Workshop on New Materials for Renewable Energy

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Nonlinear Lattice Waves: Classical and Quantum
(third part)

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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
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:

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

Small amplitude plane waves:

\[ x_l(t) \sim e^{i(\omega_q t - q l)}, \quad \omega_q^2 = V''(0) + 4 W''(0) \sin\left(\frac{q}{2}\right) \]

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 $\Omega_b$

Breathers exist in $d = 1, 2, 3, \ldots$-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 $\omega_q$ of small amplitude oscillations (phonons, magnons, whateverons)

Necessary condition for existence (Flach 1994):

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

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

Ansatz: $x_l(t) = \sum_k A_{kl} e^{i k \omega_l t}$

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

\[ \hat{H} = \hat{H}_0 + \gamma \hat{H}_1 \]

\[ \hat{H}_0 = -\sum_{j=1}^{f} b_j^+ (b_{j-1} + b_{j+1}) \]

\[ \hat{H}_1 = -\frac{1}{2} \sum_{j=1}^{f} b_j^+ b_j^+ b_j b_j \]

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: \( E = -2\cos(k) \)
Two particles: like one particle in two dimensions (and so on ...)

Choose the optimal basis! Look for symmetries and conserved quantities:
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:
\[ \tau = \exp(ik) \quad k = 2\pi\nu/f \]
\[ \nu \in \left[ -(f-1)/2, (f-1)/2 \right] \]
Then we can reduce effective d=2 problem to d=1:

Relative distance between two quanta: $j$

$$|\Psi_2\rangle = \sum_{j=1}^{(f+1)/2} v_j |\Phi_j^2\rangle$$

$$|\Phi_2^j\rangle = \frac{1}{\sqrt{f}} \sum_{s=1}^{f} \left( \frac{\hat{T}}{\tau} \right)^{s-1} |10\cdots01\cdots\rangle$$

$$\hat{H}_k |\Psi_n\rangle = E |\Psi_n\rangle$$

$$\hat{H}_k = -\left( \begin{array}{cccc}
\gamma & q\sqrt{2} & 0 & q \\
 q^*\sqrt{2} & 0 & q & 0 \\
 0 & q^* & 0 & q \\
 0 & 0 & q^* & 0 \\
 q & 0 & q & 0 \\
 0 & q & 0 & q \\
 q & 0 & q & p \\
 q & 0 & q & p
\end{array} \right)$$

$$q = 1 + \tau \quad p = \tau^{-(f+1)/2} + \tau^{-(f-1)/2}$$
Solution: two particle continuum and bound states!

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

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

exponential localization: \[ \nu = \left( \frac{1}{\sqrt{2}}, \mu, \mu^2, \mu^3, \ldots \right) \]
\[ \mu = \frac{\left[ \gamma + E_2(k) \right]e^{ik/2}}{4 \cos(k/2)} \]
\[ C_j \equiv |\nu_j|^2 = |\mu|^{2(j-1)} = e^{2\lambda(j-1)} \]

FIG. 1. Energy spectrum of the Bose-Hubbard model for different values of the interaction \( \gamma \): (a) \( \gamma = 0.1 \), (b) \( \gamma = 1.0 \), and (c) \( \gamma = 10 \). Here, \( f = 101 \).
From bosons to fermions with finite range interaction

\[ \hat{H} = \hat{H}_0 + \hat{H}_U + \hat{H}_V \]
\[ \hat{H}_0 = -\sum_{j,\sigma} \hat{a}_{j,\sigma}^+ (\hat{a}_{j-1,\sigma} + \hat{a}_{j+1,\sigma}) \]
\[ \hat{H}_U = -U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}, \quad \hat{n}_{j,\sigma} = \hat{a}_{j,\sigma}^+ \hat{a}_{j,\sigma} \]
\[ \hat{H}_V = -V \sum_j \hat{n}_j \hat{n}_{j+1} \quad \hat{n}_j = \hat{n}_{j,\uparrow} + \hat{n}_{j,\downarrow} \]

We deal with symmetric and antisymmetric states (spin exchange)

\[
H^s(i,j) = - \begin{pmatrix}
U & q\sqrt{2} \\
q^*\sqrt{2} & V & q \choose & q^* & 0 & q \choose & & \ddots & \ddots & \ddots \choose & & & q^* & 0 & q \choose & & & q^* & p
\end{pmatrix}
\]
\[
H^a(i,j) = - \begin{pmatrix}
V & q \choose & q^* & 0 & q \choose & & \ddots & \ddots & \ddots \choose & & & q^* & 0 & q \choose & & & q^* & -p
\end{pmatrix}
\]
We obtain two symmetric and one antisymmetric bound state bands.
Three and more particles – becomes increasingly difficult 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
The classical dimer

\[
H = \frac{i}{2} |\psi_1|^4 + \frac{i}{2} |\psi_2|^4 + C \left( |\psi_1|^2 |\psi_2|^2 + cc \right), \quad \dot{\psi}_{1,2} = i \frac{\partial H}{\partial \psi^{\ast}_{1,2}}
\]

\[
B = |\psi_1|^2 + |\psi_2|^2, \quad \vec{B} = 0
\]

\[
\psi_{1,2} = A_{1,2} e^{i \varphi_{1,2}}, \quad \Delta \varphi = \varphi_2 - \varphi_1, \quad s\varphi = \varphi_1 + \varphi_2
\]

\[
H = \frac{i}{2} (A_1^4 + A_2^4) + 2c A_1 A_2 \cos \Delta \varphi, \quad \vec{B} = A_1^2 + A_2^2
\]

**Isolated Periodic Orbits:** \( \text{grad } H \parallel \text{grad } B \), \( \vec{R} = (A_1 A_2 \Delta \varphi, s\varphi) \)

\[
\text{grad } H = \begin{pmatrix}
2 A_1^3 + 2c A_2 \cos \Delta \varphi \\
2 A_2^3 + 2c A_1 \cos \Delta \varphi \\
-2c A_1 A_2 \sin \Delta \varphi \\
0
\end{pmatrix}, \quad \text{grad } B = \begin{pmatrix}
2 A_1 \\
2 A_2 \\
0 \\
0
\end{pmatrix}
\]

\[\sin \Delta \varphi = 0 \Rightarrow \Delta \varphi = 0 \quad (A_1 / A_2 < 0 \text{ taken care of if })\]

\[
A_{1,2} + c A_{2,1} = \varphi A_{1,2} \quad (\varphi \text{ is some constant})
\]

\[
\psi_{1,2}(+) = A_{1,2} (+) e^{i \varphi(+)}, \quad \frac{d}{dt} |\psi_1|^2 \sim \sin \Delta \varphi = 0 \Rightarrow \left\{ \begin{array}{l}
A_{1,2} = \text{const} \\
\varphi = \omega = \varphi
\end{array} \right.
\]
Solutions:

a) \( A_1 = A_2 \Rightarrow \omega = A^2 + c \quad \uparrow \uparrow \text{ in phase} \)

b) \( A_1 = -A_2 \Rightarrow \omega = A^2 - c \quad \downarrow \downarrow \text{ out of phase} \)

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:

\( B_b = 2c, \quad E_b = 3c, \quad \omega_b = 2c \)

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

\( \uparrow, \downarrow \)
Integrating the dimer

\[ y = A_i - \frac{B}{2}, \quad H = \frac{1}{4}B^2 + y^2 + 2c\sqrt{\frac{B^2}{4} - y^2}\cos\Delta\varphi \]

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

\[ \dot{\varphi} = 0, \quad s\varphi = \frac{1}{2}B + B\cdot c\cdot \frac{\cos\Delta\varphi}{\sqrt{B^2/4 - y^2}} \]

\[ \begin{array}{l}
\dot{y} = -2\cdot c\cdot \frac{\sqrt{B^2/4 - y^2}}{y}\sin\Delta\varphi, \\
\Delta\dot{\varphi} = -2\dot{y} + \frac{2c}{\sqrt{B^2/4 - y^2}}\cos\Delta\varphi
\end{array} \]

\[ \dot{y} = -\frac{\partial V}{\partial y}, \quad V(y; E, B) = (-E + \frac{B^2}{4} + 2c^2)y^2 + \frac{1}{2}y^4 \]

![Graphs showing the potential energy function V(y; E, B) versus y]
The quantum dimer with b particles

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

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

\[ H_{nm} = \begin{cases} 
\frac{5}{4} + \frac{3}{2} b + \frac{1}{2} \left( n^2 + (b - n)^2 \right) & \text{if } n = m \\
C \sqrt{n(b + 1 - n)} & \text{if } n = m + 1 \\
C \sqrt{(n + 1)(b - n)} & \text{if } n = m - 1 \\
0 & \text{else}
\end{cases} \]
Perturbation theory of higher order for wave functions:

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

\[ \Delta E_n = 2C^2|\tilde{n}| \frac{\left(\frac{b}{2} + |\tilde{n}|\right)!}{(2|\tilde{n}| - 1)!^2 \left(\frac{b}{2} - |\tilde{n}|\right)!} \]

\[ \tilde{n} = n - \frac{b}{2} \]

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

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.
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

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

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!