The Abdus Salam
International Centre for Theoretical Physics

United Nations
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2286-11

Workshop on New Materials for Renewable Energy

31 October - 11 November 201

Nonlinear Lattice Waves: Classical and Quantum (third part)

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Nonlinear Lattice Waves: Classical and Quantum

S. Flach, MPIPKS Dresden

mpipks

Three lectures and one tutorial:

- discrete breathers – localization in real space
- q-breathers – localization in mode space
- **tutorial: quantizing discrete breathers**
- the problem of weak passwords: chaos, criticality, and p-captchas

Quantizing Discrete Breathers – Introduction and Tutorial

S. Flach, MPIPKS Dresden

mpipks

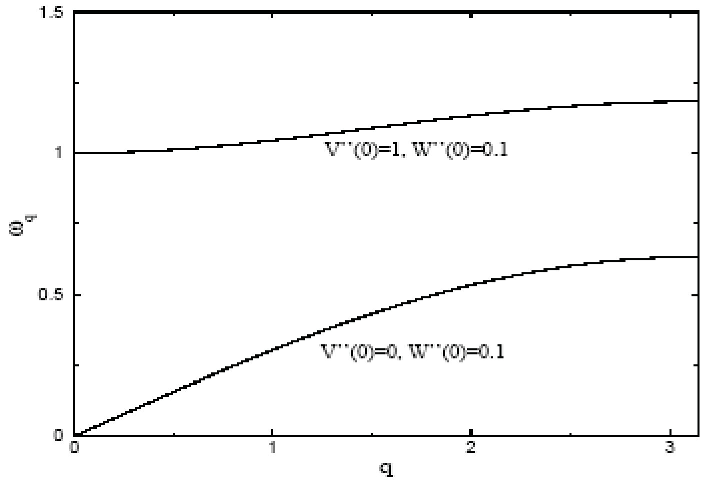
Road map:

- short recollection on classical discrete breather solutions
- some simple quantum guesses
- two interacting quantum particles in a chain
- from the dimer to the trimer
- more symmetries - more fine structure

short recollection on classical discrete breather solutions

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

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



Equations of motion:

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

Small amplitude plane waves:

$$x_l(t) \sim \mathrm{e}^{\mathrm{i}(\omega_q t - ql)} \;,\; \omega_q^2 = V''(0) + 4W''(0)\sin(\frac{q}{2})$$

Group velocity $v_g(q)$:

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

For N sites trajectories evolve in a $2N$-dimensional phase space!

Exact solutions?

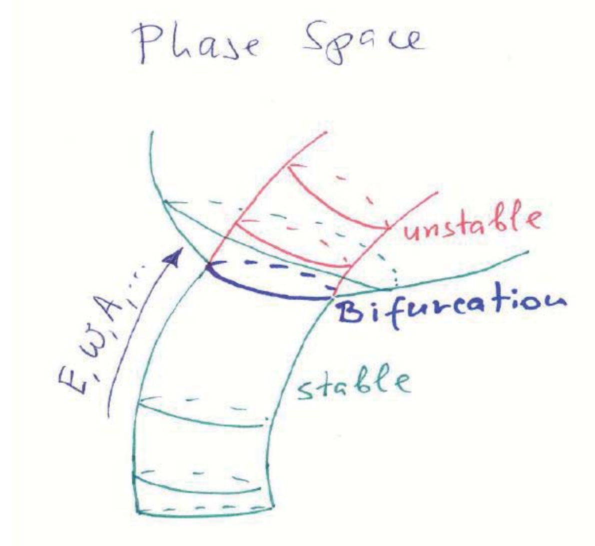
Discrete Breathers:

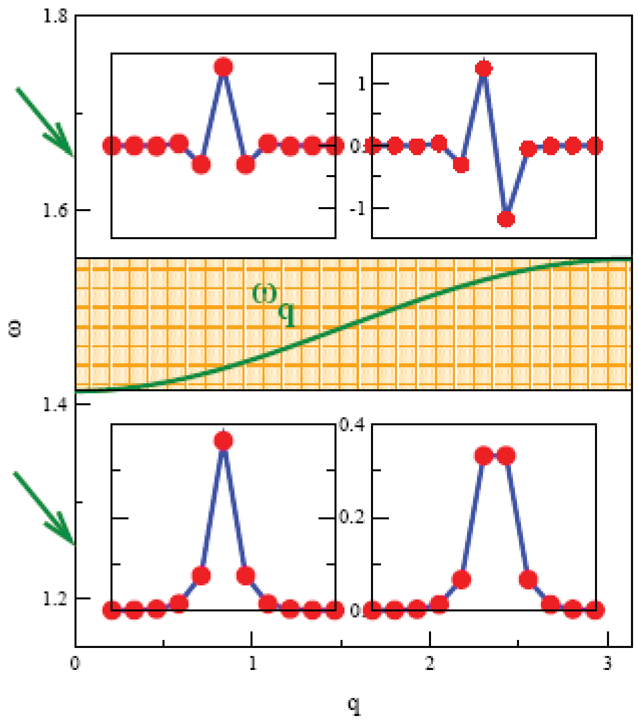
> time-periodic, spatially localized solutions of the equations of motion with finite energy (action) with frequency Ω_b

Breathers exist in
$d = 1, 2, 3, ...$-dimensional lattice models

Existence proofs: MacKay/Aubry, Flach, James, Sepulchre, ...

Are dynamically and structurally stable, form one-parameter families of solutions





Necessary ingredients:

nonlinear equations of motion and bounded spectrum ω_q of small amplitude oscillations (phonons, magnons, whateverons)

Necessary condition for existence (Flach 1994):

$$k\Omega_b \neq \omega_q \quad , \quad k = 0, 1, 2, 3, ...$$

Thus:
in general no localized exciations with quasiperiodic time dependence (Flach 1994)

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}

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

Tutorial: some simple quantum guesses

- action quantization: countable set of eigenenergies
- N-fold degeneracy due to translational invariance?
- degeneracy will be lifted!
- discrete breathers will start to tunnel along the lattice!
- therefore quantum discrete breathers are
  many quantum particle bound states

Quantum mechanics is conceptually much simpler than nonlinear classics, because it is simply linear algebra and vector spaces. But it is often much harder to perform actual calculations, both analytical and numerical, due to the huge dimensional potentially entangled Hilbert Jungle (I mean space)

Ovchinnikov 11969
Scott/Eilbeck et al 1994
Probably Landau etc

Tutorial: two interacting quantum particles in a chain: the integrable Bose Hubbard chain with periodic boundary conditions

$$\hat{H} = \hat{H}_0 + \gamma \hat{H}_1 \qquad \hat{H}_0 = -\sum_{j=1}^{f} b_j^+ (b_{j-1} + b_{j+1}) \qquad \hat{H}_1 = -\frac{1}{2}\sum_{j=1}^{f} b_j^+ b_j^+ b_j b_j$$

Bosonic particle creation and annihilation operators: $[b_i, b_j^+] = \delta_{ij}$

Hamiltonian conserves total number of particles: $\hat{N} = \sum_{j=1}^{f} b_j^+ b_j$

Number of states for N particles and f sites: (N+f-1)! / (N! (f-1)!)

Zero particles: one ground state; one particle: E=-2cos(k)

Two particles: like one particle in two dimensions (and so on ...)

Choose the optimal basis! Look for symmetries and conserved quantitites:
Here: number states and Bloch representation

$$|\Phi_n\rangle = |n_1, n_2, \ldots, n_f\rangle$$

For example $|0200000\rangle$

Translation operator: $\hat{T}|n_1, n_2, \ldots, n_f\rangle = |n_f, n_1, n_2, \ldots, n_{f-1}\rangle$

Eigenvalues: $\tau = \exp(ik) \qquad k = 2\pi\nu/f$

$$\nu \in [-(f-1)/2, (f-1)/2]$$

Then we can reduce effective d=2 problem to d=1:

Relative distance between two quanta: j

$$|\Psi_2\rangle = \sum_{j=1}^{(f+1)/2} v_j |\Phi_2^j\rangle \qquad |\Phi_2^j\rangle = \frac{1}{\sqrt{f}} \sum_{s=1}^{f} \left(\frac{\hat{T}}{\tau}\right)^{s-1} |1\underbrace{0\cdots0}_{j-1}1\cdots\rangle$$

$$\hat{H}_k |\Psi_n\rangle = E |\Psi_n\rangle \qquad \hat{H}_k = -\begin{pmatrix} \gamma & q\sqrt{2} & & & & \\ q^*\sqrt{2} & 0 & q & & & \\ & q^* & 0 & q & & \\ & & \ddots & \ddots & \ddots & \\ & & & q^* & 0 & q \\ & & & & q^* & p \end{pmatrix}$$

$$q = 1 + \tau \qquad p = \tau^{-(f+1)/2} + \tau^{-(f-1)/2}$$

Solution: two particle continuum and bound states!

continuum: $E^{0}_{k,k_1} = -2[\cos(k_1) + \cos(k_1 + k)]$

bound states: $E_2(k) = -\sqrt{\gamma^2 + 16\cos^2 k/2}$

exponential localization: $\mathbf{v} = \left(\frac{1}{\sqrt{2}}, \mu, \mu^2, \mu^3, \ldots\right)$

$$\mu = -\frac{[\gamma + E_2(k)]e^{ik/2}}{4\cos(k/2)}$$

$$C_j \equiv |v_j|^2 = |\mu|^{2(j-1)} = e^{2\lambda(j-1)}$$

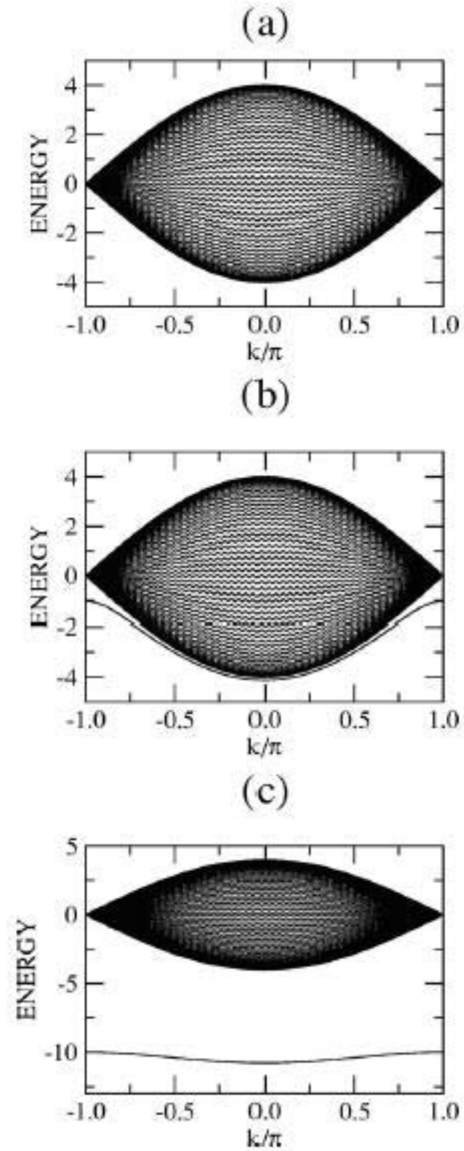


FIG. 1. Energy spectrum of the Bose-Hubbard model for different values of the interaction γ: (a) γ=0.1, (b) γ=1.0, and (c) γ=10. Here, f=101.

From bosons to fermions with finite range interaction

Nguenang,SF 2009

$$\hat{H} = \hat{H}_0 + \hat{H}_U + \hat{H}_V$$

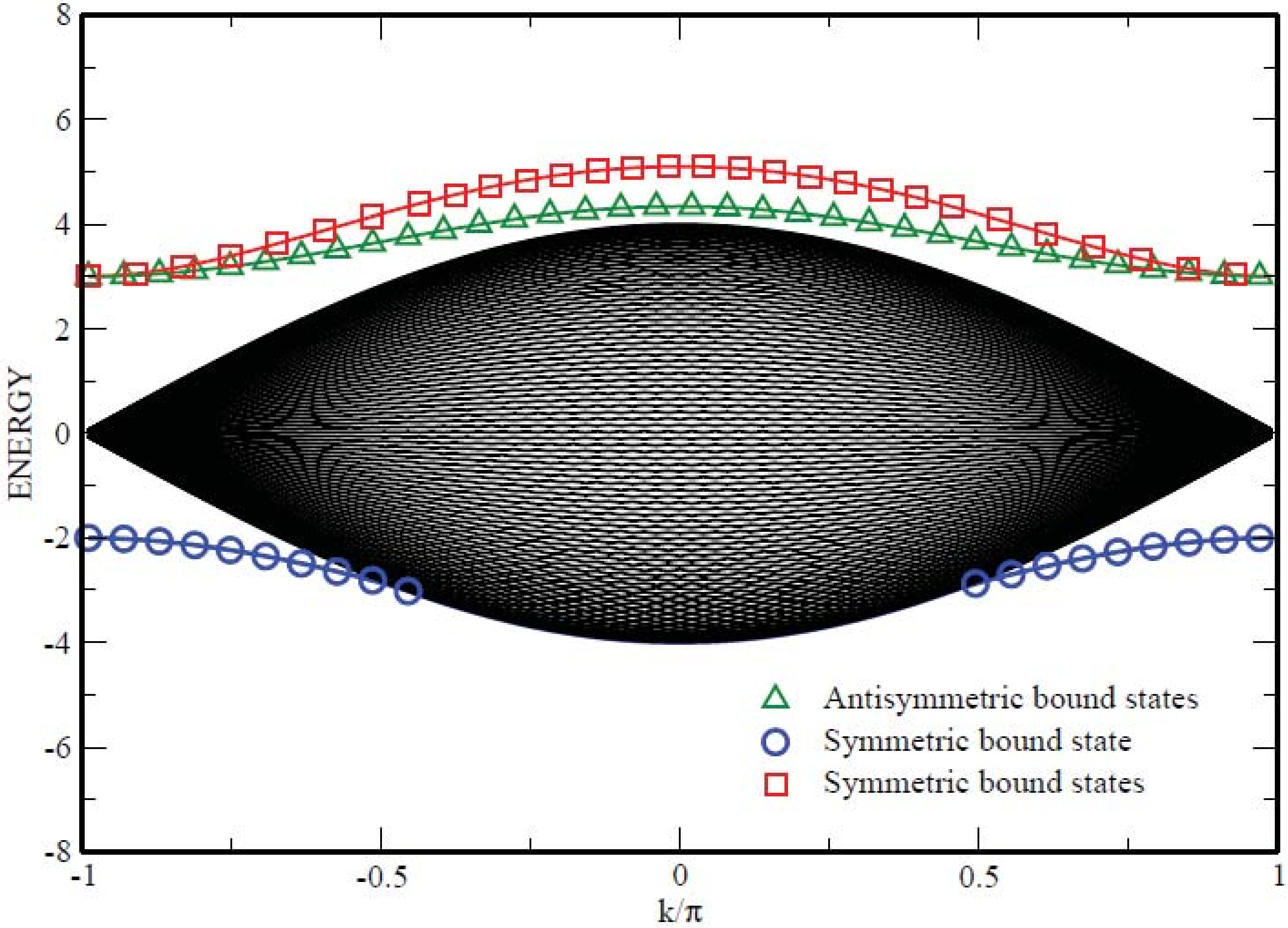
$$\hat{H}_0 = -\sum_{j,\sigma} \hat{a}^+_{j,\sigma}(\hat{a}_{j-1,\sigma} + \hat{a}_{j+1,\sigma})$$

$$\hat{H}_U = -U\sum_{j} \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}, \qquad \hat{n}_{j,\sigma} = \hat{a}^+_{j,\sigma}\hat{a}_{j,\sigma}$$

$$\hat{H}_V = -V\sum_{j} \hat{n}_j\hat{n}_{j+1} \qquad \hat{n}_j = \hat{n}_{j,\uparrow} + \hat{n}_{j,\downarrow}$$

We deal with symmetric and antisymmetric states (spin exchange)

$$H^s(i,j) = -\begin{pmatrix} U & q\sqrt{2} & & & & \\ q^*\sqrt{2} & V & q & & & \\ & q^* & 0 & q & & \\ & & \ddots & \ddots & \ddots & \\ & & & q^* & 0 & q \\ & & & & q^* & p \end{pmatrix} \qquad H^a(i,j) = -\begin{pmatrix} V & q & & & & \\ q^* & 0 & q & & & \\ & q^* & 0 & q & & \\ & & \ddots & \ddots & \ddots & \\ & & & q^* & 0 & q \\ & & & & q^* & -p \end{pmatrix}$$



We obtain two symmetric and one antisymmetric bound state bands

Tutorial: the classical and the quantum dimer – many interacting particles

Three and more particles – becomes increasingly dificult because

- **increase of dimension**
- **no additional symmetries or integrals of motion**
- **getting into Hilbert jungle**

But we can instead work with small systems:

- **two sites = dimer (up to few thousand particles)**
- **three sites = trimer (up to 50-100 particles)**
- **and can study correspondence between classical and quantum worlds**

$$H = \frac{1}{2}|\psi_1|^4 + \frac{1}{2}|\psi_2|^4 + C\cdot(\psi_1^*\psi_2 + cc), \quad \dot{\psi}_{1,2} = i\frac{\partial H}{\partial \psi_{1,2}^*}$$

$$B = |\psi_1|^2 + |\psi_2|^2, \quad \dot{B} = 0$$

$$\psi_{1,2} = A_{1,2}\cdot e^{i\varphi_{1,2}}, \quad \Delta\varphi = \varphi_2 - \varphi_1, \quad S\varphi = \varphi_1 + \varphi_2$$

$$\Downarrow$$

$$H = \frac{1}{2}(A_1^4 + A_2^4) + 2CA_1A_2\cdot\cos\Delta\varphi, \quad B = A_1^2 + A_2^2$$

Isolated Periodic Orbits: grad H ∥ grad B, $\vec{R} = (A_1, A_2, \Delta\varphi, S\varphi)$

$$\text{grad}\, H = \begin{pmatrix} 2A_1^3 + 2CA_2\cos\Delta\varphi \\ 2A_2^3 + 2CA_1\cos\Delta\varphi \\ -2CA_1A_2\sin\Delta\varphi \\ 0 \end{pmatrix}, \quad \text{grad}\, B = \begin{pmatrix} 2A_1 \\ 2A_2 \\ 0 \\ 0 \end{pmatrix}$$

$$\Downarrow$$

$\sin\Delta\varphi = 0 \Rightarrow \Delta\varphi = 0$ ($A_1/A_2 < 0$ takes care of π)

$A_{1,2}^3 + CA_{2,1} = \varkappa A_{1,2}$ ($\varkappa$ is some constant)

$$\psi_{1,2}(t) = A_{1,2}(t)\cdot e^{i\varphi(t)}, \quad \frac{d}{dt}|\psi_1|^2 \sim \sin\Delta\varphi = 0 \Rightarrow \begin{cases} A_{1,2} = \text{const} \\ \dot{\varphi} = \omega = \varkappa \end{cases}$$

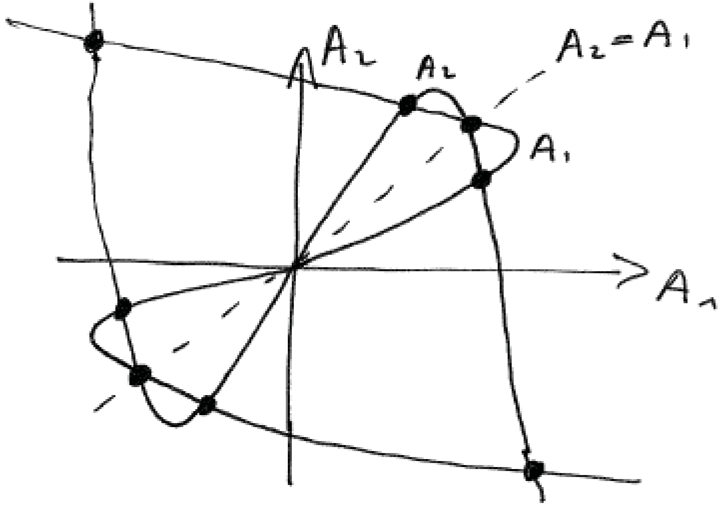
The classical dimer

Solutions :

a) $A_1 = A_2 \Rightarrow \omega = A^2 + c$ ↑↑ in phase

b) $A_1 = -A_2 \Rightarrow \omega = A^2 - c$ ↑↓ out of phase

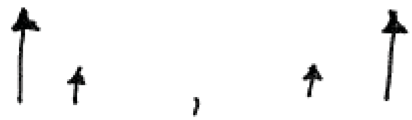
c) $A_2 = \frac{\omega}{c} A_1 - \frac{1}{c} A_1^3$, $A_1 = \frac{\omega}{c} A_2 - \frac{1}{c} A_2^3$



Bifurcation:

$B_b = 2c, \; E_b = 3c, \; \omega_b = 2c$

$$\begin{cases} A_{1,2}^2 = \frac{1}{2}\left[\omega \pm \sqrt{\omega^2 - 4c^2}\right] \\ \omega = 1 + B \end{cases}$$



Integrating the dimer

$$y = A_1^2 - \frac{B}{2}, \quad H = \frac{1}{4}B^2 + y^2 + 2C\sqrt{\frac{B^2}{4} - y^2}\cdot\cos\Delta\varphi$$

$$\Downarrow$$

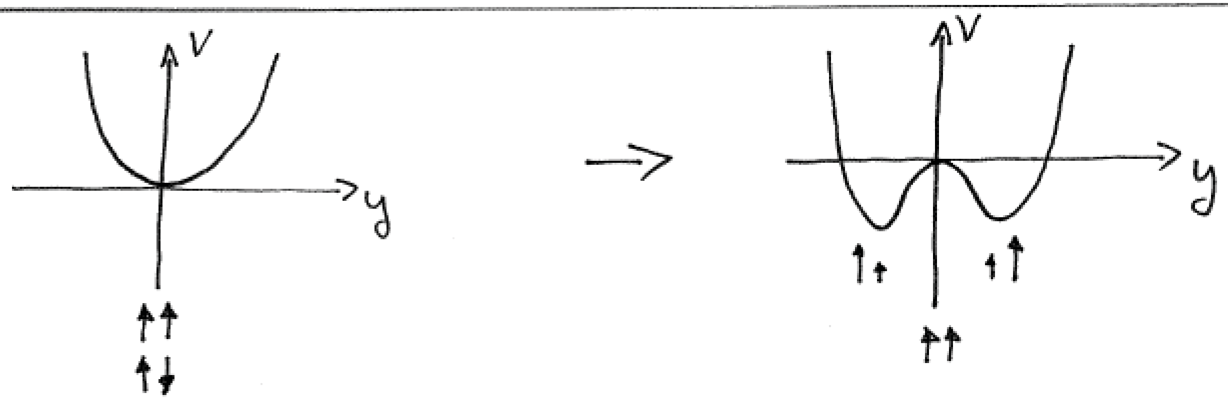
$$\dot{y} = \frac{\partial H}{\partial \Delta\varphi}, \quad \dot{\Delta\varphi} = -\frac{\partial H}{\partial y}; \quad \dot{s\varphi} = \frac{\partial H}{\partial B}, \quad \dot{B} = -\frac{\partial H}{\partial s\varphi}$$

$$\Downarrow$$

$$\begin{cases} \dot{B} = 0, \quad \dot{s\varphi} = \frac{1}{2}B + B\cdot C\cdot\frac{\cos\Delta\varphi}{\sqrt{B^2/4 - y^2}} \\ \dot{y} = -2\cdot C\cdot\sqrt{B^2/4 - y^2}\cdot\sin\Delta\varphi, \quad \dot{\Delta\varphi} = -2y + \frac{2Cy}{\sqrt{B^2/4 - y^2}}\cos\Delta\varphi \end{cases}$$

$$\Downarrow$$

$$\boxed{\ddot{y} = -\frac{\partial V}{\partial y}, \quad V(y; E, B) = \left(-E + \frac{B^2}{4} + 2C^2\right)y^2 + \frac{1}{2}y^4}$$



The quantum dimer with b particles

Aubry,SF,Kladko,Olbrich 1996

$$H = \frac{5}{4} + \frac{3}{2}\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) + \frac{1}{2}\left((a_1^\dagger a_1)^2 + (a_2^\dagger a_2)^2\right) + C\left(a_1^\dagger a_2 + a_2^\dagger a_1\right)$$

number states: $|n, (b-n)\rangle \equiv |n)$

$$H_{nm} = \begin{cases} \frac{5}{4} + \frac{3}{2}b + \frac{1}{2}\left(n^2 + (b-n)^2\right) & n = m \\ C\sqrt{n(b+1-n)} & n = m+1 \\ C\sqrt{(n+1)(b-n)} & n = m-1 \\ 0 & \text{else} \end{cases}$$

Aubry,SF,Kladko,Olbrich 1996

Perturbation theory of higher order for wave functions:

$$\Delta E_n = 2 \prod_{i=n}^{b-n-1} H_{i,(i+1)} \prod_{i=n+1}^{b-n-1} (H_{nn} - H_{ii})^{-1}$$

$$\Delta E_n = 2C^{2|\tilde{n}|} \frac{(\frac{b}{2} + |\tilde{n}|)!}{(2|\tilde{n}| - 1)!^2(\frac{b}{2} - |\tilde{n}|)!} \qquad \tilde{n} = n - b/2$$

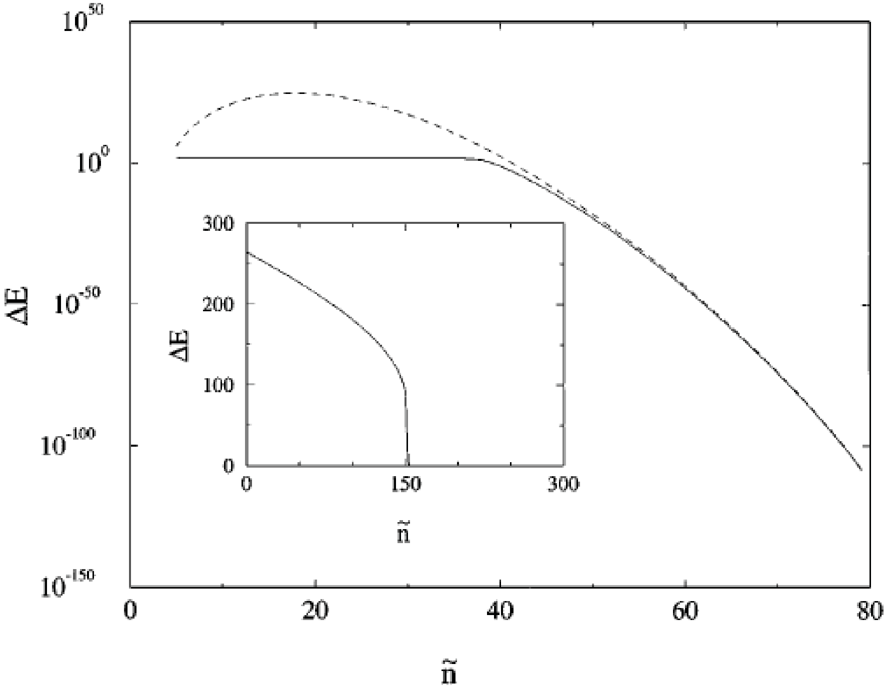


FIG. 2. Eigenvalue splittings versus quantum number $\tilde{n}$ for $b = 150$ and $C = 10$ (calculated with precision 512). Solid line—exact diagonalization, dashed line—perturbation theory

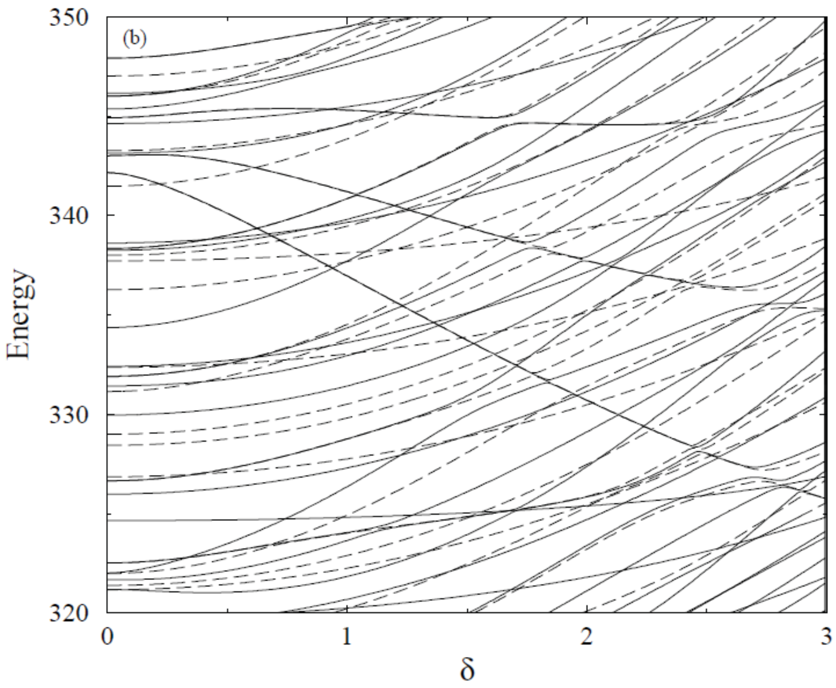
In the limit of infinite number of particles the splitting goes to zero and we recover the classical discrete breather!

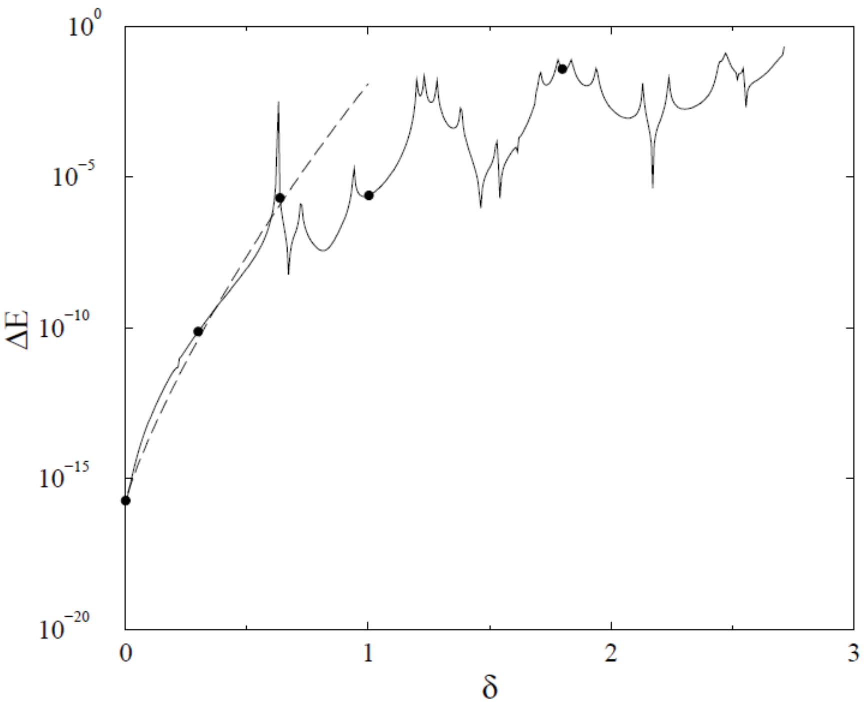
SF,Fleurov 1997

From dimer to trimer, from integrable to chaotic

$$H = \frac{15}{8} + \frac{3}{2}(a_1^\dagger a_1 + a_2^\dagger a_2 + a_3^\dagger a_3) + \frac{1}{2}\left[(a_1^\dagger a_1)^2 + (a_2^\dagger a_2)^2\right]$$
$$+C(a_1^\dagger a_2 + a_2^\dagger a_1) + \delta(a_1^\dagger a_3 + a_3^\dagger a_1 + a_2^\dagger a_3 + a_3^\dagger a_2)$$

- **bound tunneling pairs persist upon loss of integrability**
- **they collide with single states and other tunnel pairs**
- **this is visible in the energy splitting of a given tunneling pair**





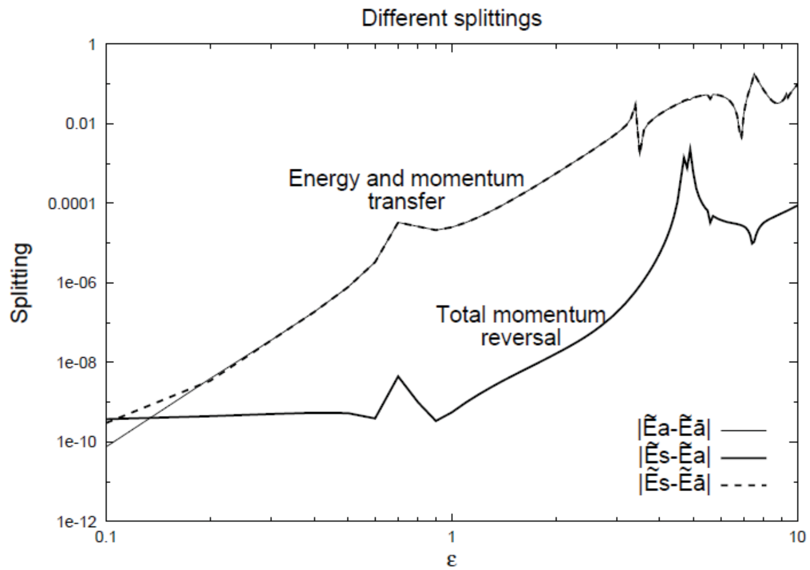
Quantum rotobreathers – more symmetries, more fine structure

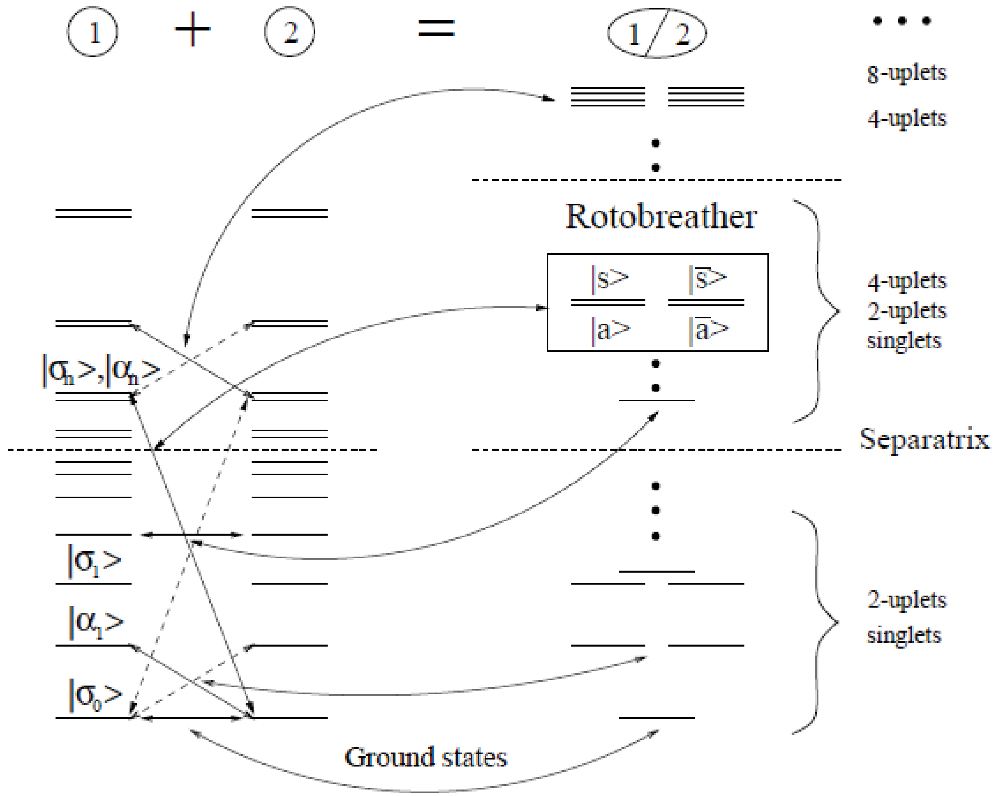
Dorignac,SF 2002

$$H = \sum_{i=1}^{2} \left\{ \frac{p_i^2}{2} + \alpha(1 - \cos x_i) \right\} + \varepsilon(1 - \cos(x_1 - x_2))$$

Symmetries:
permutation and time reversal

Solutions:
can break any of them





Instead of a conclusion

- quantum mechanics of interacting particles is simple
- quantum mechanics of interacting particles is complicated
- few particles are a nice playground for trivial and fundamental concepts in physics
- more: Josephson qubit networks
- more: correlations and entanglement
- more: fluctuations of particle number effects
- more: still to be done, your job!