Study of Lattice Vibrations: Different Perturbations and Vibrational Modes

Adhilsha A - 2011006
School of Physical Sciences, National Institute for Science Education and Research, HBNI, Jatni, India
(Dated: April 22, 2024)

In lattices where atoms are bound by the neighboring atoms and forces, the study of lattice vibrations can reveal information about the material's properties. In this project, we will study the vibrational modes of a 1D lattice of N atoms with the same mass m and nearest-neighbor interactions by employing a combination of numerical methods. By utilizing RK4 time stepping and FFT analysis, we explore the vibrational modes arising from various initial conditions and boundary constraints. Noteworthy observations include the manifestation of expected normal modes under specific perturbations and the implications of symmetric and random perturbations on mode development. Furthermore, the study underscores the method's adaptability, paving the way for effortless exploration of diverse conditions and dimensions in lattice dynamics simulations.

CONTENTS

I. INTRODUCTION

Materials science and solid-state physics are inextricably linked to lattice vibrations, which have a significant impact on the mechanical, thermal, and electrical properties of materials. The study of lattice vibrations can provide information about thermodynamics, superconductivity, phase transitions, thermal conductivity, and thermal expansion[1].

Given the importance, the many degrees of assumptions and subtleties in interaction cause numerous challenges in solving the system for vibrational modes. Such discoveries are critical for understanding material behavior under different situations, and they hold significant potential for applications ranging from nanotechnology to condensed matter physics. In such circumstances, a convenient and adaptable method for studying dynamics is highly valued.

In this project, we will be focusing on the monoatomic lattice with atoms of the same mass (monoatomic lattice) with the following objectives:

- **Insights into Vibrational Modes**: By simulating various initial conditions and boundary constraints, the project provides valuable insights into the vibrational modes of the monoatomic lattice.
- **Impact of various Perturbations:** The study investigates the effects of different perturbations, including symmetric and random perturbations, on the development of vibrational modes.
- **Study of dispersion law:** By stimulating the system with different wavenumber, we study the dispersion law through numerical methods.
- **Robustness of the Approach**: We investigate the impact of the time factor while analyzing the developing modes and the consistency across different trials.

II. THEORY

A. Lattice Vibrations

In the study of lattice dynamics, the movement of atoms is often described as harmonic waves traveling through the lattice. Each wave is fully defined by characteristics like its wavelength, angular frequency, amplitude, and direction of movement.[2] However, dealing with wavelength can be complex due to its wide range of values. To simplify this, a wave vector $\mathbf{k}$ is commonly utilized. This vector aligns with the wave's direction of propagation and is normalized to have a magnitude equal to $\frac{2\pi}{\lambda}$.

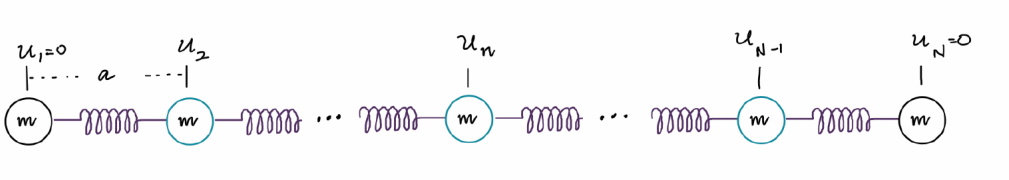

FIG. 1. Monoatomic Lattice

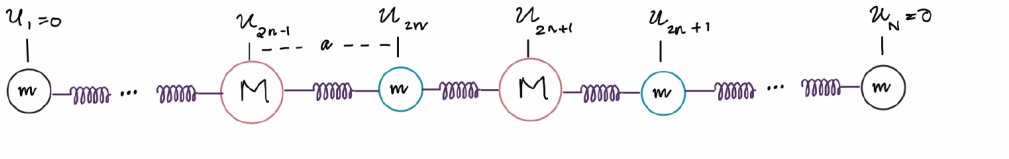

FIG. 2. Diatomic Lattice

B. Monoatomic 1D Lattice

In a monoatomic lattice, the atoms are identical, and the crystal structure is straightforward, resembling masses interconnected by springs, as depicted in Figure 1 by assuming that each atom in the lattice moves due to interactions with its nearest neighbors. For instance, in an array of coupled atoms, atom n would experience forces from the adjacent atoms $n-1$ and $n+1$[2, 3].

Let the mass of the atom be m, the equilibrium distance between any two atoms be a (Lattice Constant), U_n denotes the distance of the n^{th} atom from equilibrium position and C denotes the spring constant, then the equation of Forces acting on atom n can be written as:

$$F_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n) \tag{1}$$

With $F = ma = m\ddot{u}$, we can write the equation of motion as:

$$m\frac{d^2u_n}{dt^2} = -C(2u_n - u_{n+1} - u_{n-1}) \tag{2}$$

We can look for solutions of the following form (ansatz for normal mode):

$$u_n = Ae^{i(kna-\omega t)} \tag{3}$$

Applying equation (3) into (2), we get:

$$\begin{aligned} m\frac{d^2u_n}{dt^2} &= -C(2u_n - u_{n+1} - u_{n-1}) \\ -m\omega^2 &= -C(2 - e^{ika} - e^{-ika}) \\ -m\omega^2 &= -C(2 - 2\cos(ka)) \\ \omega^2 &= \frac{2C}{m}(1 - \cos(ka)) \end{aligned} \tag{4}$$

The corresponding dispersion law becomes:

$$\omega = \pm 2\sqrt{\frac{C}{m}}|sin(ka/2)| \tag{5}$$

For a more generalized solution to frequency for all vibrational modes, we can write the equation (2) in matrix form for N vibrating atoms with fixed boundary conditions. The equation form is:

$$\ddot{u}_n(t) = \sum_{m=1}^{N} A_{nm}u_m(t) \tag{6}$$

where the matrix A is given by:

$$A = \begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ -1 & -2 & 1 & \cdots & 0 \\ 0 & -1 & -2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -2 \end{pmatrix} \tag{7}$$

Finding the eigenvalues of this matrix, we get:

$$\omega_n = \sqrt{\frac{2K}{M}\left(1 - \cos\frac{n\pi}{N+1}\right)} \tag{8}$$

These theoretical values of normal mode frequency will be used to validate the result of our model.

We can extend this to diatomic lattice[2, 4] by changing the equation (2) as:

$$m\frac{d^2u_{2n}}{dt^2} = -C(2u_{2n} - u_{2n+1} - u_{2n-1}) \tag{9}$$

$$M\frac{d^2u_{2n+1}}{dt^2} = -C(2u_{2n+1} - u_{2n+2} - u_{2n}) \tag{10}$$

where m and M are the two different masses of atoms present as given in Figure 2.

C. Runge-Kutta 4$^{\text{th}}$ order method

The fourth-order Runge-Kutta method is a numerical technique used for solving ordinary differential equations (ODEs) of the form (notations adapted for context):

$$\frac{du_n}{dt} = f(u_n, t) \tag{11}$$

where u_n is the dependent variable, t is the independent variable (typically time), and $f(u_n, t)$ is a function that describes the rate of change of u_n with respect to t. The equation (2) is the equation in use for our implementation.

Given a time step h, we can find $u_n(t^i + h)$ from $u_n(t^i)$ from using the following steps:

$$\begin{aligned}
k_1 &= hf(t^i, u_n(t^i)).\\
k_2 &= hf\left(t^i + \frac{h}{2}, u_n(t^i) + \frac{k_1}{2}\right)\\
k_3 &= hf\left(t^i + \frac{h}{2}, u_n(t^i) + \frac{k_2}{2}\right)\\
k_4 &= hf(t^i + h, u_n(t^i) + k_3)\\
u_n t^i + h &= u_n(t^i) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned} \tag{12}$$

D. coupled RK4

In our case, the equation is of second order, and even then, $f(t^i, u_n(t^i))$ is not solely dependent on $u_n(t^i)$. To handle this, we can transform the second-order ODE into a set of $2n$ coupled first-order ODEs. This involves introducing new variables and rewriting the original equation as a system of first-order equations.

For each atom in the lattice, we introduce a new variable representing its velocity v_n, resulting in $2n$ variables in total. Many coefficients in this system will be zero, simplifying the computational burden. This transformation allows us to solve the problem numerically using techniques like the RK4 method while accurately capturing the dynamics of the system.

The equation of motion (2) becomes:

$$f_1^n(t, u, v) = \frac{du_n}{dt} = v_n \tag{13}$$

$$f_2^n(t, u, v) = \frac{dv_n}{dt} = -\frac{C}{m}(2u_n - u_{n+1} - u_{n-1}) \tag{14}$$

Here, since the equations and variables are coupled, the equations in (12) become:

$$\begin{aligned}
\overline{k_{u1}} &= hf_1(t^i, \overline{u(t^i)}, \overline{v(t^i)})\\
\overline{k_{v1}} &= hf_2(t^i, \overline{u(t^i)}, \overline{v(t^i)})\\
\overline{k_{u2}} &= hf_1\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \frac{\overline{k_{u1}}}{2}, \overline{v(t^i)} + \frac{\overline{k_{v1}}}{2}\right)\\
\overline{k_{v2}} &= hf_2\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \frac{\overline{k_{u1}}}{2}, \overline{v(t^i)} + \frac{\overline{k_{v1}}}{2}\right)\\
\overline{k_{u3}} &= hf_1\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \frac{\overline{k_{u2}}}{2}, \overline{v(t^i)} + \frac{\overline{k_{v2}}}{2}\right)\\
\overline{k_{v3}} &= hf_2\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \frac{\overline{k_{u2}}}{2}, \overline{v(t^i)} + \frac{\overline{k_{v2}}}{2}\right)\\
\overline{k_{u4}} &= hf_1(t^i + h, \overline{u(t^i)} + \overline{k_{u2}}, \overline{v(t^i)} + \overline{k_{v3}})\\
\overline{k_{v4}} &= hf_2(t^i + h, \overline{u(t^i)} + \overline{k_{u2}}, \overline{v(t^i)} + \overline{k_{v3}})\\
u_{t^i+h} &= \overline{u(t^i)} + \frac{1}{6}(\overline{k_{u1}} + 2\overline{k_{u2}} + 2\overline{k_{u3}} + \overline{k_{u4}})\\
v_{t^i+h} &= \overline{v(t^i)} + \frac{1}{6}(\overline{k_{v1}} + 2\overline{k_{v2}} + 2\overline{k_{v3}} + \overline{k_{v4}})
\end{aligned} \tag{15}$$

Each of the above quantity with an overline means its a vector of size n.

III. IMPLEMENTATION

In our implementation, we will be using the programming language `Python` using the libraries `numpy` to manage data structures, `matplotlib` package for plotting, `tqdm` to track progress and `scipy` for FFT analysis.

Both the RK4 and coupled RK4 methods are implemented from scratch, generalized to handle any dimension of 1D lattice. Considering that achieving the required resolution may necessitate small time steps, we've incorporated the option for selective data saving to alleviate the potential hassle of storing all data. This feature allows us to efficiently manage memory while retaining flexibility in data collection according to specific requirements. There is also a code specifically designed to automate the production of animations depicting lattice vibrations based on simulation results, ensuring effective visualizations.

For FFT analysis of simulation results, we will analyze individual atoms to investigate their vibrational characteristics. By performing FFT on each atom's displacement data, we extract frequency information and plot the results collectively. Additionally, we identify the dominant mode of vibration for each atom and are then compared with theoretical predictions to assess the agreement between simulation and theory. For the study of dispersion relation, we analyze how each individual atom follows the dispersion law by examining its predominant mode at each wavenumber.

See the implementation in Github.

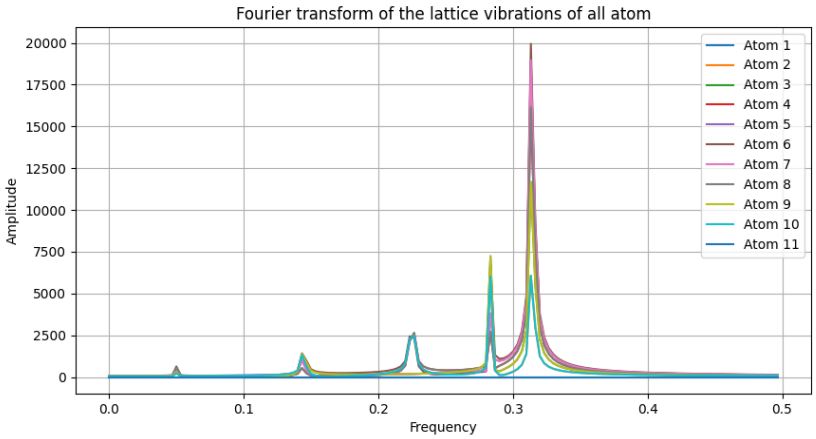

FIG. 3. FFT obtained from simulating a normal mode

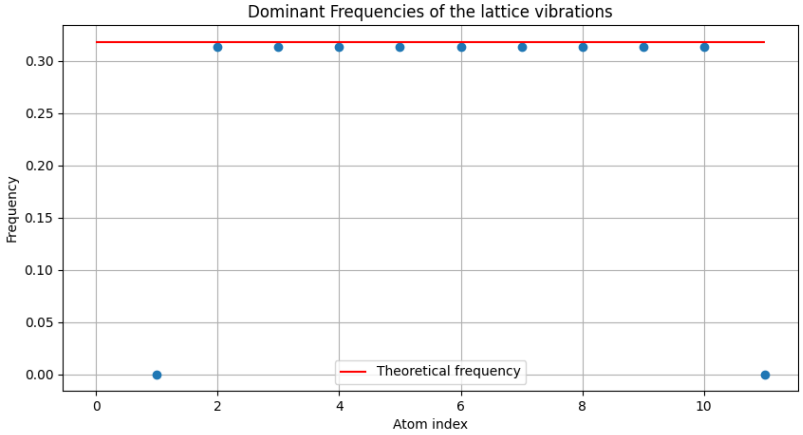

FIG. 4. Frequency of each atom compared with theoretical

IV. EXPERIMENTS AND OBSERVATIONS

For our system, the simulation was conducted using 11 atoms, with the end atoms fixed as boundary conditions, leaving 9 vibrating atoms. To simplify implementation, the parameters of the lattice, C, m, and a, were assigned a value of 1. We will be using $k = \pi/a$ for most parts other than the study of dispersion relations. Given that theoretical values are also calculated based on these parameters, this choice ensures consistency between simulation and theory. All the results, as well as different experiment settings, are stored in the Github where the animations of vibrations can also be viewed as well the parameters in use.

A. Normal Mode

To obtain normal mode, we apply the oscillation ansatz given in equations (3) with $t = 0$ and let the system evolve into the normal mode. For the same parameters of C, m, a, and N, we can calculate the theoretical normal mode frequency by using equation (4).

For our implementations, we will be using the ansatz from equation (3) to generate the time series data for each atom for the same time as the simulation and pass them through the same process of analysis to get a fair comparison. The developed normal modes are given in Figure 3, and the comparison to the theoretical frequency is given in Figure 4.

As you can see, due to the boundary conditions needed for the time evolution of a finite Lattice, the atoms close the boundaries, deviate from the expected value, and influence other atoms to develop smaller yet distinct modes.

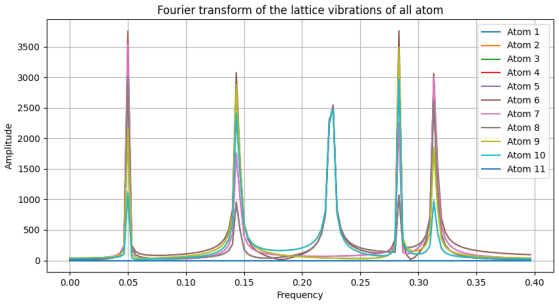

FIG. 5. FFT obtained from simulating a symmetric perturbation

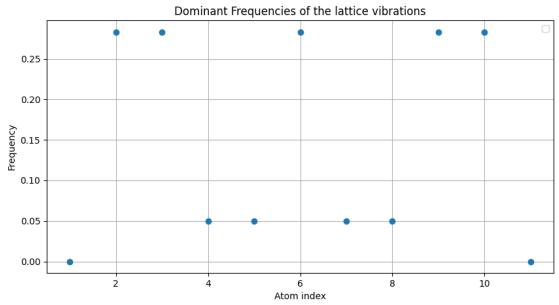

FIG. 6. Frequency of each atom compared in symmetric perturbation

B. Symmetric Perturbation

In this simulation, we perturbed only the central atom, let the vibrations spread symmetrically across the lattice, and observed the developing vibrational modes. The FFT analysis result is given in Figure 5. You can also see the symmetry in the dominant mode of each atom as shown in Figure 6.

As expected from the inherent symmetry of the system, we see modes symmetrically distributed around the central atom. Since the odd number of atoms $(2n+1)$ were let to vibrate, it was exactly $(n+1)$ modes.

C. Random Perturbation

Here, we gave three different random perturbations to the system and observed the developing vibrational modes. The FFT analysis results of these are given in Figures 7 to 9.

As you can see, for N vibrating atoms, we get N modes as expected. Furthermore, the modes developed in all three trials are the same for the same system, confirming that the modes are unique to the system of N atoms. The theoretical values given in equation (8) are also confirmed in Figure 10.

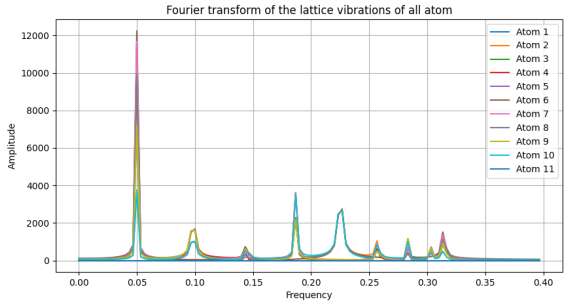

FIG. 7. FFT obtained from simulating random perturbation - trial1

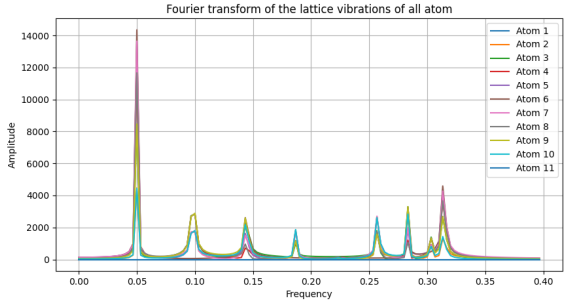

FIG. 8. FFT obtained from simulating random perturbation - trial2

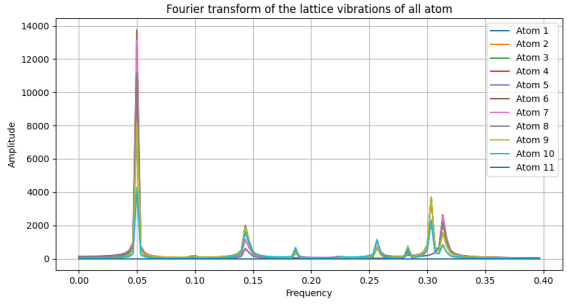

FIG. 9. FFT obtained from simulating random perturbation - trial3

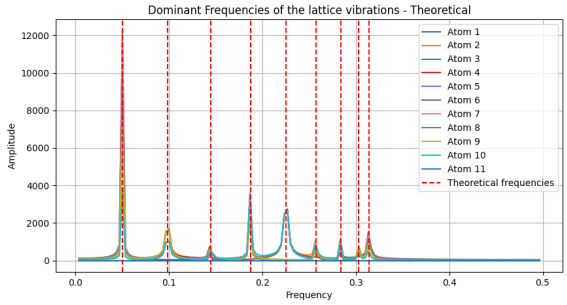

FIG. 10. Vibrational modes compared with theoretical frequencies

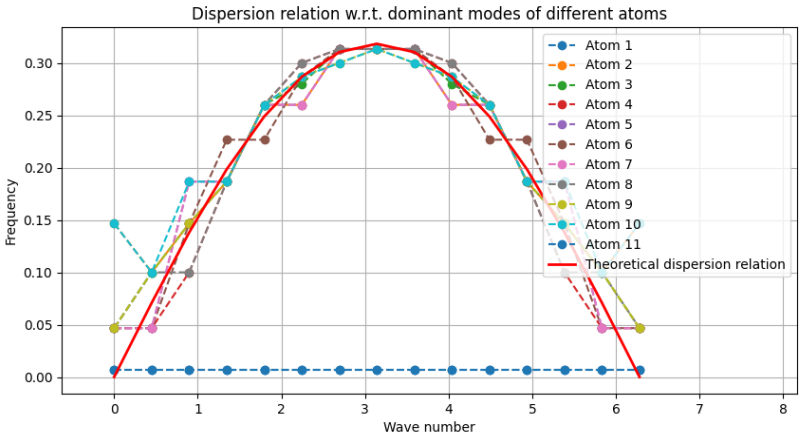

FIG. 11. Dispersion law - 9 vibrating atoms

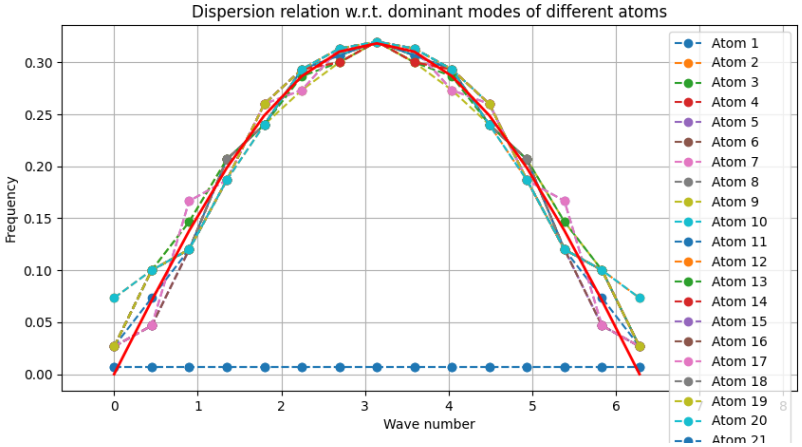

FIG. 12. Dispersion law - 19 vibrating atoms

D. Dispersion law

To obtain a curve representing the dispersion relation, we varied the wavenumber between 0 and $\frac{2\pi}{a}$, where a is the lattice spacing, and calculated the corresponding frequencies using equation (5). In our simulations, we determined the dominant modes of each atom across this range of k values and compared them with the theoretical expectations. The results are illustrated in Figure 11.

E. Consistency and Impact of Time

In the context of dispersion law, we conducted a simulation with a similar setting but with more atoms, bringing clearer results as the fixed boundary conditions affect chains less for longer. This can be seen by comparing Figure 11 to 12.

Across all trials, consistent observations reveal that peaks occur at the same frequencies for the same system, regardless of variations in the prominence of each mode. See Figures 3, 5, 7, 8, 9 and even 13 (run for much shorter time). This consistency indicates that the implementation effectively identifies the system's unique modes across diverse scenarios, ensuring robust and reliable results.

Initial trials on shorter simulations revealed similar peaks, albeit with lower peak resolution. This was attributed to insufficient time for the system to reach a balanced state among its various natural modes.

From a computational standpoint, the oscillations of each atom over shorter periods may not encompass enough information about all modes and their equilibrium states. This limitation arises because a 'complete cycle' oscillation across all modes within a frequency range is constrained by the smallest frequency and the initial perturbation.

This is clearly demonstrated in Figures 13 and 14, where the former depicts a simulation of a shorter duration compared to latter, which extends over a longer

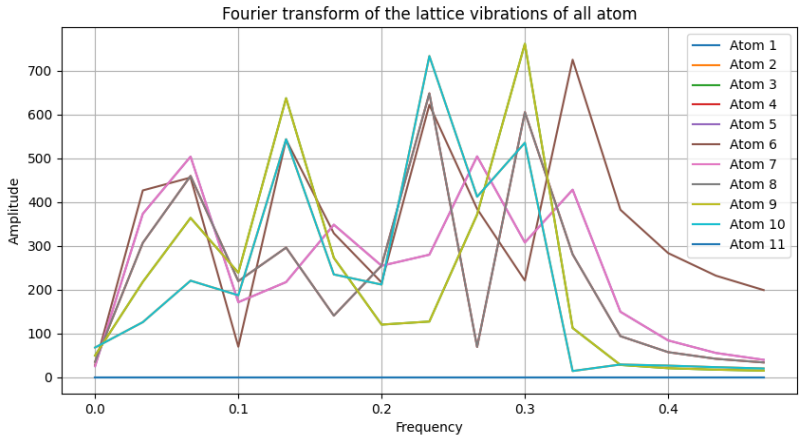

FIG. 13. FFT analysis over shorter simulation

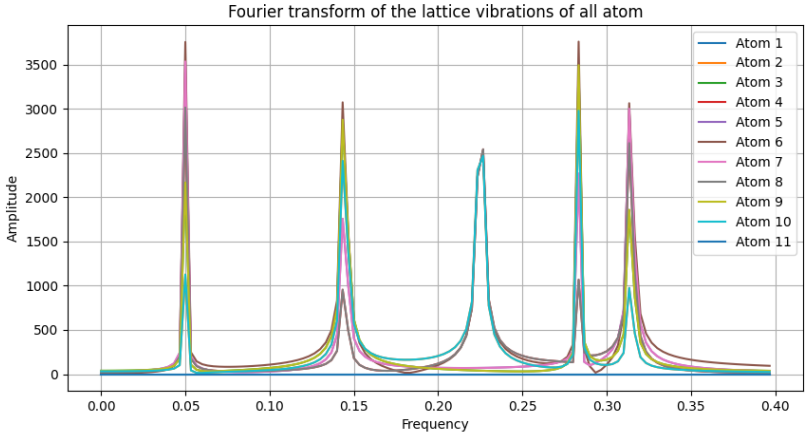

FIG. 14. FFT analysis over longer simulation

period. Despite the difference in simulation duration, all other conditions remain constant. This highlights the significance of allowing simulations adequate time to evolve, emphasizing the importance of collecting sufficient information for accurate analysis and interpretation of results.

V. RESULTS AND CONCLUSION

Given the system's normal mode oscillation ansatz given in equation (3), we were able to obtain the normal mode frequency very close the theoretical values. Symmetric perturbations yielded modes symmetrically distributed around the central atom, reflecting the system's inherent symmetry. Conversely, random perturbations lead to the emergence of all possible vibrational modes, showcasing the system's versatility and sensitivity to initial conditions. Dispersion was observed under a variation of wavenumber.

In terms of model flexibility, this approach was able to explore the dynamics of these different perturbations as well as different sizes of systems, giving consistent results across all trials while visualizing the vibrations at any given time. Observing the system for a longer period of time separates the modes as expected to obtain resolution over the smaller peaks of vibrational modes.

this study highlights the efficacy of RK4 time stepping and FFT analysis in unraveling the dynamics of lattice vibrations. The method's adaptability and versatility enable comprehensive exploration of various conditions and dimensions, offering valuable insights into material dynamics and properties.

VI. FUTURE WORKS

Future works can delve into the testing of diatomic lattice, extending the implementation to estimate bandgaps, speed of sound, etc. Additionally, expanding to higher dimensions and considering interactions beyond nearest

neighbors are avenues for further exploration.

VII. ACKNOWLEDGEMENTS

I sincerely thank Dr. Subhasis Basak for his invaluable guidance and expertise in guiding me through the details of numerical methods and computational techniques throughout this project. I also express my heartfelt appreciation to Dr. Joydeep Bhattacharya for his guidance, innovative ideas, and continuous encouragement, which shaped the direction and scope of this project.

[1] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston, New York, 1976) Chap. 22, pp. 430–431.
[2] H. J. Pain, *The Physics of Vibrations and Waves*, sixth ed. (Wiley, 2005) Chap. 4, pp. 90–95.
[3] J. D. Louck, Exact normal modes of oscillation of a linear chain of identical particles, Am. J. Phys. **30**, 585 (1962).
[4] D. K. Chaturvedi and J. S. Baijal, Normal modes of oscillation for a finite one-dimensional diatomic lattice, Am. J. Phys. **42**, 482 (1974).