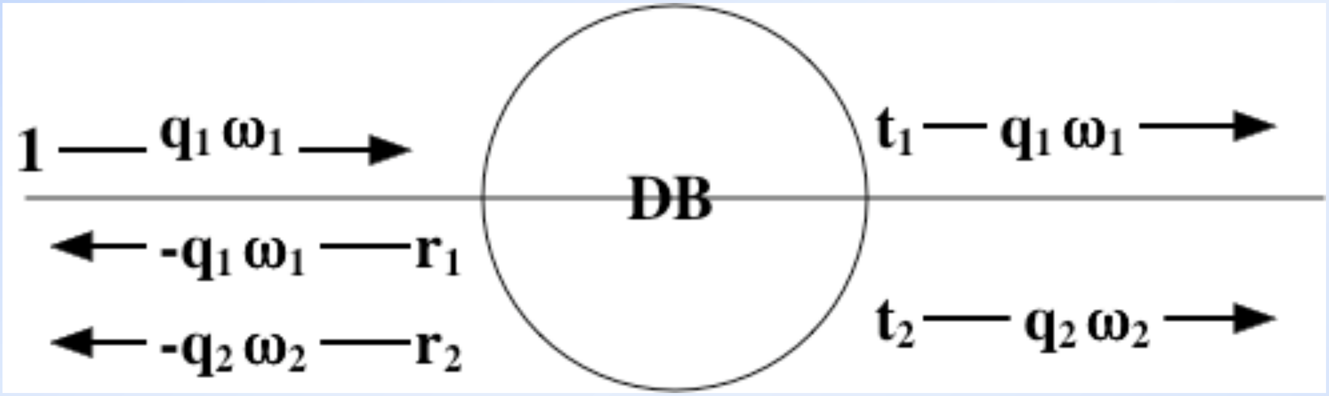
Two channel scattering



Inelastic: the DB energy decays

Higher order p: p ω(q)+k Ω belongs to the phonon spectrum
DB may grow at the expanse of the incoming phonon or decay

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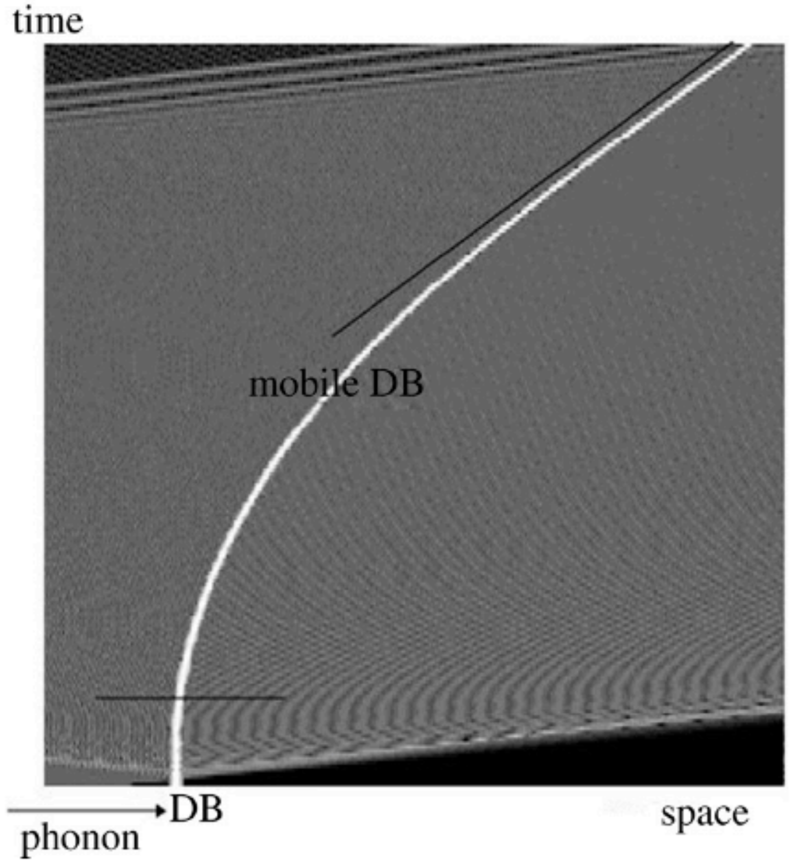


Fig. 14. Grey–white energy density versus space i and time for the KG chain with a Morse potential at $C = 0.2$. The initial conditions correspond to a DB at frequency $\Omega = 0.7$. A small amplitude travelling wave arrives from the left with wavevector $q = 0.8$ and amplitude 2×10^{-2} and scatters on the DB. The white stripe (energy density peak) corresponds to the spatial location of the DB. The energy of the DB first decays, which increases its frequency Ω. When $\Omega = 0.73$, the stationary DB becomes unstable, because of a vanishing pinning frequency, and thus starts to move and to accelerate. Next, it reaches a limiting velocity. As for Fig. 12, the system evolution was calculated with the full non-approximate equations of the KG system.

Interaction of DBs with small perturbations at higher order p is always inelastic Johansson-Aubry

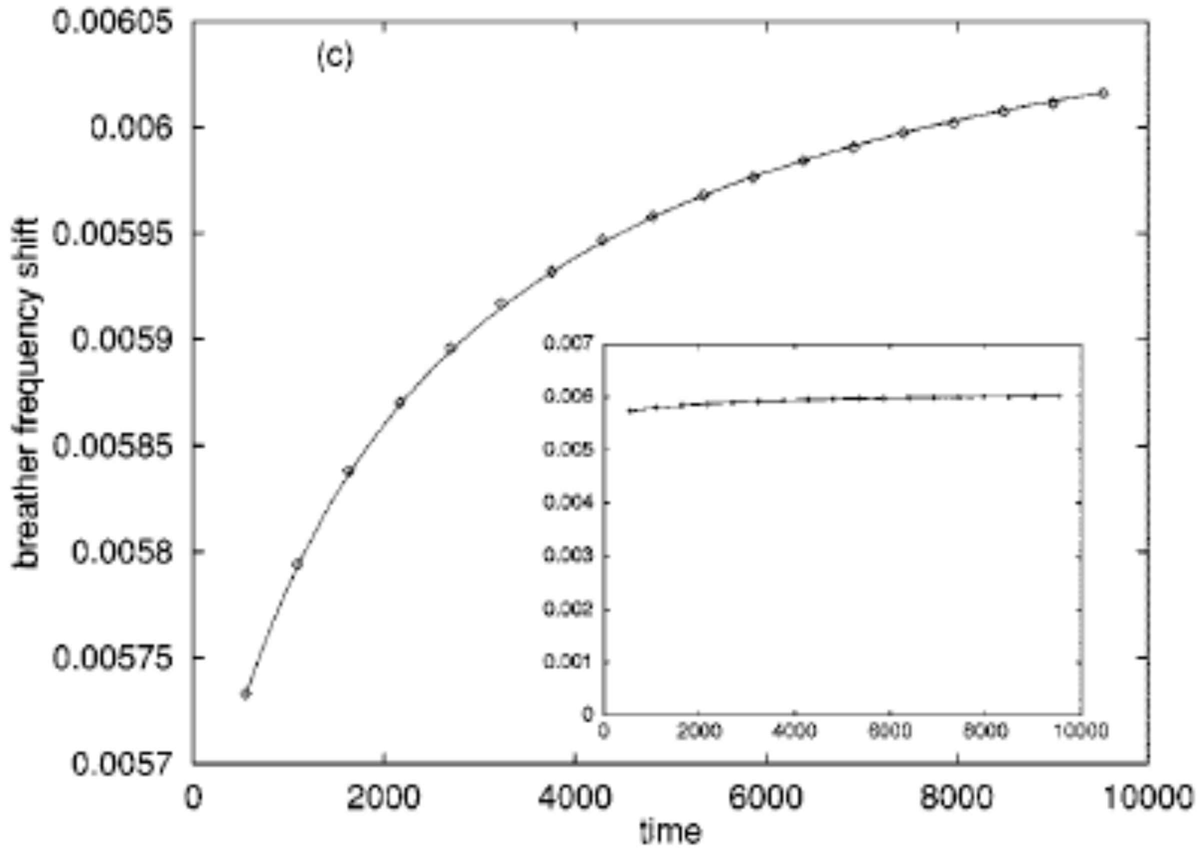
$p\omega + n\,\Omega \in$ Linear spectrum

for some p large enough $\Rightarrow$ radiation

Generate either a Growth of the DB or a Decay

Example:

$$i\,\dot{\psi}_n = \frac{\partial \mathcal{H}}{\partial \psi_n^*} = -C(\psi_{n+1} + \psi_{n-1} - 2\psi_n) - |\psi_n|^2 \psi_n \,.$$



Breathing Mode

Decay of the perturbation by radiation

and Growth of the DB

FIG. 2. Time evolution of a breather with an initial perturbation in the direction of the breathing mode. Parameters are $\Lambda=0.5$, $\omega_p \approx 0.47$, and $C=1$. (a) shows the time evolution of the central-site intensity $|\psi_{n_0}|^2$, (b) shows its time average $\langle|\psi_{n_0}|^2\rangle_t$ calculated using Eq. (29), and (c) shows the instantaneous shift of breather frequency $\Lambda(t)-\Lambda_0$. The solid line in the main figure in (c) is a fit using Eq. (40) with $a(0)=0.082$, $C_1=0.9078$, $C_2=0.069$, and $\gamma=0.067$.

time

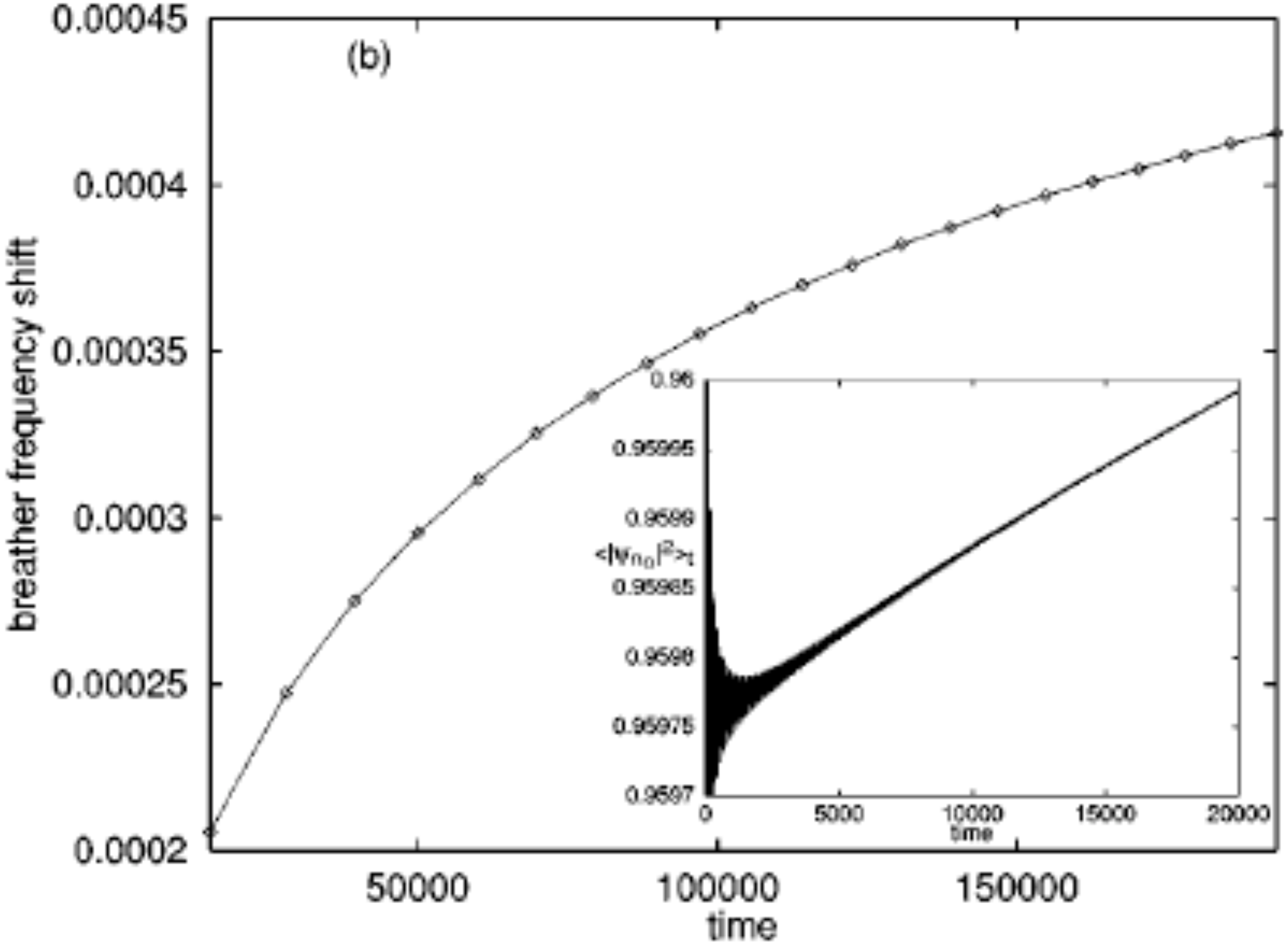


FIG. 3. Time evolution of a breather with an initial perturbation in the direction of the pinning mode. Parameters are $\Lambda=0.45$, $\omega_p \approx 0.197$, and $C=1$. (a) shows the time evolution of $|\psi_{n_0-1}|^2$, where n_0 is the central site of the breather, (b) (main figure) shows the instantaneous shift of the breather frequency $\Lambda(t)-\Lambda_0$, and the inset in (b) shows the time average $\langle|\psi_{n_0}|^2\rangle_t$.

Interaction with small amplitude extended phonons

Growth or Decay of the DB

Since the phonon has infinite energy, the process stops either by DB decay to zero or a DB instability, DB mobility etc….

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Energy Transportation by DBs

1- Mobile DBs (periodic systems)

2- MultiDBs are able to carry energy by phase torsion

3-Targeted Transfer of DBs

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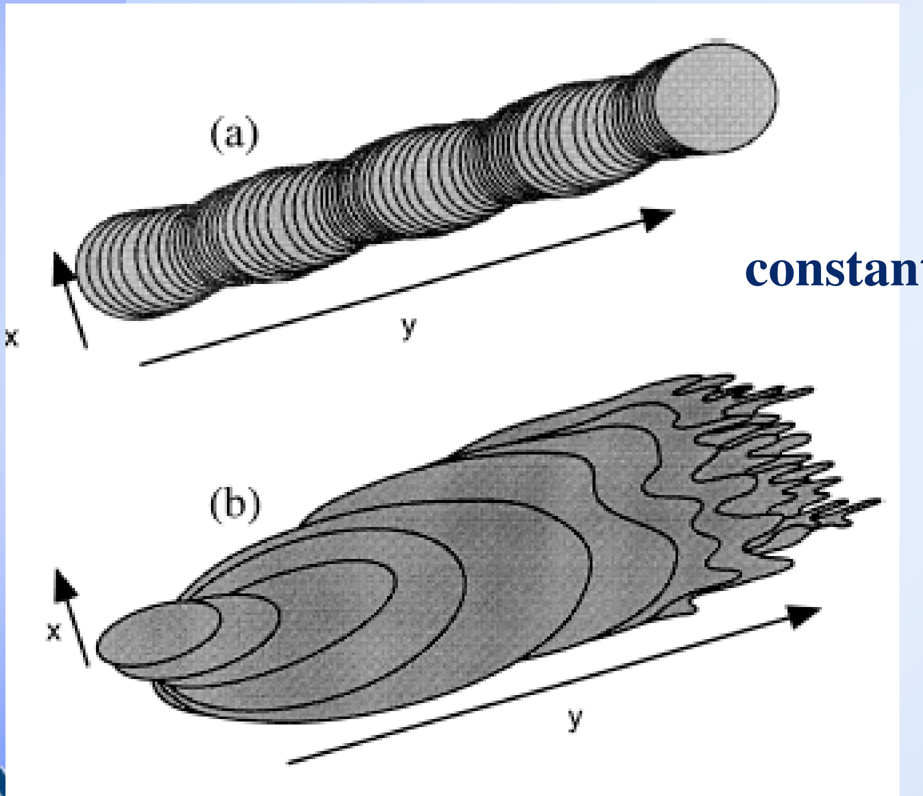
1-DB mobility

A DB is an invariant loop in the phase space
Perturbation: a mobile DBs is a slowly moving loop



constant action

Almost degenerate set of
Invariant Loops

Determine a continuum of DB at constant action under the constraint of spatial location x
Peierls-Nabarro energy profile:E(x)
The extrema of E(x) are real DB
Mobile DB E(x) is almost constant

When two Floquet eigenvalues become degenerate, there are Marginal Modes: (pseudo eigen vectors of the Floquet operator) which grows algebraically as a function of time
Pinning modes appears at an instability at $\theta=0$ and grows linearly.
Mobility appears close to DB instability threshold!

Motion of a DB by excitation of the pinning mode (kick).

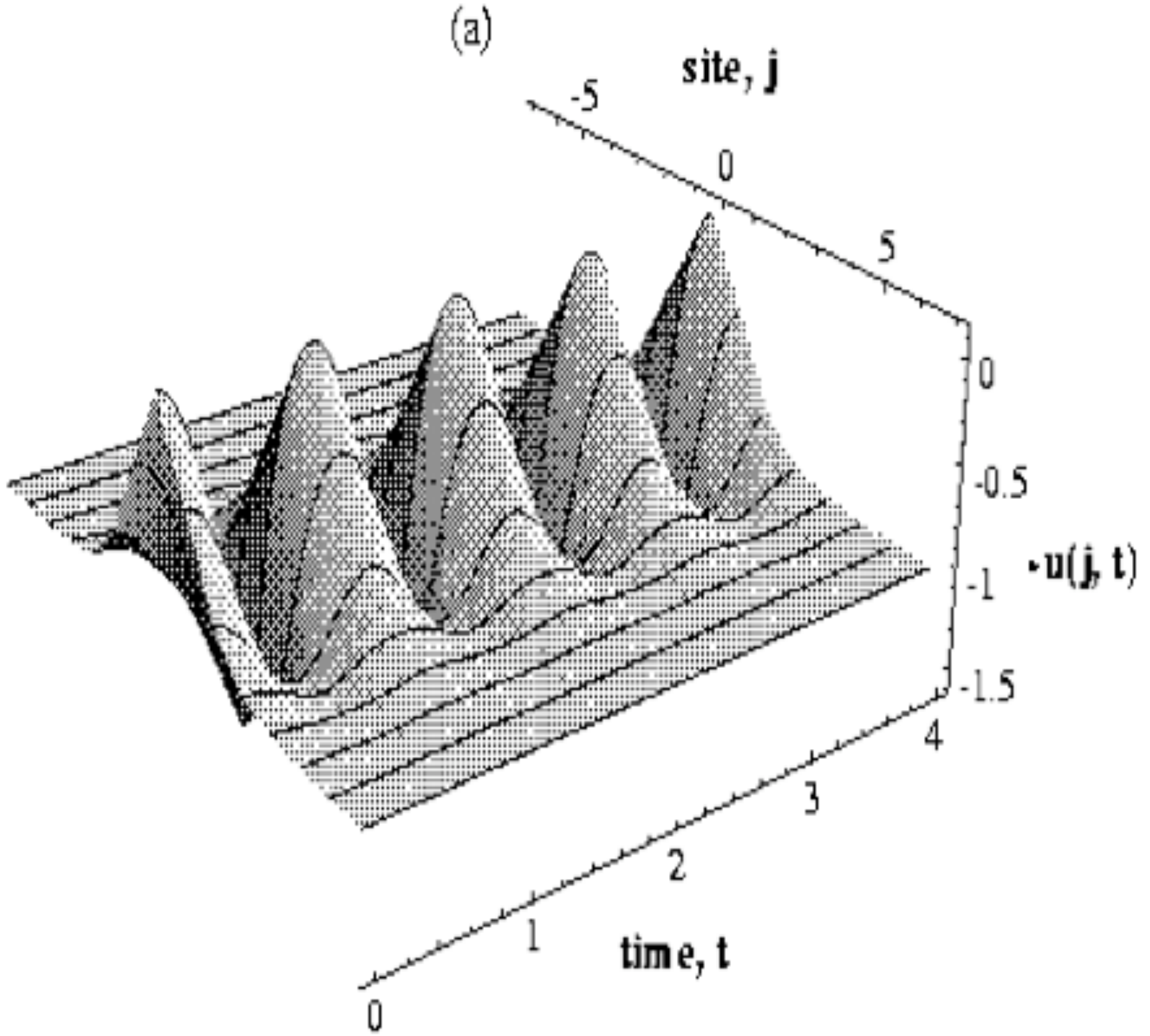
Threshold for the amplitude of the kick (PN energy profile)

However, mobility of very long distances may be obtained in some specific cases even for narrow DB (small energy dissipation).

Exact numerical solutions for moving DB (always exhibit a non vanishing tail.
Generically, there is no exact mobile DBs (which are spatially localized)
Cf. Y. Sire and G. James

Spatially extended (large) DB are usually mobile. Narrow DBs are exceptionally mobile.

Requires uniform generally 1d systems (no defects)



Morse potential $V(x) = \frac{1}{2}(e^{-x} - 1)^2$

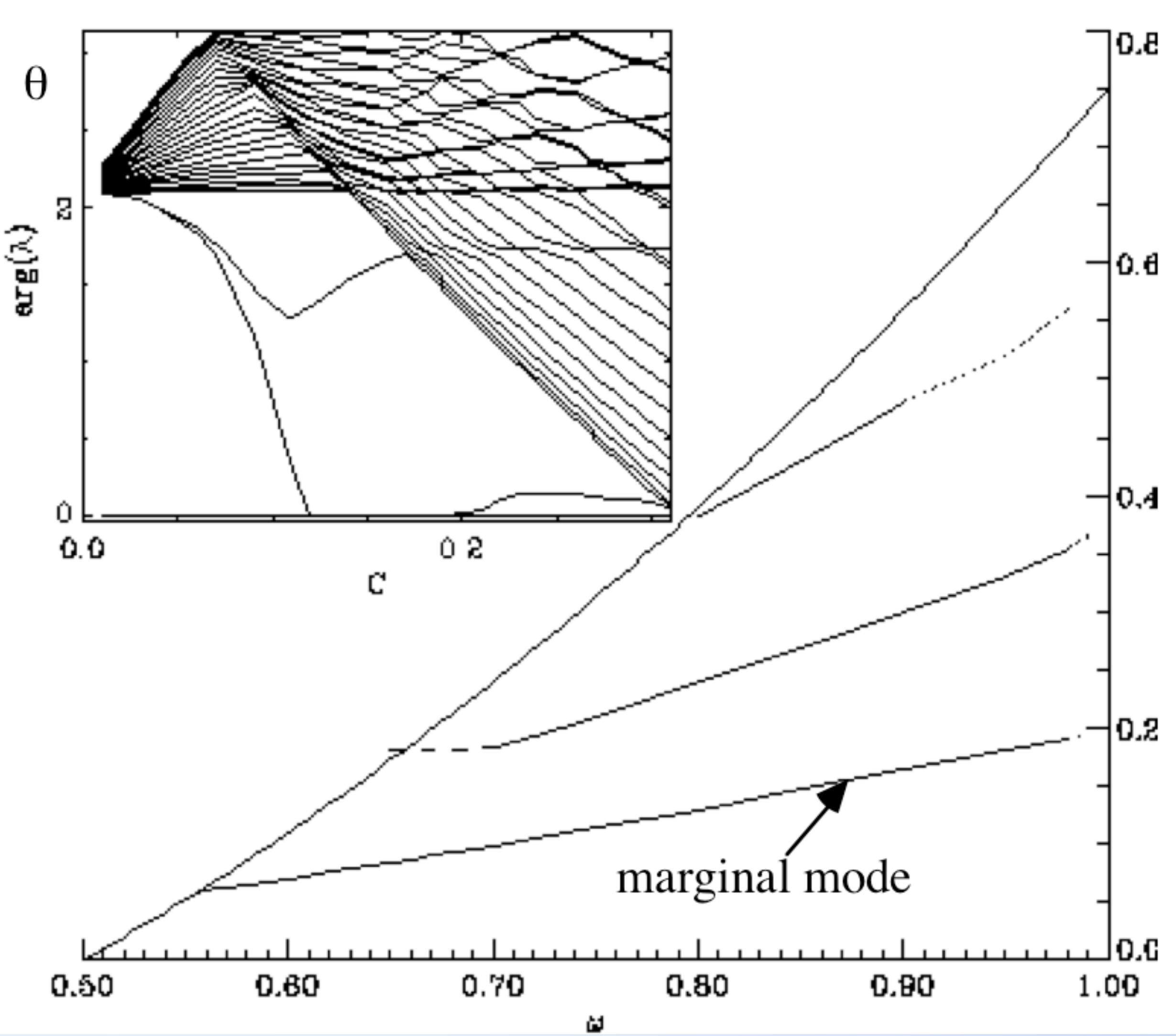
C=0.5888

$\omega_b = 0.7$

Stability inversion

Serge A

Breather ...0001000... Breather ...00011000...



Instability and pitchfork bifurcations

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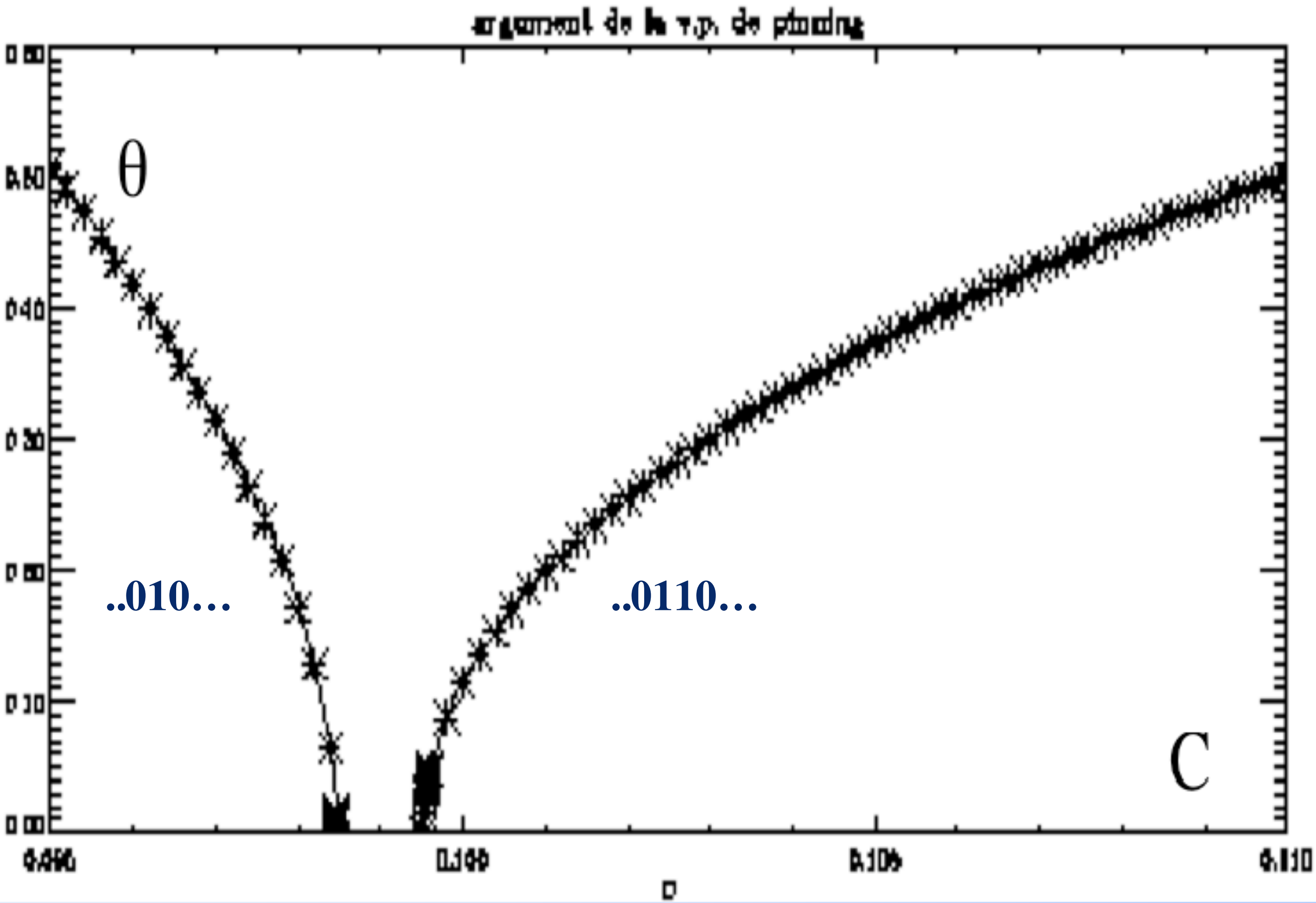
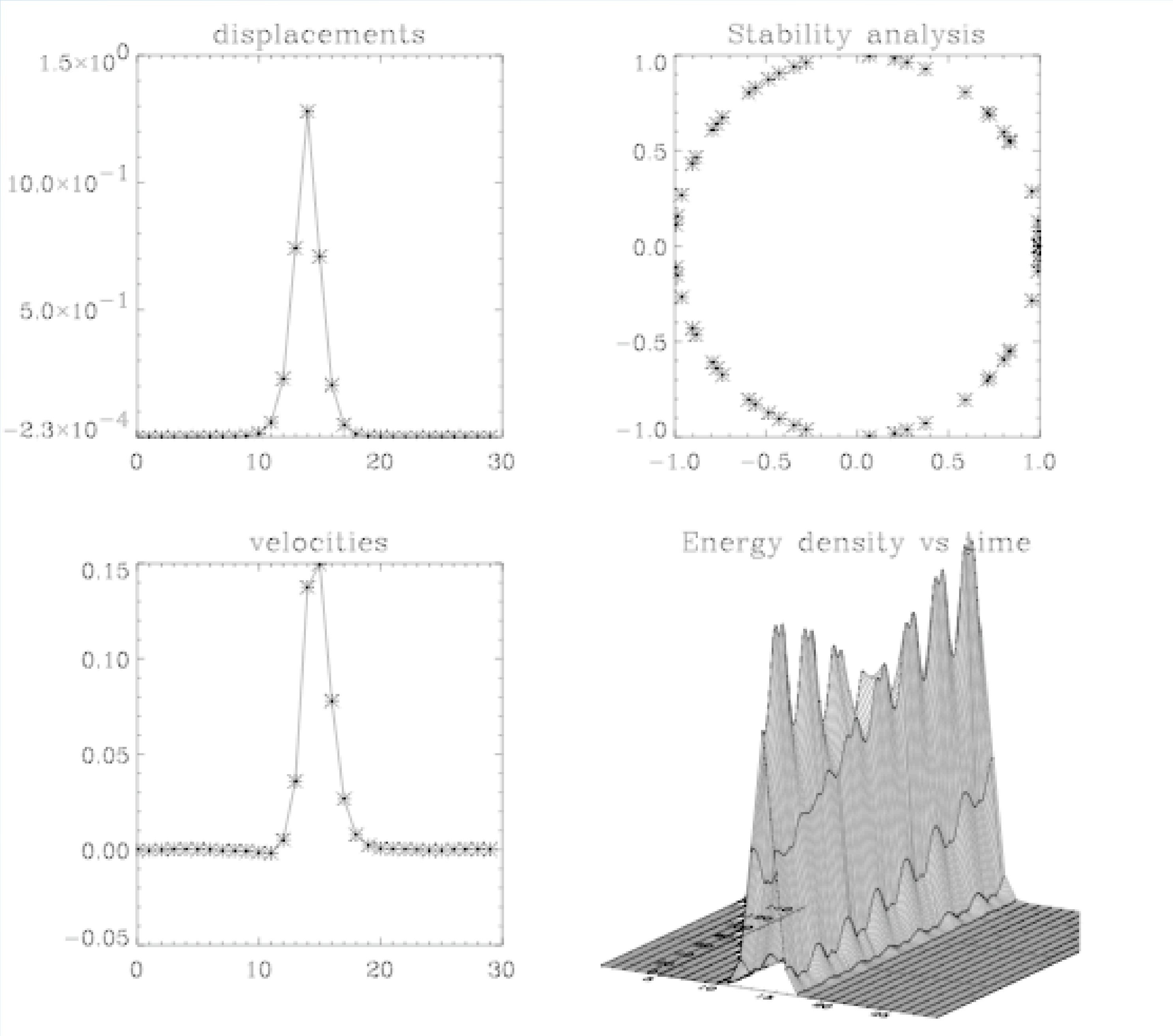
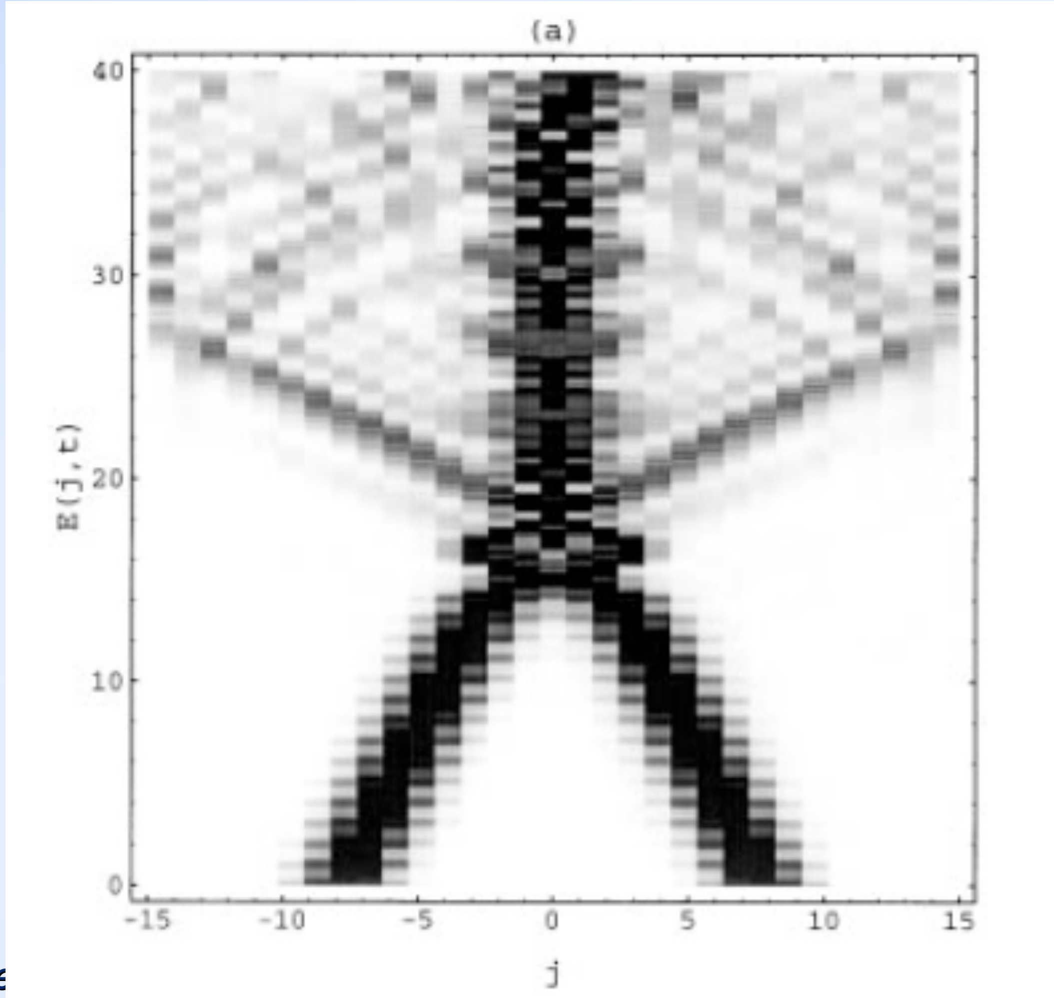

θ
..010…
..0110…
C

A (numerically) exact moving DB calculated with a Newton method



Inelastic Collision of two DBs

Ding Chen, S. A and G. P. Tsironis 1996



Se

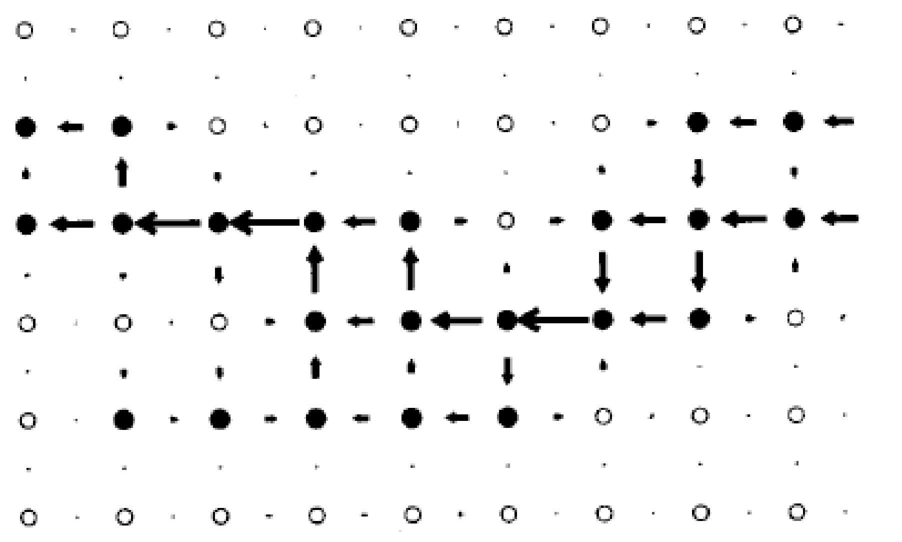
2- Energy Transportation by phase torsion of multiDBs in more than 1D

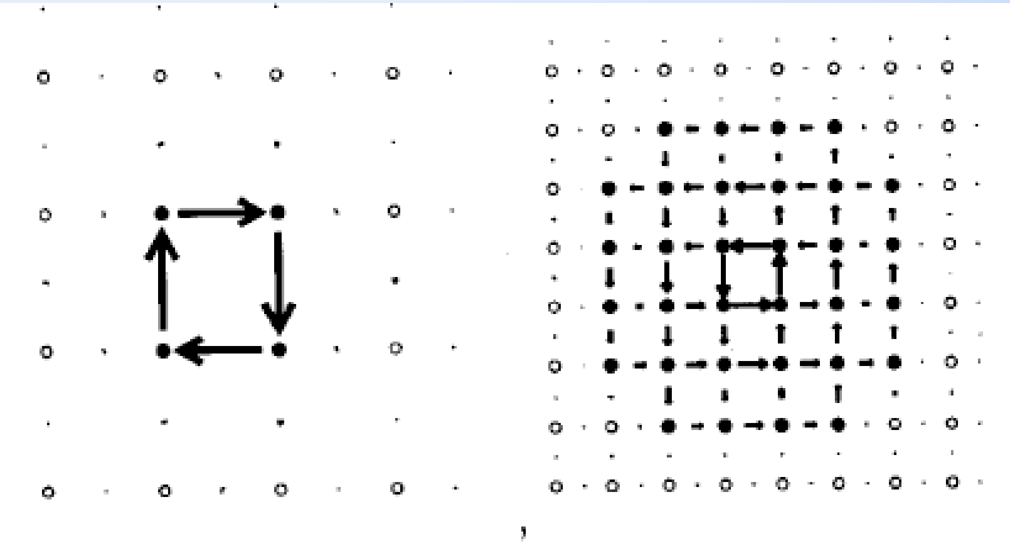
Plane waves can be viewed
as multibreather states (at all sites)
with Phase Torsion

Other multibreather states
may carry energy by phase torsion

1- Extremalize the Grand Action
at fixed phases
2- Extremalize with respect to phases

rivers





vortices

Summary of previous lecture

Existence of time-periodic spatially localised solutions in infinite arrays of coupled non linear oscillators
Proof 1 From the anticontinous limit (uncoupled oscillators)
Proof 2 By variational method

Linear stability
Bifurcation
Mobility

Physical interest: Though DBs are special solutions
Numerics show spontaneous manifestations of DBs

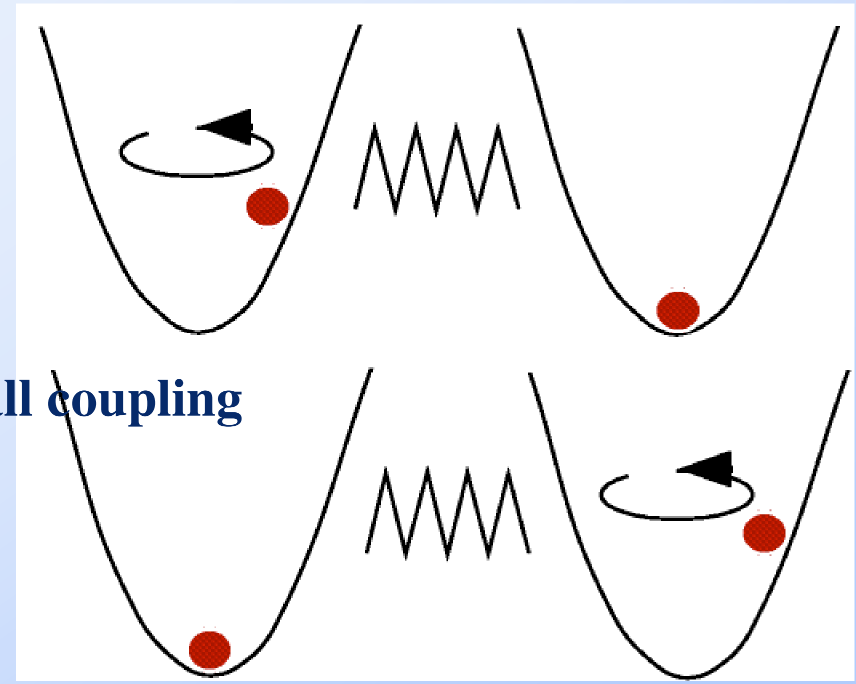
Experimental manifestations:
Bose Einstein Condensate, Coupled Optical Wave Guides,
Arrays of coupled Josephson junctions
Micromechanics (cantilever) etc ....
Biomolecules ???

Targeted Energy (or charge) Transfer

1-linear resonance Galileo (Quantum Tunneling)

The energy oscillates back and forth between the two oscillators with a long period proportional to the small coupling constant

Resonance is a Linear Phenomena



Small coupling

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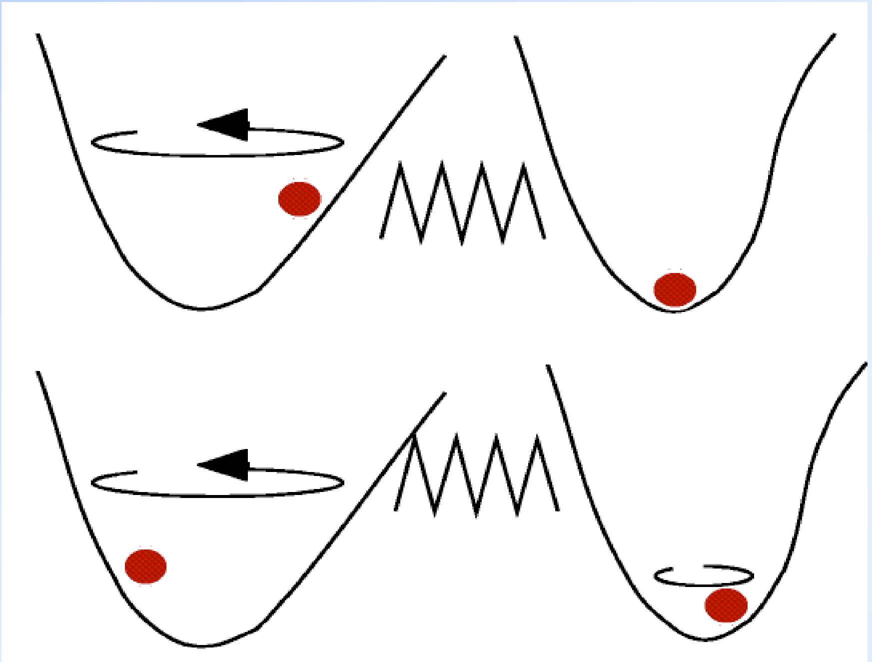
Weakly Coupled Anharmonic Oscillators (or Discrete Breathers)



Because the frequency of anharmonic oscillator depends on its energy, initial resonance is GENERALLY lost after only a small energy transfer

Only partial Energy Transfer for anharmonic resonance

A non-integrable system close to integrable (weak coupling): Quasiperiodic (KAM) solutions block energy transfer

EXCEPTIONALLY, resonance persists at all energy transfer: Targeted Energy Transfer between Conjugate Anharmonic Oscillator D and A

Action-angle variables

$I_0 = (I_D + I_A)/2$ $\quad$ $I = (I_D - I_A)/2$

$\theta_0 = \theta_D + \theta_A$ $\quad$ $\theta = \theta_D - \theta_A$

$$H(I_0, I) = \quad H_D(I_0 + I) + H_A(I_0 - I) = K$$

Nonlinear condition for TET

Find I_0 such that K does not depend on I

A continuum of loops at constant action and constant energy (as for DB mobility)

TET at weak coupling

Let us consider a weak perturbation $\lambda V(I_0,I,\theta_0,\theta)$ which couples the two anharmonic oscillators $<\lambda V(I_0,I,\theta_0,\theta)>_{\theta_0,\theta}=0$

θ_0 is a fast variable θ is a slow variable
$\lambda<V(I_0,I,\theta_0,\theta)>$ averaged over the fast variable θ_0
$= \lambda V_{eff}(I_0,I,\theta)$
of the Hamiltonian induces a complete energy transfer (at a SELECTED energy only) between Donor and Acceptor which oscillates back and forth.

$-I_0 \leq I \leq I_0$ I, θ define a sphere

Dynamics with Hamiltonian **$\lambda V_{eff}(I_0,I,\theta)$**
If $\lambda V_{eff}(I_0,I,\theta) = 0$ define a circle connecting the poles
Targeted Transfer

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An integrable model

$$\mathscr{H} = (\tfrac{1}{2}\chi_1|\psi_1|^4 + \omega_1|\psi_1|^2) + (\tfrac{1}{2}\chi_2|\psi_2|^4 + \omega_2|\psi_2|^2) - \lambda(\psi_1\psi_2^* + \psi_1^*\psi_2), \tag{8}$$

Energy $E = \mathcal{H}$ *and total norm* I_0 *are conserved*

Action-Angle representation

$I_0 = (I_1 + I_2)/2 = Cste \qquad I = (I_1 - I_2)/2 \qquad \theta = \theta_1 - \theta_2$

The phase space (I, θ) *has the topology of a sphere*

$V(I_0, I, \theta) = -2\lambda\ (I_0^2 - I^2)^{1/2} \cos\theta$

Targeted transfer for $I_0 = I_T$ *where* $H_0(I_0, I) = E_T = Cste$

Circular orbit between the poles

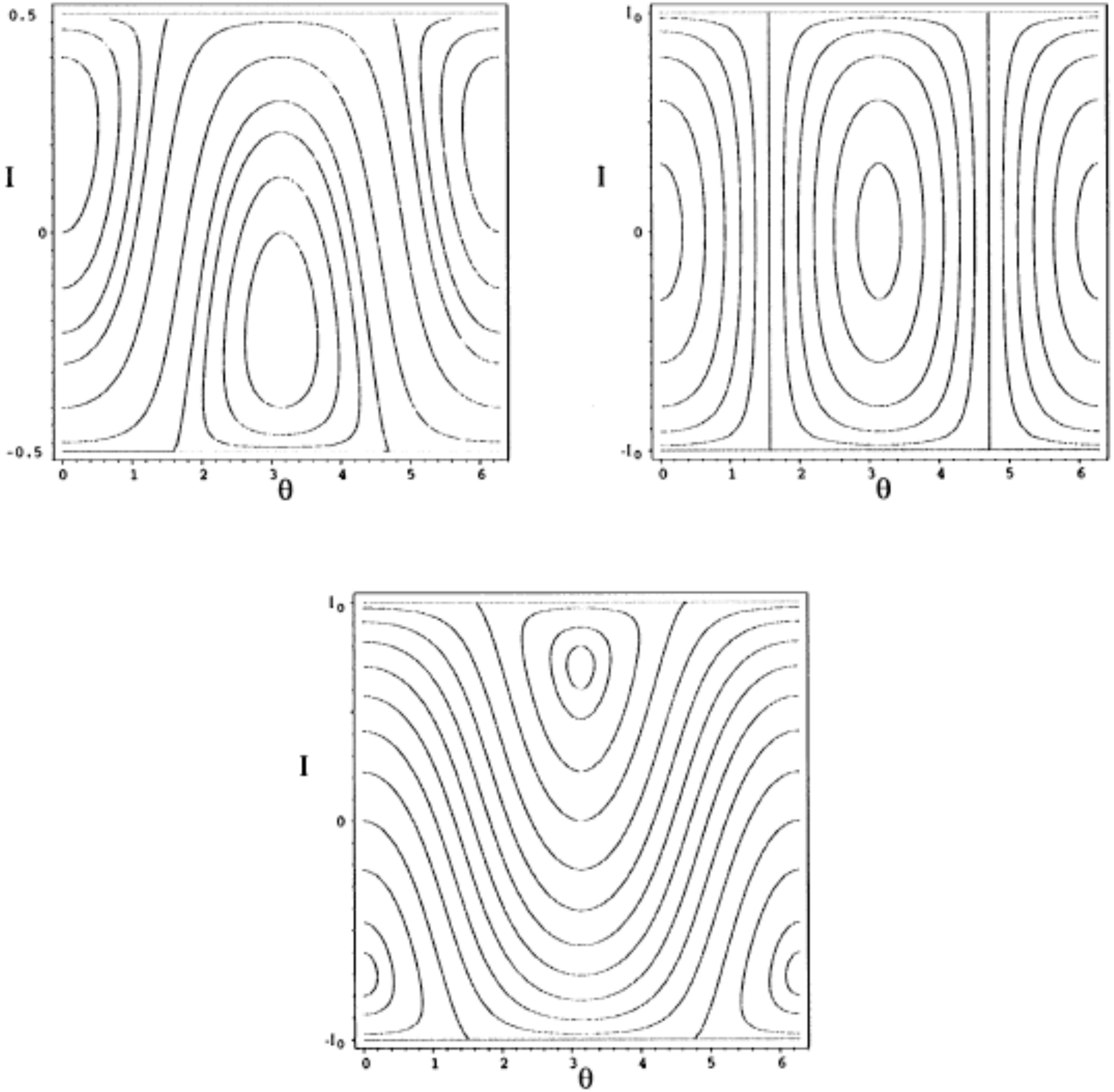


Fig. 1. Cylindrical projections of the contour lines on the sphere (I, θ) of Hamiltonian (9) for $I_0 = 0.5$ (a), $I_0 = 1.0$ (b) (ideal targeted transfer), $I_0 = 2.0$ (c). Model parameters are $\chi_0 = 0$, $\chi = 1$, $\omega_0 = 0$, $\omega = -1$, $\lambda = 1/2$.

Condition for TET $\chi_1 + \chi_2 = 0$ $\omega_1 - \omega_2 + I_0(\chi_1 - \chi_2) = 0$ Then

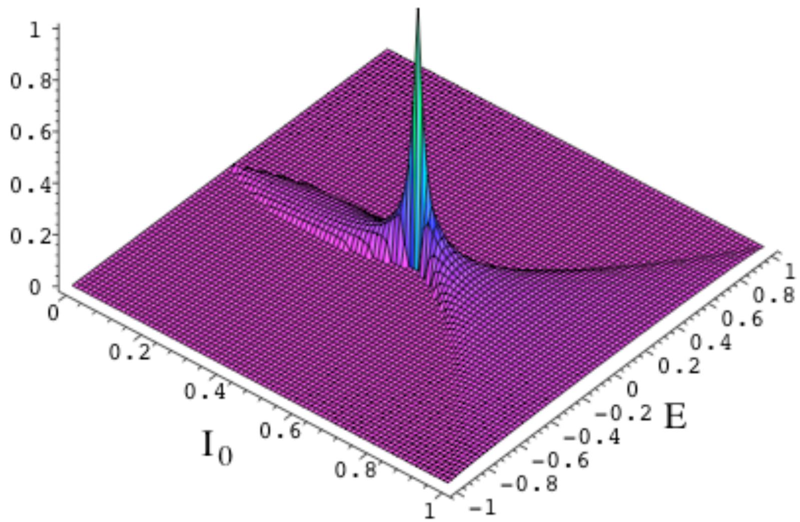
$$\psi_1(t) = \sqrt{\frac{-\omega}{\chi}} \cos \lambda t \exp - i\left(\frac{\varphi}{4\lambda} \sin 2\lambda t + \frac{\omega_0 t}{2}\right), \tag{25}$$

$$\psi_2(t) = i\sqrt{\frac{-\omega}{\chi}} \sin \lambda t \exp - i\left(\frac{\varphi}{4\lambda} \sin 2\lambda t + \frac{\omega_0 t}{2}\right). \tag{26}$$

$\omega_0 = \omega_1 + \omega_2$
$\omega = \omega_1 - \omega_2$

Maximum of $I+1/2$

Transfer Rate in action versus initial action and initial energy in a model with targeted transfer solutions.
Targeted transfer is highly selective in Energy



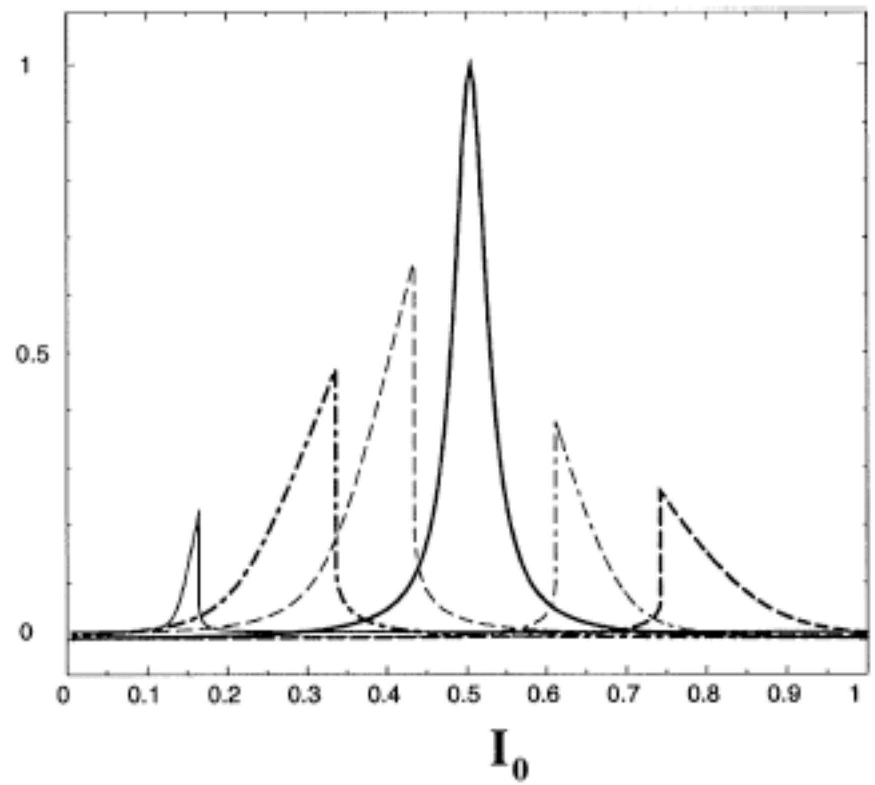


Fig. 4. Transfer rate in action versus I_0 for $\chi = 2$, $\omega = -1$, $\lambda = 0.01$ and several values of $\chi_0 = -0.8$ (thick dashed), -0.5 (thin dashed–dotted), 0 (thick full line), 0.25 (thin dashed), 0.5 (thick dashed–dotted), 5. (thin full).

Extension: Conjugate oscillators when

$$H_D(I_0 + I) + H_A(I_0 - I) = K$$

Giving an arbitrary oscillator $p^2/2+V_D(u)$, it is possible to find a conjugate oscillator $p^2/2+V_A(u)$, at total action $2I_0$

Quantization: Targeted energy transfer persists after quantization and manifest as a « path » of almost degenerate quantum states

Semiclassical quantization:
$E_{dn} + E_{A(p-n)}$ = independant of n for some p

If

$H_D(I_0+I)+ H_A(I_0-I)$ *is not strictly constant*

$\varepsilon= Var(H_D(I_0+I)+ H_A(I_0-I))$ *small*

Targeted transfer occurs for $|\lambda| > \lambda_c$ *small*

(out of band) Discrete Breathers comes as 1-parameter family
$H(I)$ $\omega(I)= dH(I)/dI$

Behave like single anharmonic oscillators

Possibility of Targeted Transfer

Role of damping: Irreversible transfer

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Targeted Transfer for Discrete Breathers

DBs comes by family. The energy E_α of a DB α is a function of its action I_α

Two systems X=D or A which are weakly coupled

$$H_X = \sum_i \Big\{ -E_{X,i}|\psi_{X,i}|^2 - \frac{1}{2}\sigma_X|\psi_{X,i}|^4 - C(\psi_{X,i}\psi^*_{X,i+1} + \psi^*_{X,i}\psi_{X,i+1}) \Big\},$$

It is rare to find two DB families α in D and β in A such that for some I_0

$\mathbf{E_\alpha(I_0+I)+ E_\alpha(I_0-I) \approx Cste}$

However by tuning models parameters one can find DBs family fulfilling this condition

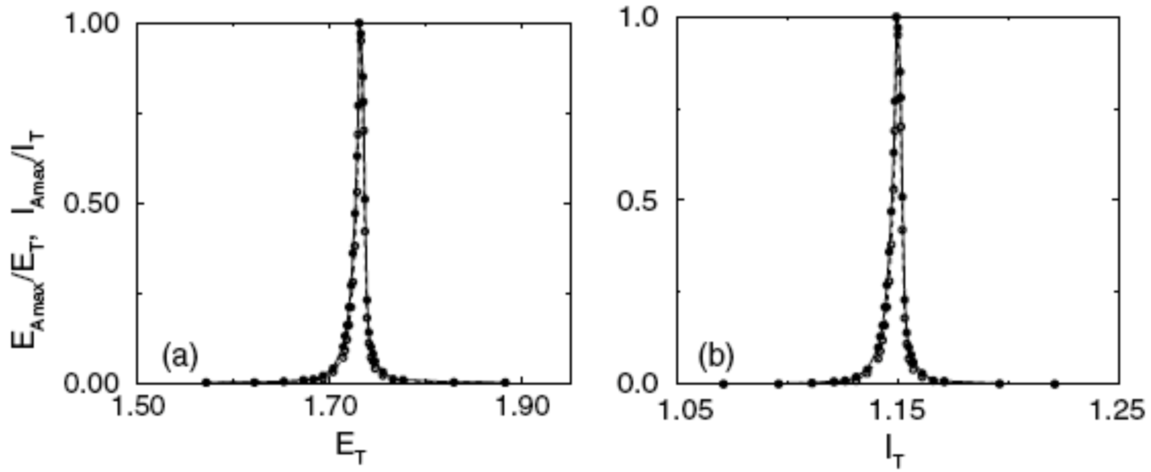

FIG. 3. The ratio of the energy and action transferred from D to A, $E_{A\max}/E_T$ and $I_{A\max}/I_T$ (solid circles connected by a solid line, empty circles connected by a dashed line, respectively), as a function of E_T in (a) and I_T in (b). The DB is initially localized on site d of D.

TET in a weakly coupled Rotor-Morse oscillator system:
A toy model for a Chemical Expressway for Ultrafast Chemical Reaction (non Brownian)
A rotor weakly coupled to a chemical bond

$$H = \frac{1}{2}\dot{u}^2 + \frac{1}{2}(1-e^{-u})^2 + \frac{J_R}{2}\dot{\theta}^2 + f(u,\theta)$$

$$f(u,\theta) = (\lambda e^{-u} + b)\cos\theta$$

Action-Angle representation

$$H = I_M - \frac{1}{2}I_M^2 + \frac{1}{2J_R}I_R^2 + 2\lambda \sum_{n=0}^{+\infty} a_n(I_M)\cos n\theta_M \cos\theta$$

Isotopic kinetic fractionation

TET for J_R=1

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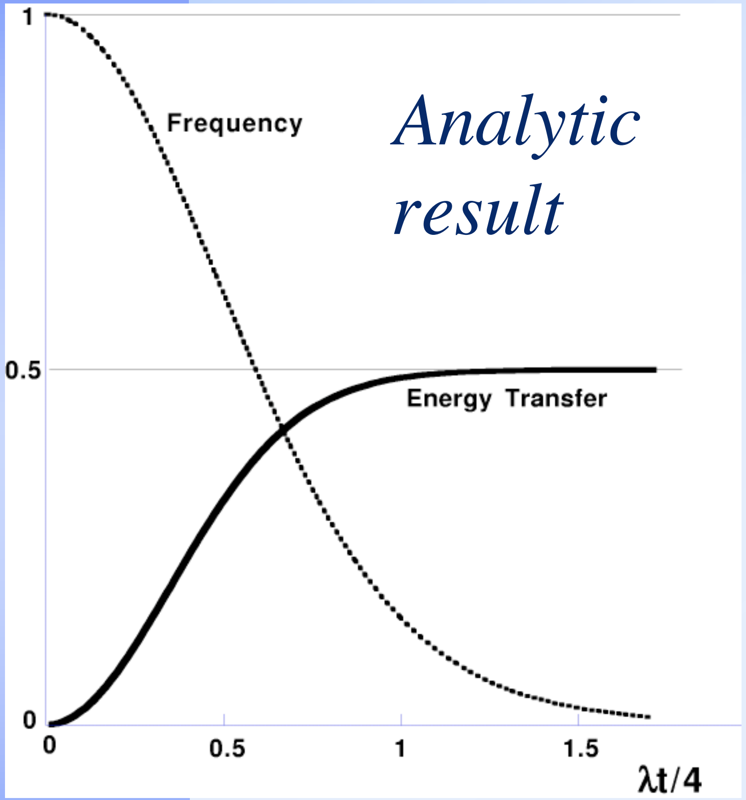
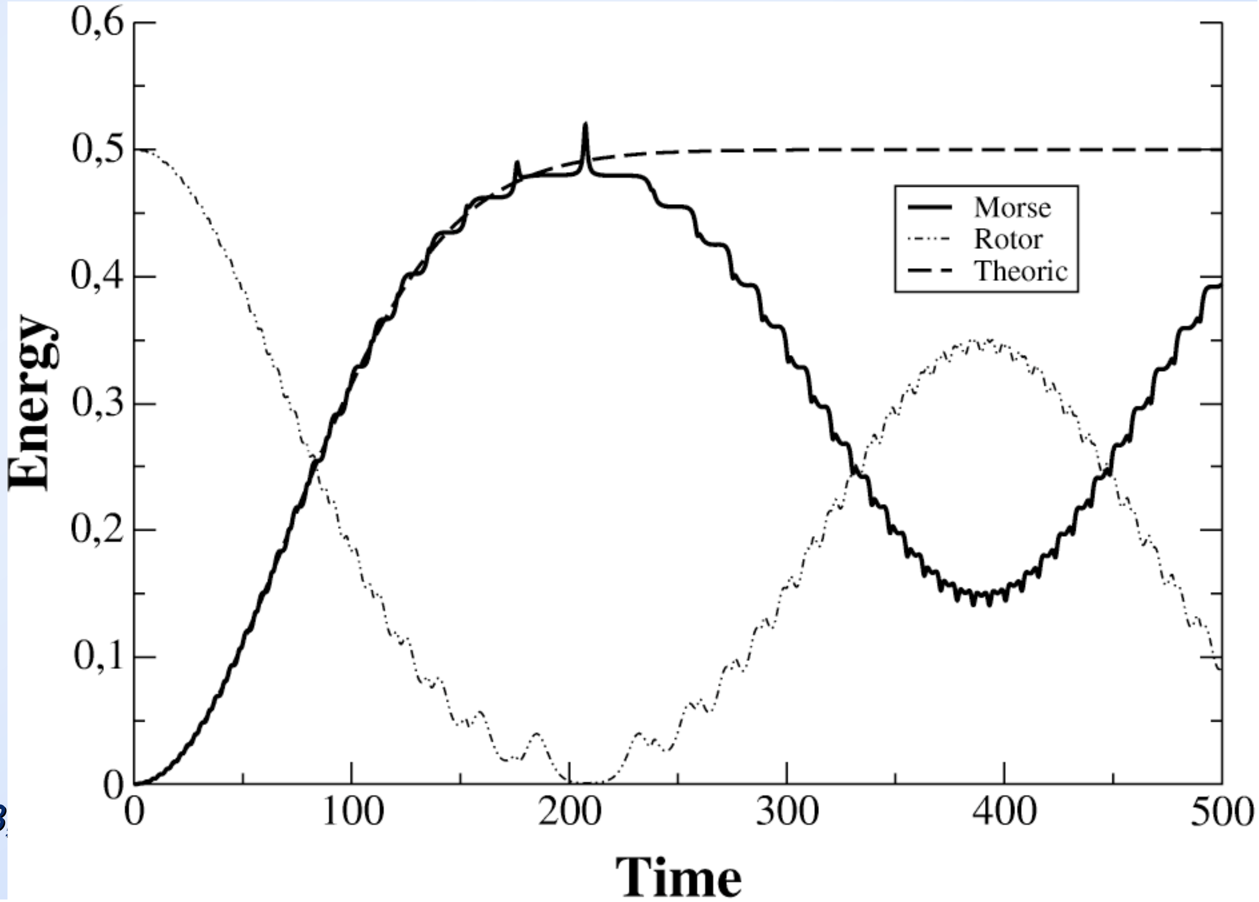


Frequency
Analytic result
Energy Transfer
1
0.5
0
0
0.5
1
1.5
λt/4

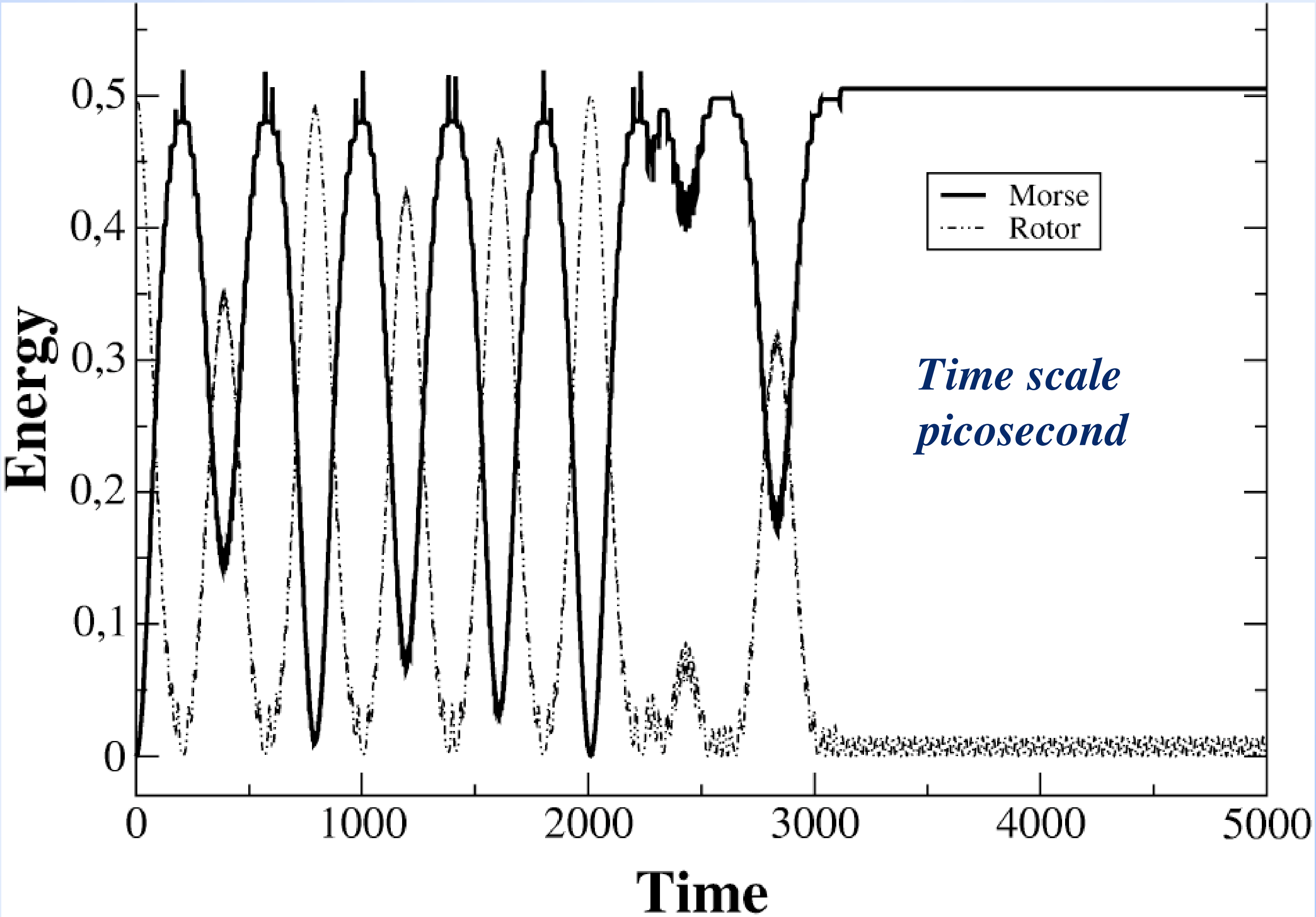


Energy
Time
Morse
Rotor
Theoric
0,6
0,5
0,4
0,3
0,2
0,1
0
0
100
200
300
400
500

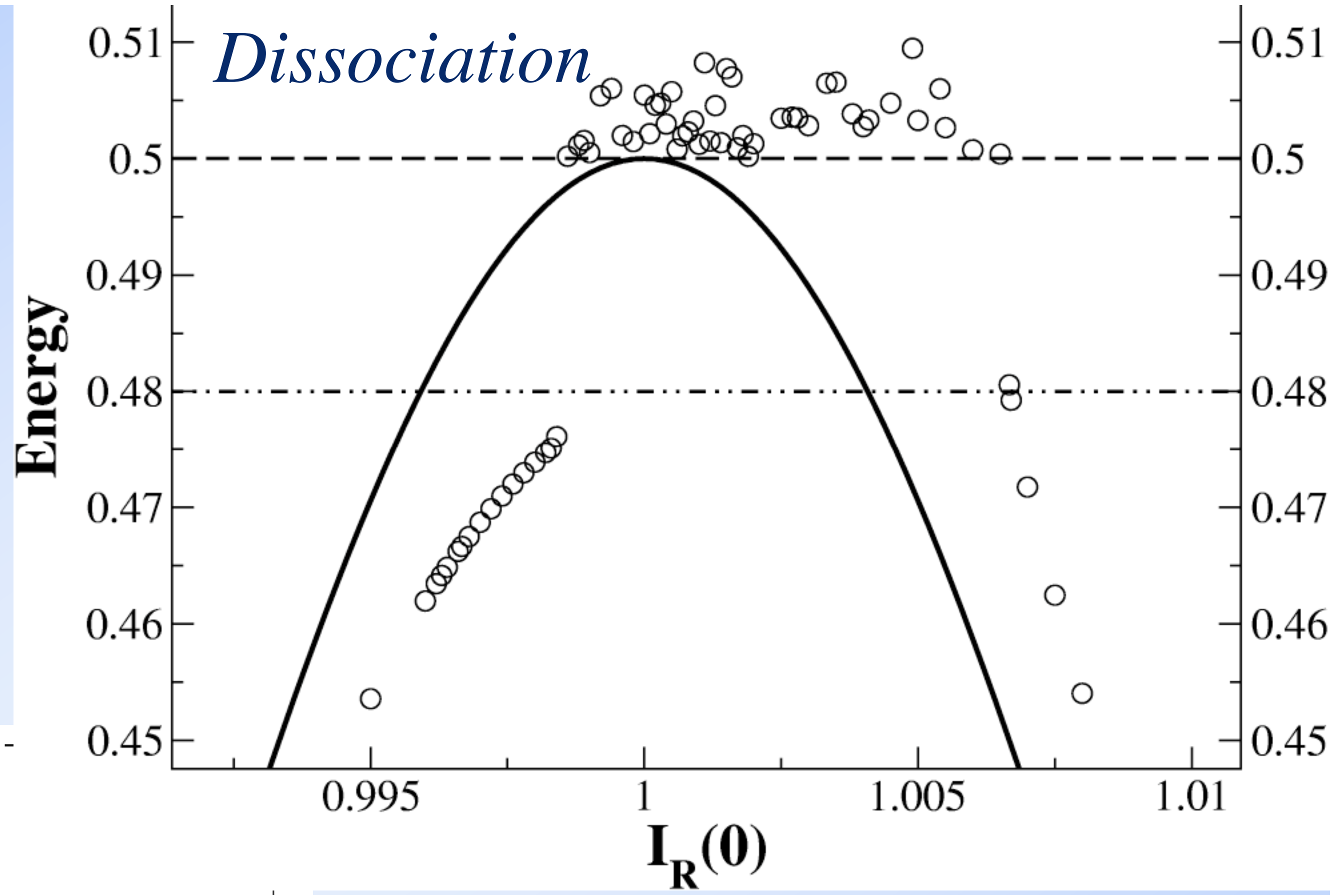
Longer term behavior: Fast Chemical Dissociation

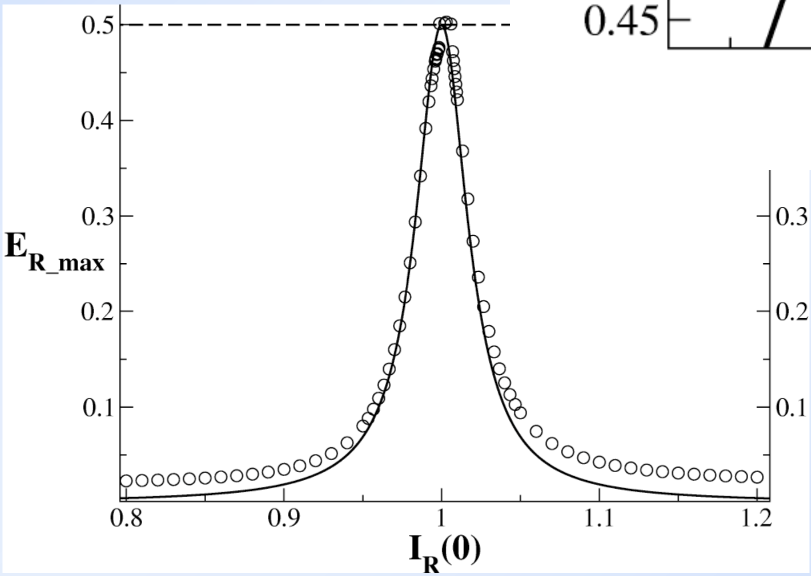
This chemical reaction is fast and work at low temperature

Usual models in Chemistry require a Brownian exploration of the phase space due to thermal noise which is slow and ineffective at low temperature



Time scale picosecond





Tip Magnification

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Targeted energy Transfer by Fermi resonance (resonance by harmonics)

The harmonic n_D of a nonlinear oscillator D is resonant with the harmonics n_A of the rest frequency of another nonlinear oscillator A.

Then nonlinearities can be tuned for having targeted energy transfer

$$\mathcal{H} = H_{\mathrm{D}}(I_{\mathrm{D}}) + H_{\mathrm{A}}(I_{\mathrm{A}}) + \lambda H_{\mathrm{V}}(I_{\mathrm{D}}, I_{\mathrm{A}}, \theta_{\mathrm{D}}, \theta_{\mathrm{A}})$$

Canonical transformation

$$\begin{pmatrix} \theta \\ \theta_0 \end{pmatrix} = \begin{pmatrix} n_{\mathrm{D}} & -n_{\mathrm{A}} \\ n_{\mathrm{A}} & n_{\mathrm{D}} \end{pmatrix} \cdot \begin{pmatrix} \theta_{\mathrm{D}} \\ \theta_{\mathrm{A}} \end{pmatrix}$$

$$\begin{pmatrix} I \\ I_0 \end{pmatrix} = \frac{1}{n_{\mathrm{D}}^2 + n_{\mathrm{A}}^2} \begin{pmatrix} n_{\mathrm{D}} & -n_{\mathrm{A}} \\ n_{\mathrm{A}} & n_{\mathrm{D}} \end{pmatrix} \cdot \begin{pmatrix} I_{\mathrm{D}} \\ I_{\mathrm{A}} \end{pmatrix}.$$

Morse-Rotor Model   Targeted Transfer by third order resonance

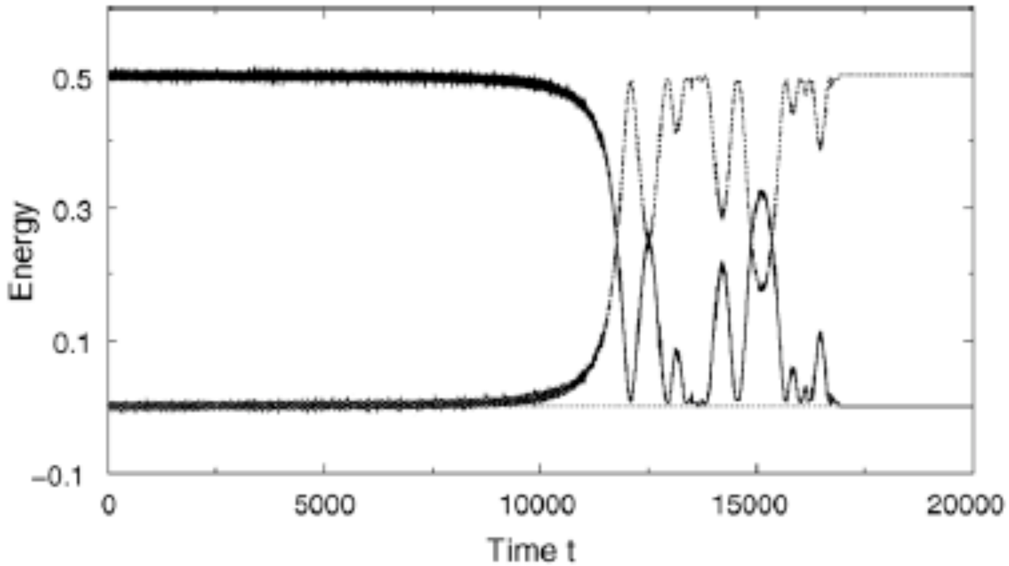

Fig. 9. Energy of the rotor (continuous line) and the Morse oscillator (thin line) vs. time for a FTET with the third harmonics ($n_M = 3$, $J_R = 1/9$) Coupling parameter is $\lambda = 7 \times 10^{-3}$. The initial conditions are $\theta_R(0) = \pi/2$, $\dot{u}(0) = 0$. $\dot{\theta}_R(0)$ and $u(0)$ are chosen in order the initial energy of the rotor is 0.999 E_F and of the Morse oscillator 0.001 E_F (the total initial energy is $E_F = 1/2$).

In ordinary chemistry, chemical reactions obey the standard Arrhenius law of chemistry
Energy barrier overcome by thermal fluctuations.
Chemical reaction are slow and stochastic (non selective)
because of the random exploration of the accessible phase space.

Biochemistry is very different because it is entirely controlled by enzymes. It is highly selective and for any chemical reaction in the cell, there is an enzyme which work for it. Those reactions are very fast and do not obey the Arrhenius law. The role of the enzyme is to depress to zero the energy barrier of a specific reaction.
Highly energetic reaction occurs with little heat generation.
Energy storage.

There is no exploration of the phase space but the use of chemical expressways.

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Ultrafast Electron Transfer (non Marcus)

Electrons (or quantum excitations) in deformable molecules=polarons

Targeted Transfer of Polarons

No Energy Barrier: Marcus Inversion point (not sufficient : Nonadiabatic model!)

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What is a polaron?

$$H = \Sigma_n (E_0 - k\, u_n)\ |\psi_n|^2 + 1/2\, u_n^{\,2} + 1/2\, p_n^{\,2}$$
$$-\Sigma_{<n,m>} C\,(\psi_n \psi_m^* + \psi_m \psi_n^*)$$
$$\Sigma_n |\psi_n|^2 = 1$$

Special localized solutions at C=0:

$\psi_n = 0$ except $n=0$ $\psi_0 = 1$

$u_n = 0$ except $n=0$ $u_n = k$

It is the ground state

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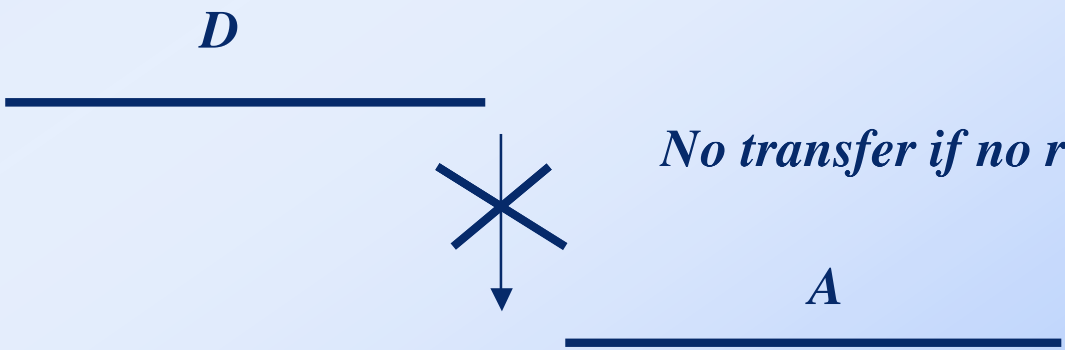
Chemical reactions corespond a reorganisation of the chemical bonds that is to electron transfers

The most elementary chemical reaction is an electron transfer.

Electrons are charged and strongly coupled to the ions.

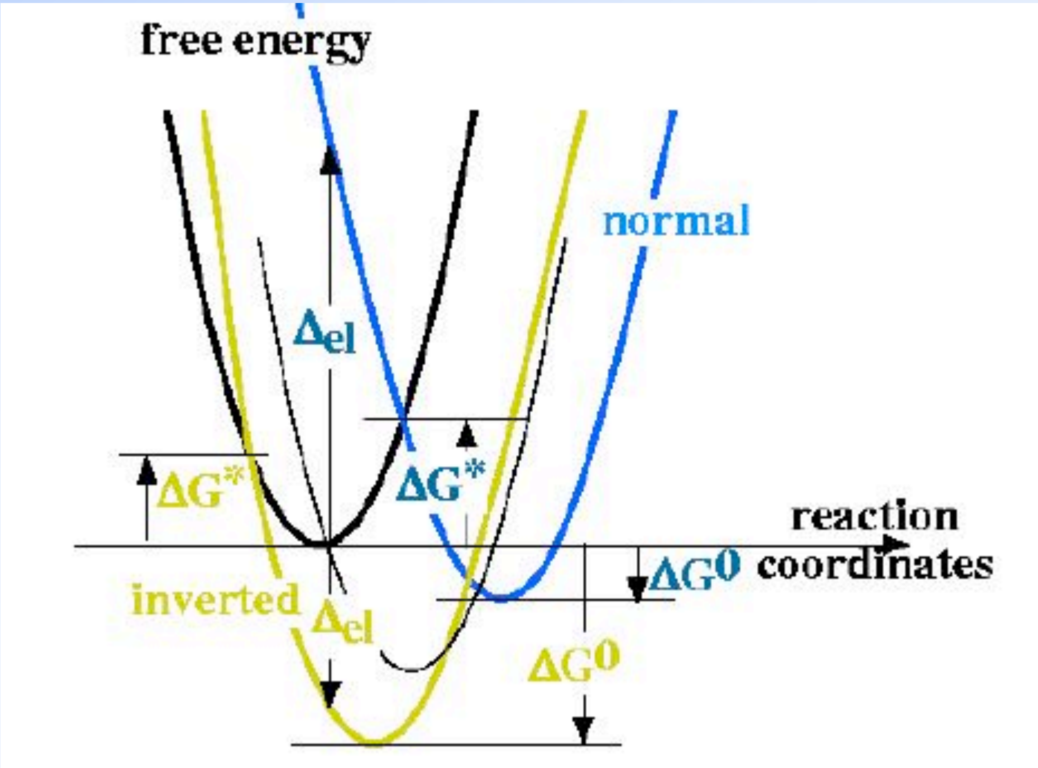
An electron+deformation is a polaron which is a nonlinear object similar to DBs



No transfer if no resonance

Standard Marcus Theory for Electron Transfer in Chemistry (adiabatic theory)

A two states system coupled to a phonon bath



Free energy versus Reaction Coordinates for several redox potentials: in the normal regime and the inverted regime

Electron transfer at (linear) resonance

The adiabatic approximation is not valid close to the inversion point because the characteristic electronic frequency Δ_{el} becomes of the order of the phonon frequencies $\hbar\omega_{ph}$.

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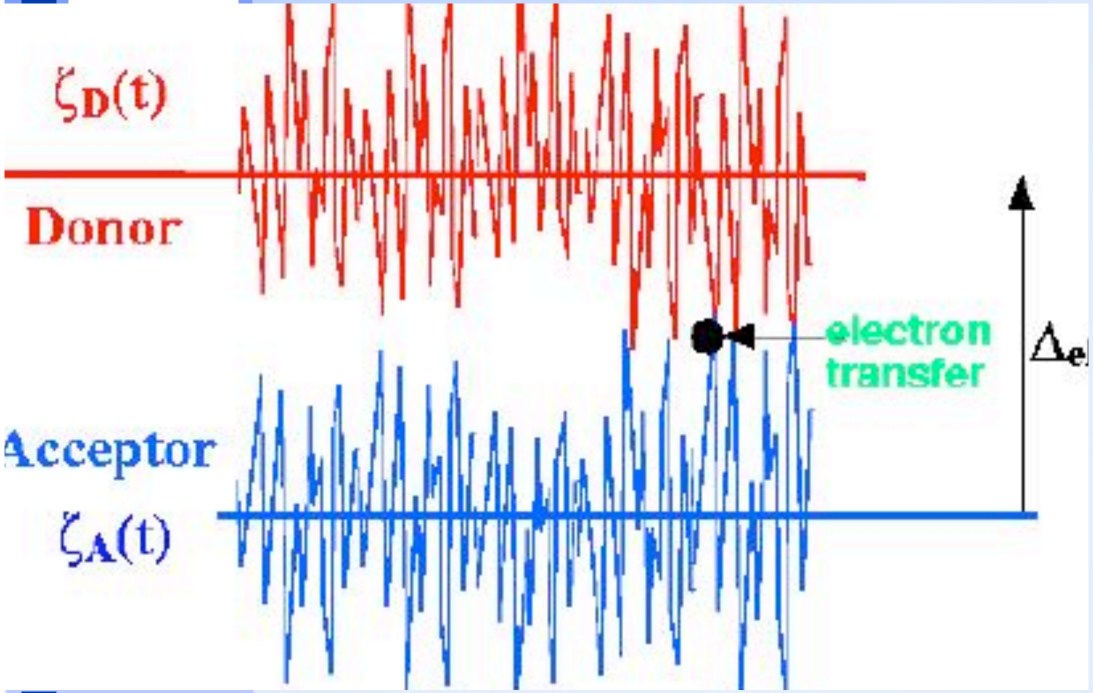
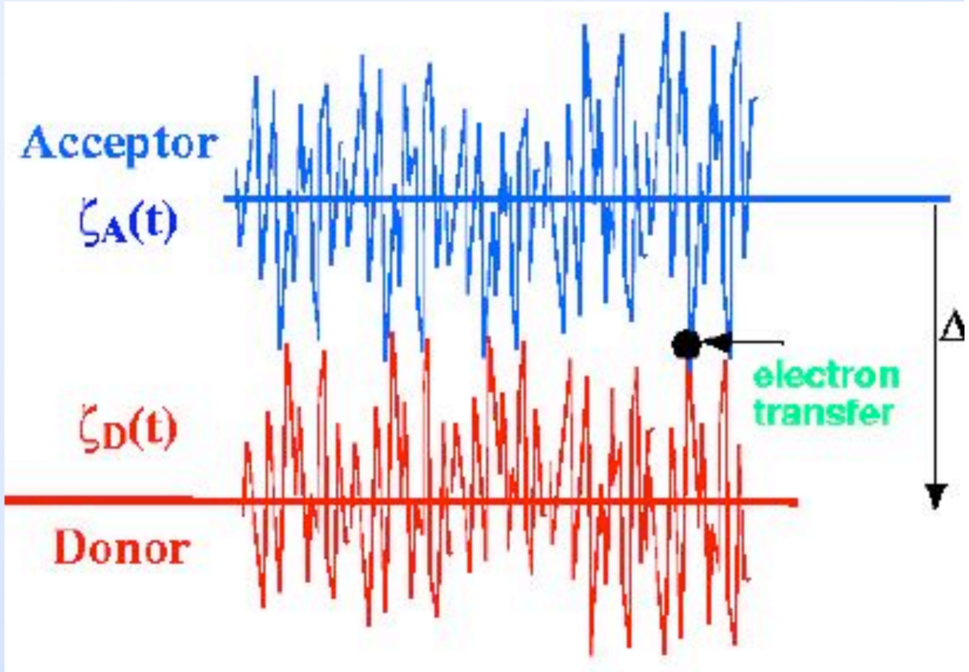


Inverted



Normal

Electron (polaron) transfer occurs by quantum tunneling of the electron when the thermal fluctuations of the environment brings the system at the top of the energy barrier (Peierls-Nabarro energy barrier) where the electronic eigenenergies are degenerate.

Standard formula for the reaction characteristic time :Arrhenius law with prefactor

$$A(T)\exp -\frac{E_{PN}}{k_B T}$$

A nonadiabatic model for electron transfer

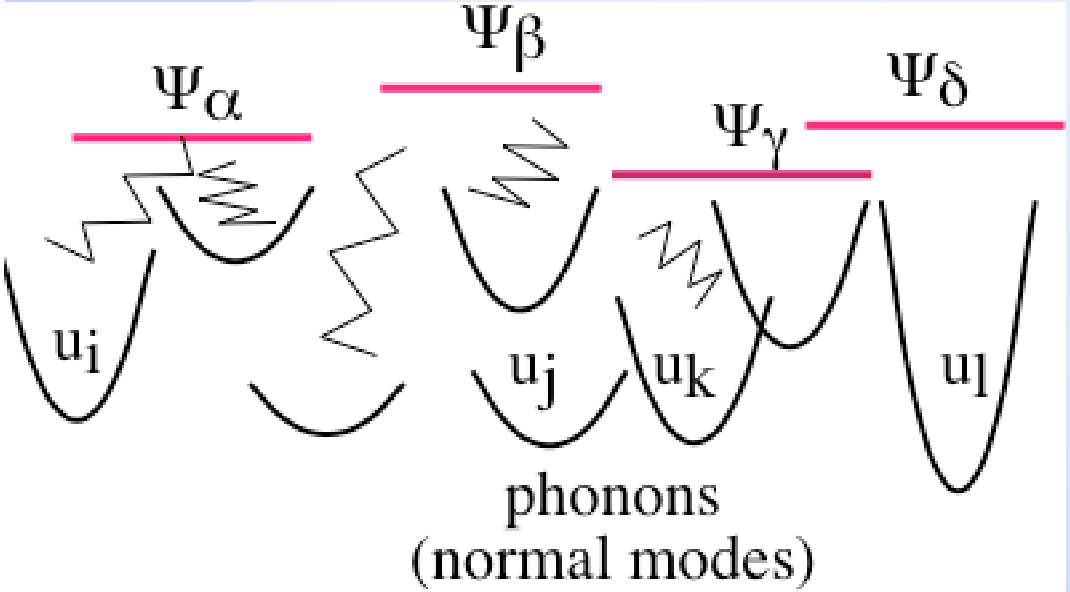
$$\mathbf{H} = H_T(\{\Psi_\alpha\}) + H_{ph}(\{|\Psi_\alpha|^2, u_i, p_i\})$$

Quantum electrons
Classical lattice

$$H_T(\{\Psi_\alpha\}) = \min_{\{u_i,p_i\}} \mathbf{H}(\{|\Psi_\alpha|^2, u_i, p_i\})$$

Anti-adiabatic Hamiltonian

$$H_{ph}(\{|\Psi_\alpha|^2, u_i, p_i\}) = \sum_i \left[\frac{1}{2m_i}p_i^2 + \frac{1}{2}m_i\omega_i^2\left(u_i - \sum_\alpha k_{i,\alpha}|\Psi_\alpha|^2\right)^2\right]$$



Harmonic normal modes coupled linearly to electronic densities on different orbitals

$$\sum_\alpha |\Psi_\alpha|^2 = 1$$

The antiadiabatic electronic Hamiltonian includes all electrostatic interactions and is anharmonic.

$$i\hbar\dot{\Psi}_\alpha = \frac{\partial H_T}{\partial \Psi^\star_\alpha} - \sum_i m_i \omega_i^2 k_{i,\alpha}(u_i - \sum_\beta k_{i,\beta}|\Psi_\beta|^2)\Psi_\alpha$$

$$\ddot{u}_i + \omega_i^2(u_i - \sum_\alpha k_{i,\alpha}|\Psi_\alpha|^2) = 0$$

$$u_i(t) = u_i^{(r)}(t) + u_i^{(n)}(t)$$

$$u_i^{(n)} = \lambda_i \cos(\omega_i t - \xi_i)$$

$$u_i^{(r)}(t) = \sum_\alpha k_{i,\alpha}\omega_i \int_{-\infty}^t |\Psi_\alpha(\tau)|^2 \sin\omega_i(t-\tau)d\tau$$

$$= \sum_\alpha k_{i,\alpha}\left(|\Psi_\alpha(t)|^2 - \int_{-\infty}^t \frac{d|\Psi_\alpha(\tau)|^2}{d\tau}\cos\omega_i(t-\tau)d\tau\right)$$

$$i\hbar\dot{\Psi}_\alpha = \frac{\partial H_T}{\partial \Psi_\alpha^\star} + \left(\int_{-\infty}^{t} \left(\sum_\beta \Gamma_{\alpha,\beta}(t-\tau)\frac{d|\Psi_\beta(\tau)|^2}{d\tau}\right)d\tau + \zeta_\alpha(t)\right)\Psi_\alpha$$

$$\Gamma_{\alpha,\beta}(t) = \sum_i m_i\omega_i^2 k_{i,\alpha}k_{i,\beta}\cos\omega_i t$$

Memory function

Cut-off at Debye frequency

$$\zeta_\alpha(t) = -\sum_i m_i\omega_i^2 k_{i,\alpha}u_i^{(n)}(t)$$

Random force

(effect of temperature)

Langevin relationship

$$<\zeta_\alpha(t+\tau)\zeta_\beta(t)>= k_B T\ \Gamma_{\alpha,\beta}(t)$$

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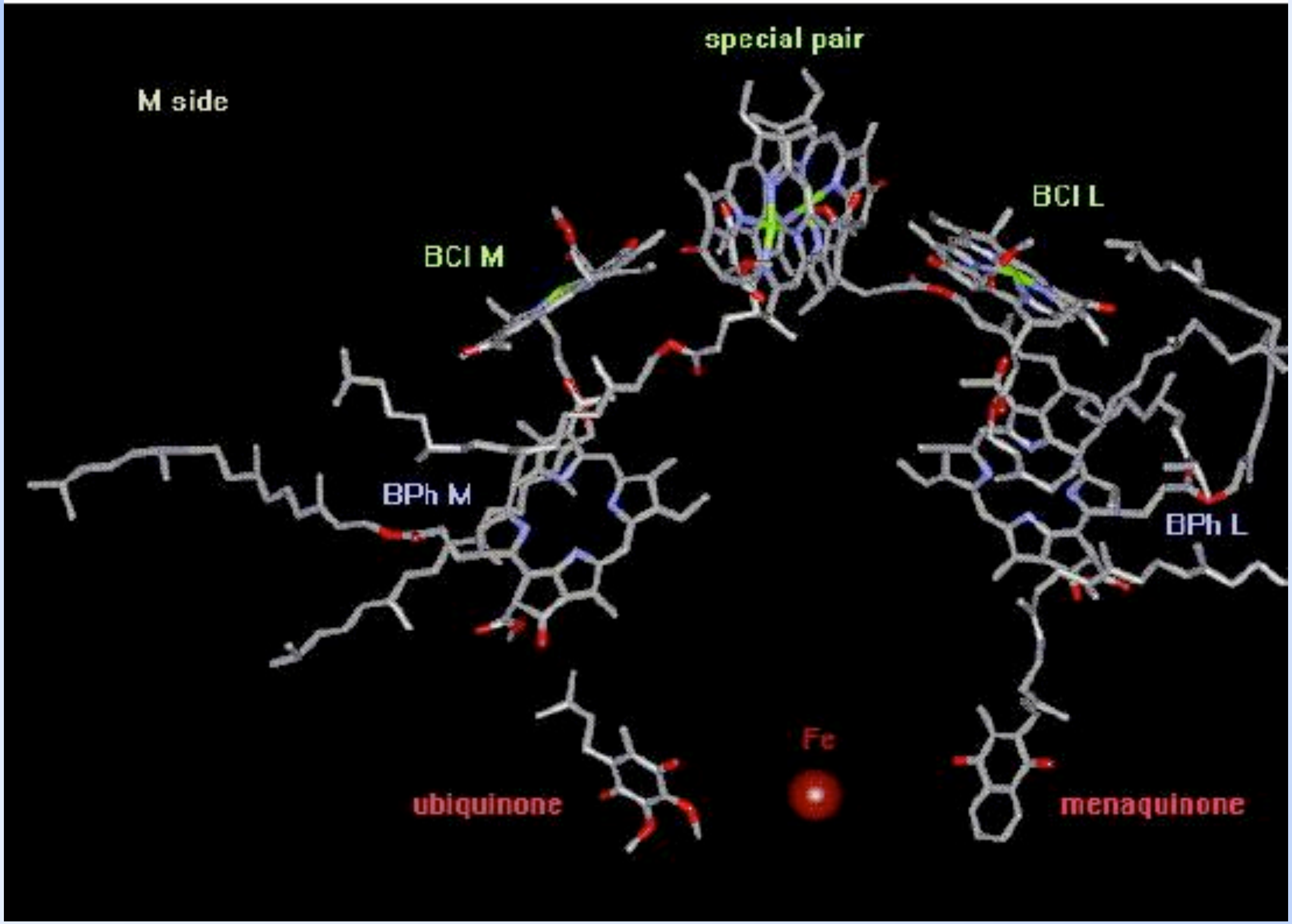

The photosynthetic reaction center

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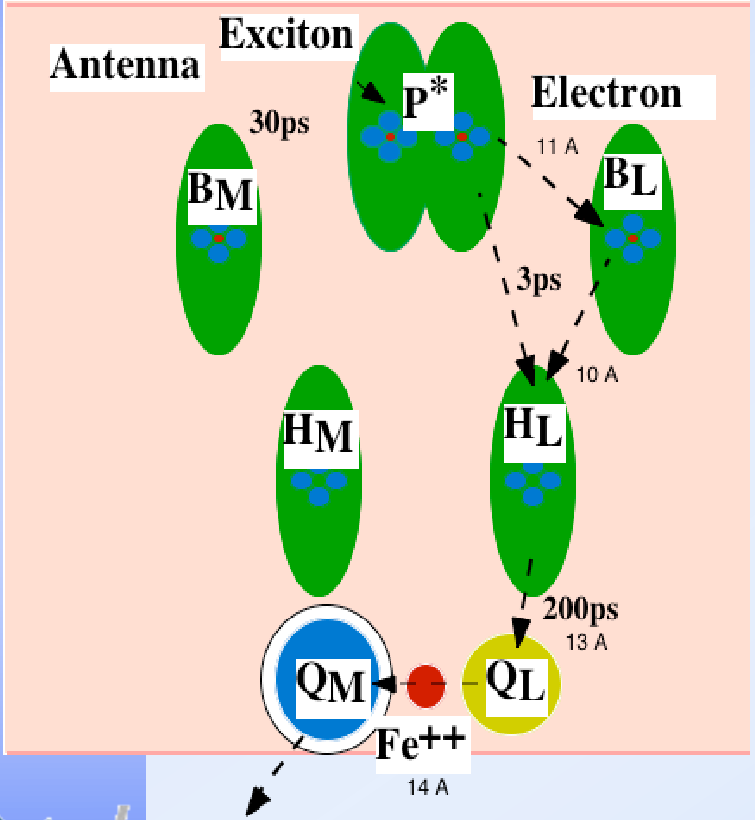
Ultrafast electron transfer in the Reaction Center:



- An exciton arrives at the bacteriochlorophyll Bchl dimer (P) $\mathbf{P} \rightarrow \mathbf{P}^*$
- An electron is transfered from $\mathbf{P}^*$ to at Bacteriopheophitin BPhea (H_L) within a half-time of 3 ps over a relatively long distance (P-H)= 17Å).
  Charge separation is stable for a few ns.
  $\mathrm{P}^*\ \mathrm{H}_L \rightarrow \mathrm{P}^+\ \mathrm{H}_L^-$
- This ultrafast ET requires the participation of the ancil-iary bacteriochlorophyll BChla (B_L), but its exact role is controversial

- High efficiency: almost 100%
- ET is **faster at low temperature** $\approx$ **1ps**
- ET is highly sensitive to certain mutations of the involved molecules and to electric field
- ET is selective among to two almost identical paths

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Simplified Model: distant sites

$$H_T(\{\Psi_\alpha\}) = \sum_\alpha H_\alpha(|\Psi_\alpha|^2) + \sum_{\alpha,\beta} \lambda_{\alpha,\beta}(\Psi_\alpha^\star \Psi_\beta + \Psi_\alpha \Psi_\beta^\star)$$

Transfer integral $\lambda_{\alpha,\beta}$ *small*

$$H_\alpha(|\Psi_\alpha|^2) = \mu_\alpha |\Psi_\alpha|^2 + \frac{1}{2}\chi_\alpha |\Psi_\alpha|^4$$

Electronic level μ_α

Nonlinear term $\chi_\alpha = \chi_\alpha^R + \chi_\alpha^C$

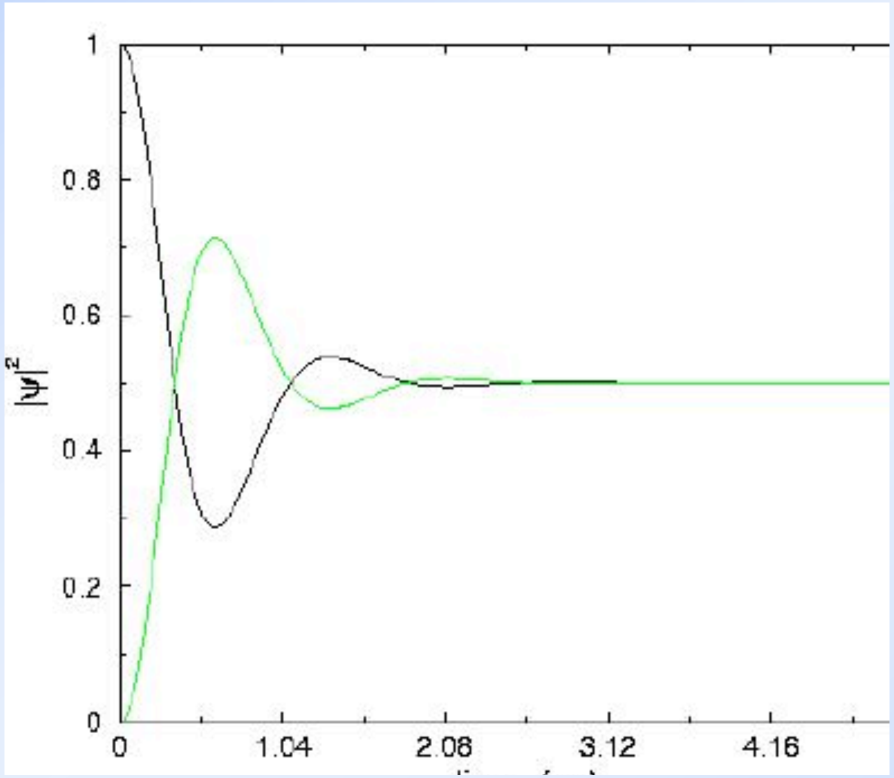
$\chi_\alpha^R = -\Sigma_\alpha m_i \omega_i^2 k_{i,\alpha}^2 < 0$ *reorganization energy*

$\chi_\alpha^C > 0$ *capacitive energy*

Catalytic Electron Transfer with a third site C

Assume $\chi_D + \chi_C = 0$ *and* $\mu_D + \chi_D = \mu_C$

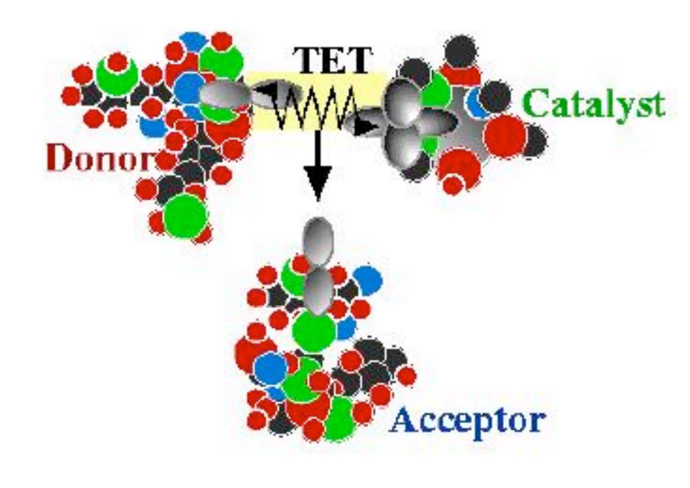
Transfer is fast from D to C but reversible (almost zero reaction energy). Slow electron oscillations

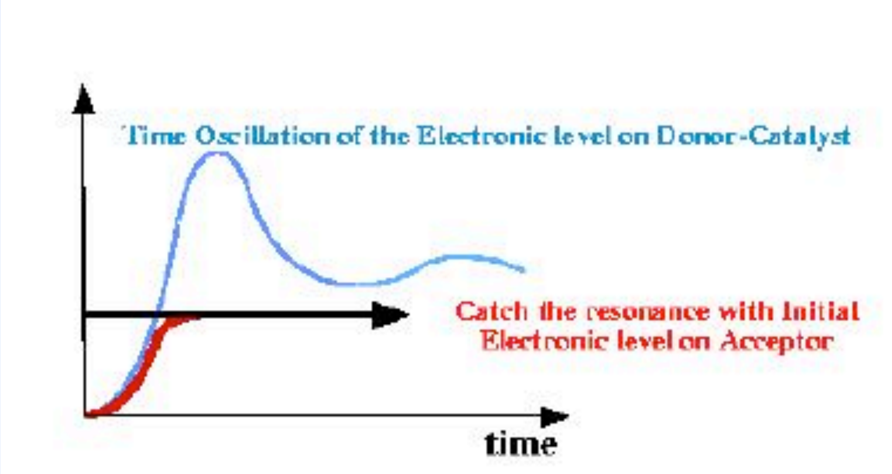


$$\mu_D = 2, \chi_D = -1, \mu_C = 1., \chi_C = -1., \lambda_{CD} = 10^{-2}, \gamma_D = \gamma_C = 1.$$

Coherent Electron-Phonon Oscillator: CEPO

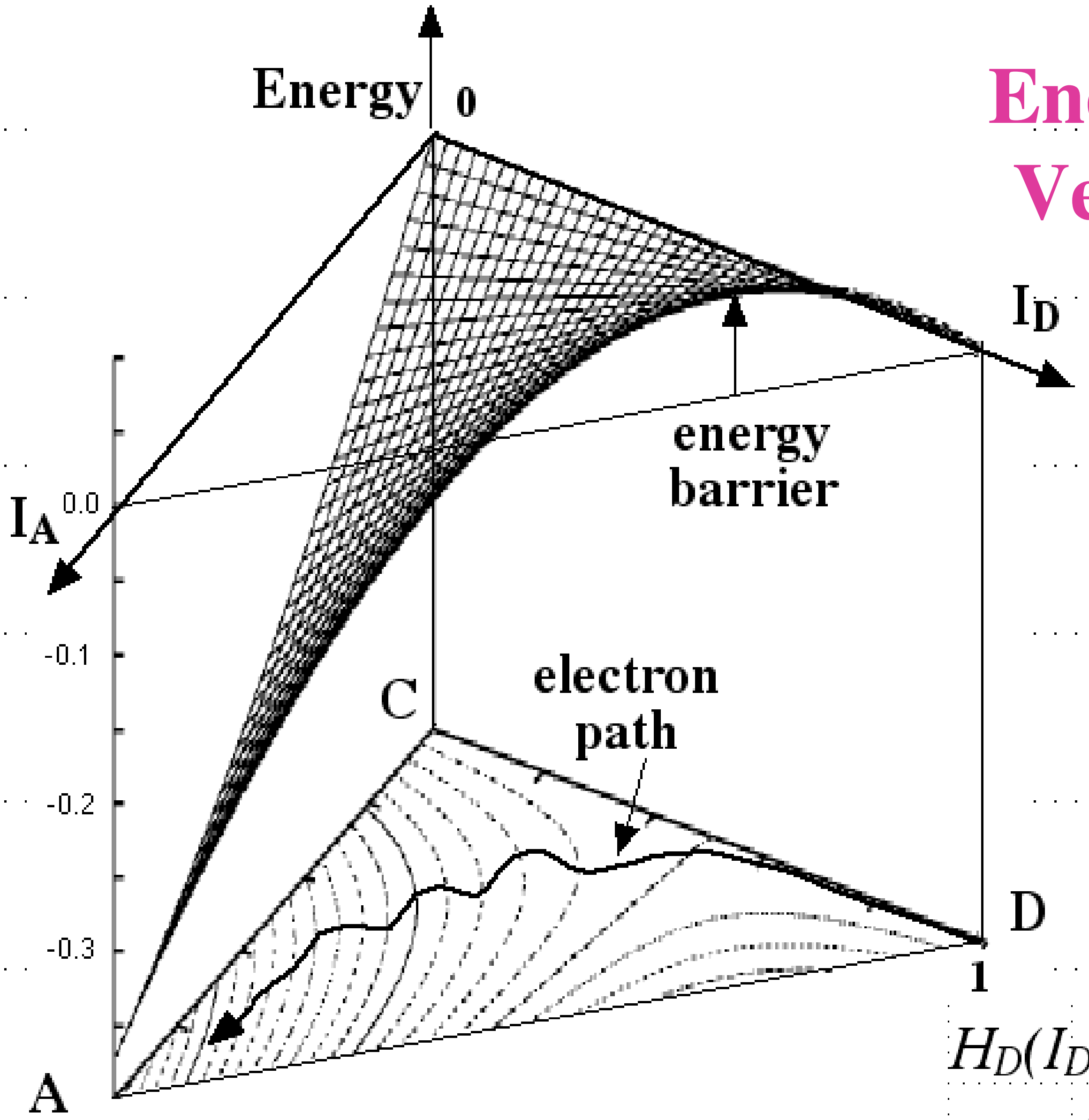
The electronic level oscillates as a function of time



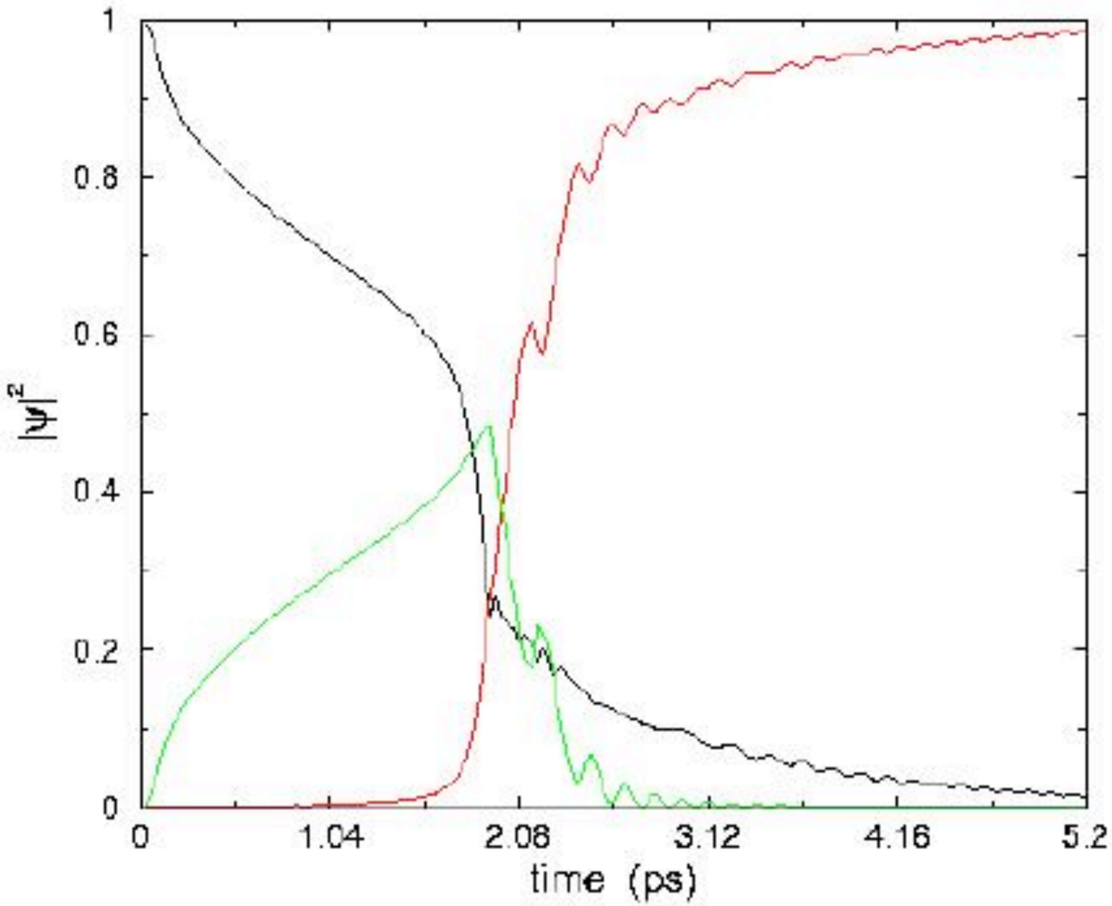


Without Catalyst: No ET possible at zero K from Donor to Acceptor.
Electron Transfer to the Acceptor is trigerred by the Catalyst.

Energy variation Versus transfer



$$H_D(I_D)+H_A(I_A)+H_C(1-I_D-I_A)$$
$$-H_D(1)-H_A(0)-H_C(0)$$
$$0\leq I_D\leq 1,\ 0\leq I_A\leq 1,\ I_D+I_A\leq 1$$



Electron density versus time on the Donor, Catalyst and Acceptor of the trimer model for $\mu_D = 2$, $\chi_D = -1$, $\mu_C = 1$, $\chi_C = 1$, $\mu_A = 1.5$, $\chi_A = -0.75$, $\lambda_{AD} = \lambda_{AC} = \lambda_{CD} = 10^{-2}$, $\gamma_D = \gamma_A = \gamma_C = 10$.

Note: The undamped trimer model is nonintegrable and chaotic.

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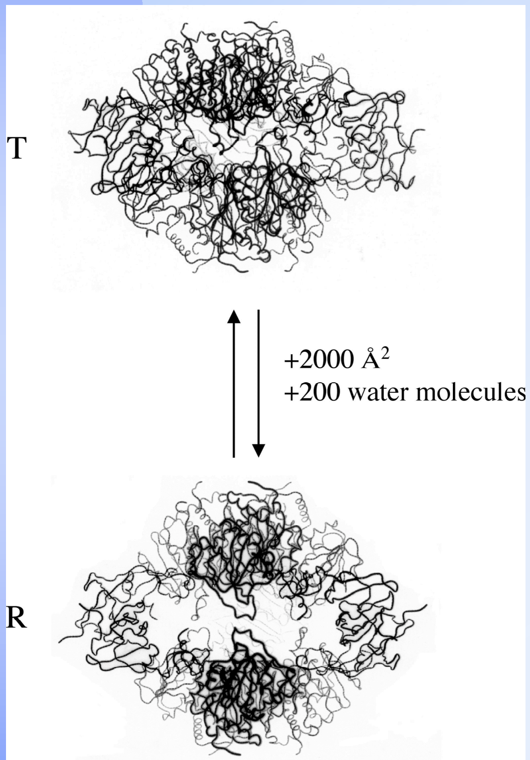
Extension of CEPO to many sites

ATcase the binding of small molecules trigger a huge change of conformation



Model: Electromechanical signal transmission

there is a highly mobile polaron along a chain of selected sites which fastly moves by electric field and change the protein conformation

Signal Transmission-Control
in allosteric enzymes

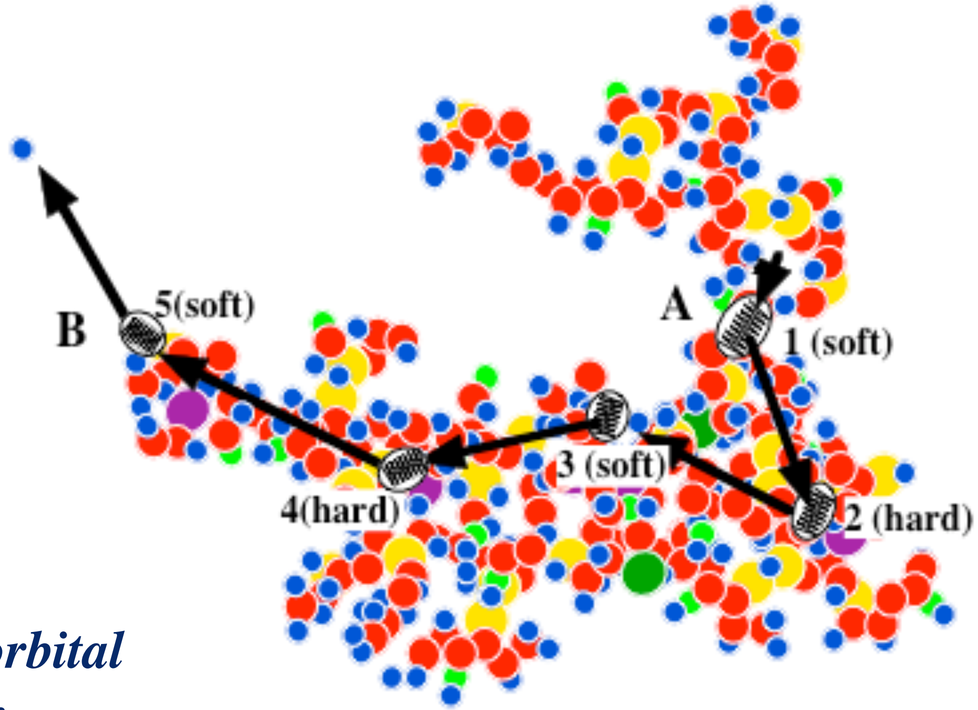
An almost degenerate path in the phase space (chemical expressway)

$$\{I_i(x)\}$$

$$\frac{\partial H_1}{\partial I_1} = \frac{\partial H_2}{\partial I_2} = ... = \frac{\partial H_p}{\partial I_p}$$

Eg. For polarons $I_i = \rho_i$

A small electrostatic change (e.g at one end) may induce large BARRIERLESS displacement of an electronic charge associated with large atomic reorganisation (eg. till the other end « ELECTROMECHANICAL SIGNAL TRANSMISSION »



Assumption: The highest occupied molecular orbital Is a polaron in Targeted transfer along a chain Of sites

Microtubule Motors:

Kinesins belong to a large family of motor proteins, most of which walk along microtubules **toward the plus end**, away from the centrosome

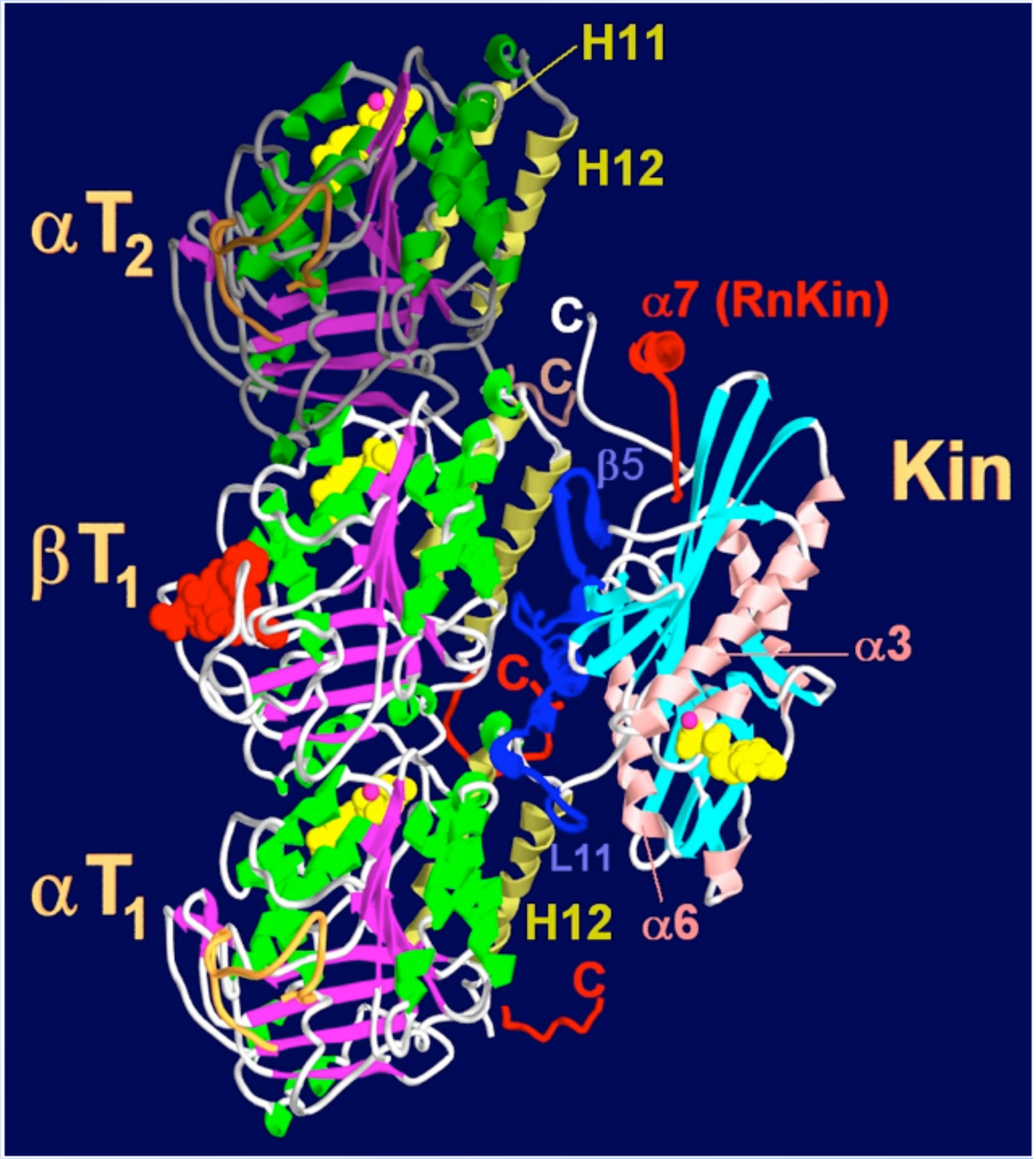
Cargo for vesicules or mitochondria which are too big to diffuse

Dyneins are other motor proteins most of which walk along microtubules **toward the minus end** (toward the centrosome).

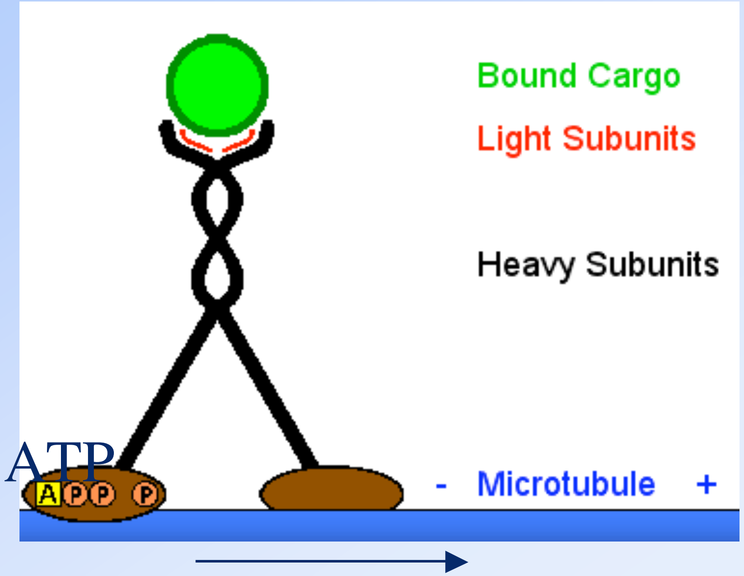
(Microtubules are polar $\Rightarrow$ Motion Directionality)

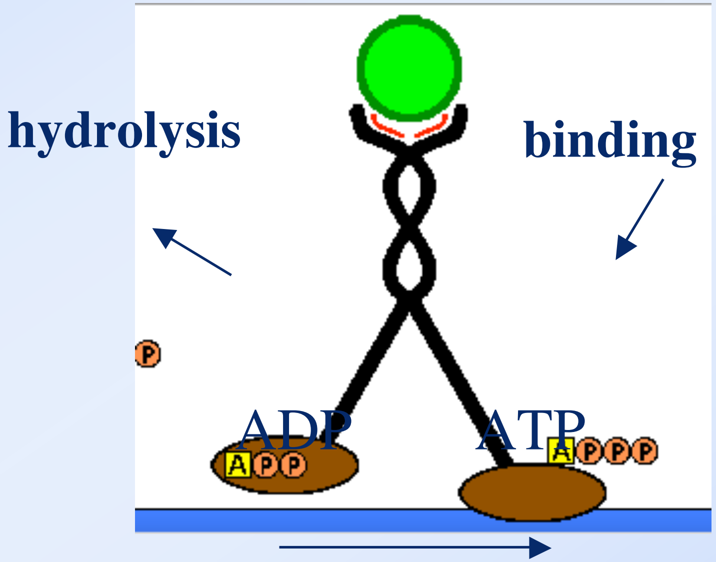
Kinesin bound
on microtubule

Microtubules
are polar chains

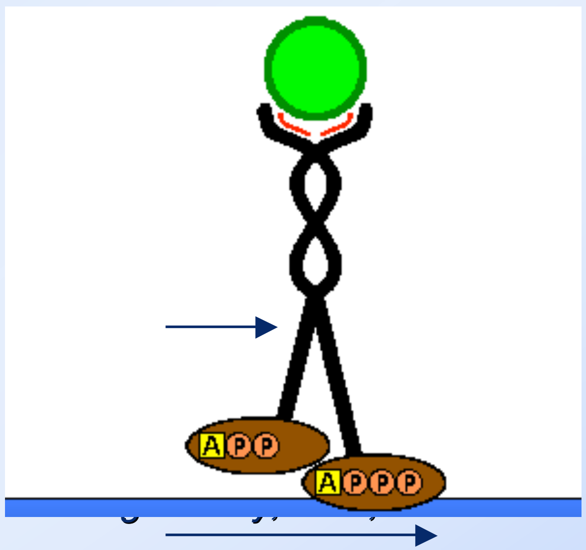


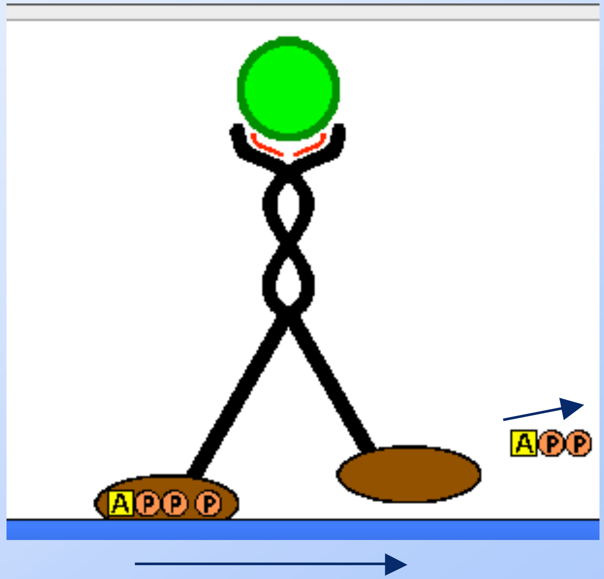
Walking Kinesin





ATP binding and Hydrolysis generates
Conformational changes which result into Motion





Molecular Motion is a consequence of the sequence of **Molecular Reorganisation** induced by a specific chemical reaction (e.g. ATP hydrolysis) **catalysed** by this molecule (biomotor).
Note the catalytic effect requires fine tuning of parameters so that small variations of the environment could induce small variations of parameters which could block the catalyst (control of the biomotor).

Efficiency in energy conversion could be close to 100%!
but thermal fluctuation (Brownian forces) reduces this efficiency

Forget first about the molecular complexity and the various molecules and situations

Goal: Make first a simple Model where we show that this is possible in principle

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A simple model for biomotors

The Catalyst is strongly coupled to one or few degrees of freedom

$$\begin{aligned} H(\{\psi_\alpha\}) = & \mu_D|\psi_D|^2 + \frac{1}{2}\chi_D|\psi_D|^4 \\ & + \mu_A|\psi_A|^2 + \frac{1}{2}\chi_A|\psi_A|^4 \\ & + \mu_C|\psi_C|^2 + \frac{1}{2}\chi'_C|\psi_C|^4 \\ & - \sum_{\alpha\neq\beta} \lambda_{\alpha\beta}\psi^\star_\alpha\psi_\beta \\ & - k(r_1 - r_2 - a)|\psi_C|^2 + \frac{K}{2}(r_1 - r_2 - a)^2 + V(r_1) + V(r_2) \end{aligned}$$

Donor D, Acceptor A   C Catalyst and motor

We couple our model for UET to a deformable molecule on a ratchet

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$$i\dot{\psi}_D = \mu_D \psi_D + \chi_D |\psi_D|^2 \psi_D - \sum_{\alpha \neq D} \lambda_{\alpha D} \psi_\alpha$$

$$i\dot{\psi}_A = \mu_A \psi_A + \chi_A |\psi_A|^2 \psi_A - \sum_{\alpha \neq A} \lambda_{\alpha A} \psi_\alpha$$

$$i\dot{\psi}_C = \mu_C \psi_C + \chi'_C |\psi_C|^2 \psi_C - k(r_1 - r_2 - a)\psi_C - \sum_{\alpha \neq C} \lambda_{\alpha C} \psi_\alpha$$

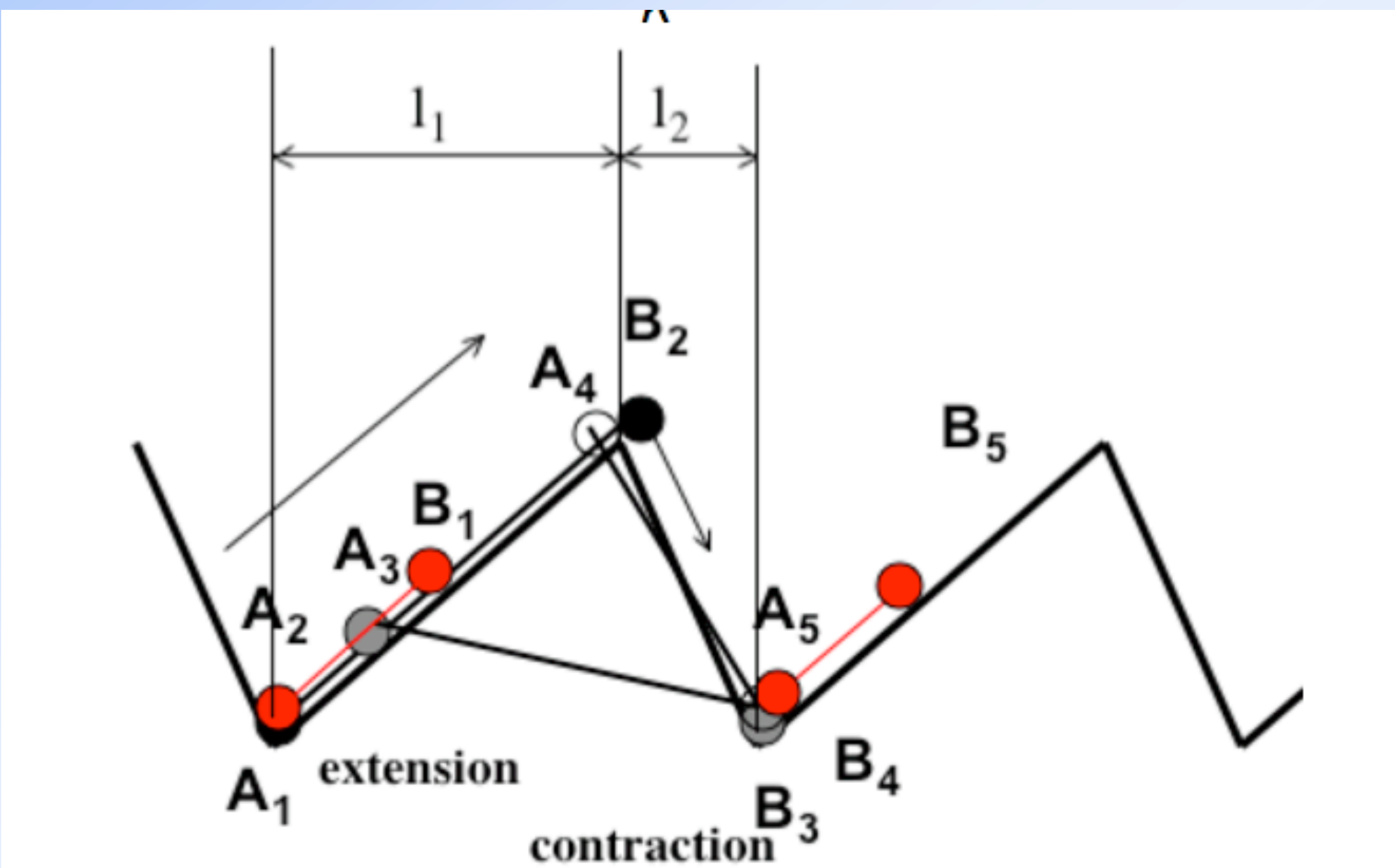
$$\dot{r}_1 = -\gamma \left(-k|\psi_C|^2 + K(r_1 - r_2 - a) + V'(r_1) \right)$$

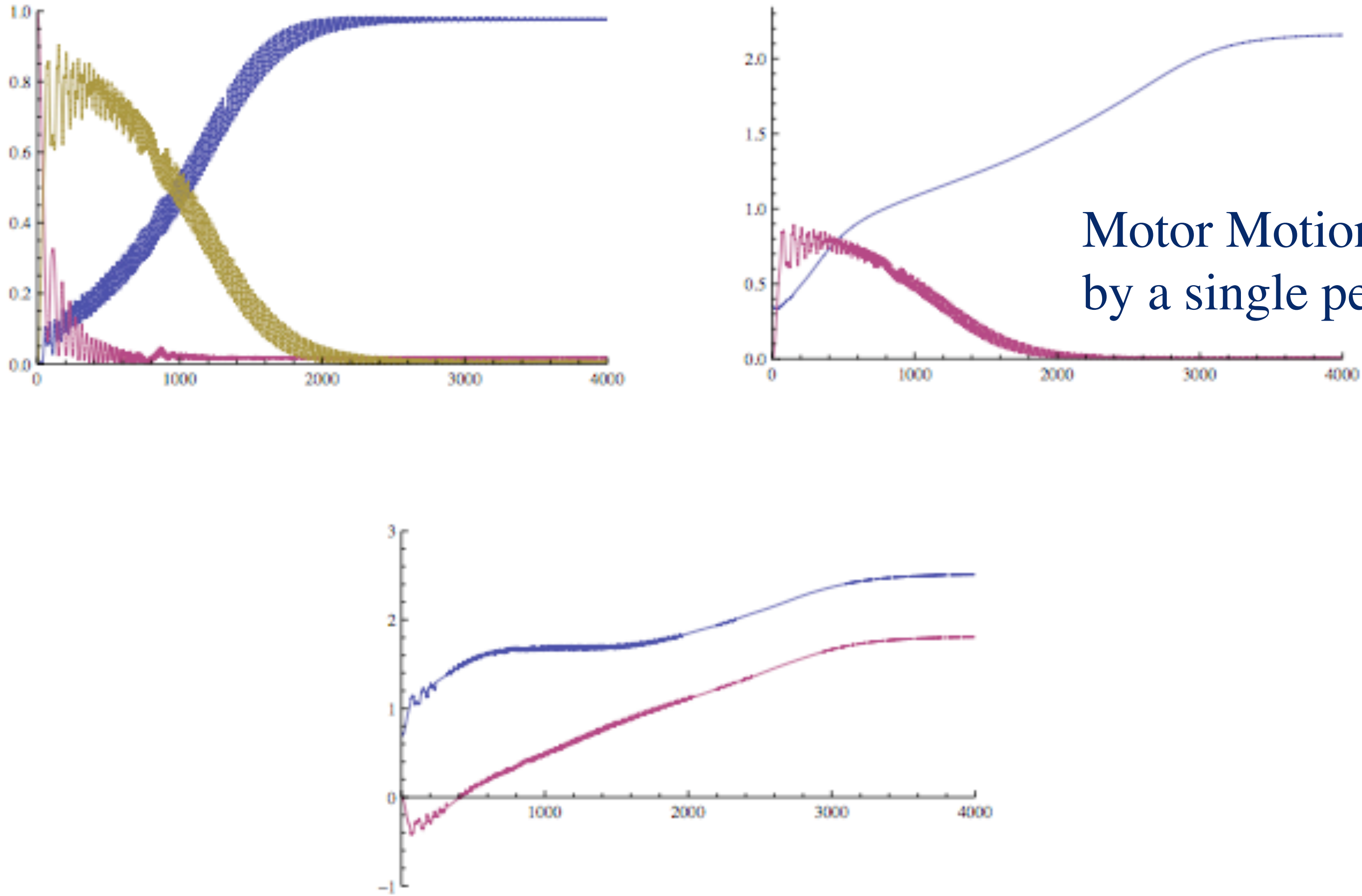
$$\dot{r}_2 = -\gamma \left(k|\psi_C|^2 - K(r_1 - r_2 - a) + V'(r_2) \right)$$

The motion of the molecule is overdamped

No extra damping

Ratchet Mechanism





Motor Motion
by a single period

Fig. 7. a) Electron densities versus time on Donor ρ_D, Acceptor ρ_A and Motor-Catalyst ρ_C when the motor is in an intermediate regime $\gamma = 0.3, k = K = 1$ and is submitted to the ratchet potential $0.001V(x)$. b) Extension $u(t)$ versus time of the Motor-Catalyst and displacement of its center of mass $R(t)$. It moves by one period of the ratchet potential during the complete cycle. c) Motion of the two head of the molecule versus time.

Course III: Random Nonlinear Networks

1-DBs in systems with discrete phonon spectrum (random etc…)
2- Open problem: Spreading of a wave packet in random nonlinear networks with discrete linear spectrum

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Existence Proofs(?) of Intraband DBs (IDBs)

Random systems: The linear spectrum may be discrete
Anderson localization implies no phonon radiation

Numerical investigations: G. Kopidakis and SA 1999-2000
Theorem: Albanèse and Frohlich 1991

Conjecture:
1- Quasi-continuation in L_2: Each Anderson mode generates a family of IDBs with frequency in a fat Cantor set (with nonvanishing measure)
2- Continuation in L_∞: Each Anderson mode becomes an extended multiDB

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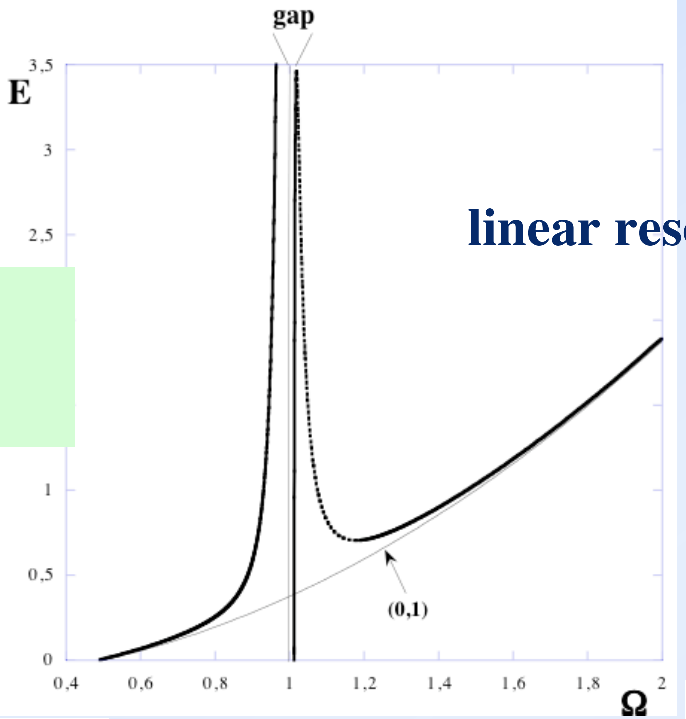
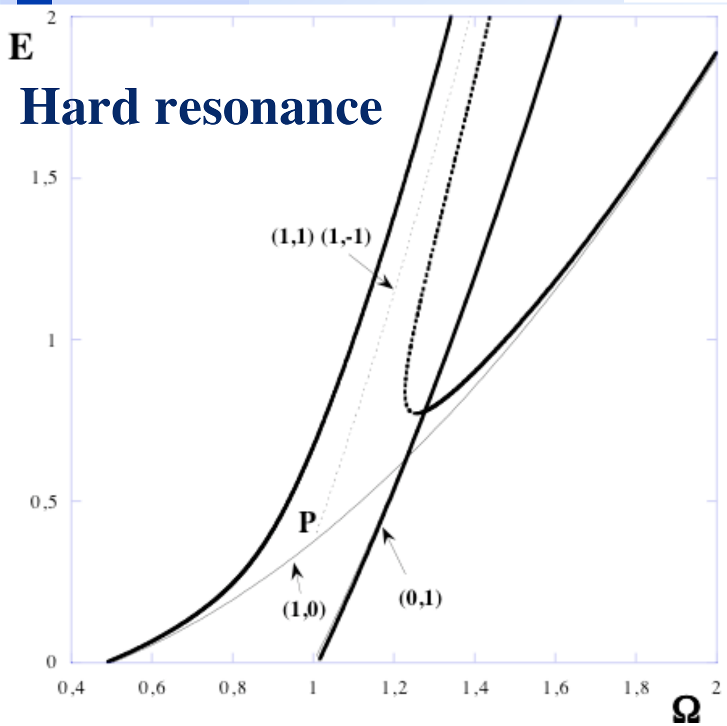
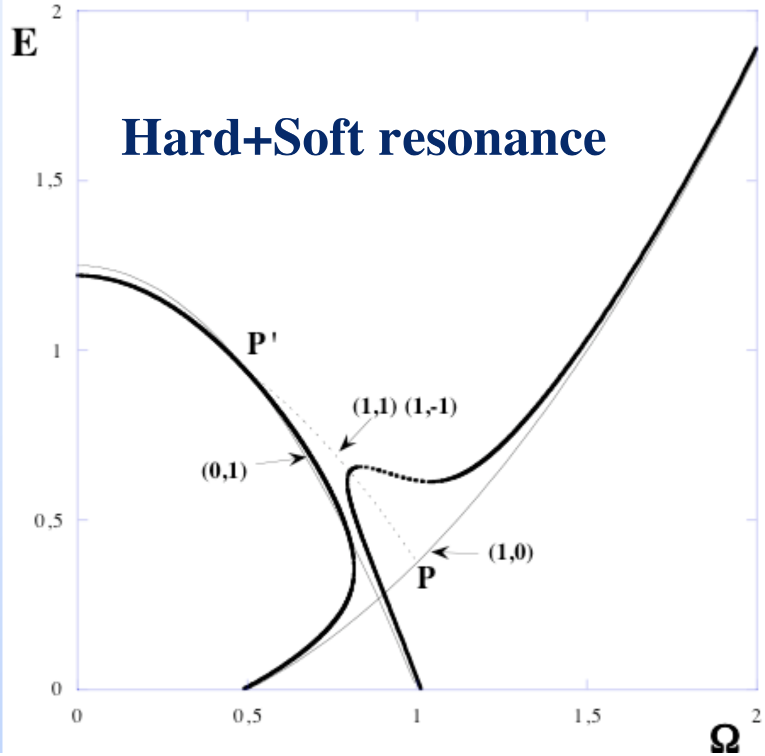
Hard DB interacting with a resonance



(exact calculation on a DNLS dimer)





Random System

$$H = \sum_i \left(\frac{\dot{u}_i^2}{2} + \frac{\omega_{i,0}^2}{2} u_i^2 + \frac{u_i^4}{4} + \frac{C}{2} (u_{i+1} - u_i)^2 \right)$$

Study on finite size with periodic boundary conditions

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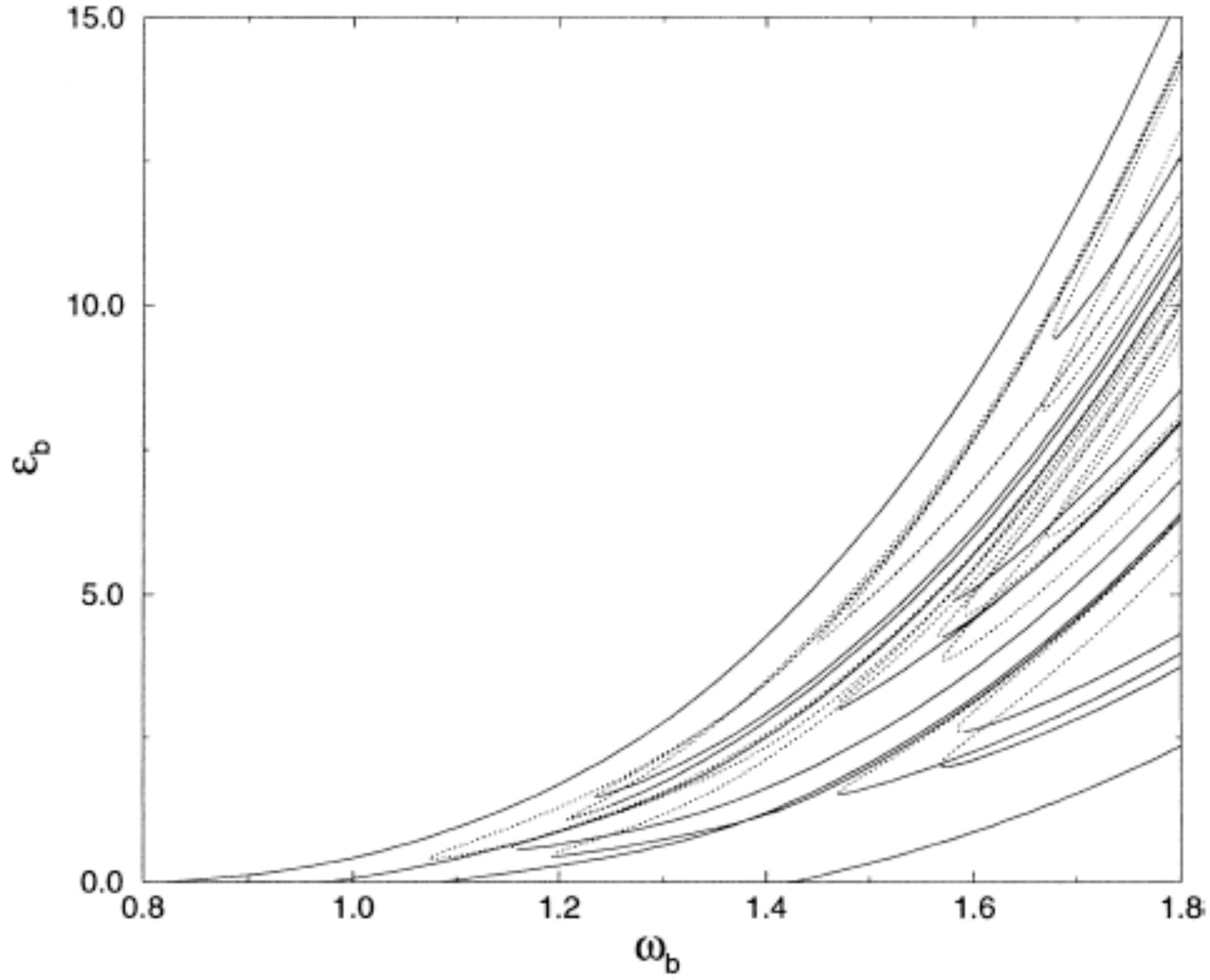

Fig. 7. Same as Fig. 5 but for a system with four sites and closed boundary conditions at $C = 0.1$. The initial local frequencies are $\omega_{1,0} = 0.75609028$, $\omega_{2,0} = 0.71504480$, $\omega_{3,0} = 1.34578317$, and $\omega_{4,0} = 0.94078505$. The frequencies of the linearized modes are $\omega_1 = 0.97307978$, $\omega_2 = 0.81573171$, $\omega_3 = 1.42488306$, and $\omega_4 = 1.08475919$.

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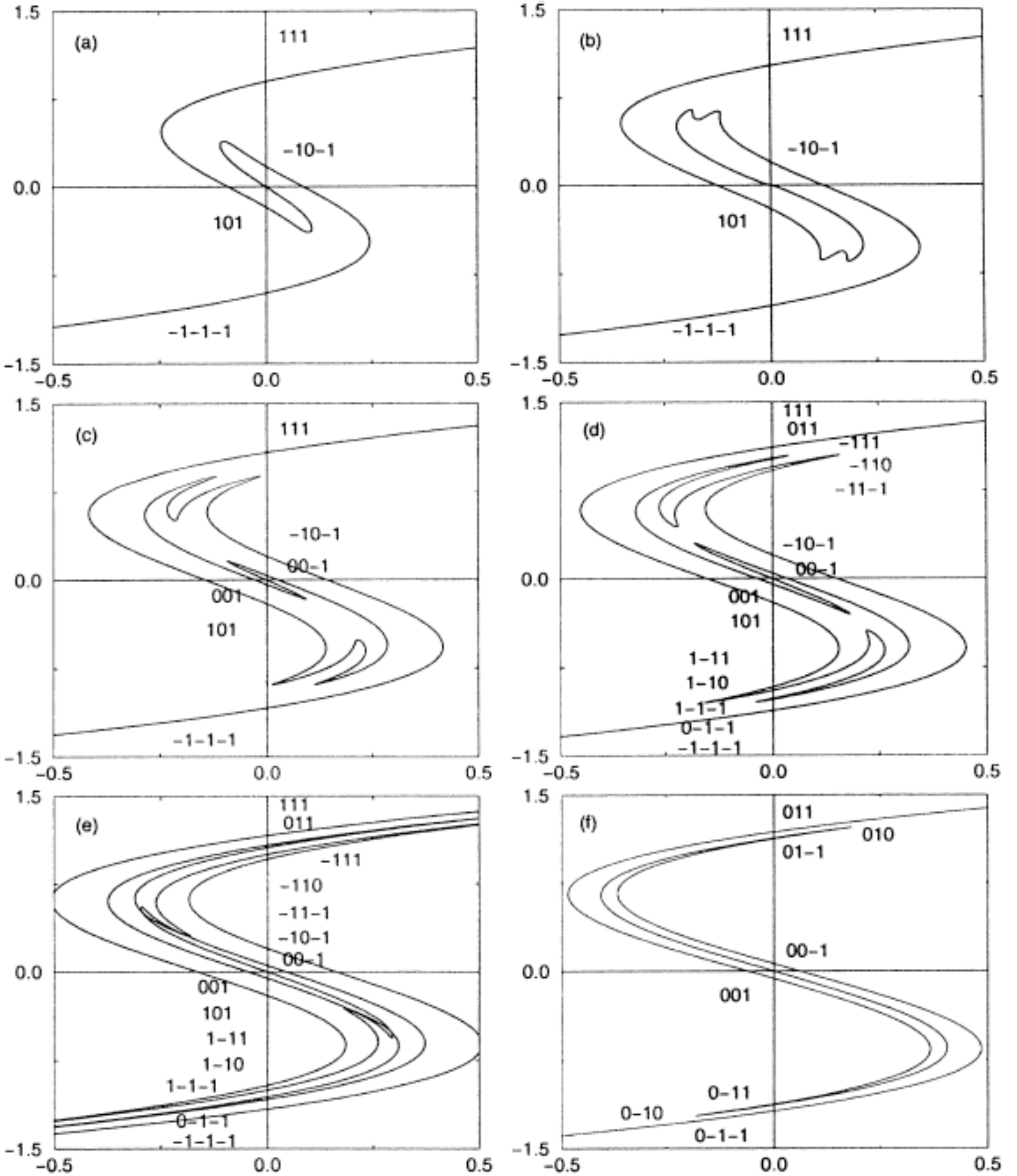
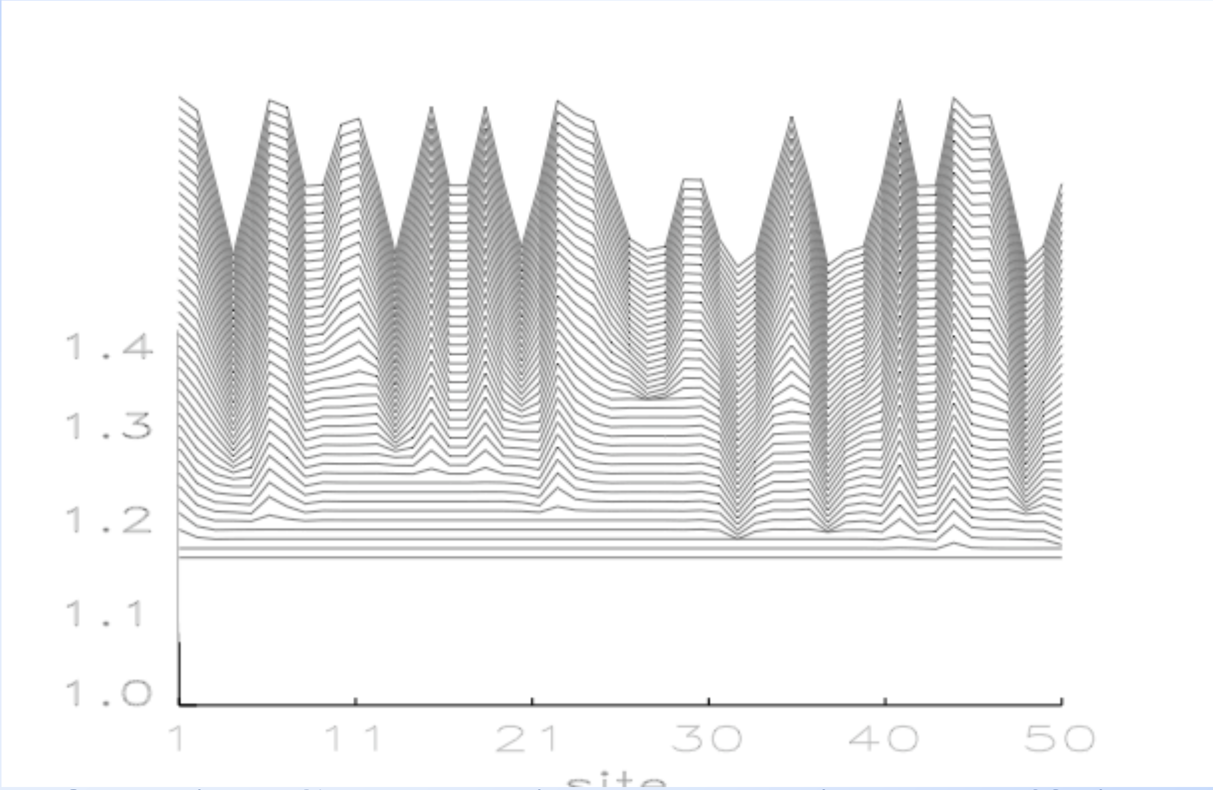


Fig. 5. Projection $(u_2(0), \lambda)$ of the NLRM with a sine force on site 2 for the three-site system described in Fig. 6 at $\omega_b = 1.08$ (a), 1.15 (b), 1.19 (c), 1.21 (d), 1.24 (e), 1.3 (f). The last curve is incomplete and only the beginning part, starting from the origin, is shown.

Anderson Mode continued as an extended multiDB with norm l_∞
(cannot be continued with norm l_2)



Quartic KG model with random linear coefficients
(G. Kopidakis S.A99)

Consequence: Nonlinearity restaures possible energy transport in models with linear discrete spectrum (at nonvanishing temperature)

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In spatially periodic systems which have an absolutely continuous linear spectrum, DBs are the only localized solutions which could be stable because they avoid linear radiation through the linear spectrum ($n\omega_b$ does not belong to the phonon spectrum for any integer n)

In nonperiodic systems where the linear spectrum is purely discrete and cannot radiate energy, this is not true.

In Systems with purely Discrete linear Spectrum, DBs are not the only spatially localized solution (l_2)

Possibility of many other localized solutions than DBs
For example: almost periodic solutions (KAM tori)
Marginal KAM tori with singular continous spectrum???

Spreading of a Wave Packet: Open questions

A FINITE ENERGY PACKET in an INFINITE SYSTEM:
« temperature 0 ». Is thermalization possible?

What is the long time behavior of an initially localized wavepacket in an infinite array of oscillators

1-Does it spread to zero amplitude (diffusion)?

2- Does it remain localized (absence of diffusion)?

3- Does a part of the energy spread and another part remains localized?

Known answers:

-Linear: **Diffusion** if the linear spectrum is **absolutely continuous** (extended eigenmodes), **no diffusion** if the spectrum is **purely discrete** **(Anderson Localization).**

-**Nonlinear** with linear absolutely continuous spectrum
Possible formation of **Discrete Breather** (Sievers and Takeno) and **partial diffusion**.

Nonlinear systems with **purely discrete** linear spectrum **.**

Most common belief on the base of numerical simulation:
The nonlinear terms couple the Anderson modes and « seems » to produce random energy transfers resulting in « subdiffusion »

The second moment of the energy distribution is expected to diverge as t^{α} with $\alpha<1$.
($\alpha=1$ for a standard diffusion or random walk)

Flaw of the numerics: Finite size and finite time,
Drastic effect of the numerical noise after long time
No universality is observed.

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Interpretation of subdiffusion:

It is assumed that because of nonlinarity, most trajectories (with probability 1) are **chaotic** and **remains so forever** (it is believed that because the system is infinite, **KAM tori are absent or negligible**).

It is assumed there is a kind of **thermalization** inside the wavepacket with broad band frequency spectrum which « heats » the cold system outside and thus spread the energy.

Subdiffusion is due to the fact the local temperature decays as the packet is spreading. The second moment behaves as t^{α}

α can be estimated with different assumptions which yields different values 1/2, 2/5, 1/3... But exponents α obtained from numerics, disagree and worst depend on system and initial conditions. α not well defined. No obvious universality!

However, KAM tori may exist in infinite nonlinear systems with non vanishing probability

Exact KAM tori in nonlinear systems with discrete linear spectrum
Nondiffusive solutions

Early rigorous results

Exact Results for Almost Periodic solutions
Fröhlich Spencer Wayne (1986) for
random Hamiltonian Systems with pair interactions

Bourgain Wang (2008) for RDNLS

Fröhlich Spencer Wayne theorem (1986)

Assumption on the Anderson base

Anderson modes have random frequencies ω_i and can be arranged on a periodic square lattice where they are only coupled between **nearest neighbours** by purely nonlinear terms

FSW model

$$H(\mathbf{P},\mathbf{Q}) = 1/2 \sum_i (P_i^2 + \omega_i^2 Q_i^2) + \varepsilon \sum_{<i,j>} f_{<i,j>}(P_i, Q_i, P_j, Q_j)$$

i belongs to a lattice Z^d

ω_i are random variables with a smooth probability density

$f_{<i,j>}$ are **nearest** neighbour coupling terms analytic of order 4

Action-angle representation

Giving an « initial state » $I^0 = \{I_i^0\}$ which **decays faster than exponential at infinity**

Then there exists ε_0 such that for $\varepsilon < \varepsilon_0$ there is a set of (nonresonant frequencies) $\Omega(I^0)$ with Prob($\Omega(\{I^0\})$) **arbitrarily close to 1**

such that if $\omega \in \Omega(I^0)$, there is a set of action-angle variables $\{I_i, \theta_i\}$ with I close to I^0

which trajectory lies on an **infinite dimensional torus** (with fundamental frequencies ω)

FSW theorem holds for random DNLS-like models (with norm conservation)

Can be extended to next nearest neighbour interactions etc...

Bourgain Wang theorem (2008) for RDNLS

$$i\hbar \frac{\partial \psi_n}{\partial t} = E_n \psi_n + \beta |\psi_n|^2 \psi_n + V(\psi_{n+1} + \psi_{n-1}),$$

Theorem (simplified):

Quasiperiodic solutions at V=0 and β=0 over a ***finite*** number of sites persist as quasiperiodic solutions (with small perturbations) with a nonvanishing probability (over outside disorder) and over a fat Cantor set of neighbouring frequencies, providing V and β be not too large.

As V and β goes to zero, this probability goes to 1 and the Cantor set goes to full measure.

Flaw: Unlike FSW, invariant tori have finite dimension in an infinite dimension phase space.

The existence of KAM tori requires a purely discrete linear spectrum

No KAM tori in spatially periodic nonlinear systems

If there would exist a localized almost periodic solution, its harmonics would be dense and would overlap the absolutely continuous spectrum and would radiate energy at infinity.

Localized Time Periodic solutions (Discrete Breathers) only are allowed if their harmonics do not overlap the phonon bands

Empirical arguments

for the existence of infinite dimension tori (almost periodic solutions) ***with finite norm (and energy)*** in the 1D Random DNLS model

More generaly in infinite systems with linear discrete spectrum (and exponential localization)

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Anderson Representation of random DNLS

$$i\dot{\psi}_n = (\epsilon_n + |\psi_n|^2)\psi_n - C(\psi_{n+1} + \psi_{n-1})$$

random

$$\psi_n(t) = \sum_p \mu_p(t)\varphi_n^{(p)}$$

New complex variables

$$\omega_p \varphi_n^{(p)} = \epsilon_n \varphi_n^{(p)} + C(\varphi_{n+1}^{(p)} + \varphi_{n-1}^{(p)})$$

$$i\dot{\mu}_p = \omega_p \mu_p + \frac{\partial \sum_n \frac{1}{2}|\psi_n|^4}{\partial \mu_p^\star} = \omega_p \mu_p + \sum_{p'} C_{p,p'}\mu_{p'}$$

The Anderson modes are coupled by nonlinear terms

norm current p —> p’

$$-J_{p\to p'} = J_{p'\to p} = 2C_{p,p'}(t)\Im(\mu_p^\star \mu_{p'})$$

$$\approx 2\chi \sum_{q,q'} \left[\left(\sum_n \phi_n^{(p)}\phi_n^{(p')}\phi_n^{(q)}\phi_n^{(q')} \right) |\mu_q(0)|\cdot|\mu_{q'}(0)|\, e^{i((\omega_q-\omega_{q'})t-(\alpha_q-\alpha_{q'}))} \right] \times |\mu_p(0)|\cdot|\mu_{p'}(0)|\sin((\omega_p-\omega_{p'})t-(\alpha_p-\alpha_{p'})),$$

Consistency of this perturbation theory (at the lowest order)
requires that the current fluxes
remains small ***at all time*** *and bounded*

$$\int J_{p\to p'}(t)\, dt \quad < \infty$$

There are resonances between four modes p,p',q,q' if

$$(\omega_q - \omega_{q'}) \pm (\omega_p - \omega_{p'}) \approx 0$$

Small denominator

$\mu_n \propto e^{-i\omega_n t}$ Consistency of Perturbation expansion (involves small denominators)

Nonresonance between modes p≠p' involving q,q':

$$|\omega_q - \omega_{q'} \pm (\omega_p - \omega_{p'})| \gtrsim \kappa \left| \chi \sum_n \phi_n^{(p)} \phi_n^{(p')} \phi_n^{(q)} \phi_n^{(q')} \right| \times |\mu_q(0)| \cdot |\mu_{q'}(0)|$$

$\varkappa >> 1$

Assume random frequencies with maximum probability density P_0

Bound for the Probability of resonance

$$\delta_{p,p',q,q'} = 2P_0\kappa \left| \chi \sum_n \phi_n^{(p)} \phi_n^{(p')} \phi_n^{(q)} \phi_n^{(q')} \right| |\mu_q(0)| \cdot |\mu_{q'}(0)|$$

If this property is fulfilled for all p,p',q,q' perturbation theory is consistent. Possibility of existence of a KAM torus

Probability to have at least one resonance

$P_R < \sum_{p\neq p',q,q'} \delta_{p\neq p',q,q'} <$ $P_0\kappa|\chi| \cdot ||\mathbf{A}|| \cdot ||\{\mu_q(0)\}||^2,$

$$||\mathbf{A}|| = \sup_{\mathbf{X}} \frac{||\mathbf{A}\cdot\mathbf{X}|||}{||\mathbf{X}||}.$$

$$A_{q,q'} \equiv \sum_{p\neq p'} |\sum_n \phi_n^{(p)}\phi_n^{(p')}\phi_n^{(q)}\phi_n^{(q')}|.$$

If **A** has a finite norm then for $||\{\mu_q(0)\}||^2 < \frac{1}{P_0\kappa|\chi| \cdot ||\mathbf{A}||},$ $P_R < 1$

The probability $P_N = 1 - P_R$ of having no resonance is strictly positive

A has a finite norm when the linear spectrum is discrete and an infinite norm when it is absolutely continuous

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Assumption: exponential localization

$$|\phi_n^{(p)}| < K\sqrt{\frac{1-\lambda^2}{1+\lambda^2}}\lambda^{|n-p|},$$

$$||\mathbf{A}|| < K^4 \frac{(1+\lambda)^6}{(1+\lambda^2)^2}\frac{1}{(1-\lambda)^2}.$$

$$||\mathbf{A}|| \lesssim 64K^4\xi^2.$$

The norm upper bound for having no resonance (and a KAM torus?) goes to zero as the localization length diverges.

If the packet is already spread μ_p is small and

$$P_N > exp\,(-\ P_0\kappa|\chi| \cdot ||\mathbf{A}|| \cdot ||\{\mu_q(0)\}||^2) > 0$$

Conjecture:

Giving a l_2 initial condition for the wave packet with a norm not too large,

And chosing randomly the disorder according to some probability law, in order the linear spectrum be purely discrete (with probability 1),

Then this initial condition has a finite probability to generate an infinite dimensional KAM torus and moreover this probability goes to 1 when the norm of the wave packet goes to zero.

(I.e. the system behave like linear for small norm wave packets)

Laboratoire Léon Brillouin

Numerical test for the existence of KAM tori

in the 1D Random DNLS model

Equivalent tests:
- Bohr recurrence
- Largest Lyapounov

No recurrence a found for large spatially periodic systems

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Almost periodic function:
Harald Bohr theorem

Definition

$F(t) = \sum_n f_n e^{i\omega_n t}$ with $\sum_n |f_n| < \infty$

Theorem:

This definition is equivalent to

$\forall \varepsilon > 0 \; \exists \; \{\tau_n\}$ (pseudo periods) such that

- $\{\tau_n\}$ is relatively dense
- $| F(t+ \tau_n) - F(t)| < \varepsilon$ for any t

Implementation for DNLS

For single site excitation at site 0, check only
$|\Psi_0(0)|^2 - |\Psi_0(t)|^2 = N - |\Psi_0(t)|^2 < \varepsilon N$
(because of norm conservation, no need to have recurrence in phase)

Choose ε no too large for having pseudoperiods of recurrence not too large

Actually it is found that if there are recurrence at relatively large ε, recurrences are found at smaller ε though more rarely. The pseudoperiods go roughly as 1/ ε

Method: Vary by small steps δ the amplitude of a single site initial condition from 0 to B. We observe for large systems and over computing time as long as possible that

Initial conditions can be classified in two categories: Recurrent or nonrecurrent

Note that Poincaré recurence theorem only holds for **finite systems** (and is not uniform). No recurrence is found for chaotic trajectories

Recurrent trajectories

-Within a given accuracy ε small, many trajectories return close to their initial condition during the whole computing time (recurrent) and within bounded pseudo periods.
-Recurrence is found for smaller ε but more sparsely.
- Trajectories repeat from the recurrence time, a new trajectory which is uniformly close from the initial one.
-Recurrence is observed simultaneously for all components of the trajectory
-Some trajectories are only recurrent up to some computing time « sticking ». They become more rare as the computing time increase. Interpretation: those trajectories belongs to thin gaps of the fat Cantor set of KAM tori.
- Recurrent trajectories have zero Lyapounov exponents.
-Conversely, all trajectories found with zero Lyapounov exponents are recurrent.

Non Recurrent trajectories

There are also many trajectories which are **not recurrent**
or **loose** recurrence after some computing time,

During the computing time.

They are (or become) apparently chaotic and (start to) spread (????).

Their Lyapounov exponents are non vanishing

Depends on disorder realisation

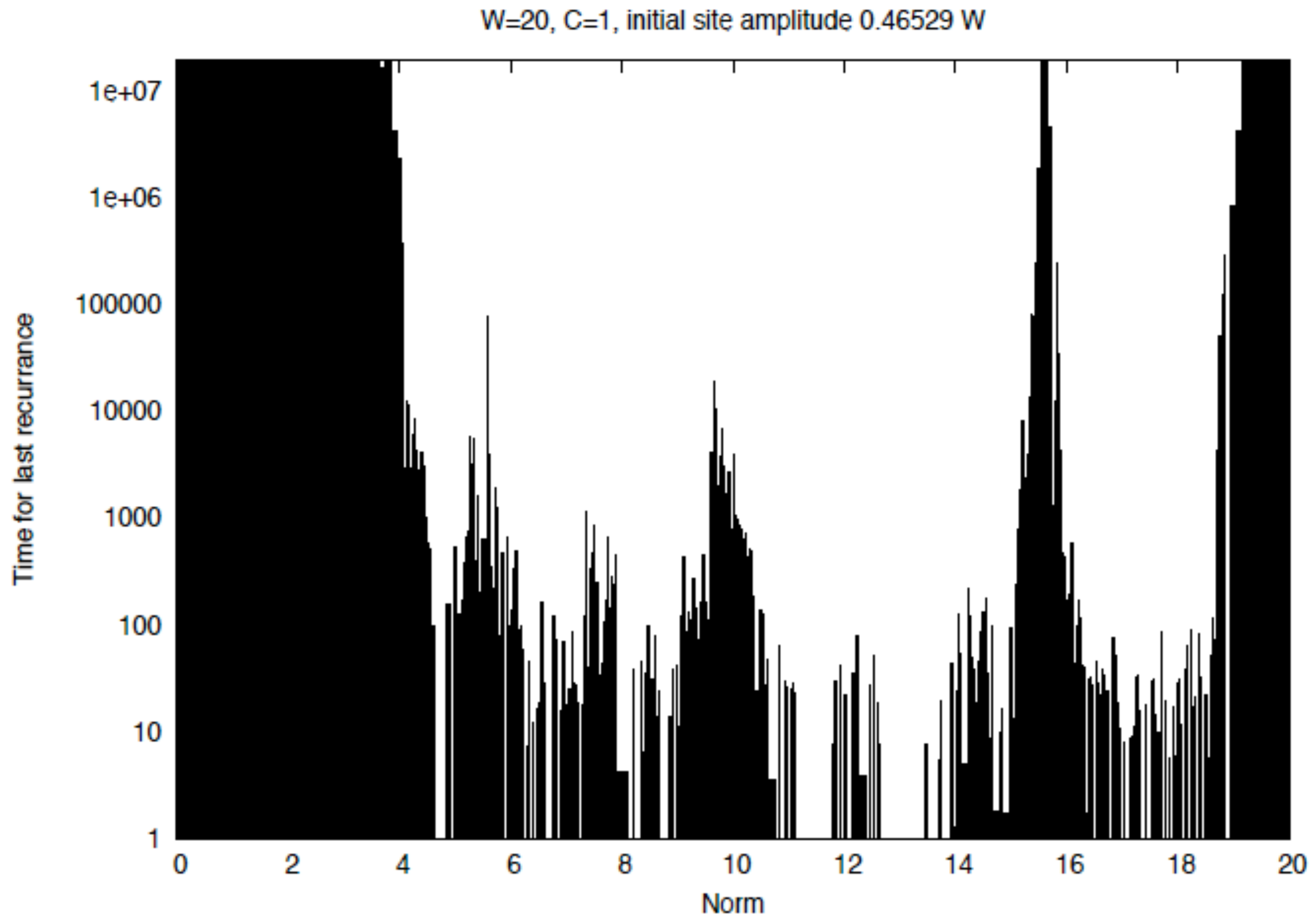


FIG. 1: Last observed time for recurrence in $|\psi_{n_0}|^2$ versus norm in a particular disorder realization. $\epsilon = 0.02\mathcal{N}, W = 20, \psi_n(0) = \sqrt{\mathcal{N}}\delta_{n,n_0}, \epsilon_{n_0} \approx 0.46529W, C = 1, \chi = -1$, system size $N = 500$.

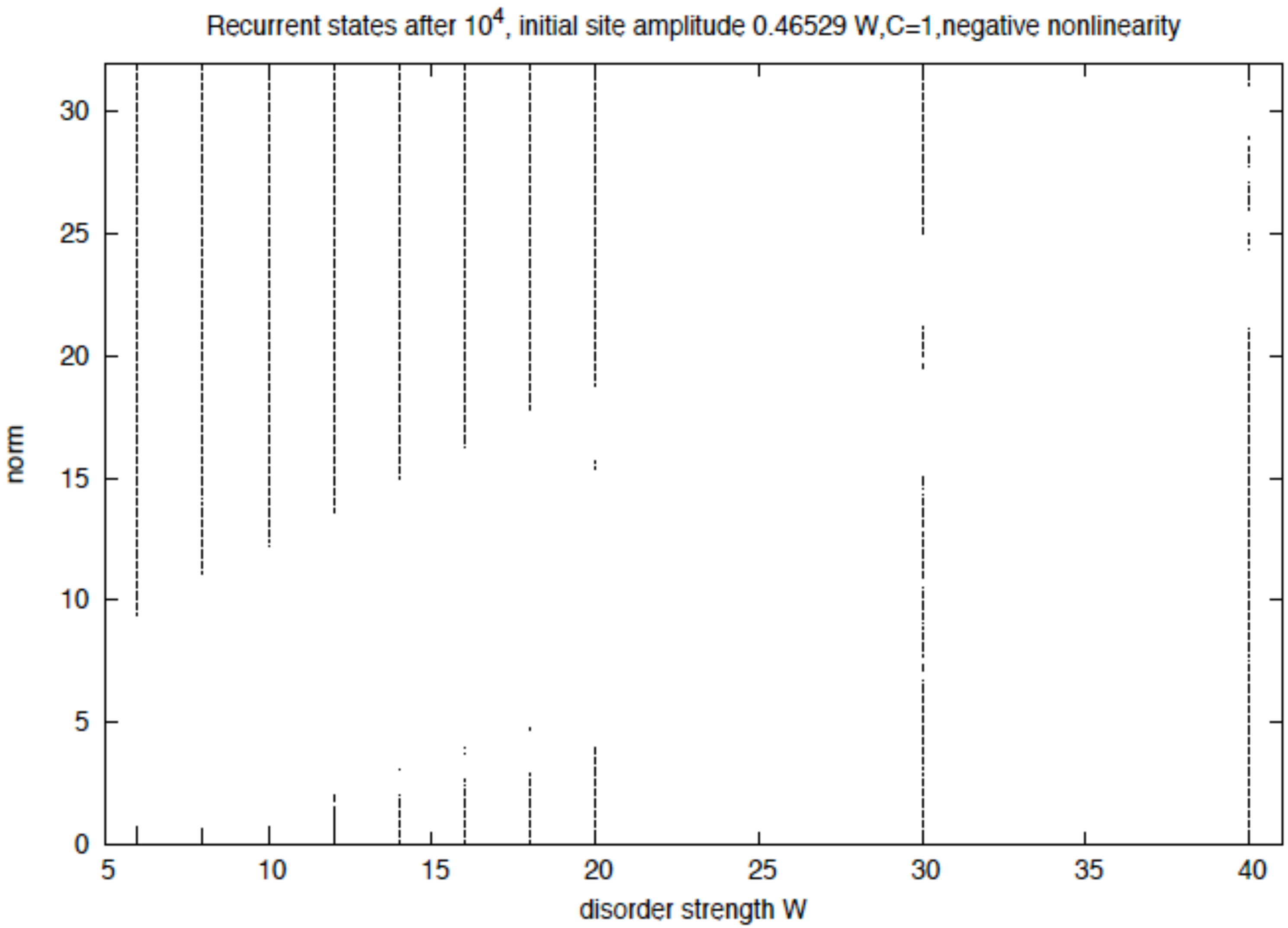


FIG. 2: Sets of T-recurrent trajectories at $T = 10^4$ for the same initial condition and disorder realization as in Fig. 1, for various disorder strengths W. Other parameters values are the same as in Fig. 1.

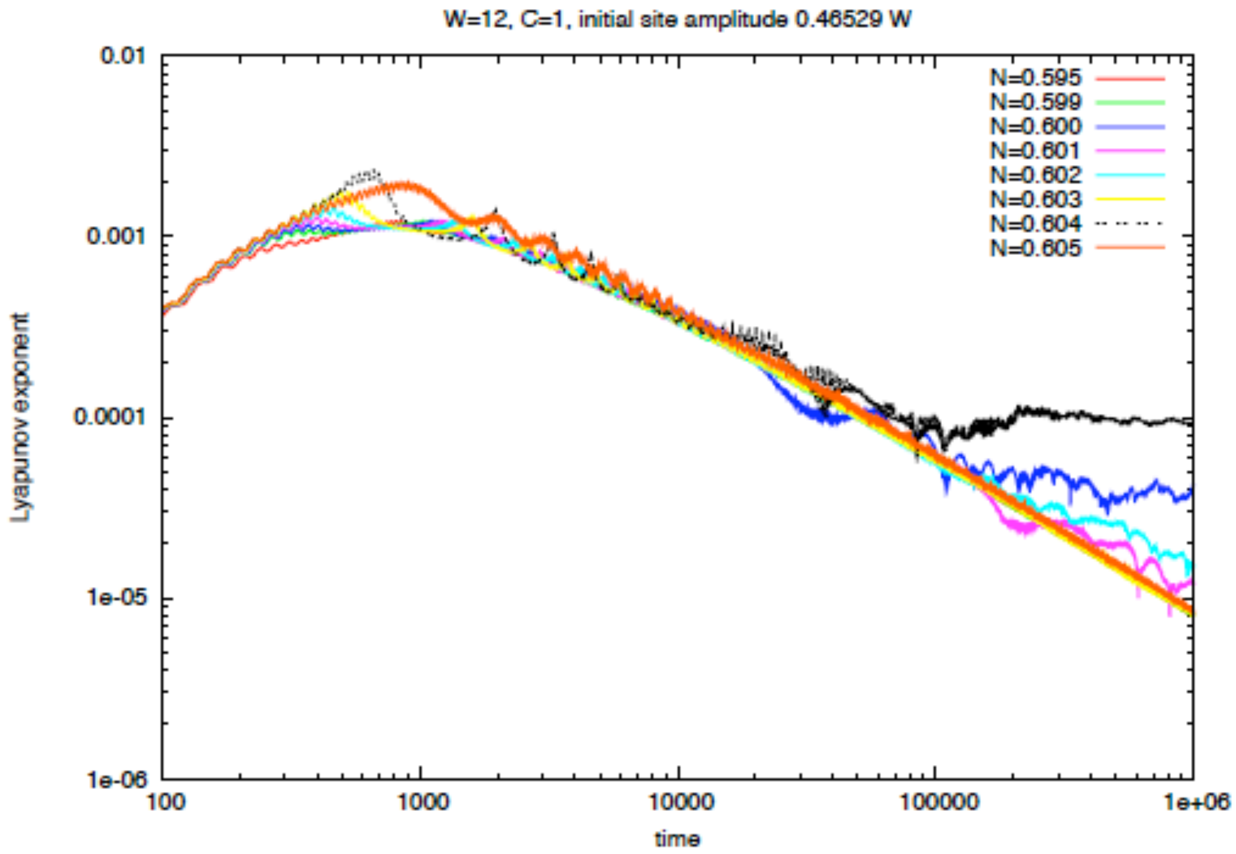


FIG. 4: Upper figure: Total norm of perturbation $\eta_n(t)$ divided by time, for solutions corresponding to single-site initial conditions ψ_n with slightly different $\mathcal{N} \approx 0.6$. Lower figure: Corresponding finite-time Lyapunov exponents. At time 10^6, the upper curves correspond, from top to bottom, to $\mathcal{N} = 0.604, 0.600, 0.602, 0.601$, while the lower curves for $\mathcal{N} = 0.595, 0.599, 0.603, 0.605$ all follow very closely a curve $\sim \log t/t$, as expected for KAM tori. Disorder strength $W = 12$, other parameters and disorder realization same as in previous figures.

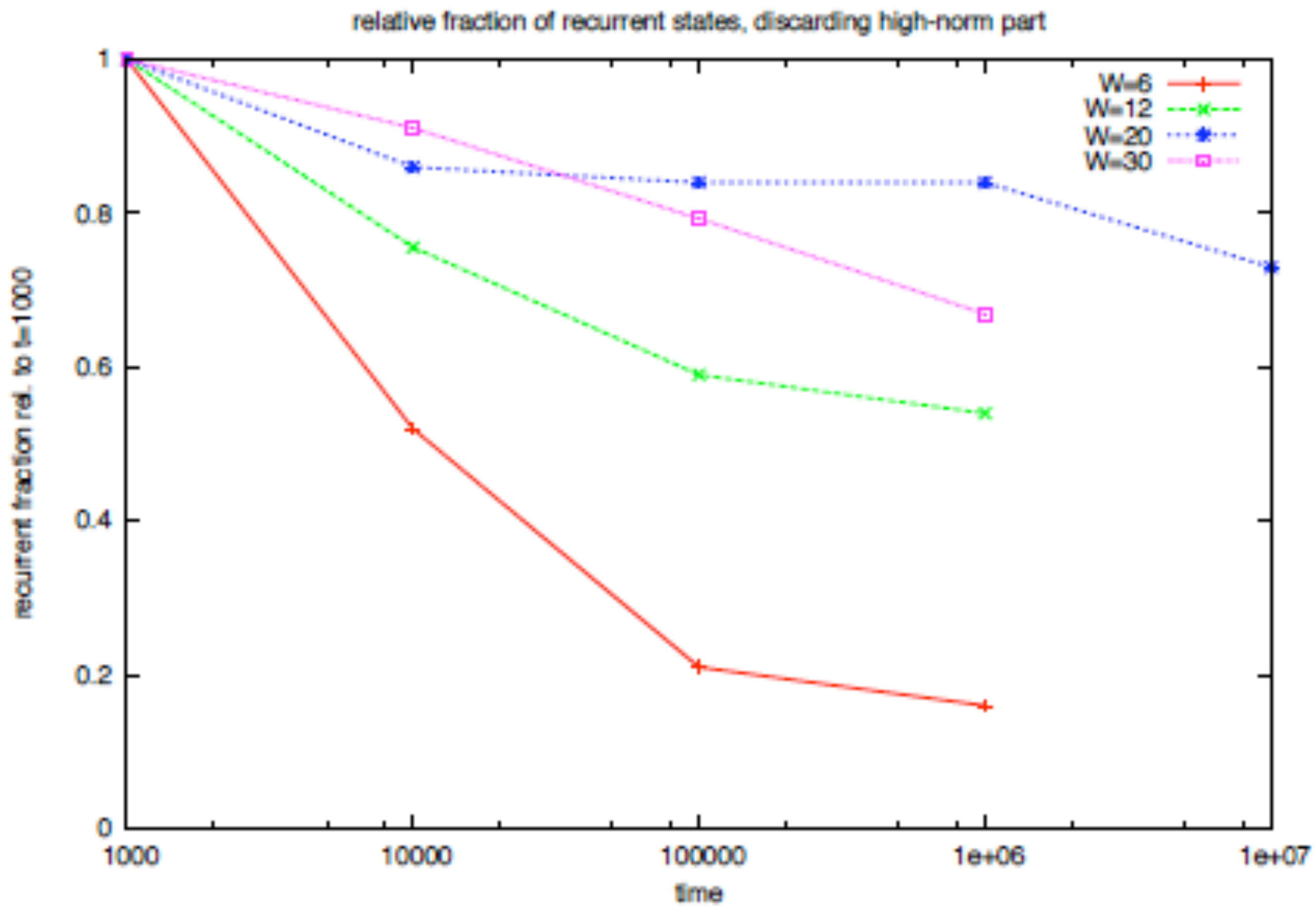


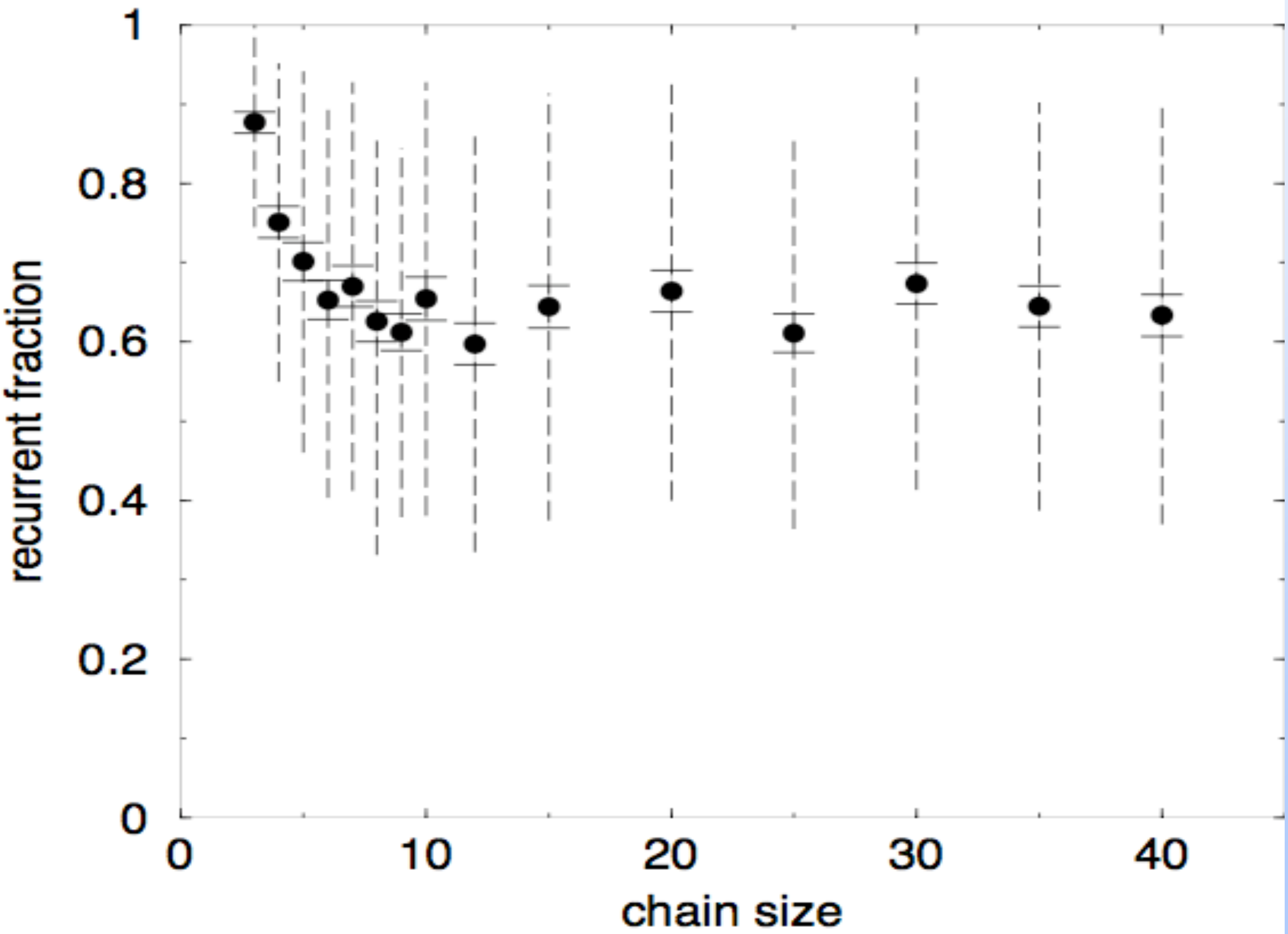
FIG. 3: Fraction of the trajectories T-recurrent at $T = 10^3$ which remain T-recurrent also at longer times, for various disorder strenghts. Trajectories from the high-norm (self-trapped) T-recurrent regime have not been included. The initial condition, disorder realization, and other parameters values are the same as in Figs. 1 - 2.

Finite size studies

When the size increases, the measure of recurrent trajectories has a clearly non vanishing asymptotic limit which is reached when the system size is sufficiently larger than the localization length (or volume).
Large fluctuations. Make disorder average for smooth graphs versus size.

If the system is periodic (no randomness), no recurrent trajectories are found as soon the system size exceeds only 10.

Averaged for 100 realizations



Conclusions for wave packets in infinite Nonlinear systems with linear Anderson localization:

There are two kinds of wavepackets both with nonvanishing probability

-wavepackets in fat Cantor sets which are almost periodic stationary states and do not spread.

--spreading chaotic wavepackets

Open problems

There are situations where wavepackets cannot spread totally or partially

-Do situations exist where they spread to zero. Blocking KAM tori. Inverse Arnold diffusion?

-If no spreading, what is the limit state?

Trajectories « initially chaotic »

(non KAM tori)

in the 1D Random DNLS model

Many trajectories are found chaotic (with sensitivity to initial conditions) and nonvanishing (transient) Lyapounov exponent.
But if the wave packet spreads, the system becomes close to linear and its Lyapounov exponent goes to zero.
In infinite system, no Poincaré recurrence
Chaos does not imply wavepacket spreading.
Self-organization?

Which « attractor » to expect for initially chaotic trajectories?

3 examples with chaos and absence or incomplete diffusion

- -large norm
- -No linear band dispersion
- -Linear system beyond a cut-off distance

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Rigorous proof for the absence of complete diffusion for a « large enough » Wavepacket

with invariance by phase rotation (implies norm l_2 conservation)

$$\psi_n \longrightarrow \psi_n e^{i\theta}$$

$$||\Psi||_2 = \left(\sum_n |\psi_n|^2\right)^{1/2} \qquad ||\Psi||_\infty = \sup_n |\psi_n|$$

quadratic

Nonlinear higher order
H_{NL} > 0 strictly positive (or negative)

$$H = H_L(\{\psi_n\}) + H_{NL}(\{\psi_n\})$$

$$H_L = \Omega_m(||\Psi||_2)^2 < \langle\Psi|\mathbf{L}|\Psi\rangle < \Omega_M(||\Psi||_2)^2 \qquad ||\mathbf{L}||_2 < +\infty$$

$$\lim_{||\Psi||_\infty \to 0} H_{NL}(\{\psi_n\})/(||\Psi||_2)^2 = 0$$

Example: $0 < H_{NL} = \sum_n |\psi_n|^4 < (\sup_n |\psi_n|)^2 \sum_n |\psi_n|^2 = (||\Psi||_\infty)^2(||\Psi||_2)^2$.

Assume the wavepacket spreads uniformy to zero:
($\lim_{t=\infty}$ $||\Psi||_\infty$ =0),
then at infinite time the nonlinear contribution H_{NL} to the energy is zero since $\lim_{||\Psi||_\infty \to 0} H_{NL}(\{\psi_n\})/||\Psi||_2^2 = 0$

and the norm $||\Psi||_2$ is time constant. Then

$$\text{At } t = +\infty,\ H = H_L < \Omega_M(||\Psi||_2)^2$$

$$\text{If at } t = 0,\ H > \Omega_M(||\Psi||_2)^2$$

energy cannot be conserved and consequently the wave packet cannot spread uniformly to zero.

Since the higher order nonlinear energy grows faster than the norm the wavepacket cannot spread uniformly to zero when its amplitude is large enough

2-A family of models without diffusion (random or not random) :

DNLS Models with Dispersionless Linear Phonons

$$H_L = \sum_n \epsilon_0 |\psi_n|^2 = \epsilon_0 (||\Psi||_2)^2$$

H_L is time constant, then H_{NL} is time constant

Any initial l_2 wavepacket cannot spread to zero independantly whether there is disorder or not

Example: FSW model

$$H = \sum_n \left(\epsilon_0 |\psi_n|^2 + \frac{\chi_n}{2} |\psi_n|^4 + C_n |\psi_n| |\psi_{n+1}| (\psi_n \psi^\star_{n+1} + \psi^\star_n \psi_{n+1}) \right)$$

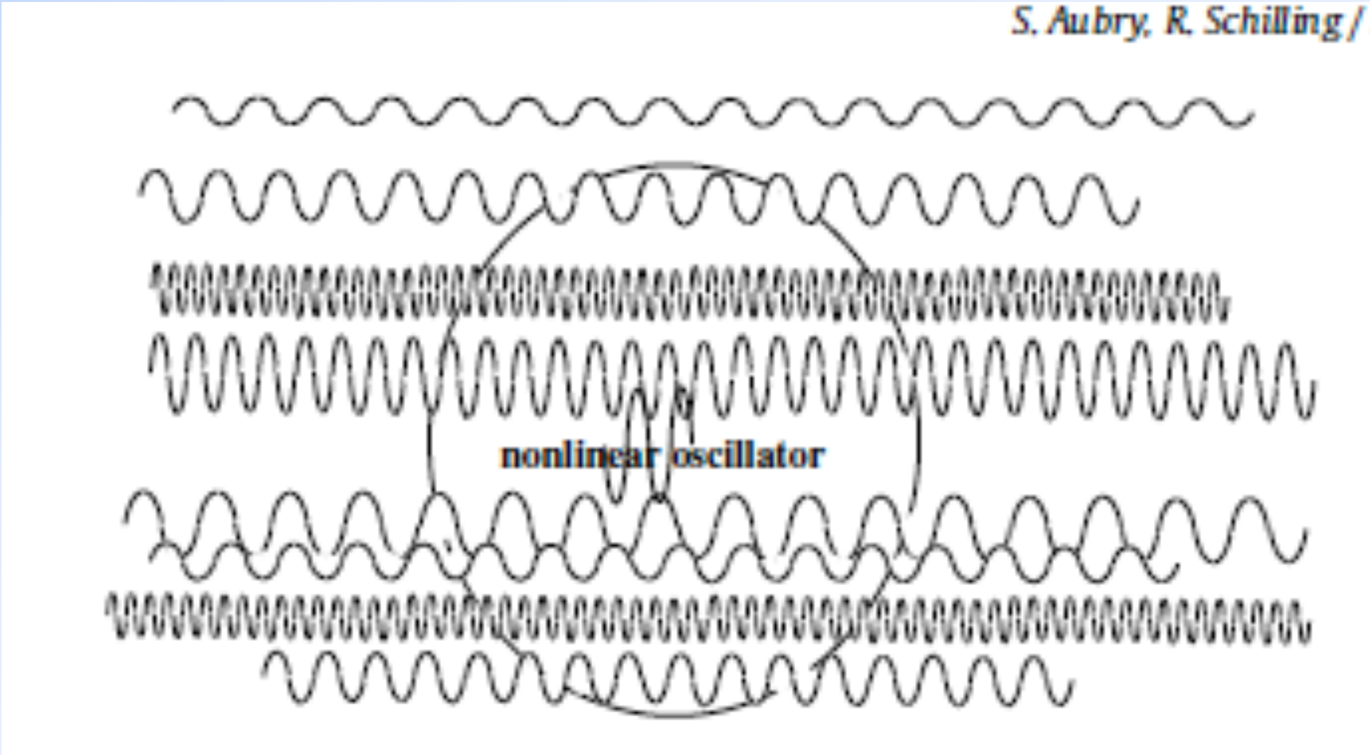
What is the long time behavior of a wavepacket if no spreading to zero is possible.

In the **Anderson base** same model, the random DNLS Model belong to this family of **NONdiffusive Hamiltonian** except that operator **L** (though it is diagonal), is not proportional to unity but is random.

Why extra randomness would generate diffusion?

Modelling Discrete Breathers

The central part of the system only is nonlinear.
Linear approximation far away



Case I

Extended phonons: Absolutely continuous spectrum

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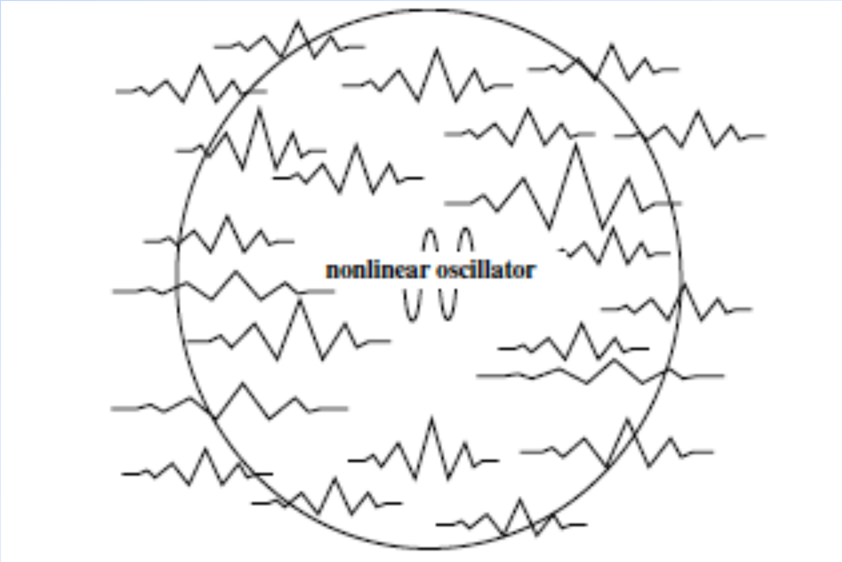
Case II



*Random systems with **complete** Anderson (Localized phonons) Purely Discrete spectrum*

There is no possible radiation from the linear part

The properties of the linear spectrum is essential

Standard Langevin Thermostat

A model for thermalization

Let us consider a dynamical system coupled to an infinite harmonic system

$$\mathcal{H} = \mathcal{H}_0(\mathbf{p}, \mathbf{q}) + \mathcal{H}_{\text{harm}}(\{u_i, p_i\}) - \lambda \mathbf{q}^t \mathbf{C} \mathbf{u}$$

Coupling matrix **C** *is short range (l_2 eg. nearest neighbors)*
equivalent to a dynamical system coupled to an infinite collection of harmonic oscillators (normal modes)

$$\mathcal{H} = \mathcal{H}_0(\mathbf{p}, \mathbf{q}) - \lambda \sum_\nu \mathbf{C}_\nu^t \mathbf{q}\, u_\nu + \sum_\nu \left(\frac{1}{2}\dot{u}_\nu^2 + \frac{1}{2}\omega_\nu^2 u_\nu^2 \right)$$

Hamilton equations

$$\ddot{\mathbf{q}} + V'(\mathbf{q}) - \lambda \sum_\nu \mathbf{C}_\nu u_\nu = 0$$

$$\ddot{u}_\nu + \omega_\nu^2 u_\nu - \lambda \mathbf{C}_\nu^{\mathrm{t}} \mathbf{q} = 0$$

General solution of the linear part

$$u_\nu(t) = u_\nu^{(0)}(t) + \lambda \frac{1}{\omega_\nu} \cdot \int_0^t \sin \omega_\nu (t - \tau) \mathbf{C}_\nu^{\mathrm{t}} \mathbf{q}(\tau)\, \mathrm{d}\tau$$

where

$$u_\nu^{(0)}(t) = \left[\frac{\lambda}{\omega_\nu^2} \mathbf{C}_\nu^{\mathrm{t}} \mathbf{q}(0) + \epsilon_\nu(0) \right] \cos \omega_\nu t + \frac{\dot{\epsilon}_\nu(0)}{\omega_\nu} \sin \omega_\nu t$$

Effective equation after eliminations of linear degrees of freedom

$$\ddot{\mathbf{q}}(t) + V'_{\mathit{eff}}(\mathbf{q}(t)) + \lambda^2 \int_0^t \mathbf{\Gamma}(t-\tau)\dot{\mathbf{q}}(\tau)\,\mathrm{d}\tau - \lambda\boldsymbol{\zeta}(t) = 0$$

$$V_{\mathit{eff}}(\mathbf{q}) = V(\mathbf{q}) - \frac{1}{2}\lambda^2 \sum_{\alpha,\beta} \Gamma_{\alpha,\beta}(0) q_\alpha q_\beta$$

Kernel (delayed interaction)

$$\Gamma_{\alpha,\beta}(t) = \sum_\nu \frac{C_{\nu,\alpha} C_{\nu,\beta}}{\omega_\nu^2} \cos \omega_\nu t$$

Thermalization of the thermostat

Langevin force

$$\langle \zeta_\alpha(0)\zeta_\beta(t)\rangle = k_B T \sum_\nu \frac{C_{\nu,\alpha} C_{\nu,\beta}}{\omega_\nu^2} \cos \omega_\nu t$$

Langevin relation

$$= k_B T\, \Gamma_{\alpha,\beta}(t)$$

Standard Langevin approximation:

the Fourier spectrum of $\mathbf{\Gamma}(t)$ is uniform on the whole real axis

$$\Gamma_{\alpha,\beta}(t) = \Gamma^{(ac)}_{\alpha,\beta}(t) = 2\gamma_{\alpha,\beta}\delta(t)$$

which yields the standard Langevin equation

$$\ddot{\mathbf{q}}(t) + V'_{eff}(\mathbf{q}(t)) + \lambda^2\boldsymbol{\gamma}\dot{\mathbf{q}}(t) - \lambda\boldsymbol{\zeta}(t) = 0$$

commonly used in physics and chemistry (eg Kramers theory)

Model for thermalization

General case: Time Fourier transform of the kernel is a positive measure

$$\tilde{\Gamma}_{\alpha,\beta}(\omega)\mathrm{d}\omega = \mathrm{d}\sigma_{\alpha,\beta}(\omega)$$
$$= \pi \sum_{\nu} \frac{C_{\nu,\alpha} C_{\nu,\beta}}{\omega_\nu^2} (\delta(\omega - \omega_\nu) + \delta(\omega + \omega_\nu))\mathrm{d}\omega.$$

$$\sigma_{\alpha,\beta}(\omega) = \int_0^{\omega} \mathrm{d}\sigma_{\alpha,\beta}(\omega')$$
$$= \frac{1}{2\,\mathrm{i}} \cdot \oint_{\mathcal{C}(\omega)} \left\langle \mathbf{C}_\alpha \left| \frac{1}{\mathbf{M}(z - \mathbf{M})} \right| \mathbf{C}_\beta \right\rangle \mathrm{d}z$$

1/2 **<u|M|u>** is the harmonic potential energy

M is positive and its eigenvalues are ω_ν^2

C(ω) is a loop in the complex plane

which contains only ω_ν^2 smaller than ω^2

The spectrum of **M** determines those of **Γ**

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Energy Dissipation at zero temperature T=0

$$E(t) = \frac{1}{2}(\dot{\mathbf{q}}(t))^2 + V_{eff}(\mathbf{q}(t)).$$

$$\dot{E}(t) = -\lambda^2 \int_0^t \dot{\mathbf{q}}(t) \cdot \boldsymbol{\Gamma}(t-\tau)\dot{\mathbf{q}}(\tau)\mathrm{d}\tau.$$

Average energy variation

$$\begin{aligned}
\frac{E(T)-E(0)}{T} &= \overline{\dot{E}}_T \\
&= -\lambda^2 \frac{1}{T}\int_0^T \mathrm{d}t \int_0^t \dot{\mathbf{q}}(t) \cdot \boldsymbol{\Gamma}(t-\tau)\dot{\mathbf{q}}(\tau)\mathrm{d}\tau \\
&= -\frac{1}{2}\lambda^2 \frac{1}{T}\int_0^T \mathrm{d}t \int_0^T \dot{\mathbf{q}}(t) \cdot \boldsymbol{\Gamma}(t-\tau)\dot{\mathbf{q}}(\tau)\mathrm{d}\tau \\
&= -\frac{1}{2}\lambda^2 \int_{-\infty}^{+\infty} \mathrm{d}t \int_{-\infty}^{+\infty} \mathbf{g}_T(t) \cdot \boldsymbol{\Gamma}(t-\tau)\mathbf{g}_T(\tau)\mathrm{d}\tau
\end{aligned}$$

$$g_{\alpha;T}(t) = \chi_T(t)\dot{q}_\alpha(t)$$

where $\chi_T(t) = 1/\sqrt{T}$ for $0 < t < T$ and $\chi_T(t) = 0$ for $t < 0$

Correlation functions

$$K_{\alpha,\beta}(\tau) = \lim_{T\to+\infty} \frac{1}{T}\int_0^T \dot{q}_\alpha(t)\dot{q}_\beta(t+\tau)dt$$

$$\tilde{K}_{\alpha,\beta}(\omega) = \int_{-\infty}^{+\infty} K_{\alpha,\beta}(\tau)e^{i\omega\tau} \, d\omega$$

Average energy dissipation (exact)

$$\boxed{\lim_{T\to+\infty} \bar{\dot{E}}_T = -\frac{\lambda^2}{4\pi}\sum_{\alpha,\beta}\int_{-\infty}^{+\infty} \tilde{\Gamma}_{\alpha,\beta}(\omega)\tilde{K}_{\beta,\alpha}(\omega)d\omega}$$

Should vanish: nonoverlap criteria

Asymptotic Solutions?

Initial condition: finite energy
The limit solutions cannot dissipate an infinite energy

$$T\dot{\bar{E}}_T = E(T) - E(0) < \infty$$

implies no overlap between positive measures

$$\tilde{K}_{\alpha,\beta}(\omega)d\omega \quad \text{et} \quad \tilde{\Gamma}_{\alpha,\beta}(\omega)d\omega$$

(disjoint supports)

If the support of measure $\Gamma(\omega)d\omega$ is the whole real axis,
only **q**(t)=0 is an asymptotic solution (standard damping)
but if not $\rightarrow\rightarrow\rightarrow\rightarrow$

Case I: Time periodic asymptotic solutions (Discrete Breathers)

$$\tilde{K}_{\alpha,\beta}(\omega) = k_{\alpha,\beta}(\delta(\omega - \Omega) + \delta(\omega + \Omega))$$ + harmonics

1-Spatially periodic systems with Bands

(absolutely continuous spectrum: the support of $\Gamma(\omega)d\omega$ consists of finite intervals)

Ω and harmonics cannot belong to the bands

Confirmation of what is known

2-Spatially random systems with Anderson localization

(discrete spectrum: the support of $\Gamma(\omega)d\omega$ consists of a countable Dense set of points)

Ω and harmonics should not be equal to eigen frequencies (and a zero measure Liouvills set)

Intraband Discrete Breathers may exist (proven) with frequency inside the spectrum (**closure of the set of eigenvalues).**

Normal Dissipation $-\langle E_T(T) \rangle$ diverges as T

Discrete spectrum thermostat:
The energy dissipation depends on the frequency of the driving force

For most frequencies $-\langle E_T(T) \rangle$ does not diverges (non resonant frequencies)

But possible subdissipative behavior (« Liouville » subset)
$-\langle E_T(T) \rangle$ diverges slower than T
And also possible superdissipative behavior (zero measure set of frequencies)
$-\langle E_T(T) \rangle$ diverges faster than T

Case2: Quasi periodic or almost periodic asymptotic solutions

$$\tilde{K}_{\alpha,\beta}(\omega) = \sum_p k_{\alpha,\beta}^{(p)} \delta(\omega - \Omega_p)$$

The series is absolutely convergent
and the set of frequencies Ω_p is dense on the real axis

Cannot exist for spatially periodic systems (phonon radiation)

But could exist for spatially random systems with Anderson localization and **purely discrete spectrum** (no mobility edge) KAM TORI?

Case 3: Fully chaotic asymptotic solutions

$\tilde{K}_{\alpha,\beta}(\omega)d\omega$ is an absolutely continuous measure

If one assume that for any ω_1 and ω_2 in the support of $\mathbf{K}(\omega)$, then $n_1\omega_1 + n_2\,\omega_2$ with n_1, n_2 integers
Is also in the support,
there is energy dissipation in all cases
(absolutely continuous, singular continuous or discrete)

Fully chaotic asymptotic solutions cannot exist
for any phonon bath with spectrum dense on intervals
absolutely continuous or discrete

Case 4: Asymptotic solutions with singular continuous spectra (weakly chaotic)

cannot exist if the phonon spectrum is absolutely continuous in some intervals

Conjecture: It could exist if the phonon spectrum is purely discrete and dense on intervals.

A nonlinear system coupled to a linear phonon bath

-could have either the rest solution 0
or only time periodic solutions (Discrete Breathers)
as asymptotic solutions

for a phonon bath with **absolutely continuous spectrum dense on some intervals**

-could have either the rest solution 0
-or time periodic solutions
-or quasiperiodic, almost periodic solutions
-or solutions with singular continuous spectra (marginally chaotic)

for a phonon bath with **purely discrete spectrum dense on some intervals**

Lemma. *Let us consider a measurable subset* $\mathcal{E} \subseteq \mathcal{R}$ *of the real line with the following property:*

$\forall \omega_1 \in \mathcal{E}$ *and* $\forall \omega_2 \in \mathcal{E}$

and $\forall n_1 \in \mathcal{Z}$ *and* $n_2 \in \mathcal{Z}$ *(integers positive or negative)*

we have $n_1\omega_1 + n_2\omega_2 \in \mathcal{E}$. (C.1)

1. *Then, either the Lebesgue measure* $\mu(\mathcal{E})$ *of* $\mathcal{E}$ *is zero or* $\mathcal{E} = \mathcal{R}$ *is the whole real line.*
2. *There exist sets* $\mathcal{E}$ *with property* (C.1) *with zero Lebesgue measure and which are uncountable.*

Perspective for Physics

Discrete Breathers (or ILM, local modes etc): Stable excitations in highly complex nonintegrable systems (finite or infinite).
(their Fourier spectrum is not dense and avoid resonances)
Essential for

1- Long time focusing (energy, charge etc…) : Retarded Thermalization.
2- Targeted Transfer: Energy, charge, signal….
and Selective transport.
3- Ultrafast chemical Expressways: Degenerate pathways in the phase space of complex (but specially built) systems may exist (DB mobility in periodic systems is a special marginal case)
4- Control: Targeted transfer is controllable by small perturbations « Breathonics », molecular transistors…. Biophysics.

Conditions: Coherent dynamics demand a relatively low temperature (cold chemistry). High temperature produces decoherence (standard models)