The Effect of Lattice Reordering on Recurrence in Disordered Fermi-Pasta-Ulam-Tsingou-α Systems

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Abstract. We study the behavior of disordered Fermi-Pasta-Ulam-Tsingou (FPUT) lattices under fixed boundary conditions, focusing on the breakdown of the well-known recurrence phenomenon. We demonstrate that this breakdown can be mitigated by reordering the lattice elements based on their tolerance values. Two reordering strategies are explored: arranging the lattices in ascending order and in a centrosymmetric order. At a fixed energy level, both approaches successfully restore recurrence for small tolerance values. However, when the tolerance values become large, these arrangements have a limited effect in preventing the breakdown of recurrence.

INTRODUCTION

The seminal work by Fermi, Pasta, Ulam, and Tsingou (FPUT) in 1950s studied a one-dimensional lattice system with nonlinear particle interactions[1]. Their primary objective was to investigate the system's tendency towards energy equipartition among its modes, a behavior they expected due to the inherent nonlinearity of the system. However, their numerical simulations revealed an unexpected phenomenon. Instead of a gradual redistribution of energy into higher modes, the system exhibited behavior where almost all energy returned to its initial configuration. This counterintuitive observation, now famously known as the FPUT recurrence, has since inspired a wealth of research across both mathematics and physics, fueling inquiries into nonlinear dynamics and integrability[2–6].

Recent research has explored the effects of disorder on the FPUT system. Nelson et al.[7] examined the disordered FPUT-α model and its impact on energy recurrences. They demonstrated that increasing disorder, through a larger tolerance in system parameters, could suppress energy recurrence and enable energy equipartition. Zulkarnain et al.[8,9], employing two-mode approximation and multiple time-scale analysis, studied the mechanisms behind this energy equipartition as tolerance increases, and further analyzed how tolerance impacts chaotic behavior in the disordered FPUT system. More recently, Li et al.[10] investigated how recurrence could be recovered even in a disordered system by reordering the lattice. Their study focused on the FPUT-β model, showing that energy recurrence could be restored by rearranging the lattice elements in either ascending order or a centrosymmetric configuration, thereby offering new insights into the role of lattice arrangement in nonlinear systems.

In this paper, we extend these investigations by analyzing the effect of lattice reordering in a disordered FPUT-α system, specifically at a fixed energy level with varying tolerance values. By adopting the initial energy of the original FPUT experiment, we assess the influence of different lattice arrangements, including both ascending and centrosymmetric configurations, on the recovery of energy recurrences. Our findings offer a broader understanding of how lattice structure impacts the dynamics of disordered nonlinear systems.

The remainder of this paper is organized as follows: in Section 2, we discuss the classical FPUT-α system and review the key results on energy recurrences. Section 3 extends this discussion to the disordered FPUT-α system. In Section 4, we investigate the impact of lattice reordering on recurrence recovery, considering various tolerance values. Finally, our conclusions are presented in Section 5.

ENERGY RECURRENCE IN THE FPUT-α SYSTEM

The Hamiltonian for the FPUT-α system can be expressed as

$$H(x,p) = \sum_{j=0}^{N} \frac{p_j^2}{2} + \sum_{j=0}^{N} \frac{1}{2}\left(x_{j+1} - x_j\right)^2 + \frac{\alpha}{3}\left(x_{j+1} - x_j\right)^3 = E, \tag{1}$$

where $x_j(t)$ and $p_j(t)$ represent the position and momentum of the j-th particle, respectively, at time t. The nonlinearity strength is controlled by the parameter $\alpha \geq 0$, and E denotes the total energy of the system. The equations of motion are written as

$$\ddot{x}_j = x_{j-1} - 2x_j + x_{j+1} + \alpha\left((x_{j+1} - x_j)^2 - (x_j - x_{j-1})^2\right), \tag{2}$$

with boundary conditions $x_0 = x_{N+1} = 0$.

By applying the normal mode transformation

$$x = AQ, \quad p = AP, \tag{3}$$

where x and p are vectors of positions and momenta, Q and P are normal mode coordinates, and the transformation matrix A is given by

$$A = \sqrt{\frac{2}{N+1}} \begin{bmatrix} \sin\left(\frac{\pi}{N+1}\right) & \dots & \sin\left(\frac{N\pi}{N+1}\right) \\ \vdots & \ddots & \vdots \\ \sin\left(\frac{N\pi}{N+1}\right) & \dots & \sin\left(\frac{N^2\pi}{N+1}\right) \end{bmatrix} \tag{4}$$

the Hamiltonian (1) becomes

$$H = \frac{1}{2}\sum_{k=1}^{N} \left(P_k^2 + \omega_k^2 Q_k^2\right) + \alpha H_3(Q_1, \dots, Q_N), \tag{5}$$

where H_3 is a nonlinear function, and the normal mode frequencies ω_k are given by

$$\omega_k = 2\sin\left(\frac{k\pi}{2(N+1)}\right). \tag{6}$$

Note that the equations of motion in normal-mode coordinates can be written as

$$Q = DQ + \alpha A^{-1}F(Q), \tag{7}$$

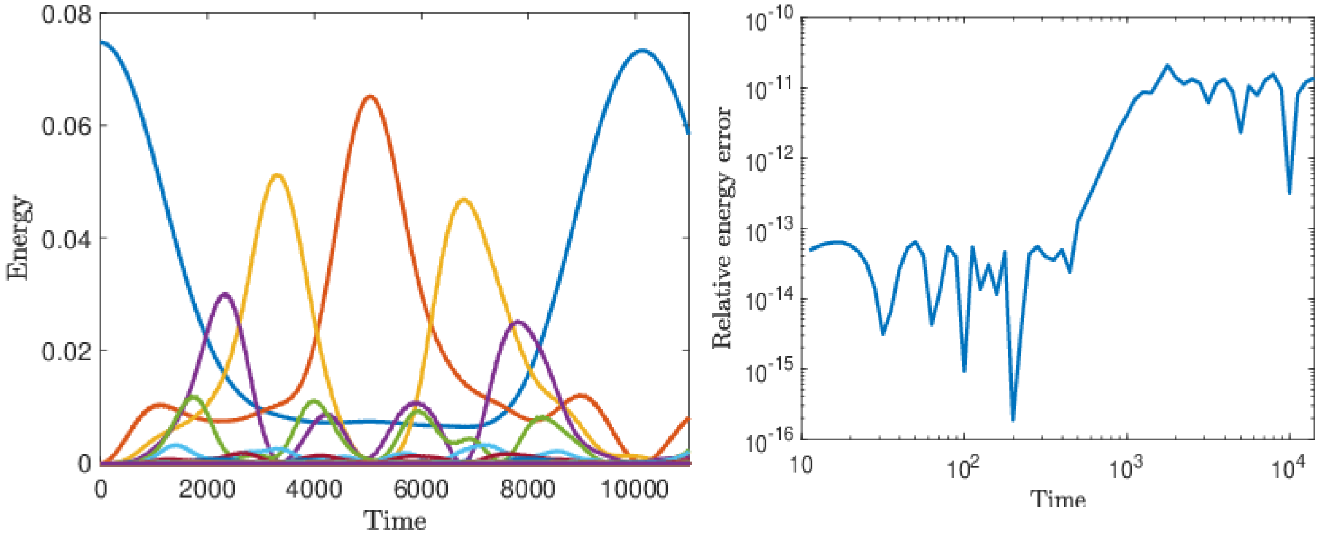
where the matrix D is diagonal, with its elements being $-\omega_k^2$, and $F(Q)$ is the nonlinear coupling terms. In this context, Q represents the spatial oscillation of each normal mode, while P corresponds to the velocity. The energy of the k-th mode is then

$$E_k = \frac{1}{2}\left(P_k^2 + \omega_k^2 Q_k^2\right). \tag{8}$$

In the linear case where $\alpha = 0$, the normal-mode transformation decouples the system, making each mode independent. However, for $\alpha > 0$, energy can transfer between the modes. In the original FPUT experiment, the first mode ($k = 1$) was excited with the following initial conditions

$$x_j = \sin\left(\frac{\pi j}{N+1}\right), \quad p_j = 0, \quad j = 1,2,\dots,N. \tag{9}$$

In normal-mode coordinate, this corresponds to $Q_1 = \sqrt{(N+1)/2}$, with $Q_k = 0$ for $k \geq 2$ and $\dot{Q}_k = 0$ for all k. Fermi, Pasta, Ulam, and Tsingou expected energy to flow from the initially excited mode into the higher modes, eventually leading to equipartition. However, they observed that the energy remained confined to the lower modes and eventually returned to the first mode, a phenomenon now known as the FPUT recurrence. This surprising result, also called the FPUT paradox, is illustrated in Fig. 1 for $N = 32$ and initial energy $E = 0.07471$. We solved Eq. (2) using a fourth-order Yoshida symplectic integrator[11] with initial conditions given by Eq. (9). The minimum energy in the first mode was found to be 0.006403, while at recurrence, the energy in the first mode reached 0.07327. Throughout the system's evolution, 91.43% of the total energy was transferred to higher-order modes. The relative energy error, defined as $\Delta E = |(E(t) - E(0))/E(0)|$, is shown in Fig. 2. The error remained below 10^{-10} with an integration time step of 10^{-2}.



(a) (b)

FIGURE 1. The FPUT-α recurrence for $N = 32$ with an initial energy of $E = 0.07471$ is shown in panel (a), with the corresponding relative energy error depicted in panel (b).

DISORDERED FPUT-α SYSTEM

We now consider the FPUT-α system with variability, where the Hamiltonian is given by

$$H(x,p) = \sum_{j=0}^{N} \frac{1}{2}\frac{p_j^2}{t_j} + \sum_{j=0}^{N} \frac{1}{2}\left(t_{j+1}x_{j+1} - t_j x_j\right)^2 + \frac{\alpha}{3}\left(t_{j+1}x_{j+1} - t_j x_j\right)^3 = E, \tag{10}$$

with fixed boundary conditions $x_0 = x_{N+1} = 0$. The parameters t_j represent the variability and are drawn randomly. For a tolerance $\tau\%$, t_j values are sampled from a Gaussian distribution with a mean of 1 and a standard deviation $\sigma = \frac{1}{3} \times 0.01\tau$. This ensures that 99.73% of t_j values fall within the range $[1 - 0.01\tau, 1 + 0.01\tau]$[7].

The resulting equations of motion are

$$\ddot{x}_j = t_{j-1}x_{j-1} - 2t_j x_j + t_{j+1}x_{j+1} + \alpha\left(\left(t_{j+1}x_{j+1} - t_j x_j\right)^2 - \left(t_j x_j - t_{j-1}x_{j-1}\right)^2\right), \tag{11}$$

and by introducing $\tilde{x}_j = t_j x_j$, this can be reformulated as

$$\frac{1}{t_j}\ddot{\tilde{x}}_j = \tilde{x}_{j-1} - 2\tilde{x}_j + \tilde{x}_{j+1} + \alpha\left(\left(\tilde{x}_{j+1} - \tilde{x}_j\right)^2 - \left(\tilde{x}_j - \tilde{x}_{j-1}\right)^2\right), \tag{12}$$

with a corresponding Hamiltonian of

$$\widehat{H}(\tilde{x},\tilde{p}) = \sum_{j=0}^{N} \frac{t_j}{2}\tilde{p}_j^2 + \sum_{j=0}^{N}\left[\frac{1}{2}\left(\tilde{x}_{j+1} - \tilde{x}_j\right)^2 + \frac{\alpha}{3}\left(\tilde{x}_{j+1} - \tilde{x}_j\right)^3\right], \tag{13}$$

where $\tilde{p}_j = p_j/t_j$. In this formulation, Eq. (12) represents a disordered FPUT lattice with mass $m_j = 1/t_j$, in line with previous work on harmonic lattices with random masses[12].

Next, we can write Eq. (11) as

$$x = Sx + \alpha F(x), \tag{14}$$

where

$$x = \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \vdots \\ \ddot{x}_N \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}, \quad S = \begin{bmatrix} -2t_1 & t_2 & 0 & \cdots & 0 \\ t_1 & -2t_2 & t_3 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \cdots & t_{N-2} & -2t_{N-1} & t_N \\ 0 & 0 & \cdots & t_{N-1} & -2t_N \end{bmatrix}, \tag{15}$$

and F is a nonlinear function. Let the matrix $V = [v_1 \; v_2 \; \cdots \; v_N]$ represent the eigenvectors of S, with corresponding eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_N$. For convenience, let us define

$$\lambda_k = -\widehat{\omega}_k^2, \quad k = 1, \ldots, N, \tag{16}$$

where $\widehat{\omega}_k \in \mathbb{R}$.

In the case where all $t_j = 1$, S simplifies to a tridiagonal matrix, and V becomes equivalent to A, with $\lambda_k = -\omega_k^2$. Using the normal-mode transformation

$$x = MQ, \tag{17}$$

$$p' = MP, \tag{18}$$

where $p_j{}' = p_j/t_j$, $M = kV$, and $k = c\widehat{\omega}_1/\sqrt{2E}$, the equations of motion transform to

$$Q = DQ + \alpha M^{-1}F(Q), \tag{19}$$

where D is a diagonal matrix containing the eigenvalues of S. As in the original FPUT experiment[1], the energy in each normal mode is given by

$$E_k = \frac{1}{2}(P_k^2 + \widehat{\omega}_k^2 Q_k^2). \tag{20}$$

We now explore the impact of variability on the evolution of normal-mode energy for a fixed energy level, using initial conditions such that only the lowest mode is excited. The initial energy is set equal to that used in the original FPUT-α system[1], where, for $N = 32$, the initial energy is defined as $E = 0.07471$. We determine a suitable constant c such that the initial conditions

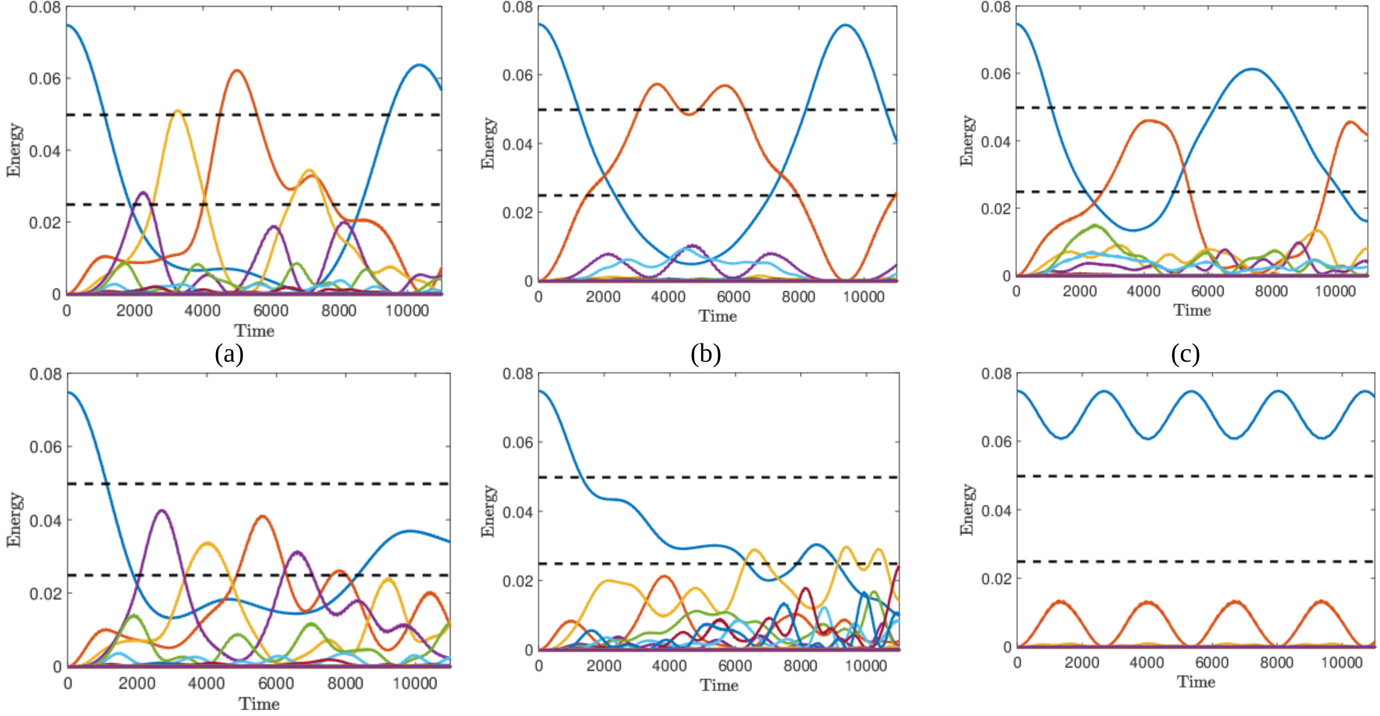
$$x(0) = cv_1, \quad p(0) = 0, \tag{21}$$

satisfy the Hamiltonian function (10). In normal-mode space, this corresponds to

$$Q_1(0) = \frac{\sqrt{2E}}{\widehat{\omega}_1}, \quad Q_k(0) = 0 \ \text{for} \ k = 2, \dots, N, \quad P_j(0) = 0 \ \text{for} \ j = 1, \dots, N. \tag{22}$$

To assess recurrence behavior, we apply two specific criteria[10]. The first criterion specifies that at least two-thirds of the initial energy should be distributed across other modes. The second criterion requires that, at the point of recurrence, at least two-thirds of the energy must return to the initial mode. These threshold values are marked as black-dashed lines in Fig. 2. For each tolerance value, we generate 50 distinct sets of t_j values, solve Eq. (11) using the initial conditions in Eq. (21), and track the associated normal-mode energy E_k in a system with $N = 32$ particles. This process is repeated for three tolerance values $\tau = 5\%$, $\tau = 50\%$, and $\tau = 95\%$, as illustrated in Fig. 2. The total initial energy is set to $E = 0.07471$, mirroring the energy in Fig. 1.

Our simulations show that for a 5% tolerance, 32 out of 50 sets demonstrate recurrence. At 50% tolerance, only 5 sets exhibit recurrence, while at the highest tolerance of 95%, recurrence is observed in just 3 sets out of 50. Representative cases of energy recurrence for each tolerance level are displayed in Figs. 2a-2c, with examples of energy equipartition shown in Figs. 2d-2f.



(a) (b) (c)

(d) (e) (f)

FIGURE 2. FPUT recurrences (panels (a)-(c)) and energy thermalisation (panels (d)-(f)) for different tolerance values: $\tau = 5\%$ in panels (a) and (d), $\tau = 50\%$ in panels (b) and (e), and $\tau = 95\%$ in panels (c) and (f). The black-dashed lines at the top and bottom represent energy levels of $2E/3$ and $E/3$, respectively.

EFFECT OF REORDERING LATTICES

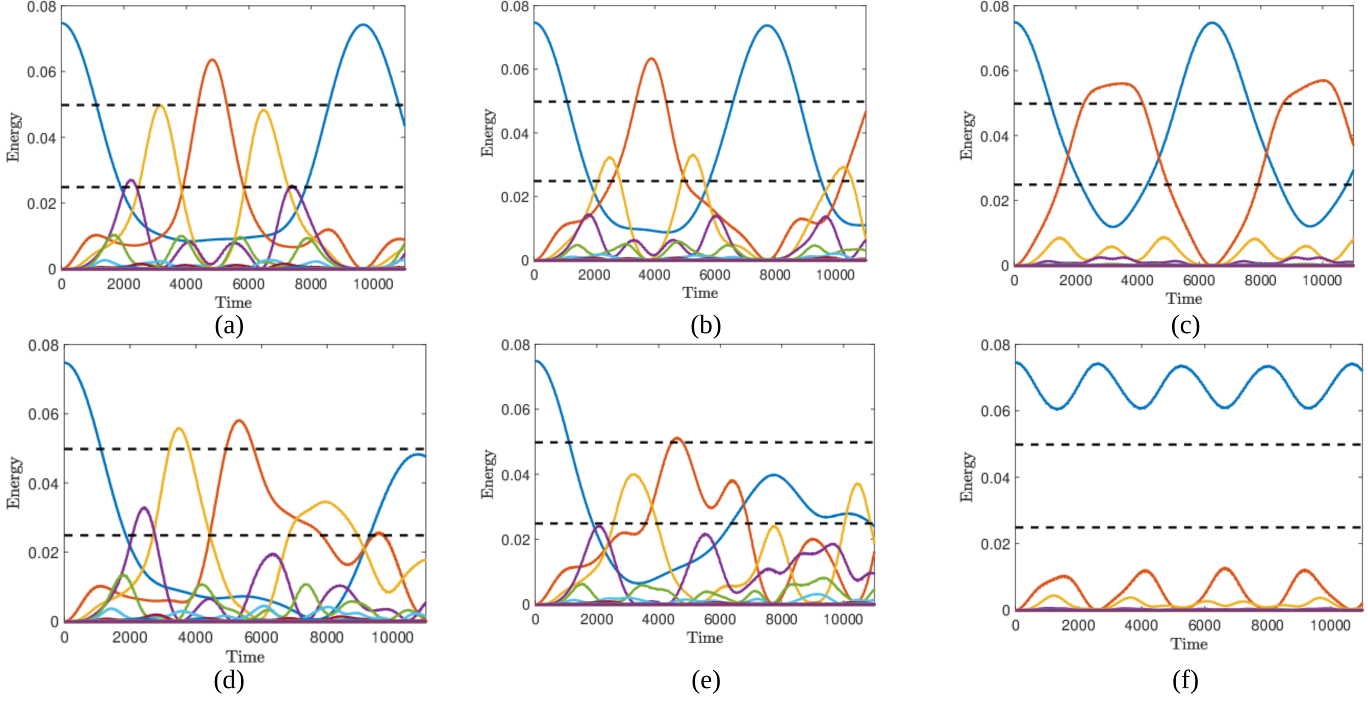
In the previous section, we randomly distributed tolerance values without a predefined lattice arrangement. Here, we examine the impact of lattice reordering on energy recurrence by arranging the lattices in ascending order of their tolerance values. We utilize the same set of 50 different t_j values as before, retaining the initial energy and conditions from the arbitrary arrangement.

Our simulations demonstrate that for a tolerance value of 5%, 45 out of 50 configurations exhibit energy recurrence. At 50% tolerance, this number reduces to 22 configurations, and further drops to 4 configurations at the 95% tolerance level. Energy recurrences and equipartitions are illustrated in Figs. 3a-3f.

Next, we explore the effect of a centrosymmetric arrangement, defined for even N. If a particle at position $N/2 - i + 1$ has a variability value differing from the mean by $+\gamma$, the particle at $N/2 + i$ differs by $-\gamma$, for $i = 1,2,\dots,N/2$. The centrosymmetric distribution is shown in Fig. 18 for $N = 32$, where the mean is 1 and centrosymmetry with respect to particle 16 and 17.

Our findings show that at a 5% tolerance, all 50 configurations achieve energy recurrence. This number decreases to 12 configurations at 50% tolerance, and further to 3 at 95%. Illustrative examples of energy recurrences at 50% and 95% tolerance levels are provided in Figs. 5a-5b, with corresponding instances of energy equipartition shown in Figs. 5c-5d.

Figure 6 displays the percentage of recurrence recovery for 5%, 50%, and 95% tolerances. The centrosymmetric order recovers 100% of recurrence at 5% tolerance, compared to 90% in ascending order, and 64% in arbitrary order. As tolerance increases, the influence of reordering diminishes. At 50%, ascending order recovers 44% while centrosymmetric order recovers only 24%. At 95%, both orders show minimal recovery, with 6% in arbitrary and centrosymmetric arrangements, and 8% in ascending order.



(a) (b) (c)

(d) (e) (f)

FIGURE 3. Illustration of FPUT recurrences (panels (a)-(c)) and energy thermalization (panels (d)-(f)) across tolerance values of 5% (panels (a) and (d)), 50% (panels (b) and (e)), and 95% (panels (c) and (f)) in ascending lattice order. The dashed lines represent $2E/3$ and $E/3$ thresholds.

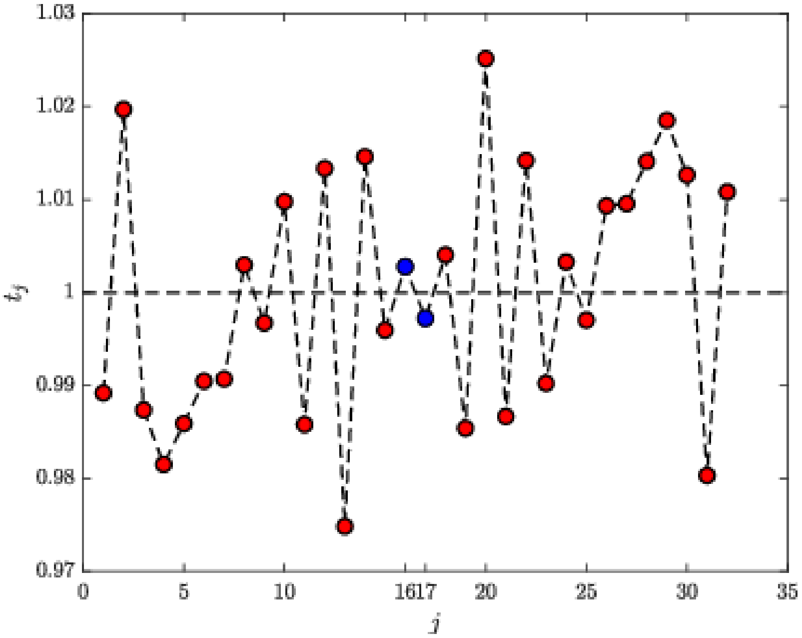
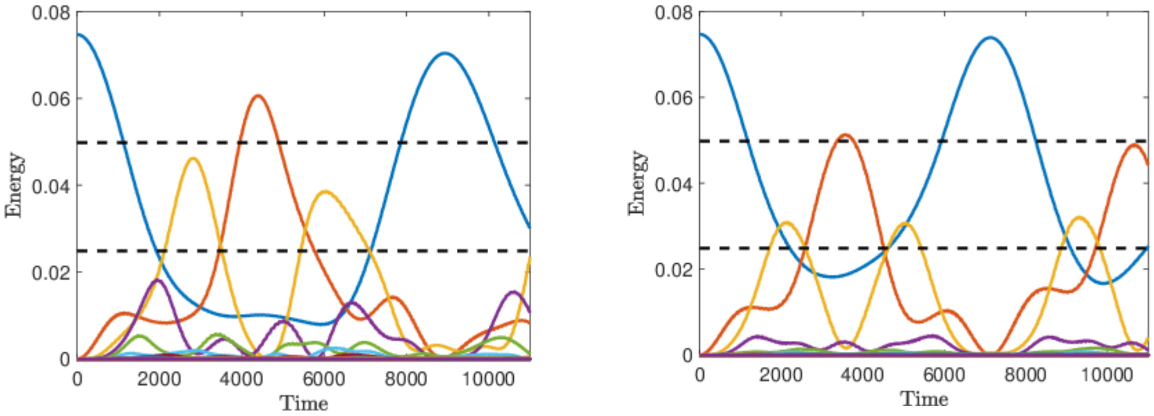
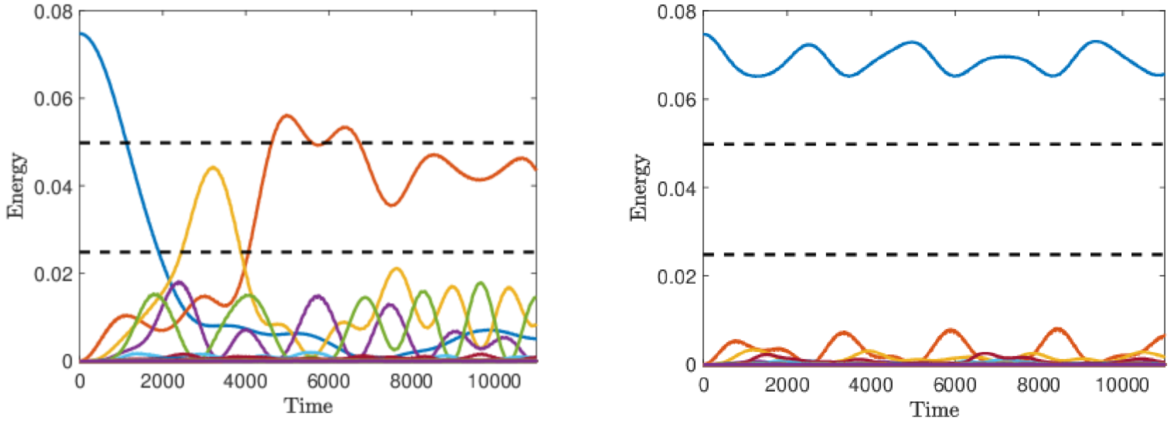


FIGURE 4: Centrosymmetric arrangement of tolerance values for a system of $N = 32$ particles.



(a)

(b)



(c) (d)

FIGURE 5. The FPUT recurrences (panels (a)-(b)) and energy thermalization (panels (c)-(d)) for tolerance values of 50% in panels (a) and (c), and 95% in panel (b) and (d), arranged in centrosymmetric order.The dashed lines represent the thresholds of $2E/3$ and $E/3$.

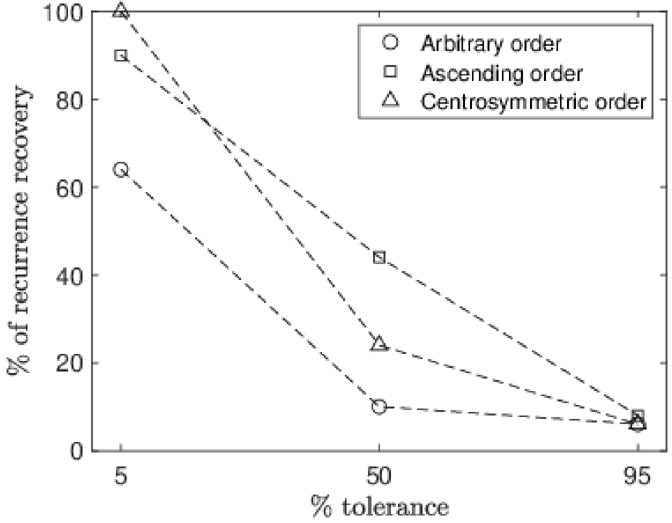


FIGURE 6. Proportion of recurrence recovery for tolerance values of 5%, 50%, and 95% across three different lattice configurations: arbitrary order, ascending order, and centrosymmetric order.

CONCLUSION

In this paper, we have examined the influence of lattice ordering on energy recurrence in the disordered Fermi-Pasta-Ulam-Tsingou-α (FPUT-α) model under varying tolerance values. Simulations revealed that reordering the lattices based on tolerance, specifically in ascending and centrosymmetric orders, significantly impacts recurrence patterns. At lower tolerance levels (5%), reordering, especially in centrosymmetric configuration, consistently recovered nearly full recurrence, as seen in up to 100% of cases. However, as tolerance levels increased to 50% and 95%, the impact of reordering diminished, with centrosymmetric arrangements showing less recurrence recovery than ascending orders at the moderate 50% tolerance. By the highest tolerance value (95%), neither arrangement consistently promoted recurrence, with rates similar to arbitrary ordering.

These findings highlight the significant initial influence of lattice ordering on recurrence behavior in systems with low tolerance values, although the effectiveness of specific arrangements declines as tolerance values increase. This indicates a complex interplay between structural configuration and tolerance in nonlinear lattice dynamics. Lattice reordering appears to be a promising method for managing recurrence in systems with low tolerance. However, its advantages decrease as tolerances grow. This study provides insights into optimizing energy recurrence in structured lattices and serves as a foundation for future research into energy distribution within complex systems.

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