Study of Lattice Vibrations:
Perturbations and Vibrational Modes
P452 Project Presentation

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22 April, 2024

Outline

1. Introduction
2. Theory
3. Implementation
4. Experiments and Observation
5. Results and Conclusion

Motivation

- Lattice vibrations - mechanical, thermal, and electrical properties of materials.[1]
- Can have/relax different levels of assumptions.
  - Uniformity of Lattice
  - Lattice defects
  - mass perturbations etc.
- **Goal**: A flexible solution that can explore the vibrational modes in this system.

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Lattice Vibrations

- characterized by Harmonic motions [5].
- described by wavelength λ, frequency ω, Amplitude A and Direction of travel (characterized by k).
- For formalizing the vibrational modes, we assume the following[4, 5]:
  - nearest neighbor interaction
    atom n interacts with $n-1$ and $n+1$ atoms.
  - The atoms are connected by springs of spring constant C
  - forces of equal strength between them - same spring constant C
  - Uniform lattice sapcing - equal inter-atomic space a

Monoatomic Lattice

A system in which all atoms have equal mass m (Figure 1).

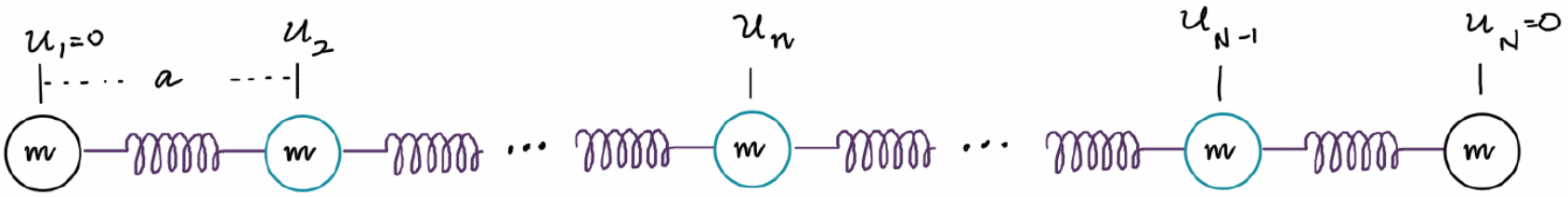

Figure: Monoatomic Lattice

u_n - distance of the n^{th} atom from equilibrium position.
Forces action on n^{th} atom is:

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

Monoatomic Lattice

The EoM is:

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

Solution form:

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

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

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

Dispersion law:

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

Monoatomic Lattice

General solution for a fixed boundary condition and N vibrating atom:

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

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 eigenvalues of this matrix, we get:

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

Vibrational modes (example)

An example of 5 Vibrating atoms with fixed boundary conditions[3].

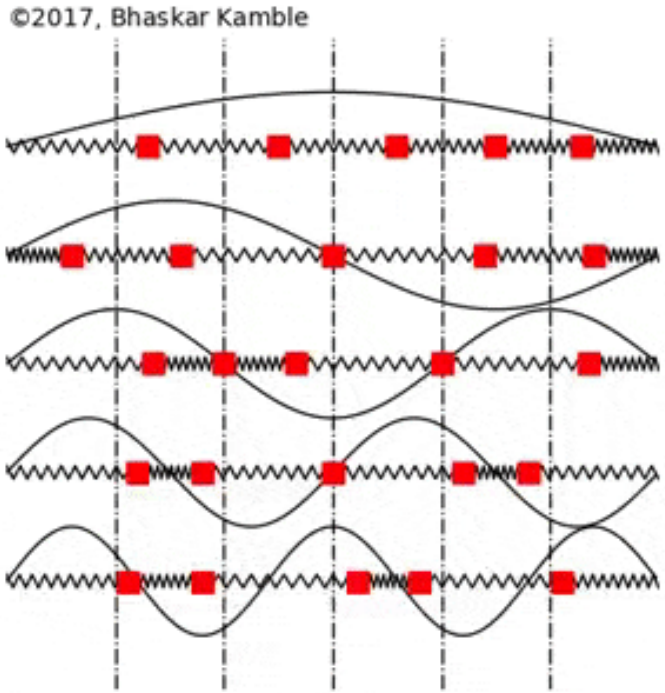

Figure: Vibrational modes

Diatomic lattice

lattice or crystal structure with two distinct types of atoms (masses m and M) periodically arranged. (Figure 3).

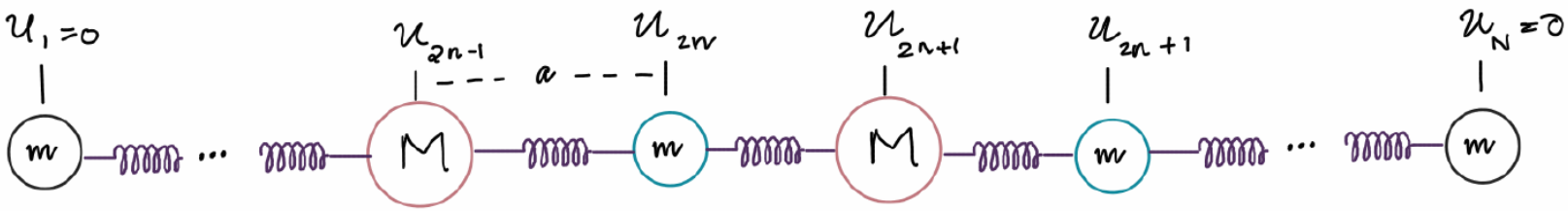

Figure: Diatomic Lattice

EoM becomes[5, 2]:

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

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

RK4 (Runge-Kutta 4^{th} order)

Solves ODEs of the form: (notations in context)

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

Given a time step h and $u_n(t^i)$:

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

Coupled RK4

Why?

- The LHS of EoM in eq (2) is a second order derivative.
- The RHS of EoM is dependent on more than one positions. (u_n interacts with u_{n+1} and u_{n-1}.

The equation of motion (2) becomes:

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

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

$$\overline{k_{u1}} = hf_1(t^i, \overline{u(t^i)}, \overline{v(t^i)})$$
$$\overline{k_{v1}} = hf_2(t^i, \overline{u(t^i)}, \overline{v(t^i)})$$

Coupled RK4

$$
\begin{aligned}
\overline{k_{u2}} &= h f_1\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \overline{k_{u1}}/2, \overline{v(t^i)} + \overline{k_{v1}}/2\right) \\
\overline{k_{v2}} &= h f_2\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \overline{k_{u1}}/2, \overline{v(t^i)} + \overline{k_{v1}}/2\right) \\
\overline{k_{u3}} &= h f_1\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \overline{k_{u2}}/2, \overline{v(t^i)} + \overline{k_{v2}}/2\right) \\
\overline{k_{v3}} &= h f_2\left(t^i + \frac{h}{2}, \overline{u(t^i)} + \overline{k_{u2}}/2, \overline{v(t^i)} + \overline{k_{v2}}/2\right) \\
\overline{k_{u4}} &= h f_1(t^i + h, \overline{u(t^i)} + \overline{k_{u2}}, \overline{v(t^i)} + \overline{k_{v3}}) \\
\overline{k_{v4}} &= h f_2(t^i + h, \overline{u(t^i)} + \overline{k_{u2}}, \overline{v(t^i)} + \overline{k_{v3}}) \\
u_{t^i+h} &= \overline{u(t^i)} + \frac{1}{6}(\overline{k_{u1}} + 2\overline{k_{u2}} + 2\overline{k_{u3}} + \overline{k_{u4}}) \\
v_{t^i+h} &= \overline{v(t^i)} + \frac{1}{6}(\overline{k_{v1}} + 2\overline{k_{v2}} + 2\overline{k_{v3}} + \overline{k_{v4}})
\end{aligned}
\tag{15}
$$

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Implementation

- Programming Language: PYTHON
- data structures: NUMPY arrays
- plots and animation: MATPLOTLIB
- Progress tracking: TQDM
- FFT analysis: SCIPY

Feautures and implementations:

- RK4, coupled RK4 generalized to handle any dimensions.
- Selective data saving for longer simulations like that of dispersion relation.
- Automated animations for N vibrating atoms
- Individual atom FFT analysis.

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Simulation Settings

- 11 atoms - ends fixed, 9 vibrating atoms
- parameters of the lattice, C, m, and $a = 1$ (simplicity)
- $k = \pi/a$ except for dispersion law.
- theoretical values are also calculated based on these parameters = consistency

All the results, as well as different experiment settings, are stored in the Github[1].

[1] https://github.com/AdhilshaA/CP_lattice_vibration_project/

Normal mode

Application of the Oscillation ansatz $Ae^{i(kna-\omega t)}$.

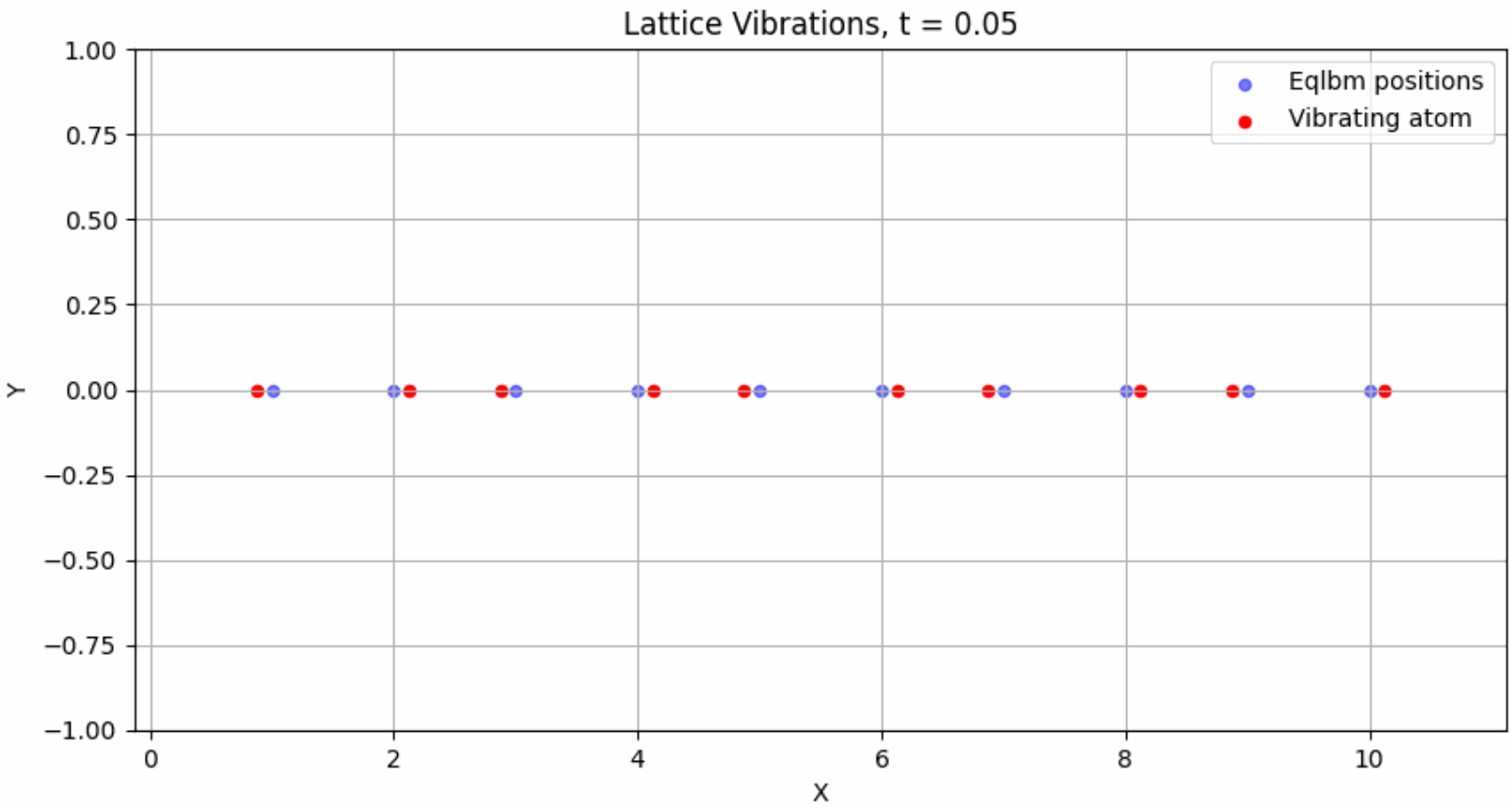

Figure: Normal mode vibrations (gif unavailable in pdf)

Normal mode

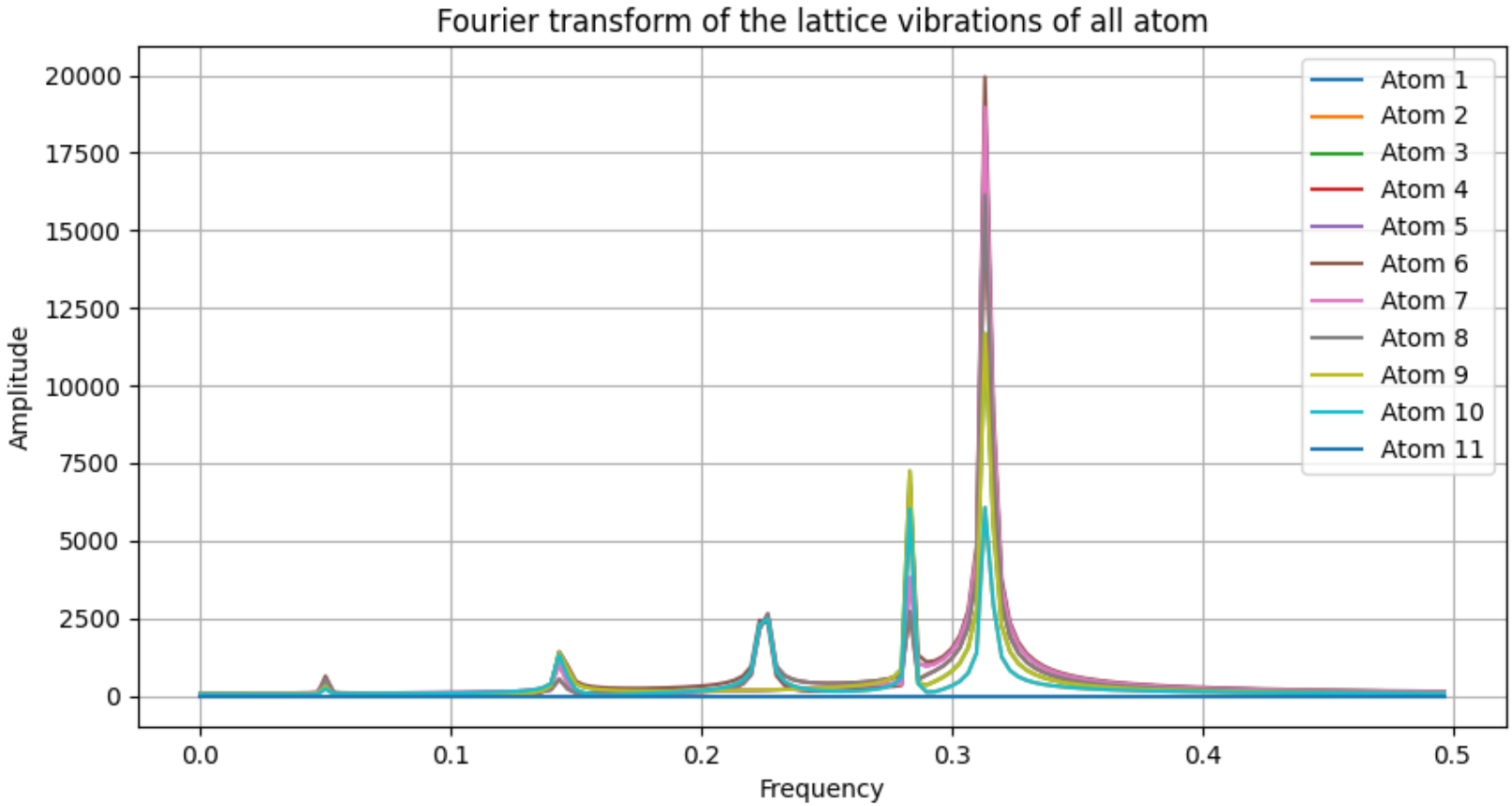

Figure: FFT obtained from simulating a normal mode

Normal mode

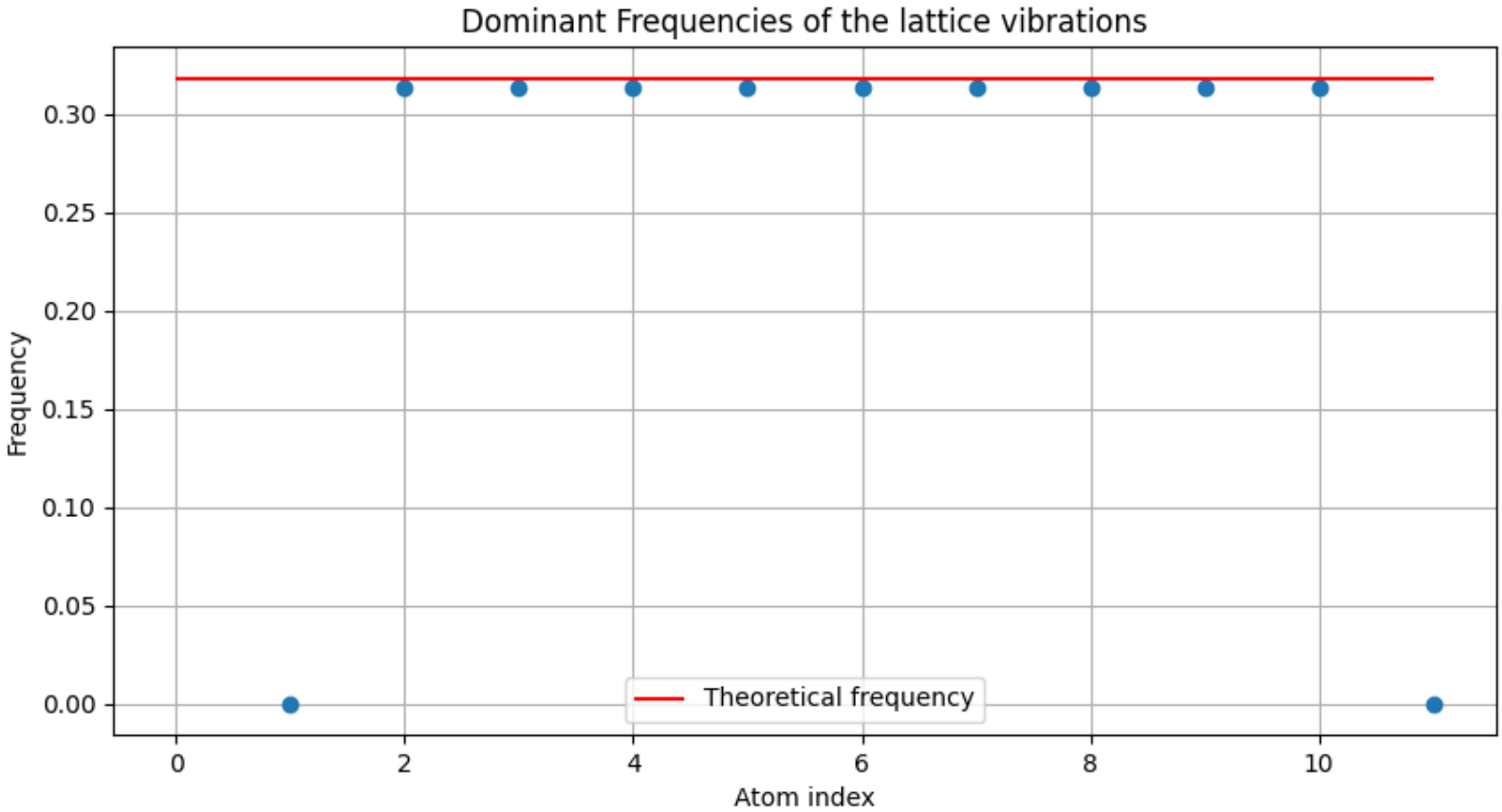

Figure: Frequency of each atom compared with theoretical

Symmetric perturbation

Only central atom is perturbed.

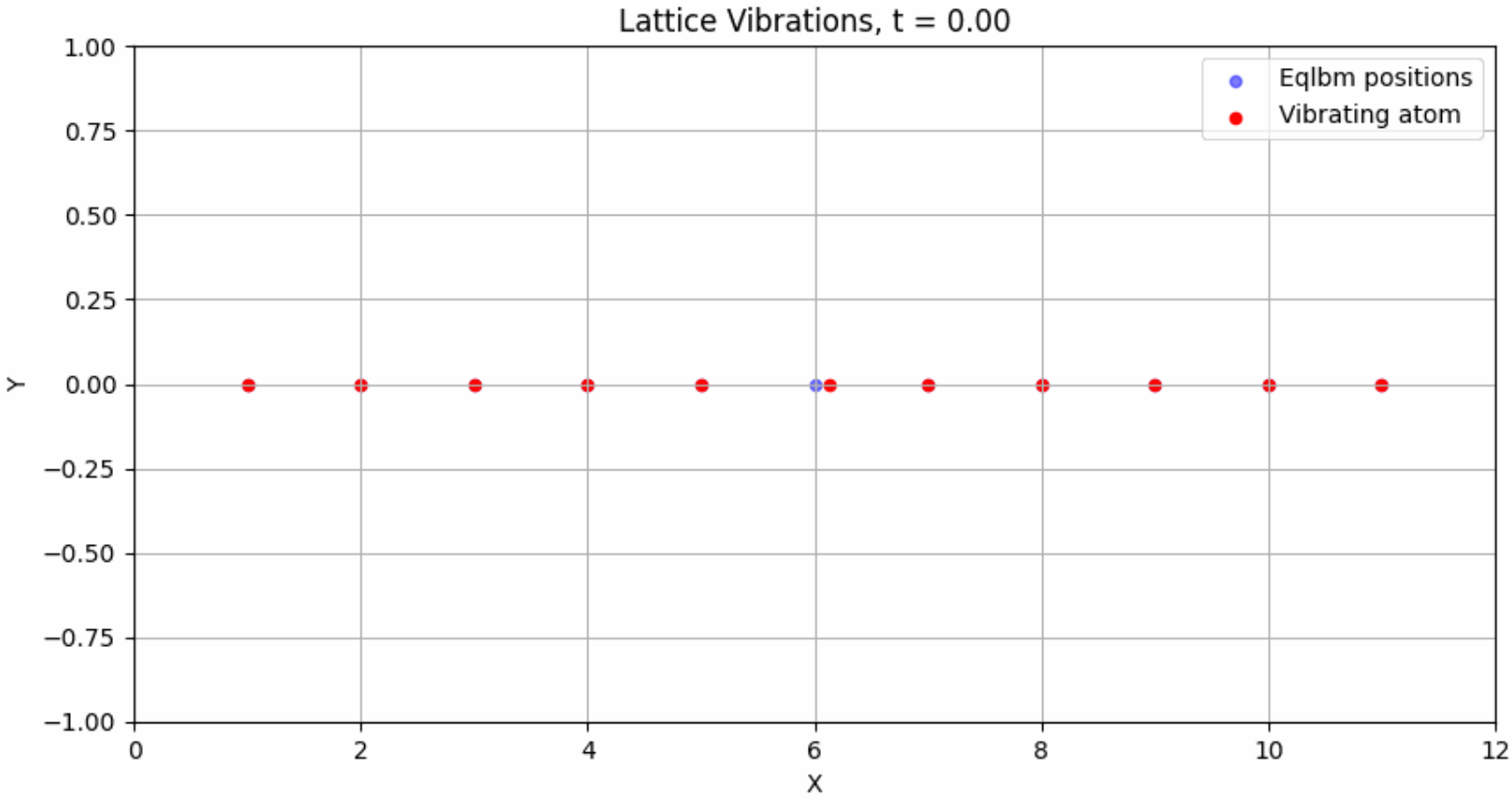

Figure: Symmetric perturbation animation (gif unavailable in pdf)

Symmetric perturbation

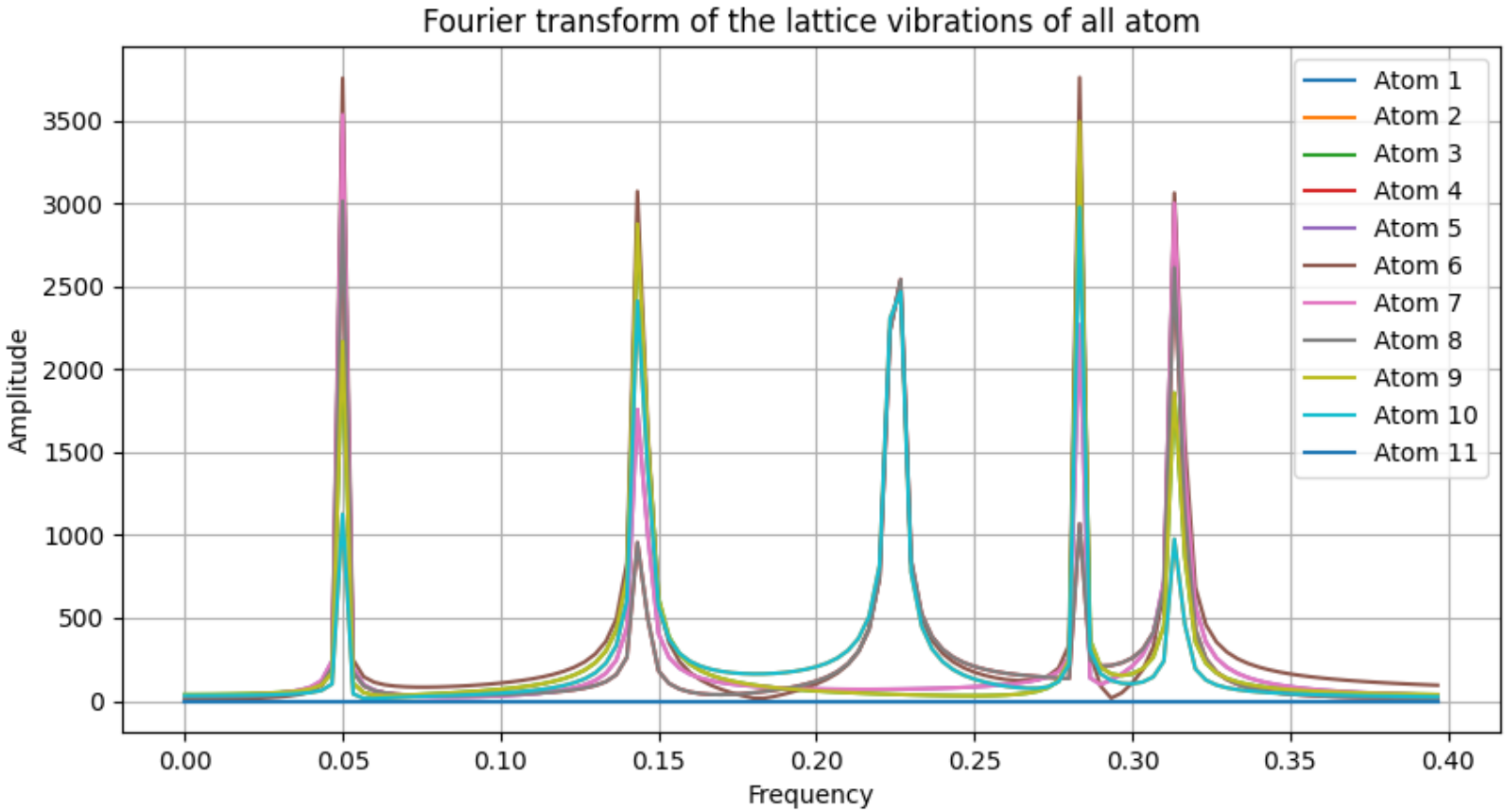

Figure: FFT obtained from simulating a symmetric perturbation

Symmetric perturbation

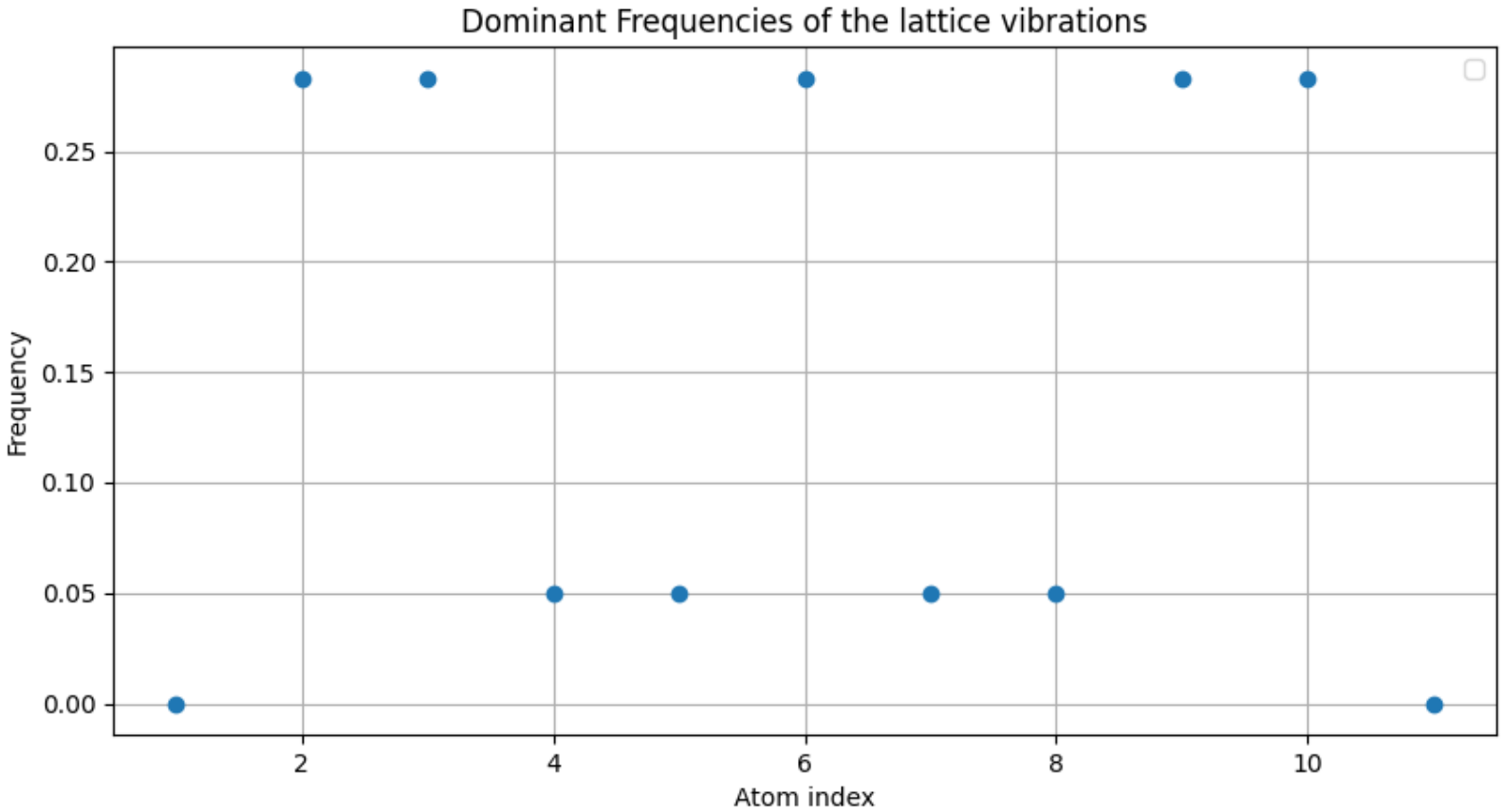

Figure: Frequency of each atom compared in symmetric perturbation

Random perturbation

Random perturbations with different seeds.

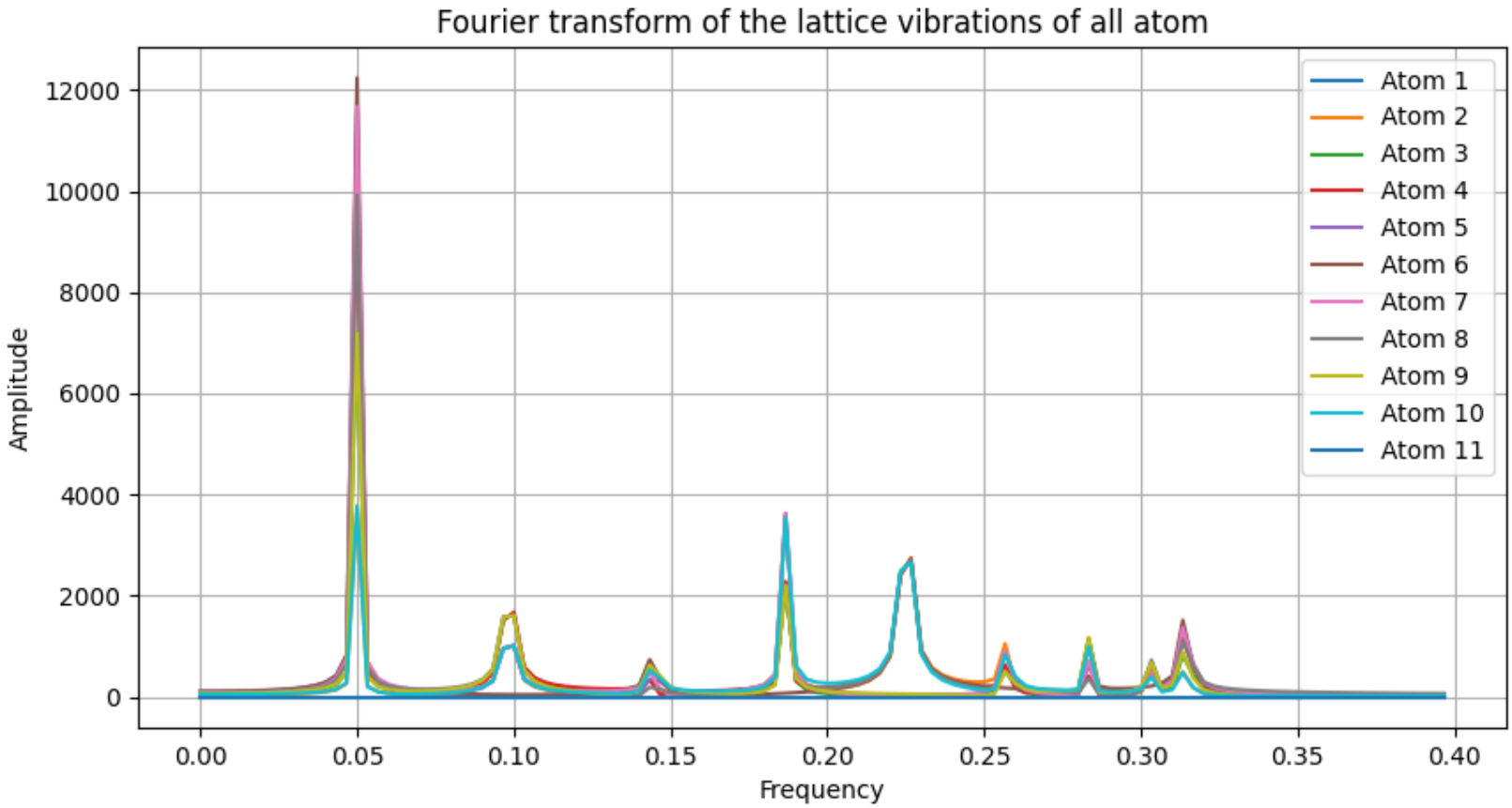

Figure: FFT obtained from simulating random perturbation - trial1

Random perturbation

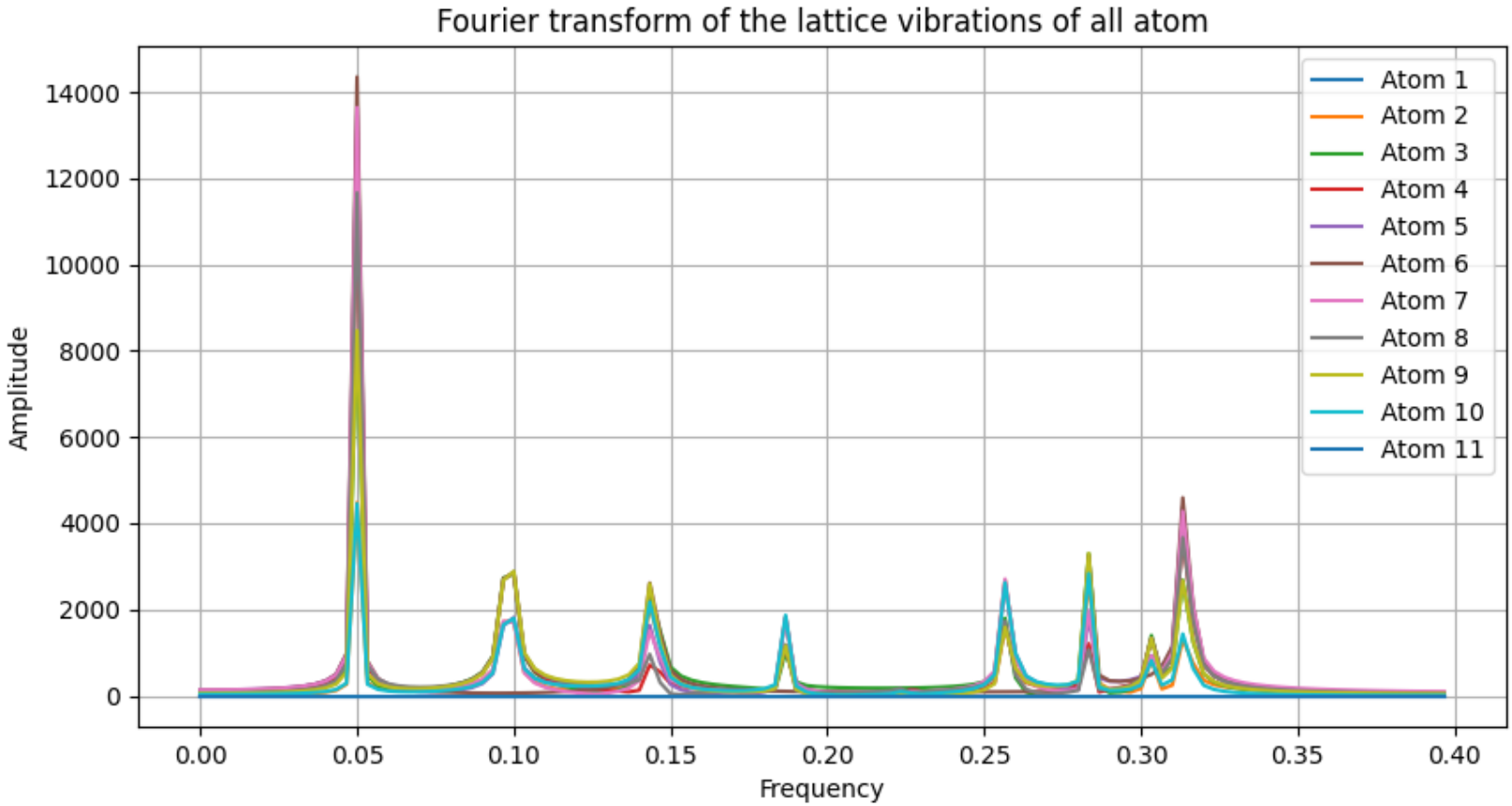

Figure: FFT obtained from simulating random perturbation - trial2

Random perturbation

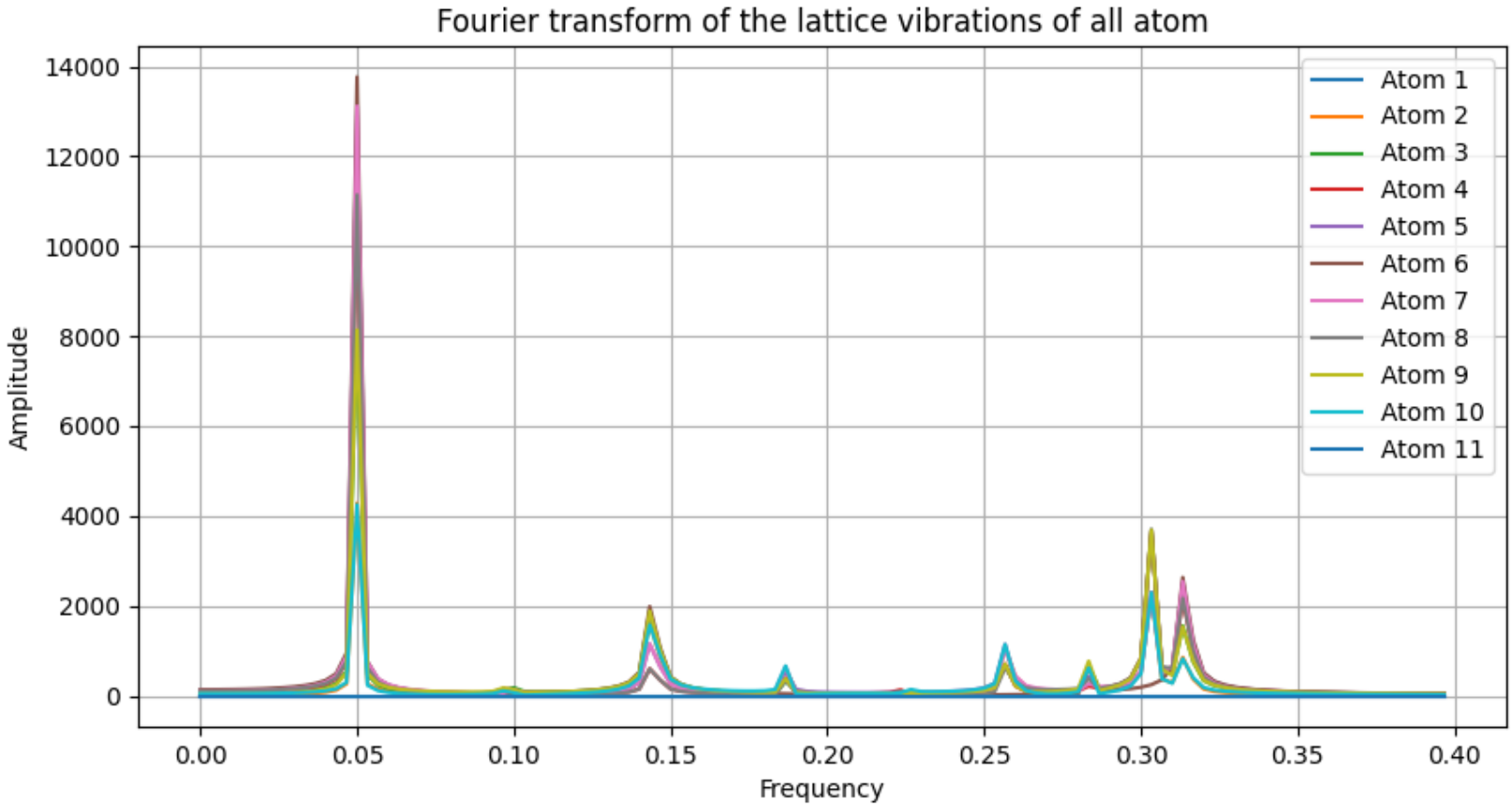

Figure: FFT obtained from simulating random perturbation - trial3

Random perturbation

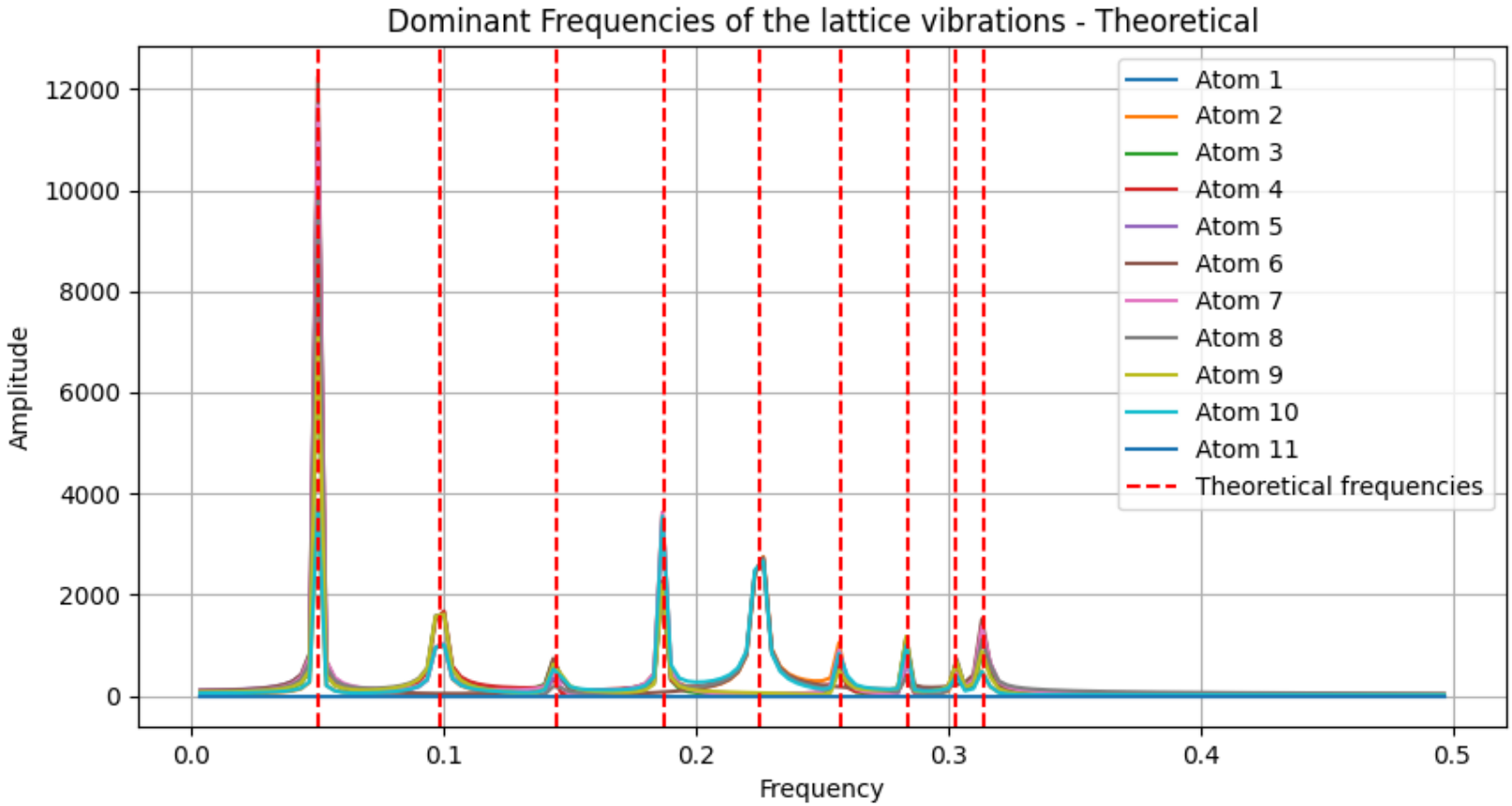

Figure: Vibrational modes compared with theoretical frequencies

Dispersion Law

Wave number k varied from 0 to $\frac{2\pi}{a}$.

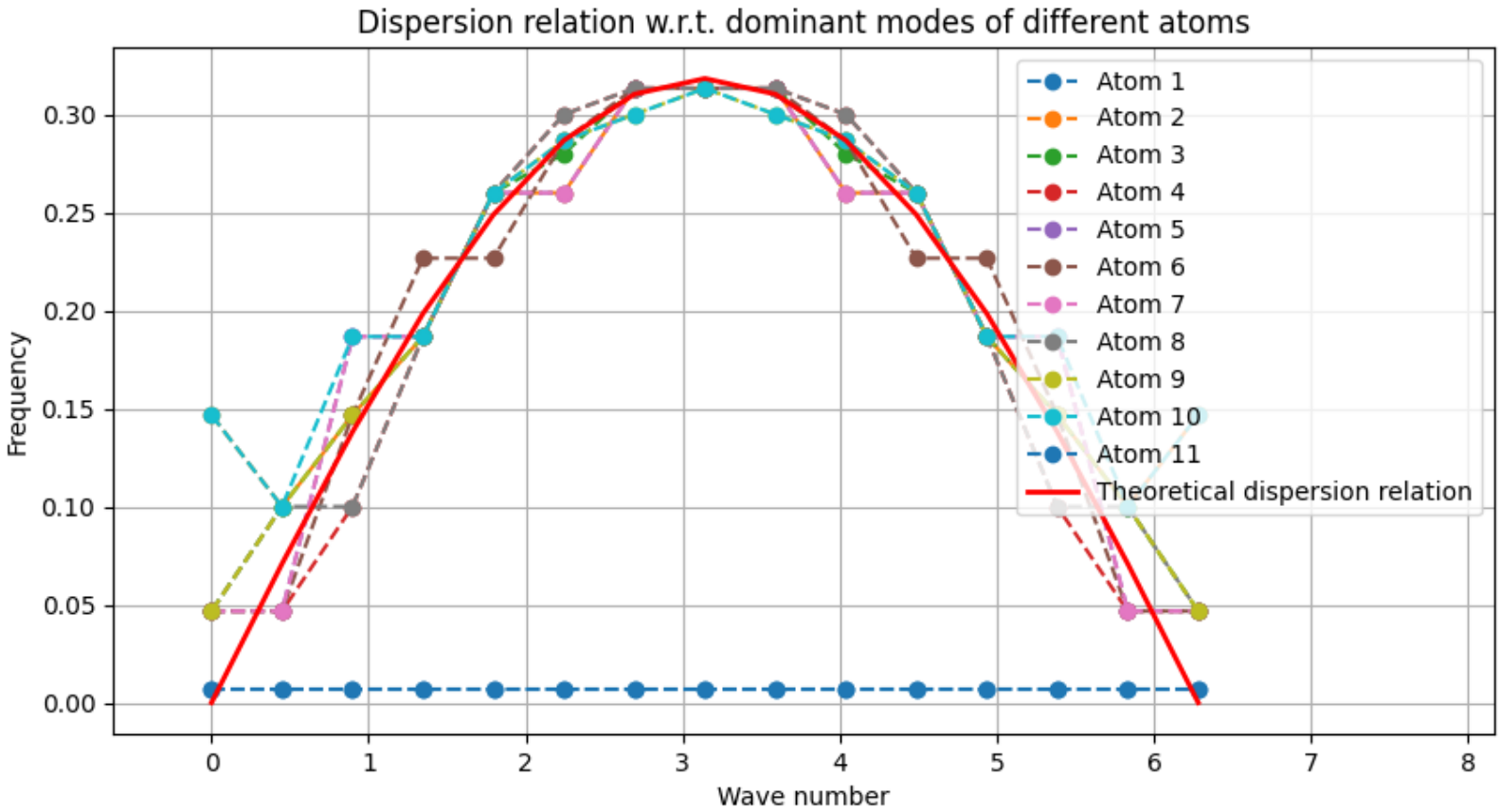

Figure: Dispersion law - 9 vibrating atoms

Dispersion Law

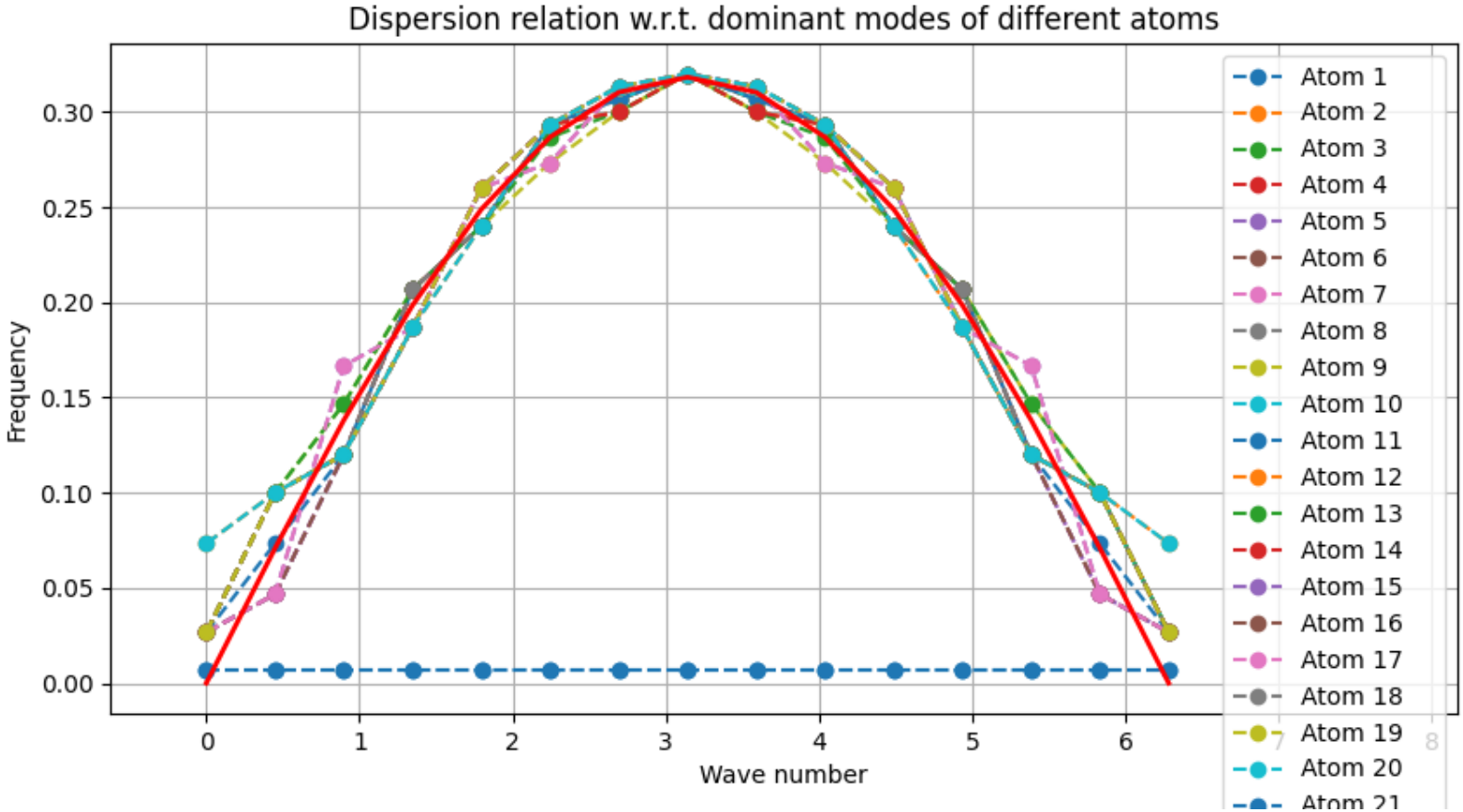

Figure: Dispersion law - 19 vibrating atoms

Impact of time

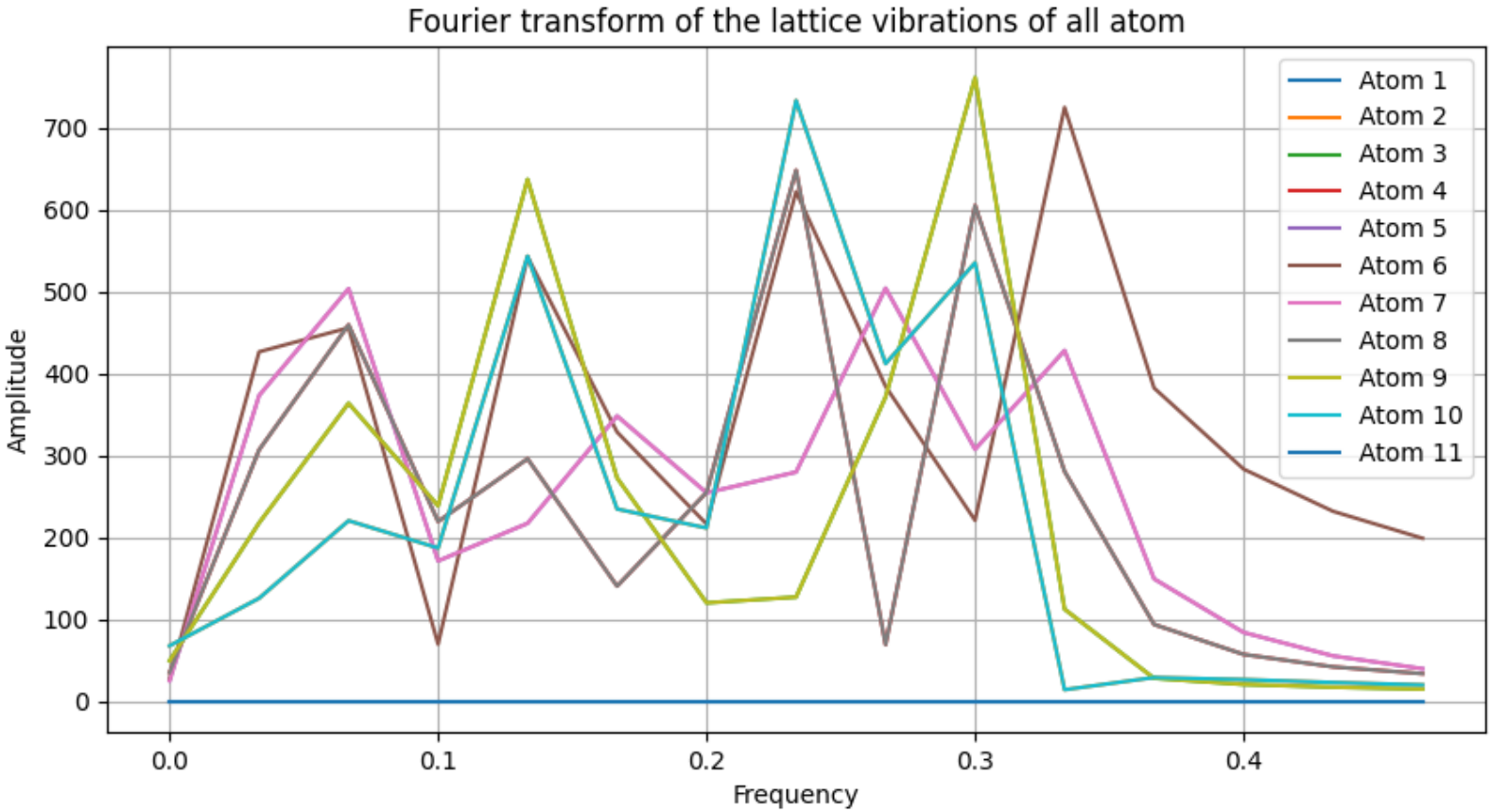

Figure: FFT analysis over shorter simulation

Impact of time

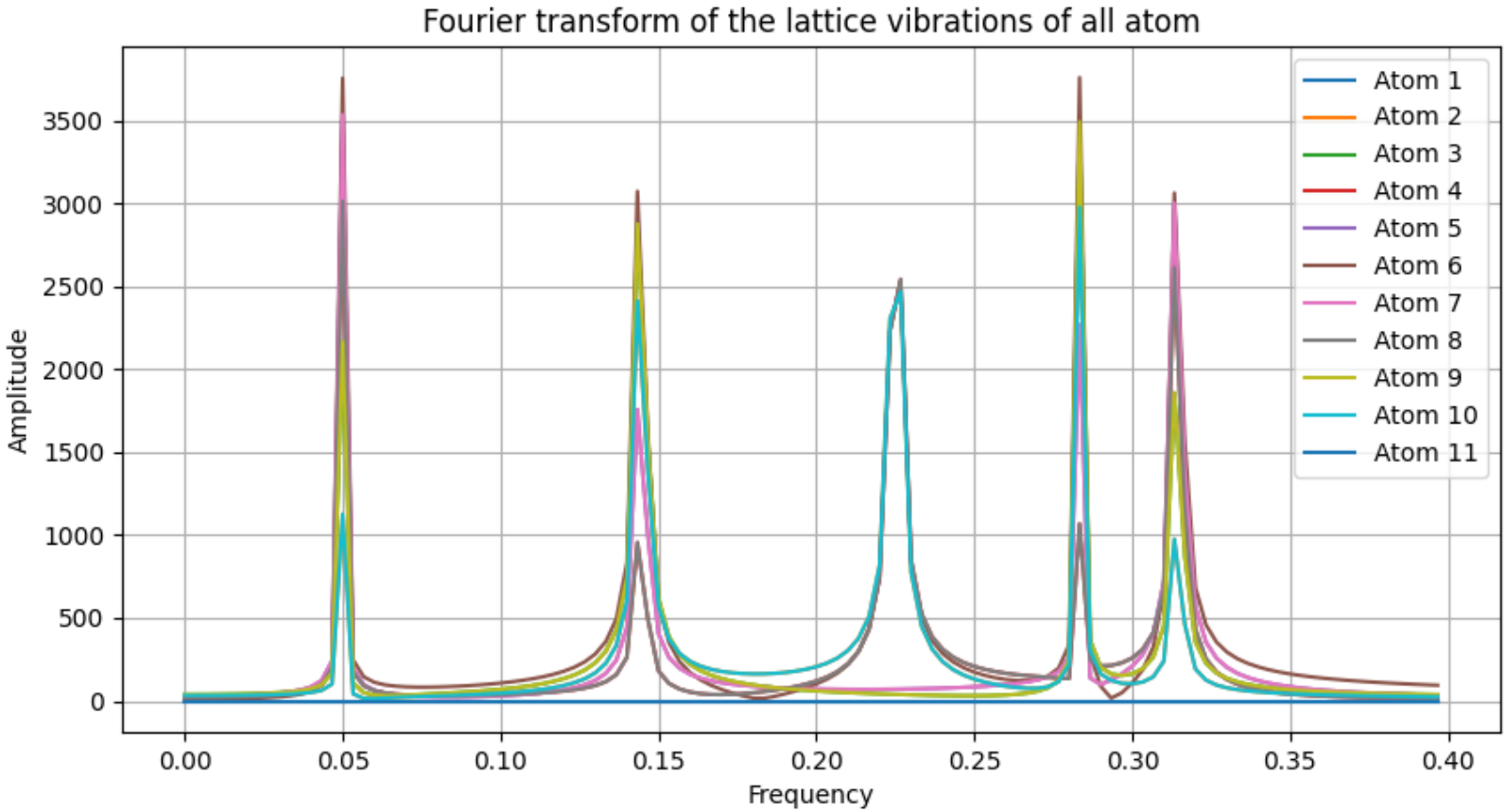

Figure: FFT analysis over longer simulation

Boundary conditions

Why it is essential for this implementation? Because this happens.

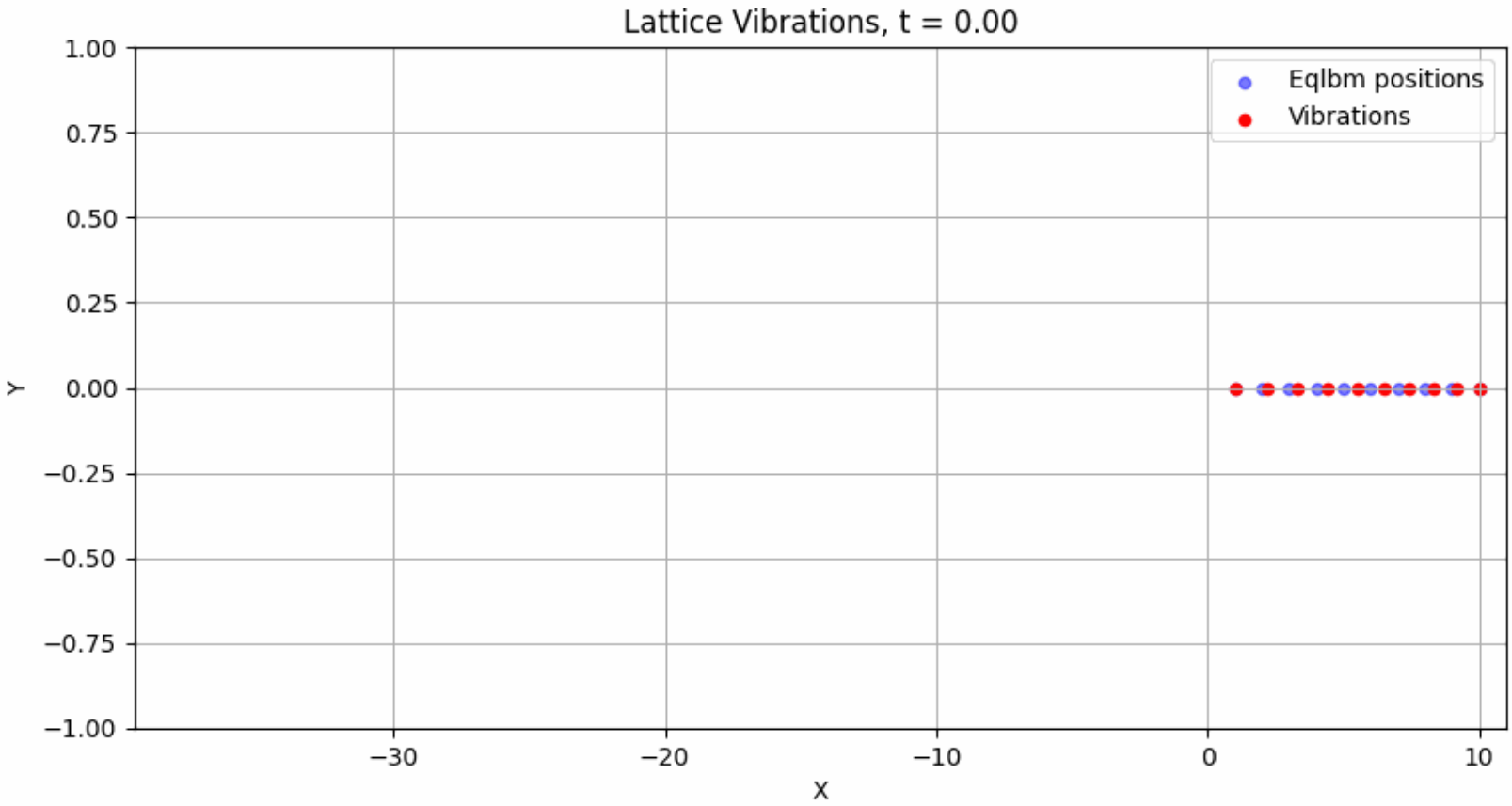

Figure: Failed Lattice vibration animation (gif not available in pdf)

Boundary conditions

In essence, the system adheres solely to the laws we establish (forces between them), beginning from the initial conditions. However, since the endpoints are unrestricted, the system has the potential to deviate significantly.

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Results and Conclusion

- Normal mode frequency very close the theoretical values.
- Symmetric perturbations yielded modes symmetrically distributed around the central atom.
- Random perturbations lead to the emergence of all possible vibrational modes.
- Dispersion law was observed through varying wavenumber.
- Observing the system for a longer period of time separates the modes.
- Model versatile to different perturbations as well as different size of systems.
- consistent results across all trials, proper visualization.

Possible Future Works

- testing of diatomic lattice
- Acoustic and Optical branches
- Estimate bandgaps, speed of sound, etc.
- Expanding Lattice to higher dimension
- Relaxation of Assumptions

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 Bhattacharjee for his guidance, innovative ideas, and continuous encouragement, which shaped the direction and scope of this project.

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