Computational studies of discrete breathers

Sergej Flach
MPIPKS Dresden
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CONTENT:

Useful on the desktop: Abramowitz/Stegun, Numerical Recipes

IMPORTANT NOTE:

For sake of simplicity in most cases one-dimensional lattice models and nearest neighbor interaction are used

Generalization to higher lattice dimensions and larger interaction ranges is STRAIGHTFORWARD

If results or methods are dimension or interaction range specific, we will inform you!

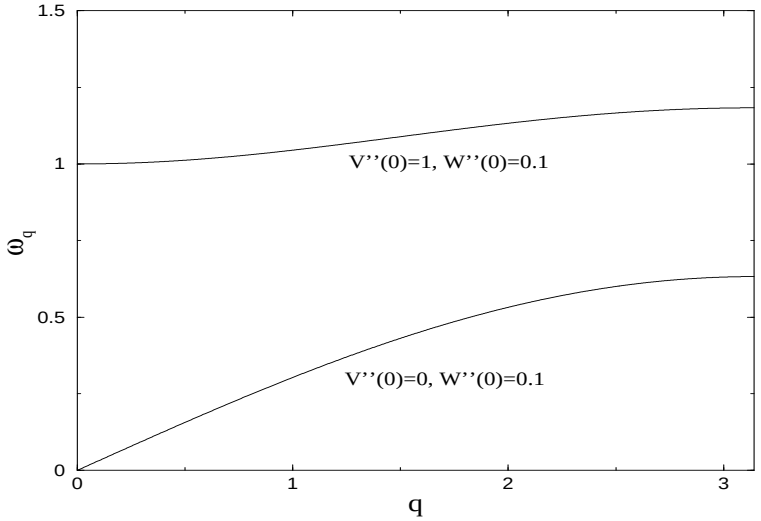
A few definitions first, using a simple model class

$$H = \sum_l \left[\frac{1}{2} p_l^2 + V(x_l) + W(x_l - x_{l-1}) \right]$$

$$V(0) = W(0) = V'(0) = W'(0) = 0$$
$$V"(0), W"(0) \geq 0$$

Equations of motion:

$$\dot{x}_l = p_l \ , \ \dot{p}_l = -V'(x_l) - W'_{l,l-1} + W'_{l+1,l}$$



Group velocity $v_g(q)$:

$$v_g(q) = \frac{\mathrm{d}\omega_q}{\mathrm{d}q}$$

Small amplitude plane waves:

$$x_l(t) \sim \mathrm{e}^{\mathrm{i}(\omega_q t - ql)} \ , \ \omega_q^2 = V"(0) + 4W"(0) \sin(\frac{q}{2})$$

So for N sites we are studying trajectories in a $2N$-dimensional phase space!

A bit on numerics of solving ODEs

$\dot{x} = f(x,t)$ - Runge-Kutta 4th order, $O(h^5)$, 4 f calculations per step

$\ddot{x} = f(x)$ - alternative symplectic Verlet (Leap-Frog) i.e.
$x(t+h) - 2x(t) + x(t-h) = h^2 f(x(t))$, $O(h^4)$, 1 f calculation per step

Always think hard before choosing an algorithm

Take into account:
- total simulation time
- maximum error
- required overall stability

Thumb rule:
- short simulations: RK4
- long simulations: symplectic

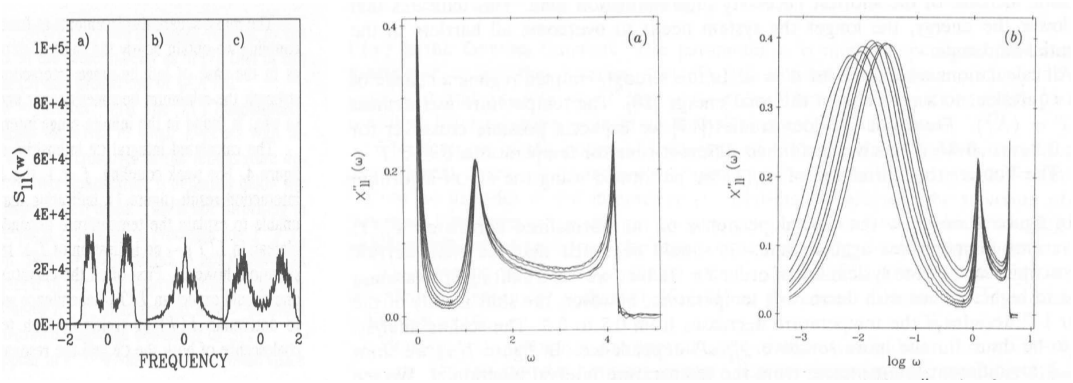
How do we make finite temperature simulations?

Main tools:

- microcanonical simulation (deterministic)
- Nose-Hoover simulation (deterministic, $N+1$)
- Langevin dynamics (stochastic)
- Monte Carlo (stochastic)

$$H = \sum_l \left(\frac{1}{2}\dot{x}_l^2 + \frac{1}{4}(x_l^2 - 1)^2 + \frac{C}{2}(x_l - x_{l-1})^2 \right)$$

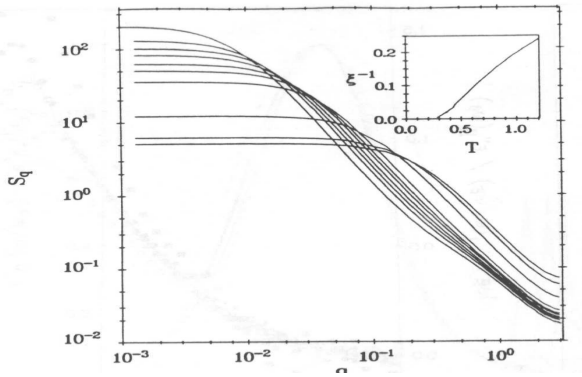
$$S_{lk}(t) = \langle x_l(t+\tau) x_k(\tau) \rangle_\tau \ , \ A(\omega) = \int_0^\infty \cos(\omega t) A(t)$$



Thumb rule:

- stochastic for excitations
- deterministic for relaxations
- Nose-Hoover ???
- Boundary conditions !
- Correlation length ξ

$$\xi^2 = -\frac{\left[\frac{\mathrm{d}^2}{\mathrm{d}q^2} S_q(t=0)\right]_{q=0}}{2 S_{q=0}(t=0)}$$



Sidenotes on spatial and temporal Fourier transforms

Spatial transforms:

$A_q = \sum_l \mathrm{e}^{\mathrm{i}q(l-k)} A_{lk}$

Temporal Fourier transforms for correlation functions:

Filon's integration formula (Abramowitz/Stegun):

$$\int_{t_0}^{t_{2n}} f(t)\cos(\omega t)\mathrm{d}t =$$

$$h\left[\alpha(\omega h)\left(f_{2n}\sin(\omega t_{2n}) - f_0\sin(\omega t_0)\right) + \beta(\omega h)C_{2n} + \gamma(\omega h)C_{2n-1}\right] + O(nh^4 f^{(3)})$$

$$C_{2n} = \sum_{i=0}^{n} f_{2i}\cos(\omega t_{2i}) - \frac{1}{2}\left[f_{2n}\cos(\omega t_{2n}) + f_0\cos(\omega t_0)\right]$$

$$C_{2n-1} = \sum_{i=1}^{n} f_{2i-1}\cos(\omega t_{2i-1})$$

$$\alpha(z) = \frac{1}{z} + \frac{\sin 2z}{2z^2} - \frac{2\sin^2 z}{z^3}\ ,\ \beta(z) = 2\left(\frac{1+\cos^2 z}{z^2} - \frac{\sin 2z}{z^3}\right)\ ,\ \gamma(z) = 4\left(\frac{\sin z}{z^3} - \frac{\cos z}{z^2}\right)$$

Temporal Fourier transforms for analytical time-periodic functions:

Simple trapezoidal rule does it with exponential accuracy!

$$A(t) = A(t+T)\ ,\ \omega = \frac{2\pi}{T}$$

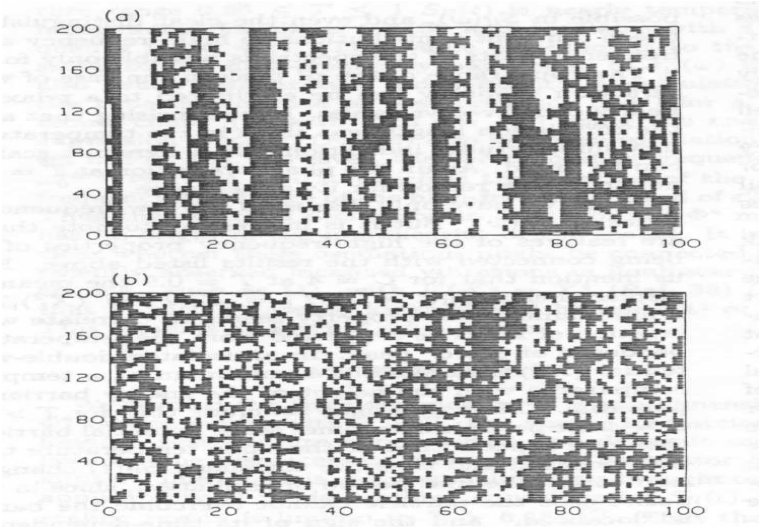
$$A(k\omega) = \int_0^T \cos(k\omega t) A(t) \mathrm{d}t = h \sum_{i=1}^{n=T/h} \cos(k\omega i h) A(ih) + O(\mathrm{e}^{-\ldots/h})$$

How to observe breathers in simple numerical runs

• fast workstation, or (even better) vector computer:

• thermal equilibrium (finite temperature), interaction not too large (?),

• observe permanent creation and annihilation of localized excitations, life times approx. 10 times the internal oscillation periods



• Excitation of slightly perturbed standing wave with $\lambda \gg 1$:

• modulational instability, wave decays into separate spatial regions(distance $\sim \lambda$) with large amplitude localized excitations! (Peyrard 1998)

188 M. Peyrard / Physica D 119 (1998) 184–199

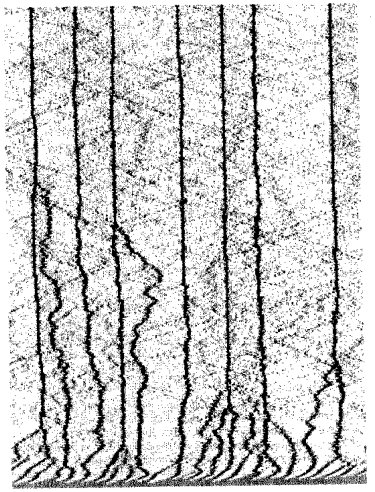
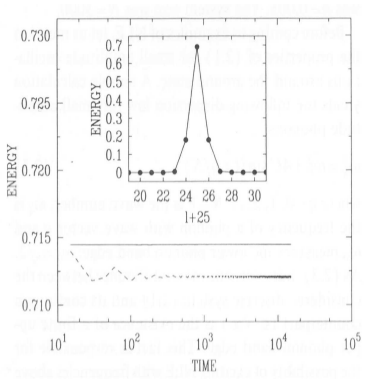
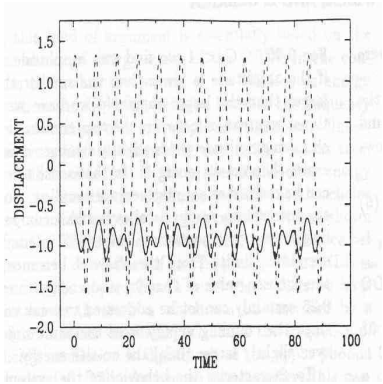


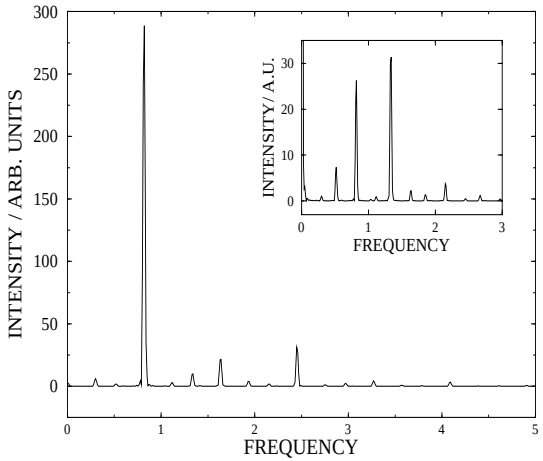
Fig. 2. Long term evolution of the energy density along the chain for an initial condition corresponding to a noisy wave given by Eq. (7). The horizontal axis indicates the position along the chain and the vertical axis corresponds to time, going upward. The energy density at site n is shown by a gray scale from $E_n = 0$ (white) to the maximum E_n recorded during the simulation (black).

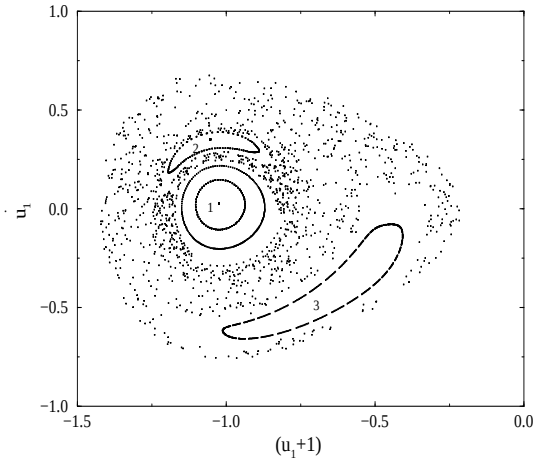
Targetted initial conditions

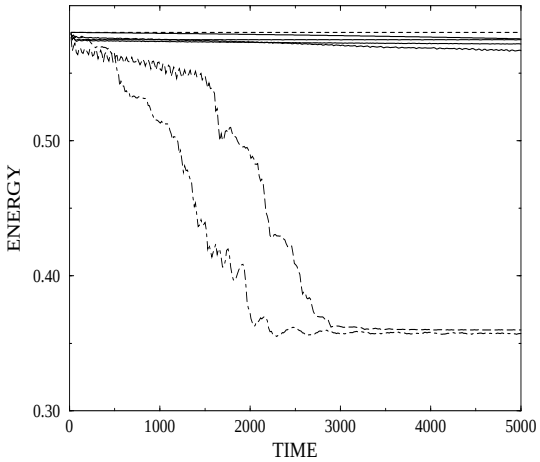




- simply all oscillators at rest (equilibrium)
- local excitations of a few oscillators
- rather arbitrary initial conditions:
- localized exciations exist for large times (how long?)





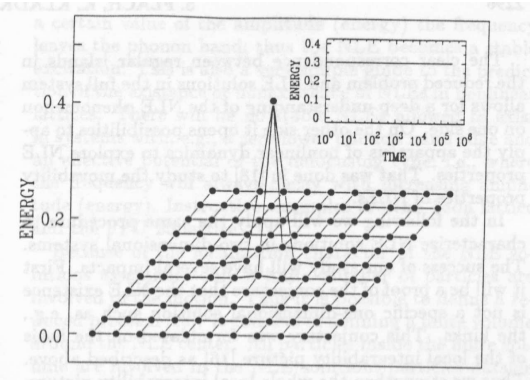


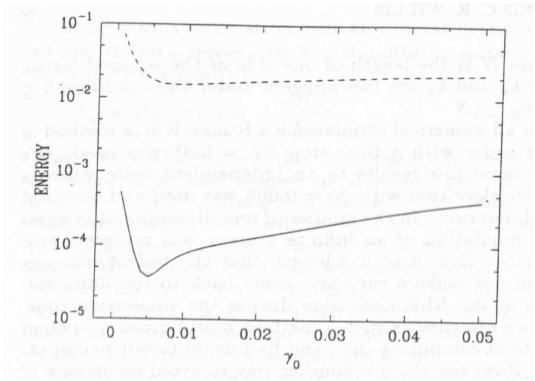
How about simulation entertainment?

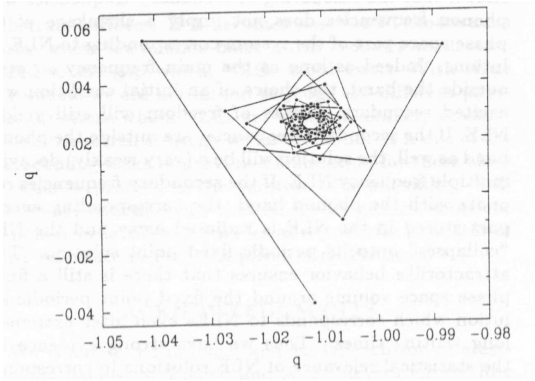
A set of useful utilities:

- PGPLOT (Fortran, C)
- JAVA
- MATLAB, etc

How about numerical runs in higher lattice dimensions?







lattice size 20×20 plus 10 rows on each side with linearly increasing friction $\sim -\dot{x}_l$
makes 1600 sites!
Zero or infinite friction give perfect transmission or reflection
Optimize numerically for linearized equations with local initial condition,
measure remaining energy after some proper large time (here $t = 2000$).

How useful are Poincare maps?
A lot if the dynamics is evolving on a low-dimensional manifold
Very instructive for 3-dimensional phase space $(3 = 4 - 1)$
Deals with projections of a 2d manifold on a 2d manifold embedded in a 3d space
Lots of tricky effects, read the books or try by yourself!

Obtaining breathers up to machine precision

Time-periodic localized excitations persist
quasi-periodic excitations radiate
Reason: resonances with ω_q!

Ansatz: $x_l(t) = \sum_k A_{kl} \mathrm{e}^{ik\omega_b t}$
Insert into EoM, assume localization, go into tails, linearize w.r.t. A_{kl}

$$H = \sum_l \left[\frac{1}{2} p_l^2 + V(x_l) + W(x_l - x_{l-1}) \right]$$

$$V(z) = \sum_{\alpha=2,3,\ldots} \frac{v_\alpha}{\alpha} z^\alpha \ , \ W(z) = \sum_{\alpha=2,3,\ldots} \frac{w_\alpha}{\alpha} z^\alpha$$

$$\ddot{x}_l = -v_2 x_l - w_2(2x_l - x_{l-1} - x_{l+1}) + F_l^{nl}(x_{l'})$$

$$) = - \sum_{\alpha=3,4,\ldots} \left[v_\alpha x_l^{\alpha-1} + w_\alpha ((x_l - x_{l-1})^{\alpha-1} - (x_{l+1} - x_l)^{\alpha-1}) \right] \ , \ F_l^{(nl)}(t) = \sum_{k=-\infty}^{+\infty} F_{kl}^{(nl)} \mathrm{e}^{ik\omega_b t}$$

$$k^2 \omega_b^2 A_{kl} = v_2 A_{kl} + w_2(2A_{kl} - A_{k,l-1} - A_{k,l+1}) + F_{kl}^{(nl)}$$

Thus for $k\omega b \neq \omega q$ linearized equations allow for localization $A_{k,|l|\to\infty} \to 0$
This is generically possible for nonlinear spatially discrete systems, because ω_q is bounded, as opposed to spatially continuous systems.
For the same reasons quasiperiodic excitations will typically radiate even in spatially discrete systems because $k_1\omega_{b1} + k_2\omega_{b2} = \omega_q$ can be realized!

Designing a map Nr.1 to find solutions

$$A_{kl}^{(i+1)} = \frac{1}{k^2\omega_b^2}\left[(v_2+2w_2)A_{kl}^{(i)} - w_2(A_{k,l-1}^{(i)} + A_{k,l+1}^{(i)}) + F_{kl}^{(nl)}(A_{k'l'}^{(i)})\right] \ , \ \lambda_{kl} = \frac{v_2}{k^2\omega_b^2}$$

$$A_{kl}^{(i+1)} = \frac{1}{v_2}\left[(k^2\omega_b^2 - 2w_2)A_{kl}^{(i)} + w_2(A_{k,l-1}^{(i)} + A_{k,l+1}^{(i)}) - F_{kl}^{(nl)}(A_{k'l'}^{(i)})\right] \ , \ \lambda_{kl} = \frac{k^2\omega_b^2}{v_2}$$

So choose $\lambda > 1$ for $l = 0, k = \pm 1$ and $\lambda < 1$ otherwise!

For low order polynomial potential functions e.g.:

$$F_{kl}^{(nl)} = \sum_{\alpha=3,4,\ldots} v_\alpha \sum_{k_1,k_2,\ldots,k_{\alpha-1}=-\infty}^{+\infty} A_{k_1 l}A_{k_2 l}\ldots A_{k_{\alpha-1} l}\delta_{k,(k_1+k_2+\ldots+k_{\alpha-1})}$$

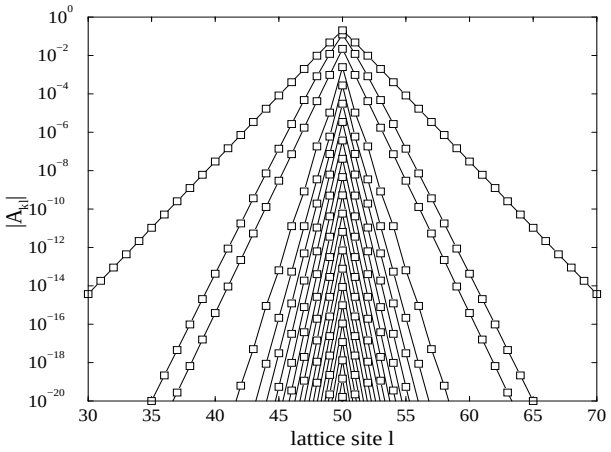
Otherwise integrate numerically at each step:

$$F_{kl}^{(nl)} = \frac{1}{T_1}\int_{-T/2}^{T_2} F_l^{(nl)}(t)\mathrm{e}^{-ik\omega_1 t}\mathrm{d}t$$

Stop the iteration when e.g.

$$\sum_{k,l} |A_{kl}^{(i)} - A_{kl}^{(i-1)}| < 10^{-10}$$

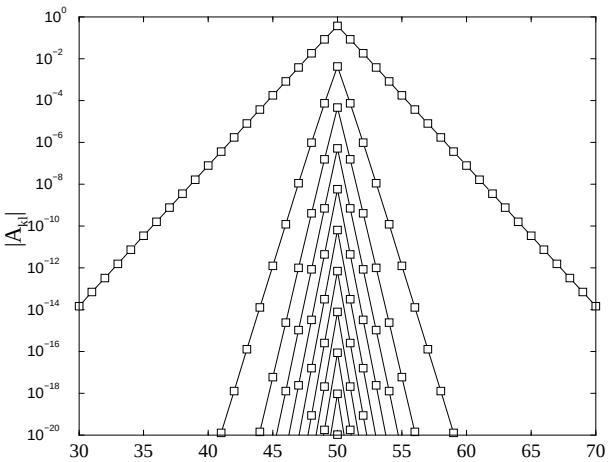
$v_2 = 2\ ,\ v_3 = -3\ ,\ v_4 = 1\ ,\ w_2 = 0.1$



k	num.result	linearization
0	-1.3202	-1.3415
1	-0.6904	-0.6898
2	-1.3796	-1.6588
3	-2.0748	-2.1143
4	-2.3957	-2.3951
5	-2.6018	-2.6026
6	-2.7663	-2.7682
$\vdots$	$\vdots$	$\vdots$

$\omega_b = 1.3$

$v_2 = 1\ ,\ v_4 = 1\ ,\ w_2 = 0.1$



k	num.result	linearization
1	-0.6722	-0.6709
3	-1.9910	-2.1464
5	-2.6103	-2.6133
7	-2.9114	-2.9117
9	-3.1324	-3.1325
$\vdots$	$\vdots$	$\vdots$

Why do we compute with double precision the localized tails pretty exact down to 10^{-307}, by just using a standard Fortran compiler?

Because double precision does not mean 10^{-16} but a cutoff after 16 digits. So if we start with initial guesses exactly zero and localize around zero, then the only obstacle to be perfect is the maximum power the compiler reserves for the exponential representation of floating point numbers :-)))

Rotating Wave Approximation:
cutoff in k-space!
Example: $\ddot{x} = -V'(x)\ ,\ V(x) = \frac{1}{2m}x^{2m}$

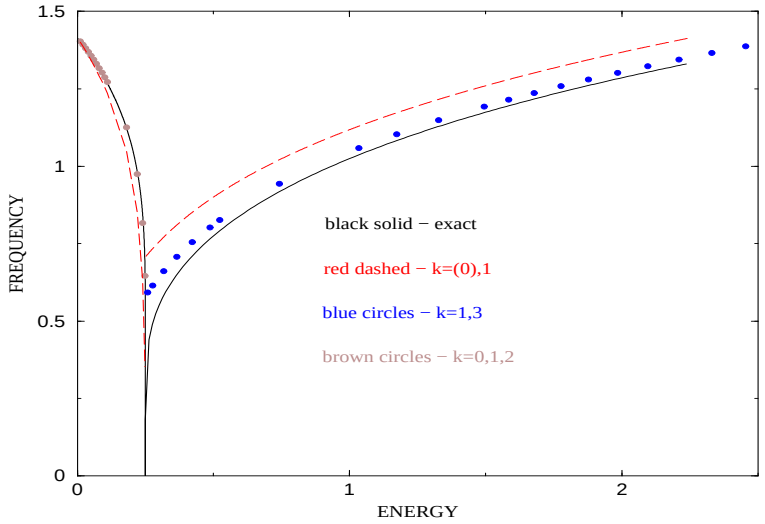
$$\omega = \frac{1}{2}\sqrt{2\pi}(2m)^{1-1/2m}\cdot\frac{\Gamma(1/2m+1/2)}{\Gamma(1/2m)}\cdot E^{1/2-1/2m}$$

RWA with $k = \pm 1$ only:

$$\omega_1 = 2^{1-m}\cdot(2m)^{1/2-1/2m}\cdot\sqrt{\frac{(2m-1)!}{m!(m-1)!}}\cdot E^{1/2-1/2m}$$

$m = 2 : 2.3\%$ error!

$V(x) = \frac{1}{4}(x^2-1)^2$:



A special case of (nearly) homogeneous potential functions

$$H = \sum_l \left[\frac{1}{2}p_l^2 + \frac{v_2}{2}x_l^2\right] + POT \ , \ POT = \sum_l \left[\frac{v_{2m}}{2m}x_l^{2m} + \frac{w_{2m}}{2m}(x_l - x_{l-1})^{2m}\right] \ , \ m = 2, 3, 4, ...$$

$$\ddot{x}_l + v_2 x_l = -v_{2m}x_l^{2m-1} - w_{2m}(x_l - x_{l-1})^{2m-1} + w_{2m}(x_{l+1} - x_l)^{2m-1}$$

Time space separation: $x_l(t) = A_l G(t)$

$$\frac{\ddot{G} + v_2 G}{G^{2m-1}} = -\kappa = \frac{1}{A_l}\left[-v_{2m}A_l^{2m-1} - w_{2m}(A_l - A_{l-1})^{2m-1} + w_{2m}(A_{l+1} - A_l)^{2m-1}\right]$$

$\kappa > 0$ is a separation parameter, can be choosen freely.

Time dependence $\ddot{G} = -v_2 G - \kappa G^{2m-1}$: single anharmonic oscillator

Spatial profile:

$$\kappa A_l = \frac{\partial POT}{\partial x_l}|_{\{x_{l'} \equiv A_{l'}\}} \ , \ \frac{\partial S}{\partial A_l} = 0 \ , \ S = \frac{1}{2}\kappa \sum_l A_l^2 - POT(\{x_l' \equiv A_l'\})$$

Breathers are saddles of S!

Method Nr.2: Saddles on the rim!

choose direction in N-dimensional space of all A_l, e.g. $(\ldots 0001000\ldots)$, $(\ldots 0001001000\ldots)$

Start from space origin P0 $A_l = 0$, depart with small steps in chosen direction,

compute S

It will first increase and then pass through a maximum P1

Now we are on the rim

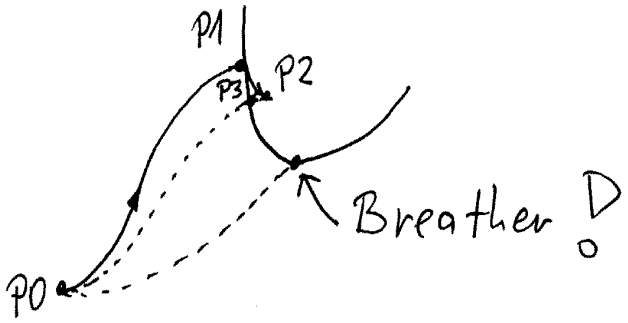
Compute the gradient of S here and make a small step in opposite direction to P2

Maximise S on the line P0-P2 to be on the rim again.

Repeat until you reach a saddle!

A very simple and efficient way to compute different types of breathers,

multibreathers etc in arbitrary dimensional lattices



Method Nr.3: Homoclinic orbits (only in $d = 1$ and with short range interaction)!

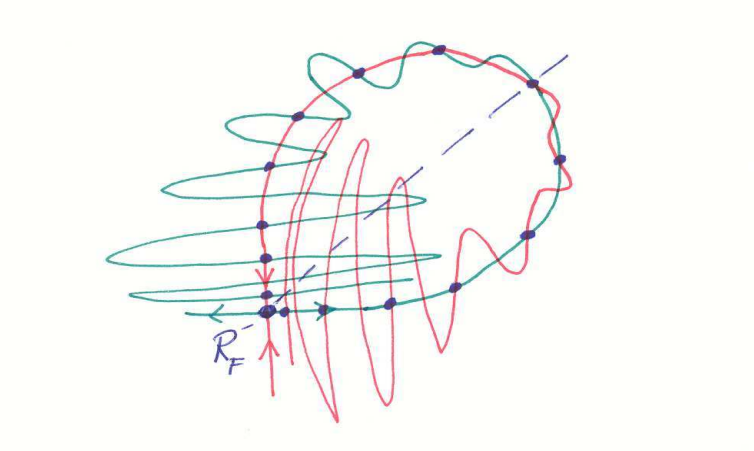
$$A_{l+1} =$$

$$A_l + \left[v_{2m} A_l^{2m-1} + w_{2m} (A_l - A_{l-1})^{2m-1} - \kappa A_l \right]^{\frac{1}{2m-1}}$$

2d map with $\vec{R}_l = (x_l, y_l) = (A_{l-1}, A_l)$:

$$x_{l+1} = y_l$$

$$y_{l+1} = y_l + \left[v_{2m} y_l^{2m-1} + w_{2m} (y_l - x_l)^{2m-1} - \kappa y_l \right]^{\frac{1}{2m-1}}$$



Fixpoint: $\vec{R}_F = (0, 0)$

(un)stable 1d manifold:

(backward) iteration converges to $\vec{R}_F$

Manifold intersections:

homoclinic points!

Iterated for- or backward yield

homoclinic orbits. i.e. breathers!

Reflection symmetry:

one homoclinic point on $x = y$

depends parametrically on κ

Simple numerical search by e.g. fixing

$x_0 = y_0$ and varying κ

Can be used for a formal

existence proof!

Existence of multibreathers follows from

generic intersection structure

Using the phase space

So far: periodic orbits as solutions of algebraic equations
Variables: Fourier coefficients or simply amplitudes

Of course we can use more general methods of solving algebraic equations, e.g. various gradient methods or Newton routines

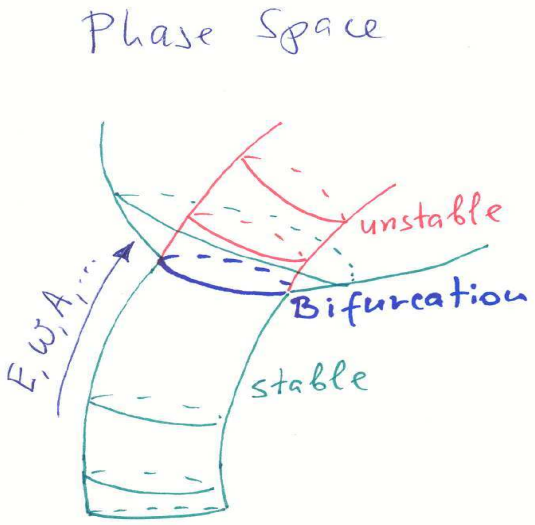
We need always a good initial guess (start close to a case where you know the solution!)

Gradient methods: more sophisticated in programming
Newton routines: may suffer from long times needed to invert matrices, danger when close to a noninvertable case (bifurcations!)
(recall: $f(x=s)=0\ ,\ f(x)=f(x_0)+f'(x_0)(x-x_0)+hot$
$x_{n+1}=x_n-f(x_n)/f'(x_n)$)

If besides the Hamiltonian H we have another conserved quantity B, then the manifolds of some isolated periodic orbits may satisfy the parallelity of gradients, i.e. $grad(H) \parallel grad(B)$

Periodic orbit:
loop in phase space

Isolated periodic orbit (PO):
neighbourhood in phase space free of POs with identical conserved quantities (as opposed to POs on resonant tori)



Method Nr.4: NEWTON in phase space

Integrate a given initial condition $\vec{\vec{R}}$ with $x_l(t=0) \equiv X_l$, $p_l(t=0) \equiv P_l$ over a certain time T:

$$x_l(T) \equiv I_l^x(\{X_{l'}, P_{l'}\}, T)$$

$$p_l(T) \equiv I_l^p(\{X_{l'}, P_{l'}\}, T)$$

Consider the functions

$$F_l^x = I_l^x - X_l \ , \ F_l^p = I_l^p - P_l$$

If $\vec{\vec{R}}$ belongs to a PO with period T then

$$F_l^x = F_l^p = 0$$

For a Newton routine to converge:
remove all degeneracies!
If $\vec{\vec{R}}$ belongs to the PO, then a 1d manifold of points belong to the PO
Degeneracy removed by one additional condition, e.g. $P_M = 0$
So for N degrees of freedom zeroes of $2N-1$ coupled equations of $2N-1$ variables!
Make sure that a zero of these $2N-1$ equations with the additional initial condition $P_M = 0$ uniqely fixes $p_M(T) = 0$, e.g. through energy conservation.

Define

$$\vec{R} = (X_1, X_2, ..., X_M, ..., X_N, P_1, ..., P_{M-2}, P_{M-1}, P_{M+1}, P_{M+2}, ..., P_N)$$
$$\vec{F} = (F_1^x, F_2^x, ..., F_M^x, ..., F_N^x, F_1^p, ..., F_{M-2}^p, F_{M-1}^p, F_{M+1}^p, F_{M+2}^p, ..., F_N^p)$$
$$\vec{F} = \vec{R}(T) - \vec{R}$$

Given an initial guess $\vec{R}^{(0)}$ expand

$$F_n(\vec{R}) = F_n(\vec{R}^{(0)}) + \sum_m \frac{\partial F_n}{\partial R_m}|_{\vec{R}^{(0)}}(R_m - R_m^{(0)})$$

$$\vec{F}(\vec{R}) = \vec{F}(\vec{R}^{(0)}) + \mathcal{M}(\vec{R} - \vec{R}^{(0)})$$
$$\mathcal{M}_{nm} = \frac{\partial F_n}{\partial R_m}|_{\vec{R}^{(0)}} = \frac{\partial R_n(T)}{\partial R_m}|_{\vec{R}^{(0)}} - \delta_{nm}$$

One Newton step: $\vec{R}$ such that $\vec{F} = 0$:

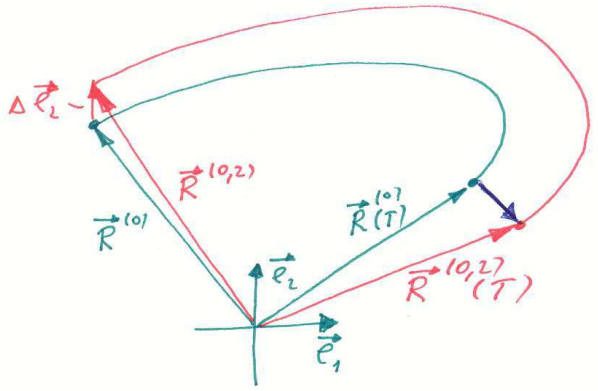
$$\vec{R} = \vec{R}^{(0)} - \mathcal{M}^{-1}\vec{F}(\vec{R}^{(0)})$$

Repeat until $|\vec{F}|$ *or* $max|F_n| < \epsilon$

How to compute $\mathcal{M}$:

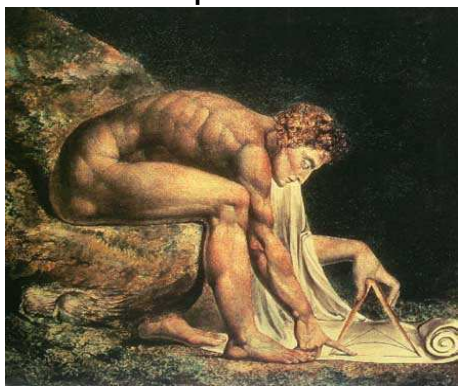
$$\vec{R}^{(0,m)} = \vec{R}^{(0)} + \Delta\vec{e}_m$$

$$\mathcal{M}_{nm} = \frac{1}{\Delta}\left(F_n(\vec{R}^{(0,m)}) - F_n(\vec{R}^{(0)})\right)$$
$$\mathcal{M}_{nm} = \frac{1}{\Delta}\left(R_n^{(0,m)}(T) - R_n^{(0)}(T)\right) - \delta_{nm}$$



Advantages of Newton:
exponential convergence $|\vec{F}|_{n_{it}+1} \sim |\vec{F}|_{n_{it}}$
easy to program
we may use one Newton matrix for several iterations

Disadvantages of Newton:
computational time $\sim N^2$
matrix inversion sensitive to bifuractions
may need subtle routines (singular value decomposition, dealing with sparse matrices etc)
Blake's representation of Newton:



Method Nr.5:
STEEPEST DESCENT in phase space

$$g(\vec{\tilde{R}}) = \sum_l \left[F_l^x F_l^x + F_l^p F_l^p\right]$$

$$(\nabla g)_n = \frac{\partial g}{\partial \tilde{R}_n}$$

Start in phase space, go in direction opposite to the gradient!

Advantages of Descent
computational time $\sim N$
insensitive to bifurcations

Disadvantages of Descent
more clumsy to program
slower convergence
distinguish zero minimima from nearly zero minima?

Some aspects of symmetries

Equations of motion are invariant under some symmetry operations:

continuous time-shift symmetry $t \longrightarrow t + \tau$
time reversal symmetry $t \longrightarrow -t \ , \ p_l \longrightarrow -p_l$
Parity symmetry $x_l \longrightarrow -x_l \ , \ p_l \longrightarrow -p_l$
discrete translational symmetry on the lattice
other discrete permutational lattice symmetries which leave the lattice invariant
(spatial reflections etc)

Each discrete symmetry implies that given a trajectory in phase space,
a new trajectory is generated by applying the symmetry operation
If the new manifold equals the original one, then the trajectory is invariant under the symmetry
Otherwise it is not invariant
Note that the symmetry operation on the phase space does not involve time!

In linear equation systems symmetry breaking is possible only in the presence of degeneracies
In nonlinear equation systems symmetry breaking is common

Example: a plane wave in a harmonic chain is not invariant under time reversal, because of degeneracy

A breather is per definition not invariant under discrete translational symmetry

If it is invariant under other symmetries, this can be used to substantially lower the numerical effort!

For time-reversal breathers it is possible to find an origin in time when
$x_l(t) = x_l(-t)$, $p_l(t) = -p_l(-t)$, saves 50% computational time!

Time-reversal parity-invariant breathers:
$x_l(t + T/2) = -x_l(t)$, $p_l(t + T/2) = -p_l(t)$, saves 75% computational time!

Computing lattice permutational invariant breathers may substantially lower the computational effort by finding the irreducible breather section, especially in higher lattice dimensions!

Breathers which are not invariant under time reversal posess a nonzero energy flux:
possible in d=2 and larger!

Perturbing breathers

Suppose we found a breather solution $x_l(t)$.
Now we add a small perturbation $\epsilon_l(t)$ to it and linearize the resulting equations for $\epsilon_l(t)$:

$$\ddot{\epsilon}_l = -\sum_m \frac{\partial^2 H}{\partial x_l \partial x_m}|_{\{x_{l'}(t)\}} \epsilon_m$$

This problem corresponds to a time-dependent Hamiltonian $\tilde{H}(t)$

$$\tilde{H}(t) = \sum_l \left[\frac{1}{2}\pi_l^2 + \frac{1}{2}\sum_m \frac{\partial^2 H}{\partial x_l \partial x_m}|_{\{x_{l'}(t)\}} \epsilon_l \epsilon_m \right]$$

$$\dot{\epsilon}_l = \frac{\partial \tilde{H}}{\partial \pi_l} \ , \ \dot{\pi}_l = -\frac{\partial \tilde{H}}{\partial \epsilon_l}$$

There is a conservation law $\dot{I} = 0$

$$I = \sum_l \left[\pi_l'(t)\epsilon_l(t) - \pi_l(t)\epsilon_l'(t) \right]$$

For simplicity we drop the lattice index here.
Define the matrix $\mathcal{J}$

$$\mathcal{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

and the evolution matrix $\mathcal{U}(t)$

$$\begin{pmatrix} \pi(t) \\ \epsilon(t) \end{pmatrix} = \mathcal{U}(t) \begin{pmatrix} \pi(0) \\ \epsilon(0) \end{pmatrix}$$

It follows

$$I = (\pi(t), \epsilon(t))\, \mathcal{J} \begin{pmatrix} \pi'(t) \\ \epsilon'(t) \end{pmatrix}$$

$$I = (\pi(0), \epsilon(0))\, \mathcal{U}^T(t) \mathcal{J} \mathcal{U}(t) \begin{pmatrix} \pi'(0) \\ \epsilon'(0) \end{pmatrix}$$

$$\rightarrow \mathcal{U}^T(t) \mathcal{J} \mathcal{U}(t) = \mathcal{J}$$

Thus $\mathcal{U}(t)$ is symplectic!

$$\mathcal{U}y = \lambda y \ , \ \mathcal{U}^T y = \lambda y$$

$$\mathcal{U}y' = \frac{1}{\lambda} y' \ , \ y' = \mathcal{J}^{-1} y = -\mathcal{J} y$$

If $\mathcal{U}$ is real and (λ, y) are an eigenvalue and eigenvector, so are

$$(\lambda^*, y^*) \ , \ (\frac{1}{\lambda}, \mathcal{J}y) \ , \ (\frac{1}{\lambda^*}, \mathcal{J}y^*)$$

Consider now the mapping over one period for a breather, which defines the Floquet Matrix $\mathcal{F}$

$$\mathcal{U}(t) = \mathcal{U}(t + T_b) \ , \ \mathcal{U}(T_b) \equiv \mathcal{F}$$

Bloch's Theorem: all Floquet eigenstates with $\lambda = \mathrm{e}^{i\omega\nu T_b}$ when taken as initial conditions correspond to

$$\epsilon_l(t) = \mathrm{e}^{i\omega\nu t} \Delta_l^{(\nu)}(t) \ , \ \Delta_l^{(\nu)}(t) = \Delta_l^{(\nu)}(t + T_b)$$

A breather is linearly stable when all Floquet eigenvalues reside on the unit circle, i.e. have absolute value 1

One Floquet eigenvalue is always located at $\lambda = +1$

Its eigenvector is tangent to the periodic orbit

As eigenvalues come in pairs, there are two eigenvalues at $\lambda = +1$.

Upon changing a control parameter the Floquet eigenvalues may move on the unit circle, collide and leave the circle

Then a breather turns from linearly stable to linearly unstable

Aubry's Band Theory does just that (helps to find Krein signatures, relate pairs or quadruplets of eigenvalues etc):

$$\ddot{\epsilon}_l = -\sum_m \frac{\partial^2 H}{\partial x_l \partial x_m}|_{\{x_{l'}(t)\}} \epsilon_m + E\epsilon_l$$

The different kinds of Floquet eigenvectors

Eigenvectors (simply the perturbations at time $t = 0$: $\vec{F} = (\epsilon_1, \epsilon_2, ..., \epsilon_N, \pi_1, \pi_2, ..., \pi_N)$ can be localized or delocalized in the lattice space

Finite number of localized states
Large number $\sim 2N$ of delocalized states
Delocalized states are just plane waves far from the breather

Obtaining the Floquet matrix: similar to the Newton matrix!

Before diagonalizing: make sure to use all possible symmetries to reduce the Floquet matrix to its noninteracting irreducible parts!

What is it useful for?

Characterizing breathers: can be stable, unstable
Eigenvalue collisions mark bifurcations (of new periodic orbits!)
Bifurcations correspond to resonances!

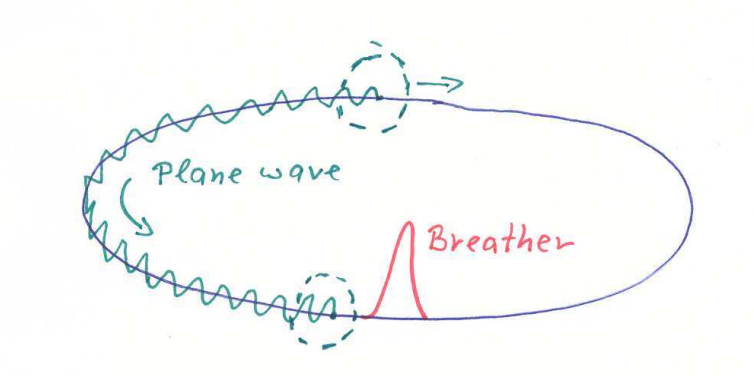
Search for bifuractions which may yield 'moving breathers'

By choosing proper boundary conditions study scattering of plane waves by breathers!
Relate the eigenvalue structure of the Floquet matrix to the scattering results
Understand as much as possible what is lost by linearizing the phase space flow

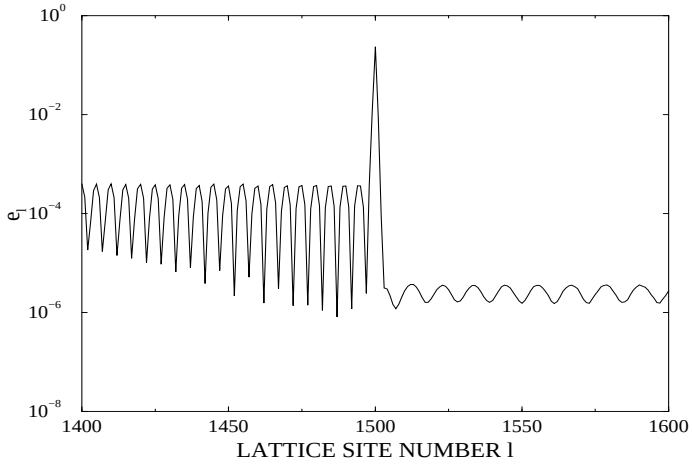
Scattering of plane waves by discrete breathers in 1d

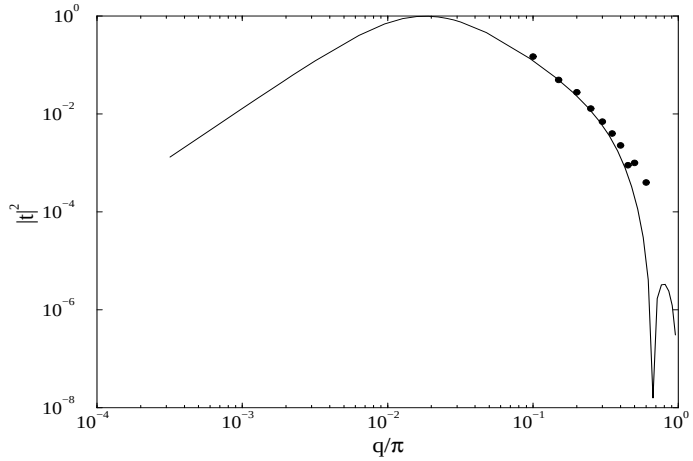
Simulation using full equations
Initial condition: breather plus plane wave packet
Packet: either gaussian or
half chain plane wave with sharp cuts (better!)

Wait until stationary pattern around breather appears
But not longer than $\frac{N}{2max(v_g)}$
Choose amplitude of plane wave not too large (nonlinear corrections) and not too small (as compared to the breather solution errors)



KG chain with $q = 0.2\pi$:

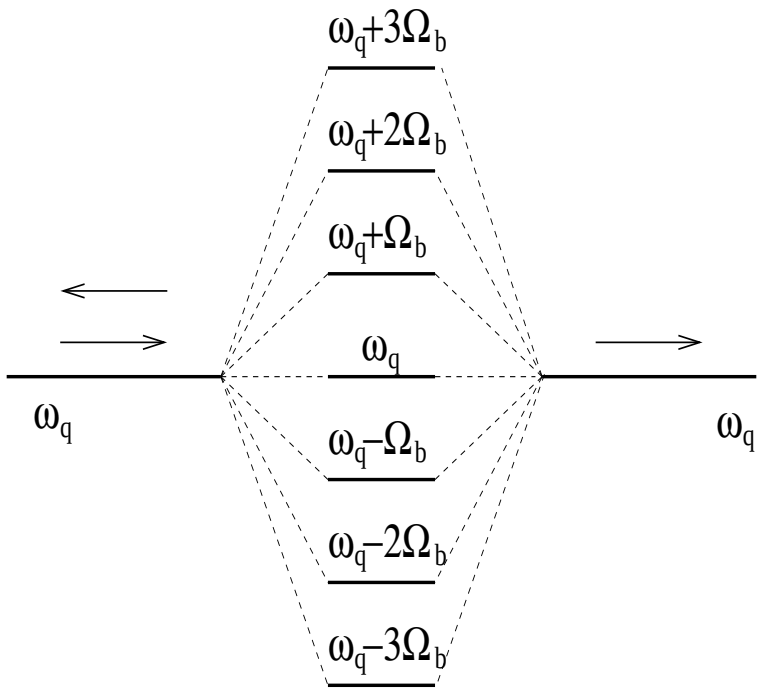




Computing transmission up to machine precision

Scattering goes through the extended Floquet states:

$$\epsilon_l(t) = \sum_{k=-\infty}^{\infty} e_{lk} \mathrm{e}^{\mathrm{i}(\omega_q + k\Omega_b)t}$$



Scattering by exact breather solutions:
elastic one-channel or
inelastic f-channel scattering (number of open channels less or equal to the number of DOF per lattice site)

Minimum lattice size: check the localization length of all closed channels (can be quite different from the localization length of the breather!)

Numerical Scheme for one-channel scattering: zeroes of $\mathbf{G}$:

$$\mathbf{G}(\vec{\epsilon}(0), \dot{\vec{\epsilon}}(0)) = \begin{pmatrix} \vec{\epsilon}(0) \\ \dot{\vec{\epsilon}}(0) \end{pmatrix} - e^{i\omega_q T_b} \begin{pmatrix} \vec{\epsilon}(T_b) \\ \dot{\vec{\epsilon}}(T_b) \end{pmatrix}$$

Lattice:

$$-N, (-N+1), ..., -1, 0, 1, ...(N-1), N$$

Boundary conditions:

$$\epsilon_{N+1} = e^{-i\omega q t} \ , \ \epsilon_{-N-1} = (A+iB)e^{-i\omega q t}$$

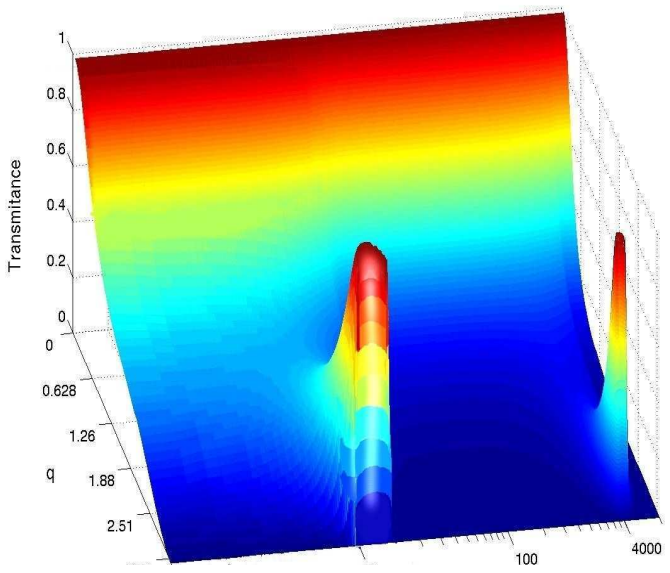
Step Nr.1:
Fixing for the moment A, B, use standard Newton to find zeroes of $\mathbf{G}$.

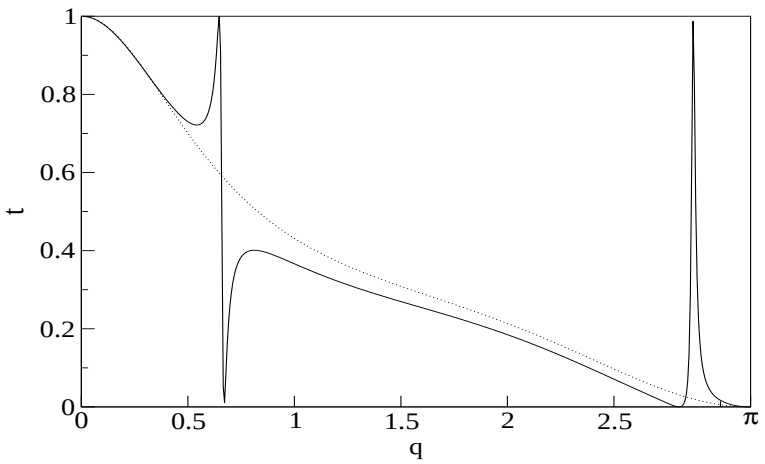
Step Nr.2:
find values for A, B such that $\epsilon_N = e^{-iq-i\omega q t}$

Use the notation $\epsilon_l(t) = \zeta_l(t)e^{-i\omega q t}$.
Then the transmission coefficient is given by

$$t_q = \frac{4\sin^2 q}{|(A+iB)e^{-iq} - \zeta_{-N}|^2}$$

FPU chains:





Instead of a closing

Dissipative systems:
Breather families get 'quantized' into attractors which are surrounded by basins of attraction
Phonons are damped out, thus possible quasiperiodic and even chaotic in time 'breathers', and even moving breathers
Possible hysteresis between different breather states upon looping control parameters

Quantum systems
Eigenvalue problems plus eigenfunctions
Provide with information on breather tunneling
Eigenfunction can be 'mapped' onto classical phase space to observe correspondence with classical trajectories

What all this could be good for in the future:
Everything concerning nonequilibrium processes
Relaxation in quantum systems
Energy concentration via relaxation
Description of chemical processes