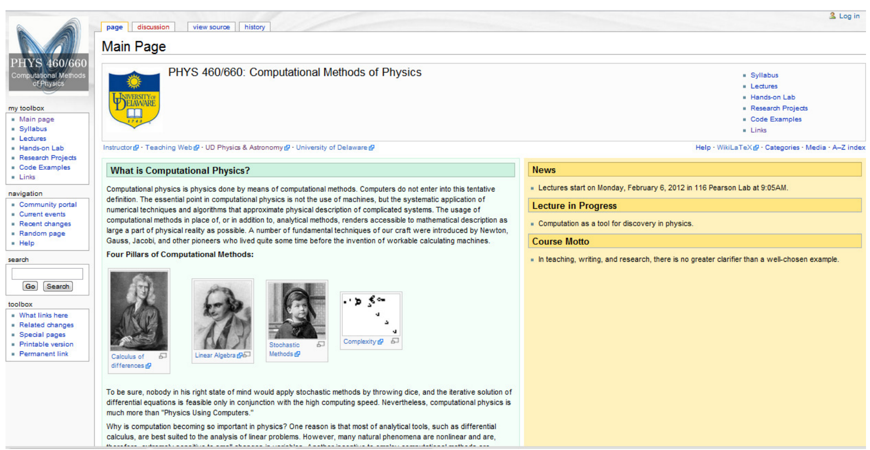
Numerical Investigation of Vibrational Eigenmodes: From Glasses to Fermi-Past-Ulam Problem

Branislav K. Nikolić

Department of Physics & Astronomy, University of Delaware, Newark, DE 19716, U.S.A.

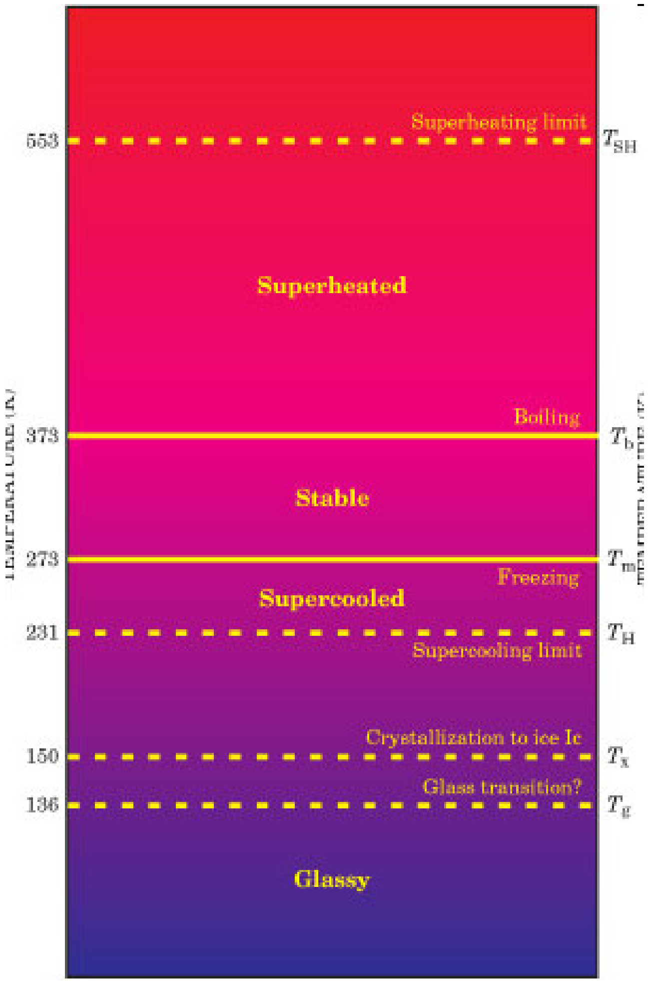
PHYS 460/660: Computational Methods of Physics

http://wiki.physics.udel.edu/phys660

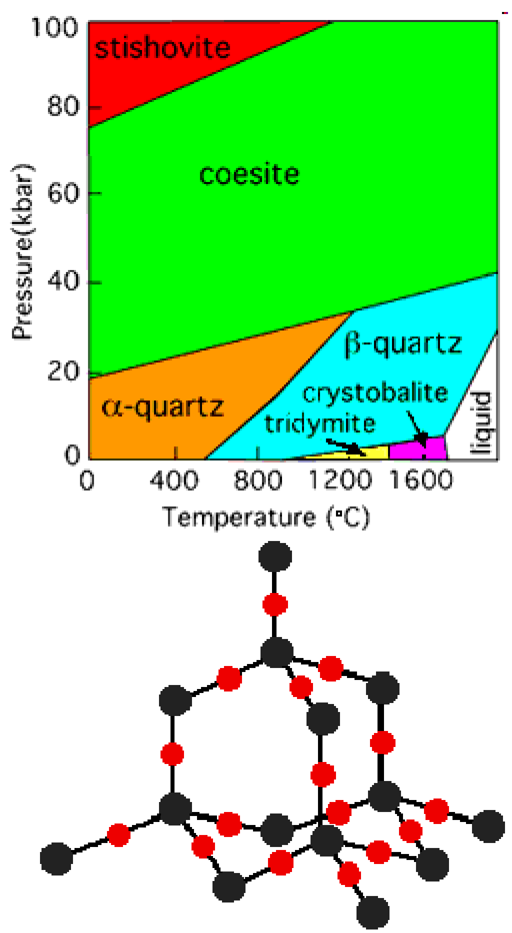


Solid State Physics: Crystals vs. Glasses

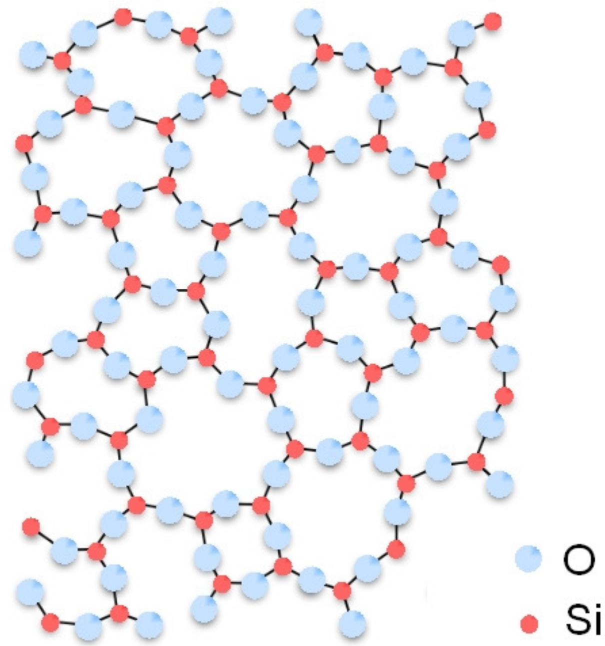
Crystalline vs. glassy water



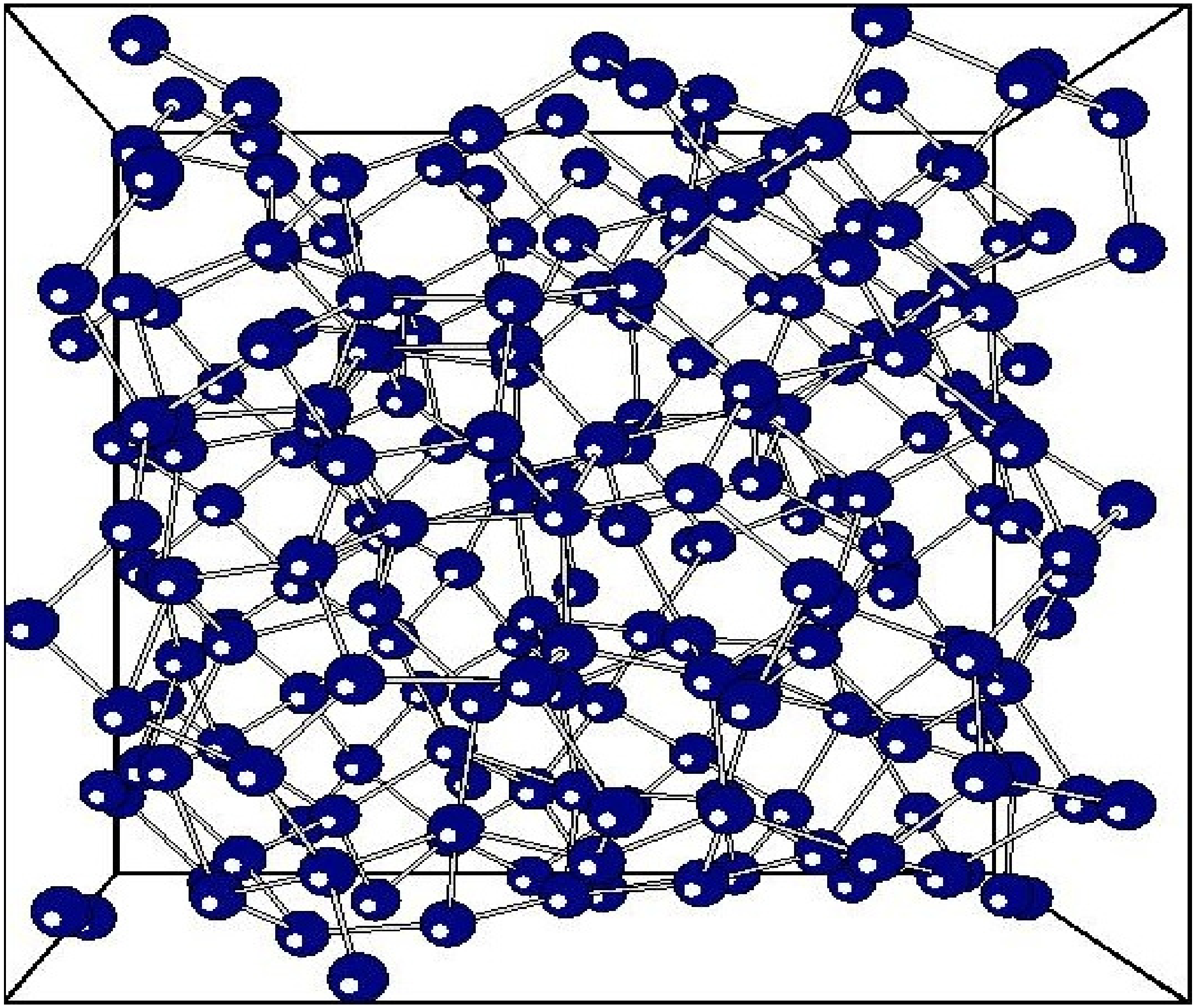
Crystalline SiO_2



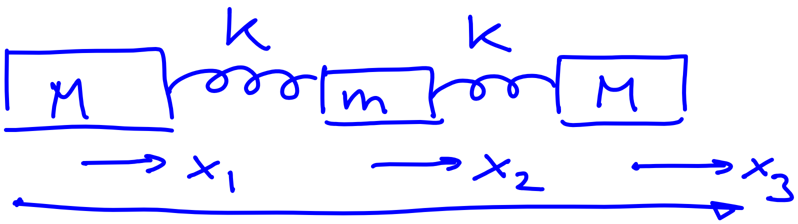
"Glass" (window):



Amorphous Silicon: Topological Disorder



Vibrational Eigenmodes in Classical Mechanics



$$M\ddot{x}_1 = -k\,(x_1 - x_2)$$
$$M\ddot{x}_2 = -k\,(x_2 - x_1) - k\,(x_2 - x_3)$$
$$M\ddot{x}_3 = -k\,(x_3 - x_2)$$

$x_i = x_i^0 \cos(\omega t + \varphi) \Rightarrow$ all masses vibrate with same frequency in the normal mode

plug into Newton 2nd law equations $\Downarrow$

$\omega = 0 \Rightarrow x_1^0 = x_2^0 = x_3^0$

$\omega^2 = k/M \Rightarrow x_1^0 = -x_3^0,\ x_2^0 = 0$

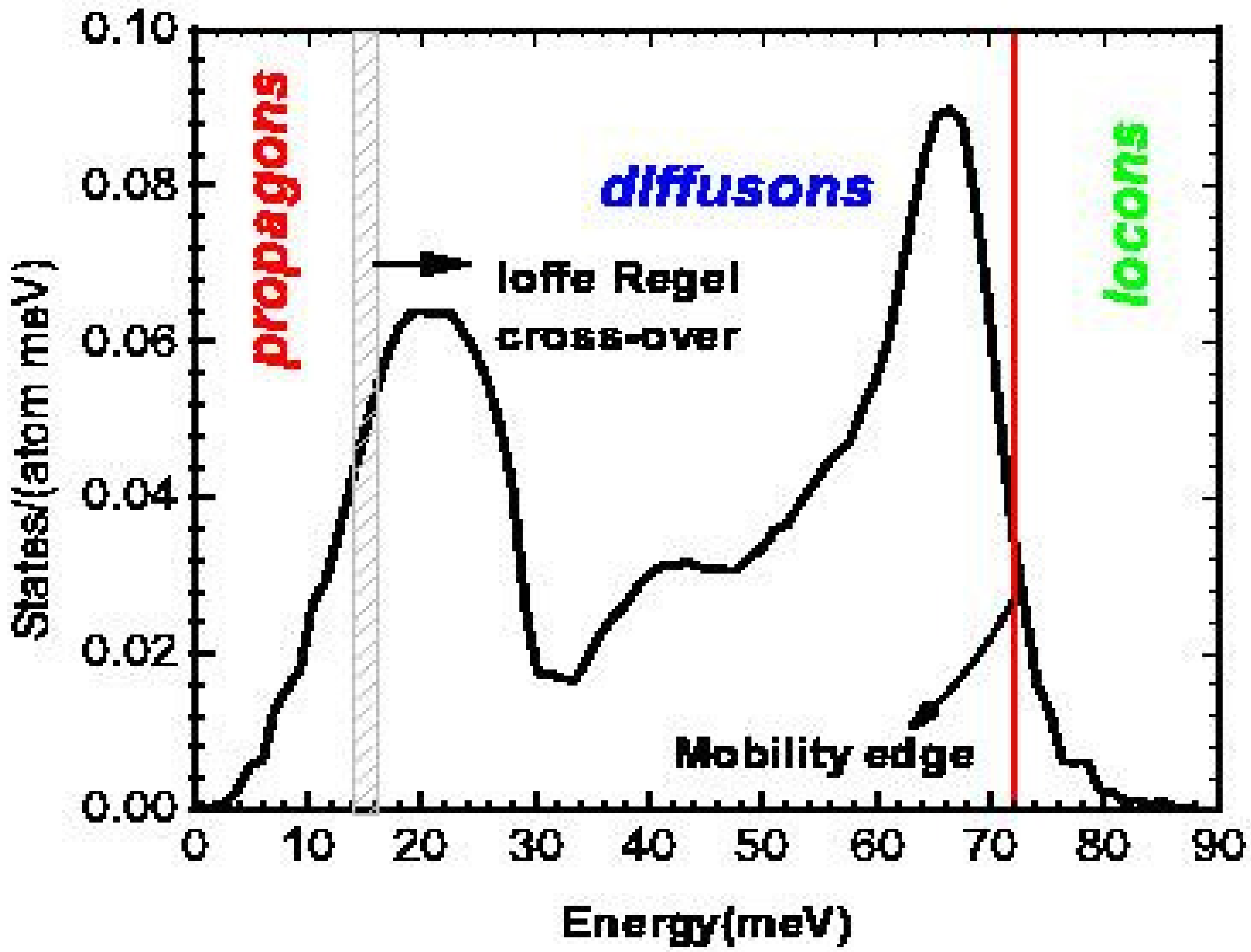
$\omega^2 = k/M + 2k/m \Rightarrow x_1^0 = x_3^0$, $x_2^0 = -\frac{2M}{m} x_1^0$

$$\begin{pmatrix} \frac{k}{M} & -\frac{k}{M} & 0 \\ -\frac{k}{m} & \frac{2k}{m} & -\frac{k}{m} \\ 0 & -k/M & k/M \end{pmatrix} \begin{pmatrix} x_1^0 \\ x_2^0 \\ x_3^0 \end{pmatrix} = \omega^2 \begin{pmatrix} x_1^0 \\ x_2^0 \\ x_3^0 \end{pmatrix} \longrightarrow \underbrace{\begin{vmatrix} \frac{k}{M} - \omega^2 & -\frac{k}{M} & 0 \\ -\frac{k}{m} & \frac{2k}{m} - \omega^2 & -\frac{k}{m} \\ 0 & -k/M & \frac{k}{M} - \omega^2 \end{vmatrix} = 0}_{\text{condition for non-trivial solution of the eigenproblem}}$$

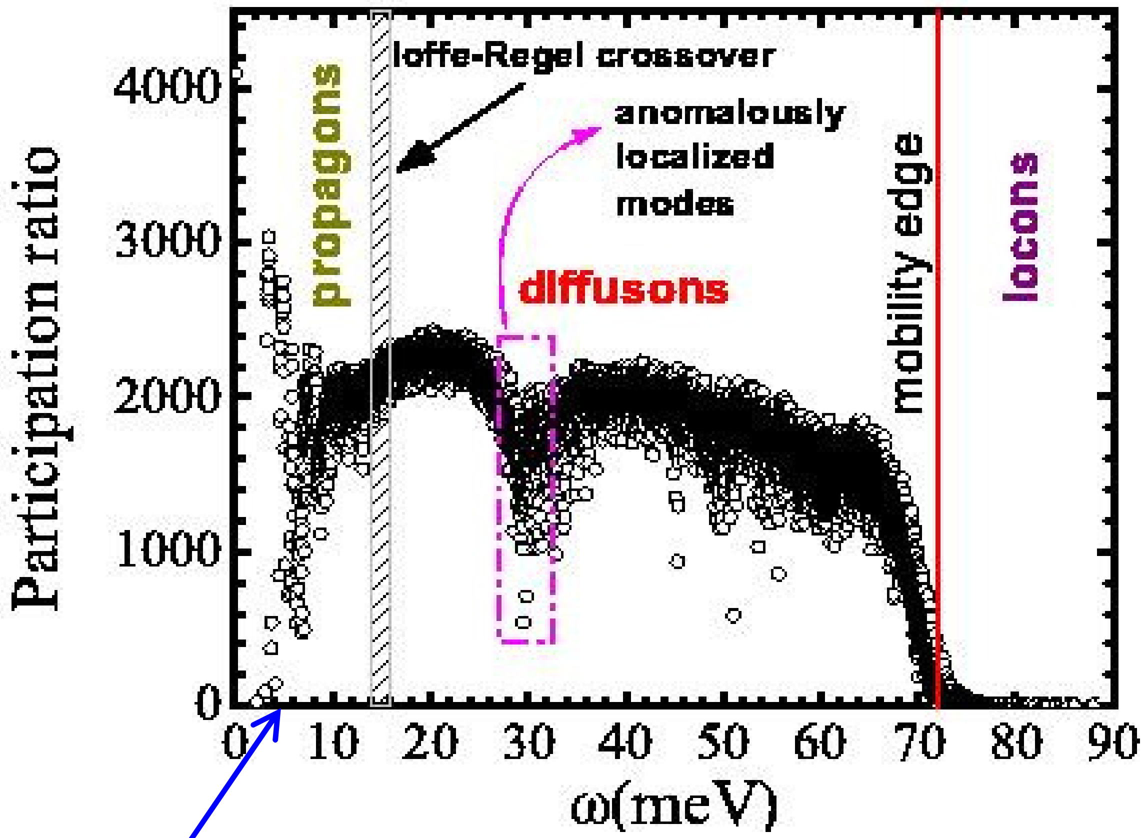
$$\omega^2\left(\frac{k}{M} - \omega^2\right)\left(\omega^2 - \frac{2k}{m} - \frac{k}{M}\right) = 0$$

$$\omega = 0;\ k/M;\ \frac{k}{M} + \frac{2k}{m}$$

Density of States in a-Si



Participation Ratio of Eigenmodes in a-Si



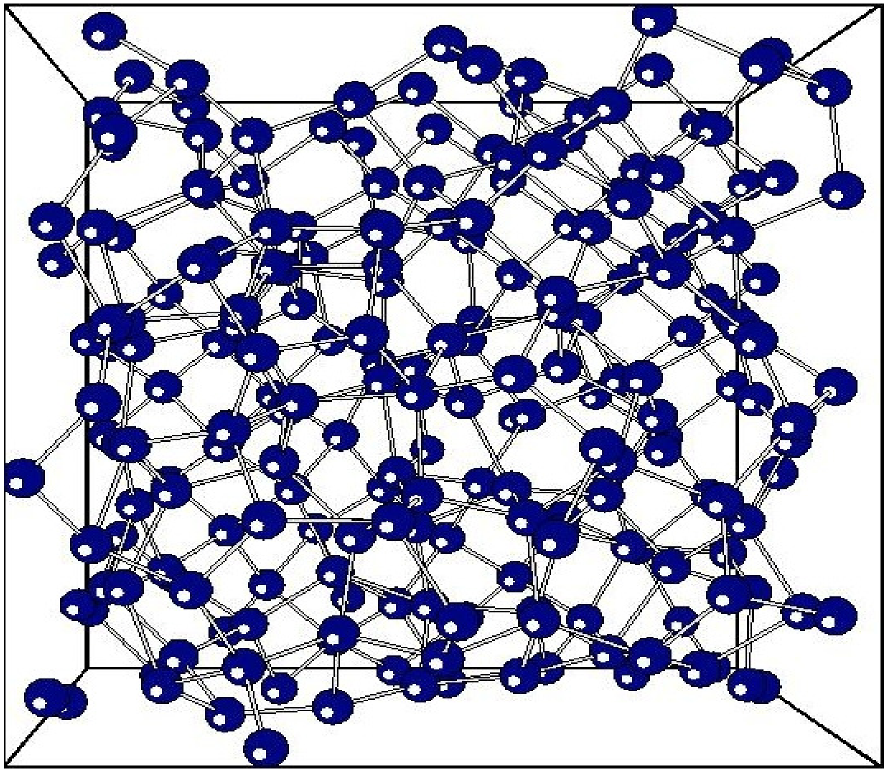
The participation ratio essentially counts **how many atoms in a given sample are vibrating** for a given vibrational mode:

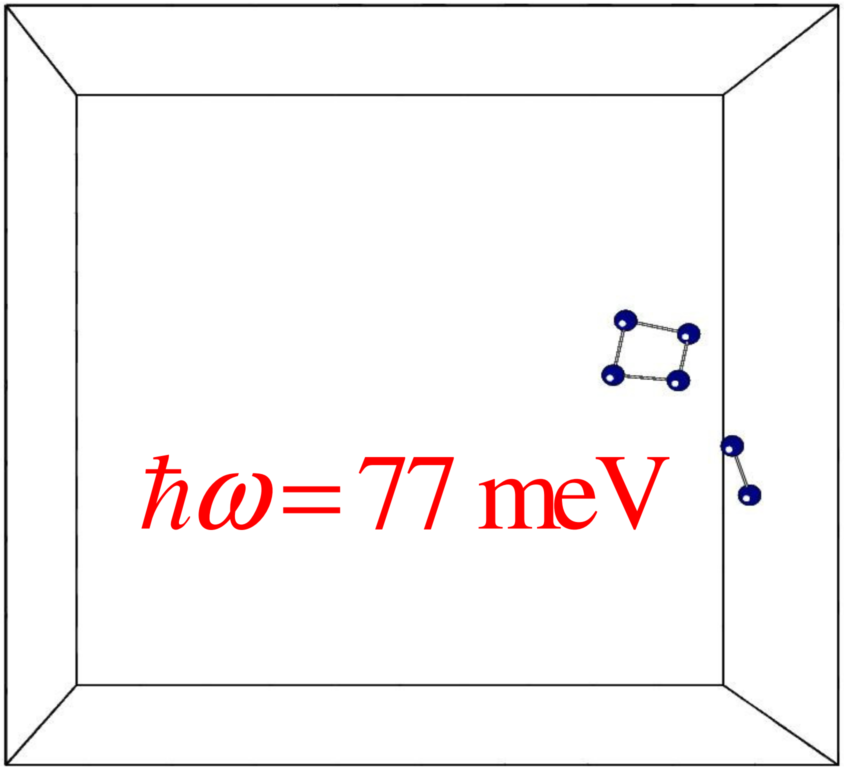
- **Extended modes** have P=N (=number of atoms), so that 1/P is small (1/N).
- **Localized modes** can have P of order 1, and their 1/P can be therefore quite large (up to 1).

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

NOTE: At the lowest frequencies some of the modes are resonant (quasilocalized) and their P can be surprisingly small.

Participation Ratio for Locons in Pictures





❑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.

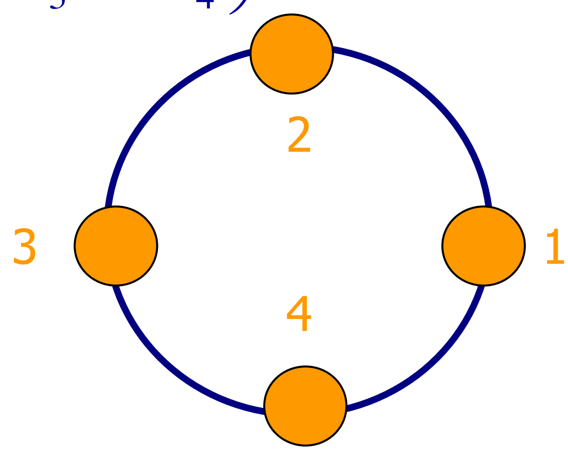
Test Example: 4-atom Chain with Periodic B.C.

- Four Newton Second Law Equations cast in a matrix form:

$$M\frac{d^2u_j(t)}{dt^2} = -k_j[u_j(t)-u_{j+1}(t)] - k_{j-1}[u_j(t)-u_{j-1}(t)] = -\left\{-k_{j-1}u_{j-1}(t) + (k_{j-1}+k_j)u_j(t) - k_j u_{j+1}(t)\right\}$$

$$\frac{d^2|U\rangle}{dt^2} = -\begin{pmatrix} K_4+K_1 & -K_1 & 0 & -K_4 \\ -K_1 & K_1+K_2 & -K_2 & 0 \\ 0 & -K_2 & K_2+K_3 & -K_3 \\ -K_4 & 0 & -K_3 & K_3+K_4 \end{pmatrix} \bullet |U\rangle$$

$$K_n = \frac{k_n}{M}; \quad |U\rangle = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}; \quad \langle U|\mathbf{K}|U\rangle = \frac{2V}{M}$$



Test Example: Normal Modes of 4-Atom Ordered Chain

$$\text{Ordered Chain}: \underbrace{K_1 = K_2 = K_3 = K_4}_{\Downarrow}$$

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

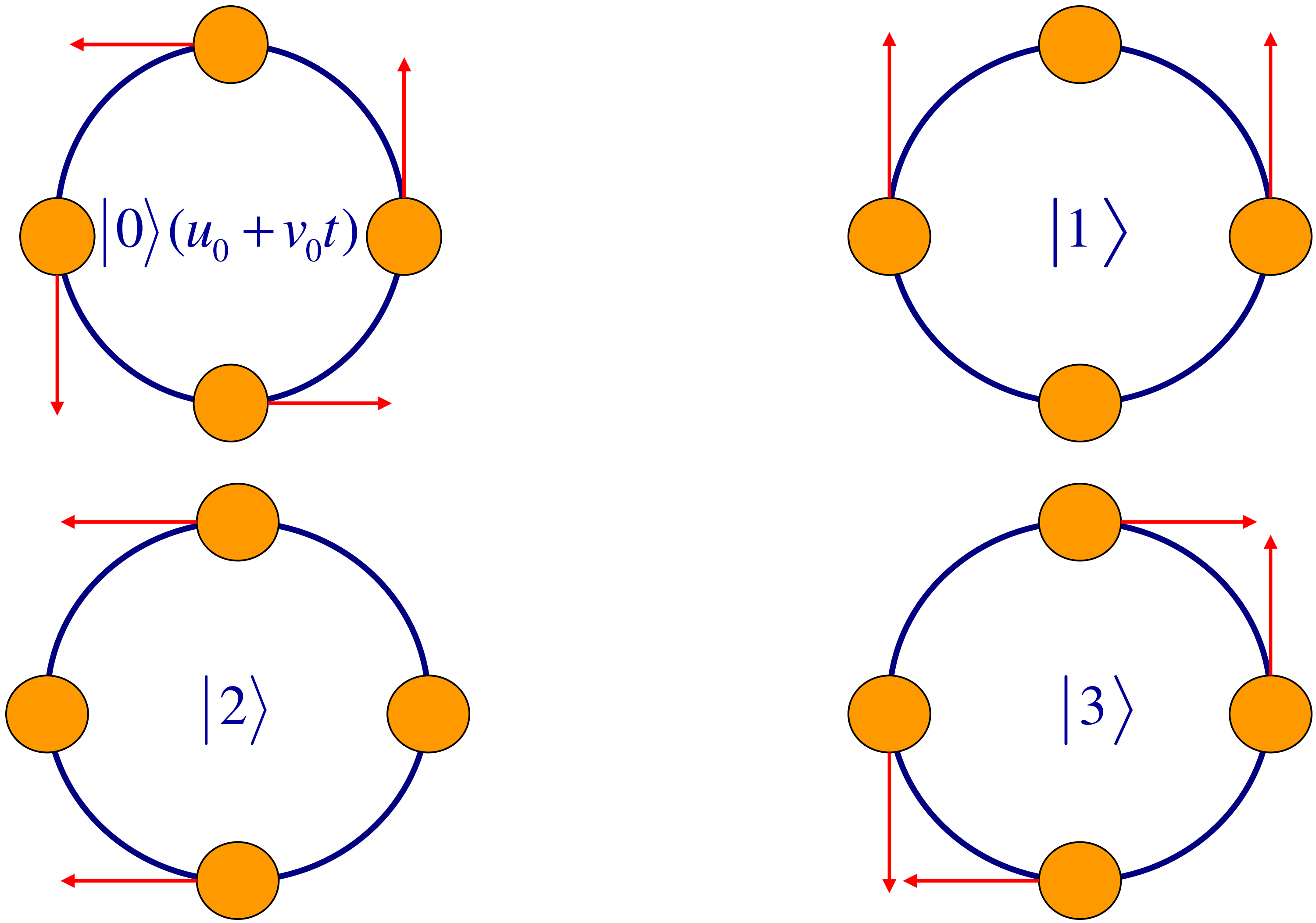
$$\omega_0 = 0, \omega_1 = \sqrt{2}, \omega_2 = \sqrt{2}, \omega_3 = 2$$

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

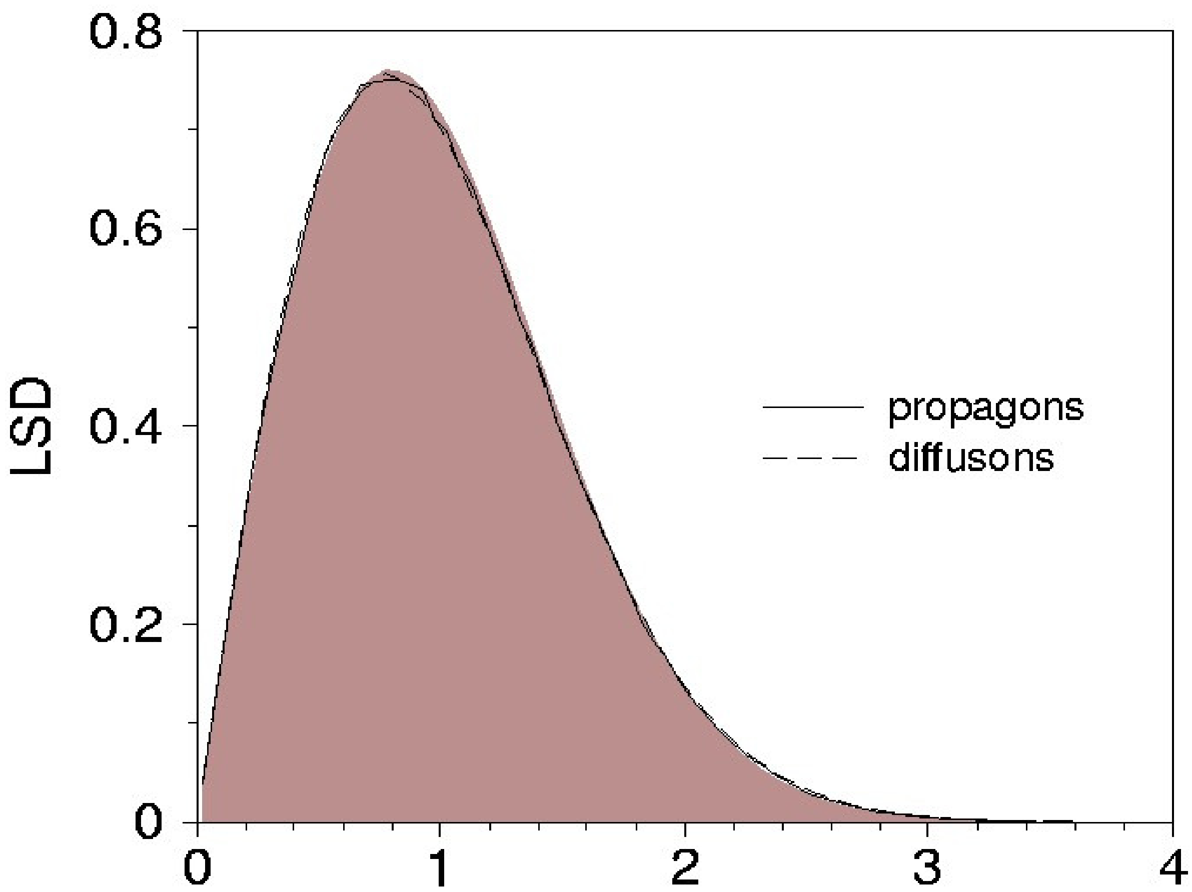
$$|U(t)\rangle = \sum_\mu \left[|\mu\rangle\langle\mu|U(0)\rangle \cos(\omega_\mu t) + |\mu\rangle\langle\mu|V(0)\rangle \frac{\sin(\omega_\mu t)}{\omega_\mu} \right]$$

$$|V(t)\rangle = \sum_\mu \left[|\mu\rangle\langle\mu|V(0)\rangle \cos(\omega_\mu t) - |\mu\rangle\langle\mu|U(0)\rangle \omega_\mu \sin(\omega_\mu t) \right]$$

Test Example: Normal Modes of Ordered 4-Atom Chain in Pictures



Code Verification for Disordered Chains: Use Results of Random Matrix Theory



Random Matrix Theory describes spectral properties (eigenenergies or eigenfrequncies) 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?

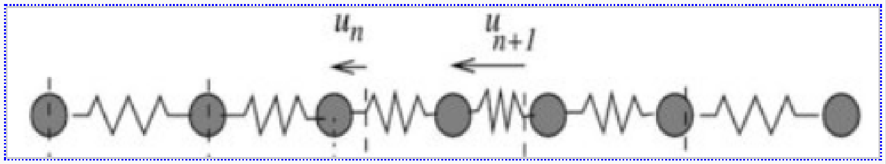


Figure 1: Schematic picture of the FPU model: masses that can move only in one dimension are coupled by *nonlinear* springs. u_n is the relative displacement with respect to the equilibrium position of the n -th mass. The two ends of the chain were assumed to be fixed, i.e., $u_0 = u_N = 0$.

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α-FPU

$$+\alpha\left[\left(u_{j+1}(t)-u_j(t)\right)^2-\left(u_j(t)-u_{j-1}(t)\right)^2\right]$$

$$M\frac{d^2u_j(t)}{dt^2} = K[u \ldots u_j(t)+u_{j-1}(t)]$$

$$+\beta\left[\left(u_{j+1}(t)-u_j(t)\right)^3-\left(u_j(t)-u_{j-1}(t)\right)^3\right]$$

β-FPU

FPU Paradox Explained: Solitons, Strong Stochasticity Threshold, and Chaotic Breathers

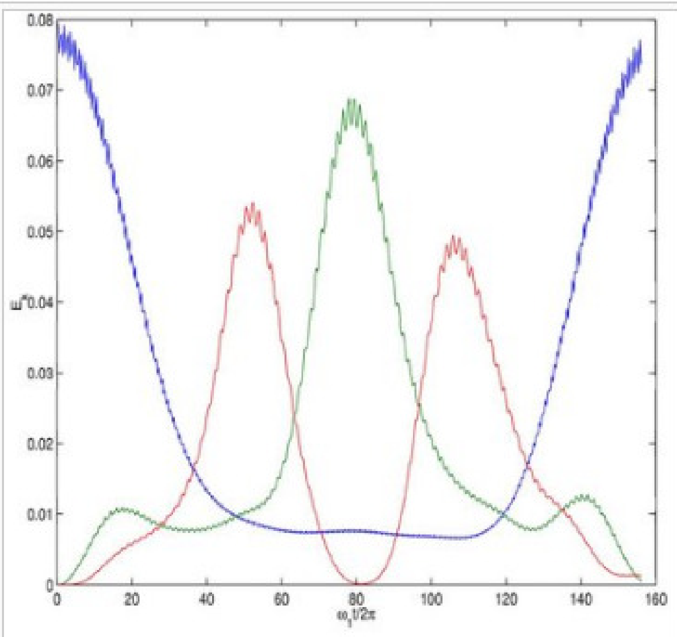
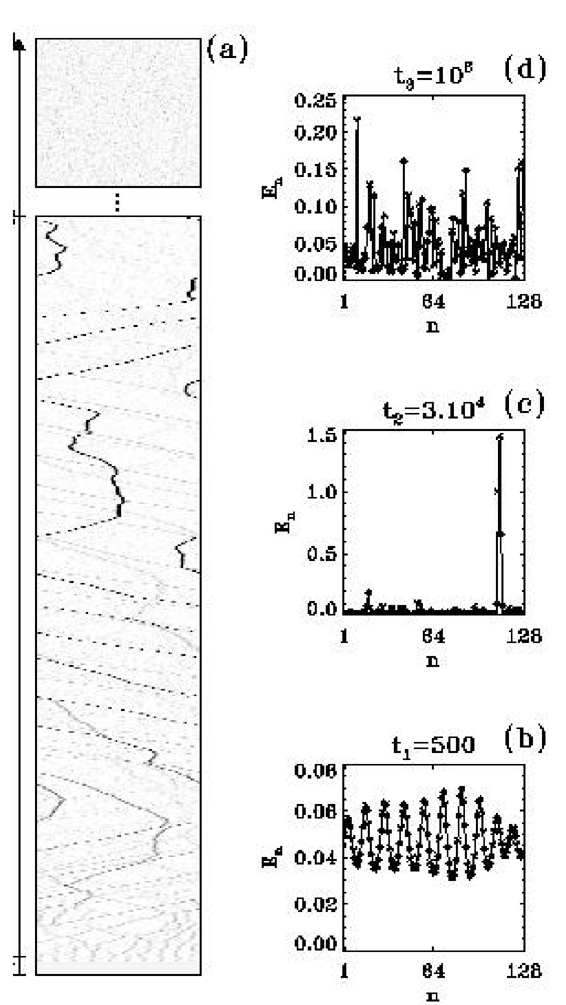


Figure 2: FPU recurrence for a FPU-α model with $N = 32$ masses and fixed ends. The plot shows the time evolution of the energy (kinetic + potential) $E_k = (\dot{A}_k^2 + \omega_k^2 A_k^2)/2$ of each of the three lowest normal modes, related to the displacements through $A_k = \sqrt{2/(N+1)} \sum_{n=1}^{N} u_n \sin(nk\pi/(N+1))$ 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.

Zabusky-Kruskal-Toda Lattice Soliton:

$$T \simeq 0.76 \frac{N^{5/2}}{\sqrt{A\alpha}}$$



How to Generate Ergodicity in Part III (FPU) of Project 3: Evading q-Breathers

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

S. Flach[a)]
Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

M. V. Ivanchenko
Department of Applied Mathematics, University of Leeds, Leeds, LS2 9JT, United Kingdom

O. I. Kanakov and K. G. Mishagin
Department of Radiophysics, Nizhny Novgorod University, Gagarin Avenue 23, 603950 Nizhny Novgorod, Russia

$$x_n(t) = \sqrt{\frac{2}{N+1}} \sum_{q=1}^{N} Q_q(t) \sin\left(\frac{\pi q n}{N+1}\right)$$

$$\ddot{Q}_q + \omega_q^2 Q_q = -\frac{\alpha}{\sqrt{2(N+1)}} \sum_{l,m=1}^{N} \omega_q \omega_l \omega_m B_{q,l,m} Q_l Q_m$$

$$B_{q,l,m} = \sum \left(\delta_{q \pm l \pm m, 0} - \delta_{q \pm l \pm m, 2(N+1)}\right)$$

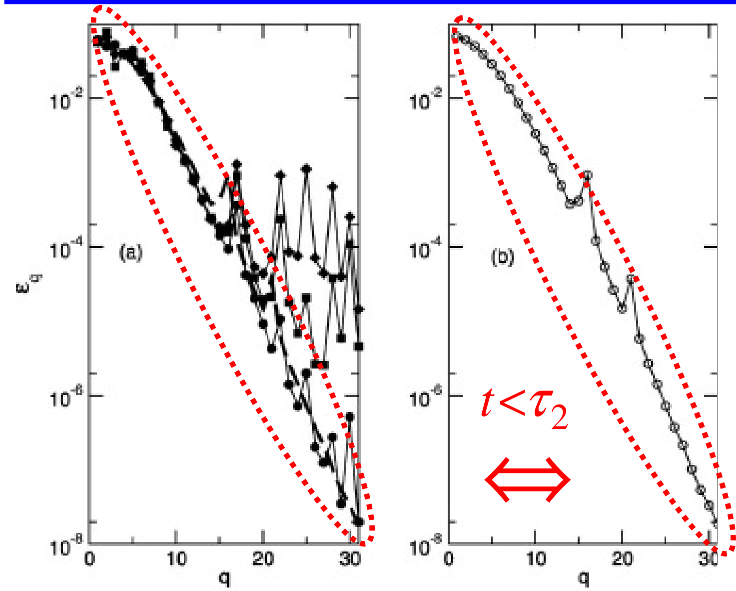

Fig. 2. (a) Distributions of the mode energy densities for the FPU trajectory with $q_0=1$, $N=31$, $\alpha=0.33$, and $E=0.32$. Circles: $t=10^4$, squares: $t=10^5$, diamonds: $t=10^6$. The dashed line is the q-breather from (b) for comparison. (b) Distributions of the mode energy densities for the q-breather with the same parameters as in (a) (see Ref. 12).

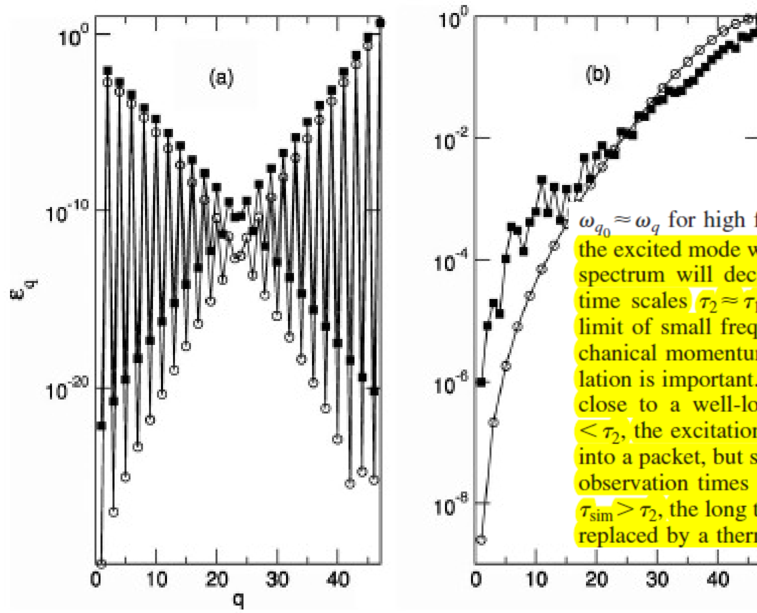

Fig. 5. Energy density distribution for the FPU trajectory (squares, $t=10^5$) and q-breather (circles) for $N=47$, $E=4.7$, and $q_0=47$. (a) $\alpha=0.25$ and (b) $\beta=0.25$ (see Ref. 12).

$\omega_{q_0} \approx \omega_q$ for high frequency modes. Thus it is expected that the excited mode with a wave number close to an edge of the spectrum will decay into many other modes, and the two time scales $\tau_2 \approx \tau_1$. These time scales must diverge in the limit of small frequencies, due to conservation of total mechanical momentum. Hence the time scale τ_{sim} of the simulation is important. Suppose we excite a normal mode that is close to a well-localized q-breather when $\tau_2 \gg \tau_1$. If $\tau_{\text{sim}} < \tau_2$, the excitation of this normal mode will quickly spread into a packet, but stay localized in normal mode space for all observation times (this localization is the FPU problem). If $\tau_{\text{sim}} > \tau_2$, the long time of nonequipartition will be eventually replaced by a thermalized state.

Nonlinear Springs: Solve ODE via Verlet Numerical Algorithm

- Verlet method → Symmetric (forward and backward) propagation:

$$\underbrace{\begin{aligned} x(t_n+\Delta t) &= x(t_n)+\frac{dx}{dt}\Delta t+\frac{1}{2}\frac{d^2x}{dt^2}(\Delta t)^2+\frac{1}{6}\frac{d^3x}{dt^3}(\Delta t)^3+\ldots \\ x(t_n-\Delta t) &= x(t_n)-\frac{dx}{dt}\Delta t+\frac{1}{2}\frac{d^2x}{dt^2}(\Delta t)^2-\frac{1}{6}\frac{d^3x}{dt^3}(\Delta t)^3+\ldots \end{aligned}}_{\Downarrow}$$

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

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

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