Vibrational Eigenmodes: From Glasses to Fermi-Pasta-Ulam Problem

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PHYS 460/660: Computational Methods of Physics
Fig. 1.3. (a) Arrangement of atoms in liquid argon. (b) Probability \( p(r) \) for a liquid (dashed line) and for a gas (solid line). (c) Probability \( p(r) \) for a simple crystal.
Solid State: Crystals vs. Glasses

Temperature ranges for water

Crystalline SiO$_2$

“Glass” (window):

- stishovite
- coesite
- $\beta$-quartz
- $\alpha$-quartz
- crystobalite
- tridymite
- liquid

O
Si

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Amorphous Silicon: Topological Disorder
Density of States in a-Si

![Diagram of Density of States in a-Si](image)
The participation ratio essentially counts how many atoms in a given sample are vibrating for a given vibrational mode:

- **Extended modes** have $P=N$ (=number of atoms), so that $1/P$ is small ($1/N$).

- **Localized modes** can have $P$ of order 1, and their $1/P$ can be therefore quite large (up to 1).

The mobility edge in amorphous silicon is 72 meV (the vertical line), as seen in the top figure--above the mobility edge $P$ rapidly decreases!

At the lowest frequencies some of the modes are resonant (quasilocalized) and their $P$ can be surprisingly small.
On the right is the same model but only the atoms that “participate” in the vibration of a given locon (frequency 77 meV) are shown. The normal mode is localized at the group of 6 atoms. Locons can be usually found at places of higher-than-average coordination.
**Test Example: 4-atom Chain with Periodic B.C.**

- **Four Newton's Second Law Equations cast in a Matrix Form:**

  \[
  \begin{align*}
  M \frac{d^2 u_j(t)}{dt^2} &= -k_j[u_j(t) - u_{j+1}(t)] - k_{j-1}[u_j(t) - u_{j-1}(t)] = -(k_{j-1}u_{j-1}(t) + (k_{j-1} + k_j)u_j(t) - k_ju_{j+1}(t)) \\
  \frac{d^2 |U\rangle}{dt^2} &= - \begin{pmatrix}
  K_4 + K_1 & -K_1 & 0 & -K_4 \\
  -K_1 & K_1 + K_2 & -K_2 & 0 \\
  0 & -K_2 & K_2 + K_3 & -K_3 \\
  -K_4 & 0 & -K_3 & K_3 + K_4
  \end{pmatrix} \cdot |U\rangle \\
  K_n &= \frac{k_n}{M}; \quad |U\rangle = \begin{pmatrix}
  u_1 \\
  u_2 \\
  u_3 \\
  u_4
  \end{pmatrix}; \quad \langle U | K | U \rangle = \frac{2V}{M}
  \end{align*}
\]
Test Example: Normal Modes of 4-atom Ordered Chain

Ordered Chain: \( K_1 = K_2 = K_3 = K_4 \)

\[
|0\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix},
|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix},
|2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix},
|3\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}
\]

\( \omega_0 = 0, \omega_1 = \sqrt{2}, \omega_2 = \sqrt{2}, \omega_3 = 2 \)

\[ A_\mu |\mu\rangle \cos(\omega_\mu t + \phi_\mu) \]

\[
|U(t)\rangle = \sum_\mu \left[ |\mu\rangle \langle \mu |U(0)\rangle \cos(\omega_\mu t) + |\mu\rangle \langle \mu |V(0)\rangle \frac{\sin(\omega_\mu t)}{\omega_\mu} \right]
\]

\[
|V(t)\rangle = \sum_\mu \left[ |\mu\rangle \langle \mu |V(0)\rangle \cos(\omega_\mu t) - |\mu\rangle \langle \mu |U(0)\rangle \omega_\mu \sin(\omega_\mu t) \right]
\]
Test Example: Normal Modes in Pictures

\[ |0\rangle (u_0 + v_0 t) \]

\[ |1\rangle \]

\[ |2\rangle \]

\[ |3\rangle \]
Random Matrix Theory describes spectral properties (eigenenergies or eigenfrequencies) of:

- Quantum Chaos,
- Wave Chaos,
- Complex Many-Body Systems (QCD, nucleons).

Level Spacing Distribution (LSD) obeys Wigner-Dyson Statistics:

\[ P_{WD}(s) = \frac{\pi s}{2} e^{-\frac{\pi s^2}{4}} \]
**Fermi-Pasta-Ulam Problem** (1955 MANIAC):
Nonlinear Springs → Chaos + Ergodicity?

![Schematic picture of the FPU model](image)

**Figure 1:** Schematic picture of the FPU model: masses that can move only in one dimension are coupled by nonlinear springs. $u_n$ is the relative displacement with respect to the equilibrium position of the $n$-th mass. The two ends of the chain were assumed to be fixed, i.e., $u_0 = u_N = 0$.

\[
M \frac{d^2 u_j(t)}{dt^2} = K\left[u_j(t) + u_{j+1}(t) + u_{j-1}(t)\right] + \alpha \left[(u_{j+1}(t) - u_j(t))^2 - (u_j(t) - u_{j-1}(t))^2\right] + \beta \left[(u_{j+1}(t) - u_j(t))^3 - (u_j(t) - u_{j-1}(t))^3\right]
\]
Zabusky-Kruskal-Toda Lattice Soliton:

\[ T \approx 0.76 \frac{N^{5/2}}{\sqrt{A\alpha}} \]

Figure 2: FPU recurrence for a FPU-\( \alpha \) model with \( N = 32 \) masses and fixed ends. The plot shows the time evolution of the energy (kinetic + potential) \( E_k = \frac{A_k^2 + \omega_k^2 A_k^2}{2} \) of each of the three lowest normal modes, related to the displacements through

\[ A_k = \sqrt{\frac{2}{N+1}} \sum_{n=1}^{N} u_n \sin(nk\pi/(N+1)) \]

with the frequencies \( \omega_k^2 = 4\sin^2(k\pi/(2N+2)) \). Initially, only mode \( k = 1 \) (blue) is excited. After flowing to other modes, \( k = 2 \) (green), \( k = 3 \) (red), etc., the energy almost fully returns to mode \( k = 1 \); this was a surprise! This picture might be easily reproduced using the MATLAB code provided below.
How to Generate Ergodicity in FPU Part of Project 3

Periodic orbits, localization in normal mode space, and the Fermi–Pasta–Ulam problem

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Fig. 2. (a) Distributions of the mode energy densities for the FPU trajectory with $q_{c}=1$, $N=31$, $a=0.33$, and $E=0.32$. Circles: $t=10^4$, squares: $t=10^5$, diamonds: $t=10^6$. The dashed line is the $q$-breather from (b) for comparison. (b) Distributions of the mode energy densities for the $q$-breather with the same parameters as in (a) (see Ref. 12).

Fig. 5. Energy density distribution for the FPU trajectory (squares, $t=10^6$) and $q$-breather (circles) for $N=47$, $E=47$, and $q_{c}=47$. (a) $a=0.25$ and (b) $\beta=0.25$ (see Ref. 12).
Nonlinear Springs: Solve ODE via Numerical Methods

- Verlet method \(\rightarrow\) **Symmetric** (Forward and Backward) Propagation:

\[
x(t_n + \Delta t) = x(t_n) + \frac{dx}{dt} \Delta t + \frac{1}{2} \frac{d^2 x}{dt^2} (\Delta t)^2 + \frac{1}{6} \frac{d^3 x}{dt^3} (\Delta t)^3 + \ldots
\]

\[
x(t_n - \Delta t) = x(t_n) - \frac{dx}{dt} \Delta t + \frac{1}{2} \frac{d^2 x}{dt^2} (\Delta t)^2 - \frac{1}{6} \frac{d^3 x}{dt^3} (\Delta t)^3 + \ldots
\]

\[
x_{n+1} = 2x_n - x_{n-1} + \frac{d^2 x}{dt^2} (\Delta t)^2 + O([\Delta t]^4)
\]

\[
u_{n+1}(i) = 2u_n(i) - u_{n-1}(i) + \frac{1}{m} F_n (\Delta t)^2
\]

no self-start \(\Rightarrow u_2(i) = u_1(i) + v \Delta t\) (use e.g. Euler)