The Fermi-Pasta-Ulam-Tsingou Analysis

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Abstract

This report investigates the dynamics of a one-dimensional lattice of masses coupled by nonlinear springs, known as the Fermi-Pasta-Ulam-Tsingou (FPUT) problem. Using a symplectic Leapfrog integration scheme, we analyze the evolution of the system for both linear and nonlinear interaction potentials. We validate the numerical method against an exact analytical solution for a single mass. For the linear chain, we observe persistent standing waves with no energy exchange between modes. In the nonlinear regime, we observe the coupling of spatial modes and the distortion of the wave, yet contrary to the expectation of rapid thermalization, the system exhibits the quasi-periodic recurrence of its initial state (FPUT recurrence). We further explore the stability limits of the integration scheme and the effects of "softening" springs with negative nonlinearity.

Methods

1.1 Governing Equations

The system consists of a chain of N particles with unit mass, connected by springs. The displacement of the i-th particle from equilibrium is denoted by $x_i(t)$. The equations of motion are given by a system of cooped second-order differential equations:

$\ddot{x}_i = K(x_{i+1} - 2x_i + x_{i-1})[1 + \alpha(x_{i+1} - x_{i-1})]$ Where K is the spring constant and α is the nonlinearity parameter. Fixed boundary conditions are applied using dummy masses such that $x_0(t) = 0$ and $x_{N+1}(t) = 0$

1.2 Numerical Integration

We employ the Leapfrog method, a second-order explicit symplectic integrator, to discretize the system in time. The update rule for the position at step $n + 1$ is derived from the central difference approximation of the second derivative: $x_i^{n+1} = 2x_i^n - x_i^{n-1} + \Delta t^2 \cdot f_i(x^n)$. Where f_i represents the force term on the right-hand side of the governing equation. To initialize the multi-step scheme, the first time step is approximated using linear extrapolation:$x_i^1 = x_i^0 + v_i^0 \Delta t$

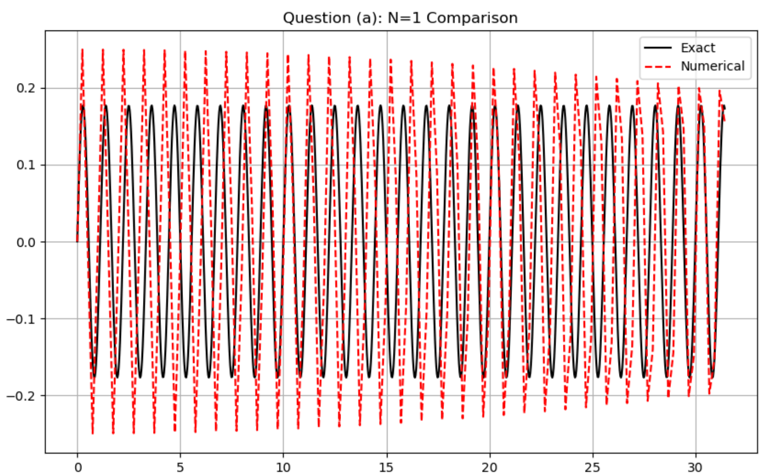
1.3 Stability and Time Stepping

For the linear case $(\alpha = 0)$, numerical stability requires the time step Δt to satisfy the Courant-Friedrichs-Lewy (CFL) condition, roughly bounded by$\frac{1}{\sqrt{K}}$. We define the time step using a safety factor C: $\Delta t = \frac{C}{\sqrt{K}}$ where $C \leq 1$ typically ensures stability. For linear cases the local stiffness of the system chances with displacement potentially requiring stricter safety factor $(C < 1)$.

Results and Findings

2.1 Validation: The Linear Oscillator $(N = 1)$

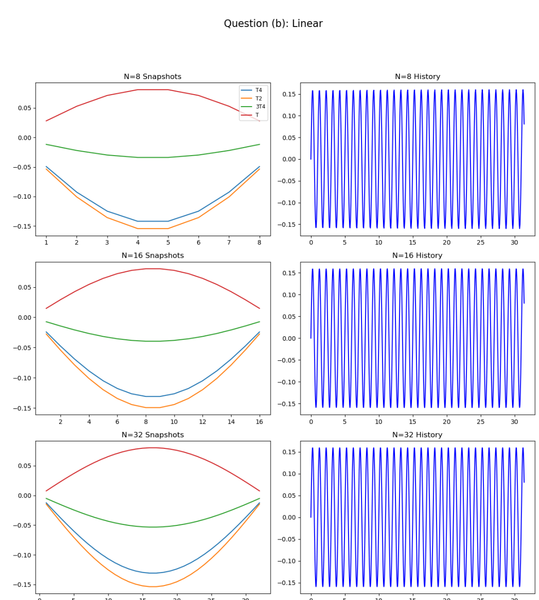
To validate the Fortran implementation, we simulated the case of a single mass $(N = 1)$ with $\alpha = 0$. In this configuration, the system reduces to a simple harmonic oscillator $\ddot{x} = - 2Kx$.



Given the initial $x(0) = 0$ and $v(0) = 1$, the exact analytical solution is: $x(t) = \frac{1}{\sqrt{2K}} sin(\sqrt{2K}t)$

Figure 1: Comparison of the numerical solution (dashed red) and the exact analytical solution (solid black) for a single linear oscillator $(N = 1)$. The numerical solution accurately captures the frequency of the oscillation, with phase alignment maintained throughout the simulation (Figure 1). However, a constant amplitude error is observed. This discrepancy arises from the first-order linear extrapolation used to initialize the Leapfrog scheme. This initialization ignores the immediate force acting on the particle at $t = 0$, introducing a small energy error that persists due to the symplectic nature of the integrator.

2.2 The Linear Chain $(\alpha = 0)$



We simulated a linear chain for $N = \{8, 16, 32\}$ with an initial excitation corresponding to the fundamental mode $(k = 1)$. **Figure 2:** Dynamics of the linear chain$(\alpha = 0)$ for varying N. Left column: Snapshots of the system state at different times. Right column: Time history of the middle mass displacement.

As expected for a linear system, the normal modes are uncoupled. Figure 2 shows that the system maintains its initial sinusoidal shape indefinitely. The snapshots overlap perfectly, indicating a standing wave. The history of the middle mass shows a clean, unmodulated oscillation with constant amplitude. The behavior is consistent across all resolutions, confirming that the scaling $K \propto (N + 1)^2$ correctly preserves the continuum wave physics.

2.3 Nonlinear Dynamics: FPUT Recurrence $(\alpha > 0)$

We introduced a nonlinear "hardening" term with $\alpha = \frac{N}{10}$. This nonlinearity couples the spatial modes, allowing energy to transfer from the fundamental mode to higher-frequency modes.

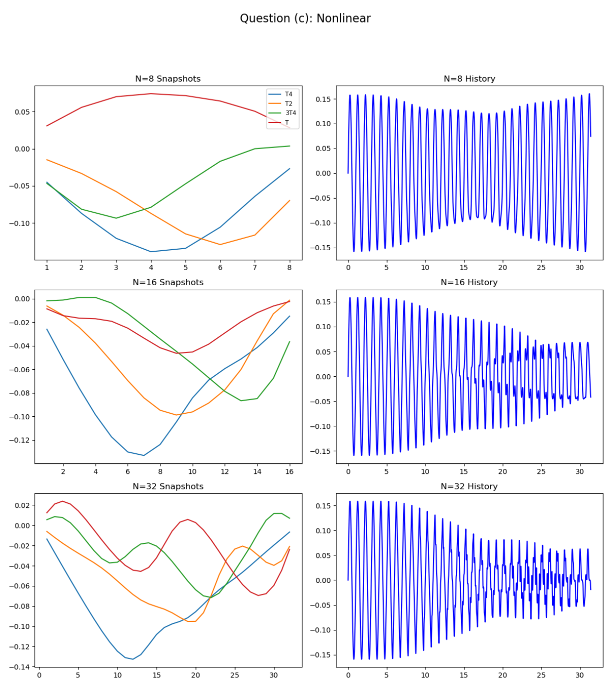
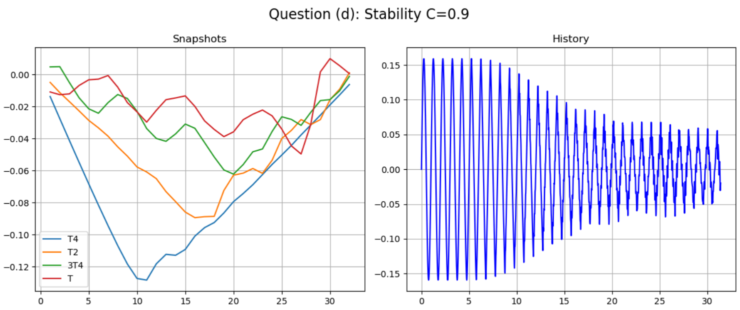


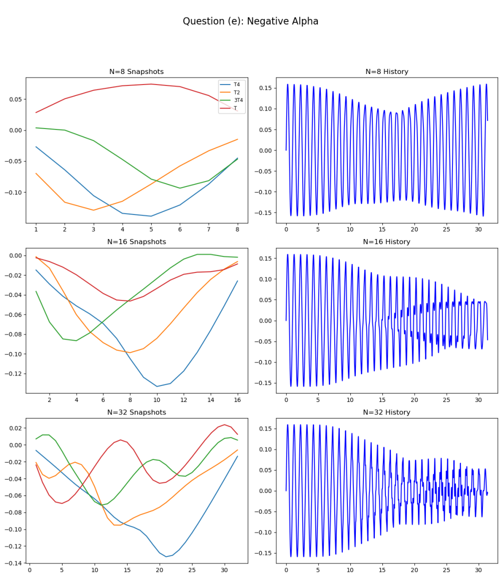
Figure 3: Dynamics of the nonlinear FPUT chain $(\alpha > 0)$. Note the distortion of the wave shapes (left) and the amplitude modulation or "beating" in the history plots (right), indicative of energy recurrence. The results in Figure 3 clearly demonstrate the breakdown of the superposition principle. The snapshots show the waveform distorting, developing ripples as higher harmonic modes are excited—an effect most pronounced for $N = 32$ where α is largest. Crucially, the system does not thermalize into random noise. Instead, the history plots reveal a "beating" pattern where the energy moves away from the initial mode and then coherently returns, a phenomenon known as FPUT recurrence.

2.4 Stability Analysis



We investigated the stability limit of the Leapfrog scheme by increasing the safety factor C to 0.9 for the strongest nonlinearity tested ($N = 32,\ \alpha = 3.2$) **Figure 4:** Stability test for $N = 32$ with $\alpha = 3.2$ and safety factor $C = 0.9$. The simulation remains stable with bounded oscillations. While the "hardening" springs increase the effective stiffness of the system at large displacements, Figure 4 shows that the simulation remains stable at $C = 0.9$. The trajectories remain bounded and smooth. However, theoretical analysis suggests that values of C approaching or exceeding 1.0 would violate the stability condition during the moments of maximum displacement, leading to numerical overflow.

2.5 Softening Spring ($\alpha < 0$)



Finally, we investigated "softening" springs by setting $\alpha = -\frac{N}{10}$. In this regime, the restoring force weakens as the spring stretches. **Figure 5:** Dynamics of the nonlinear chain with "softening" springs ($\alpha < 0$). Similar to the positive case, the system exhibits mode coupling and recurrence without instability. Despite the potential for instability (if the restoring force were to reverse), the system remained bounded for all tested cases (Figure 5). Qualitatively, the behavior mirrors the positive α case: the fundamental wave distorts due to mode coupling, and the history plots show the characteristic FPUT recurrence beating pattern. This confirms that the lack of thermalization is a robust feature of the system, independent of the sign of the nonlinearity.

Conclusion

The numerical simulations successfully reproduced the classic behavior of the Fermi-Pasta-Ulam-Tsingou problem. While the linear system behaved as an integrable set of independent oscillators, the introduction of nonlinearity facilitated energy exchange between spatial modes. However, contrary to the ergodic hypothesis, the energy did not equipartition among all modes on the observed time scales. Instead, the system exhibited quasi-periodic recurrence, where the initial state is nearly restored. These findings highlight the rich and counter-intuitive dynamics of nonlinear lattices, where integrability can persist or "ghosts" of stable orbits can prevent rapid thermalization.