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

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Outline

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- **Goal**: A flexible solution that can explore the vibrational modes in this system.

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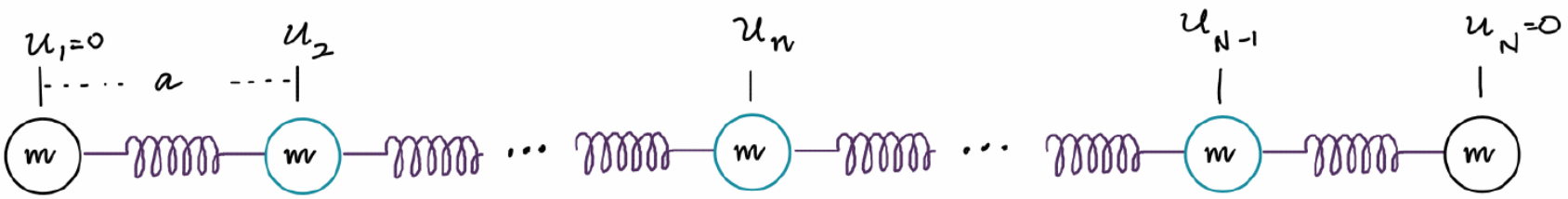

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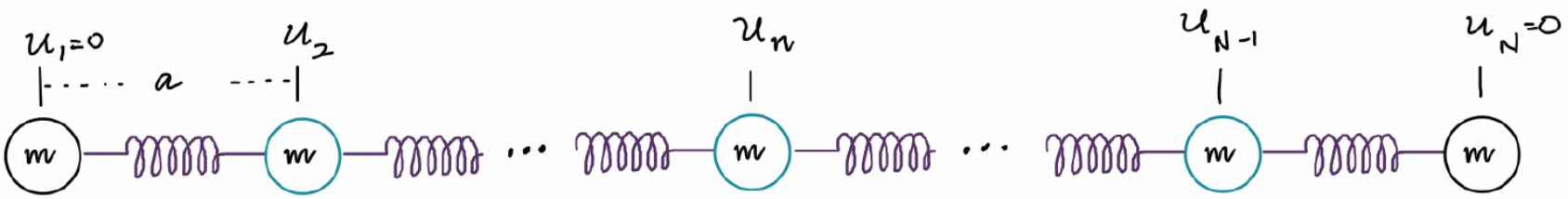

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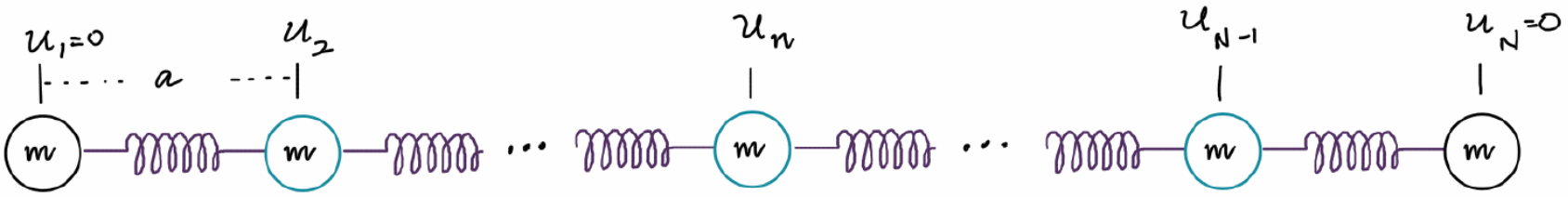

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Forces action on n^{th} atom is:

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

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

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Dispersion law:

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

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

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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].

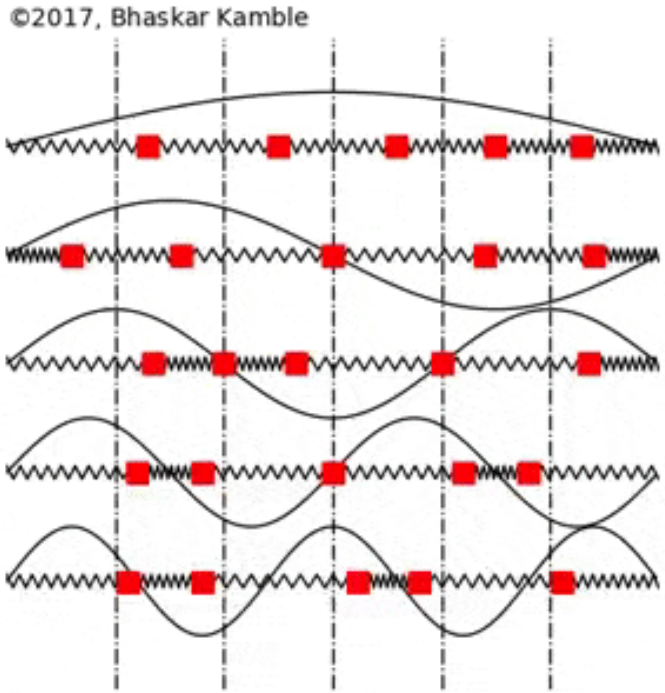

Figure: Vibrational modes

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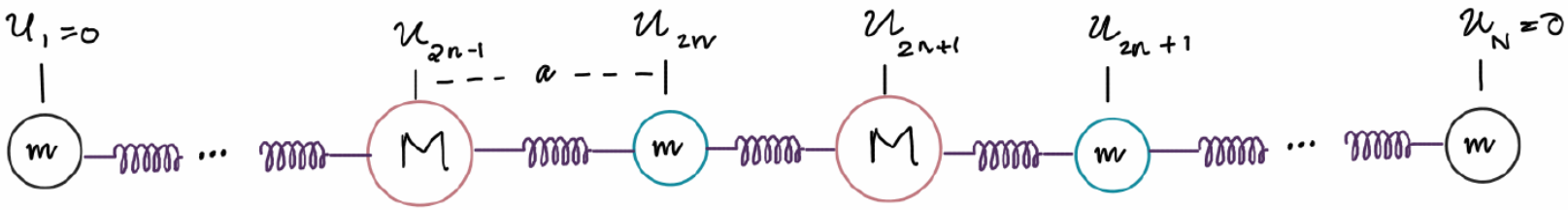

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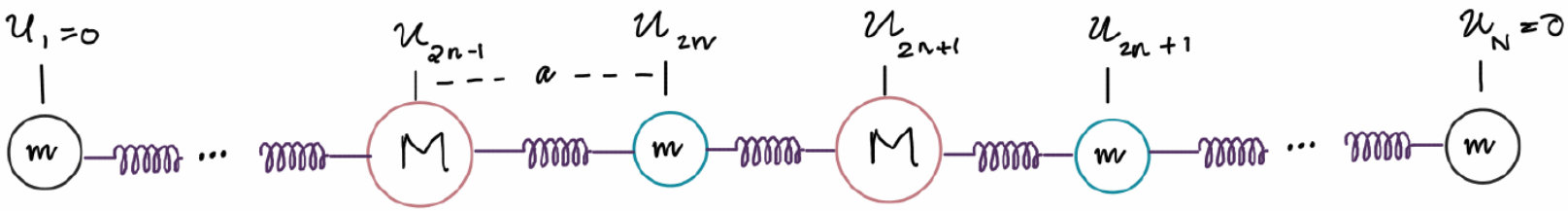

Figure: Diatomic Lattice

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)

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

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

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

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

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

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$$
\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) \\
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\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

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- 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/

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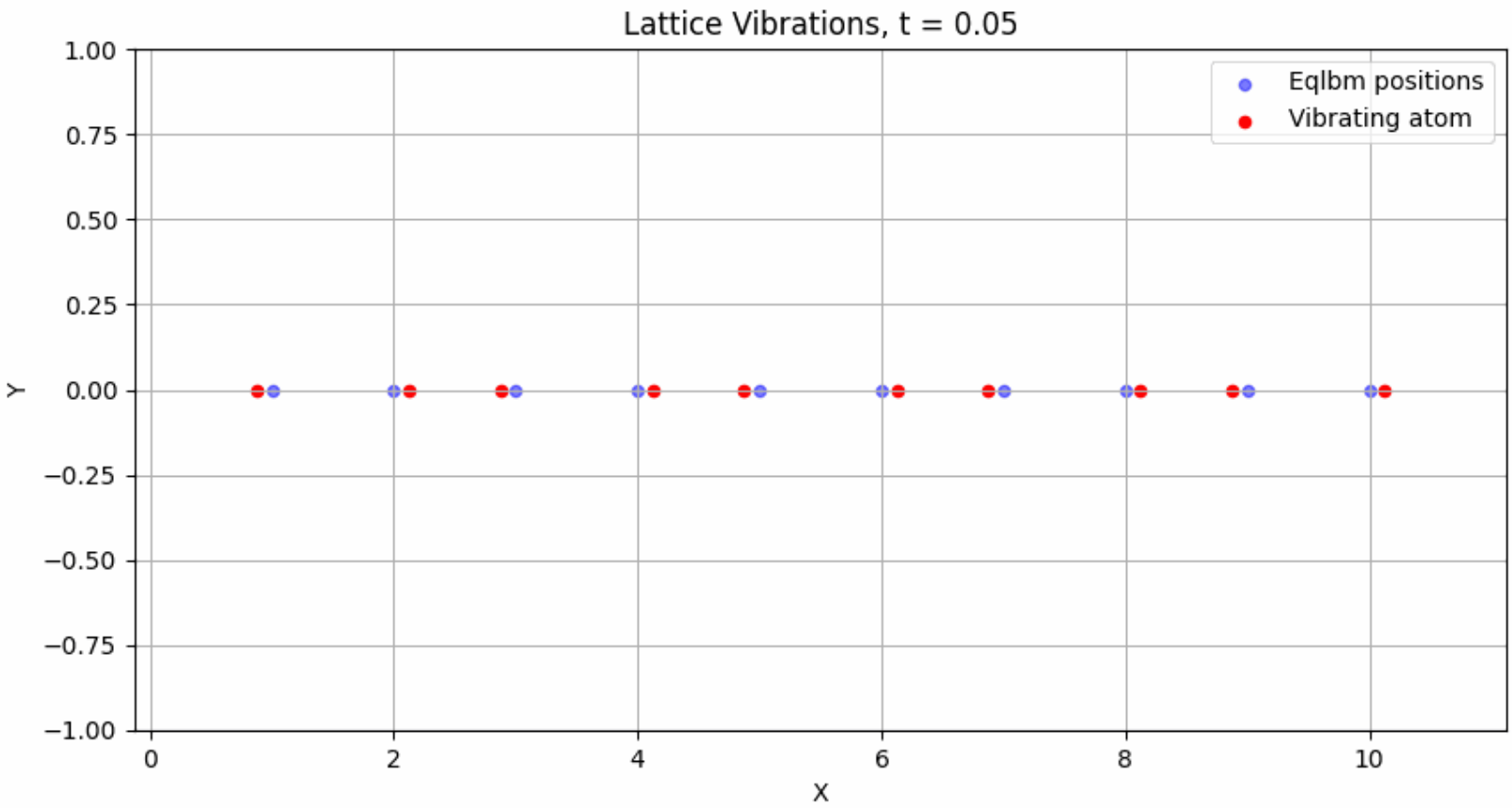

Figure: Normal mode vibrations (gif unavailable in pdf)

Normal mode

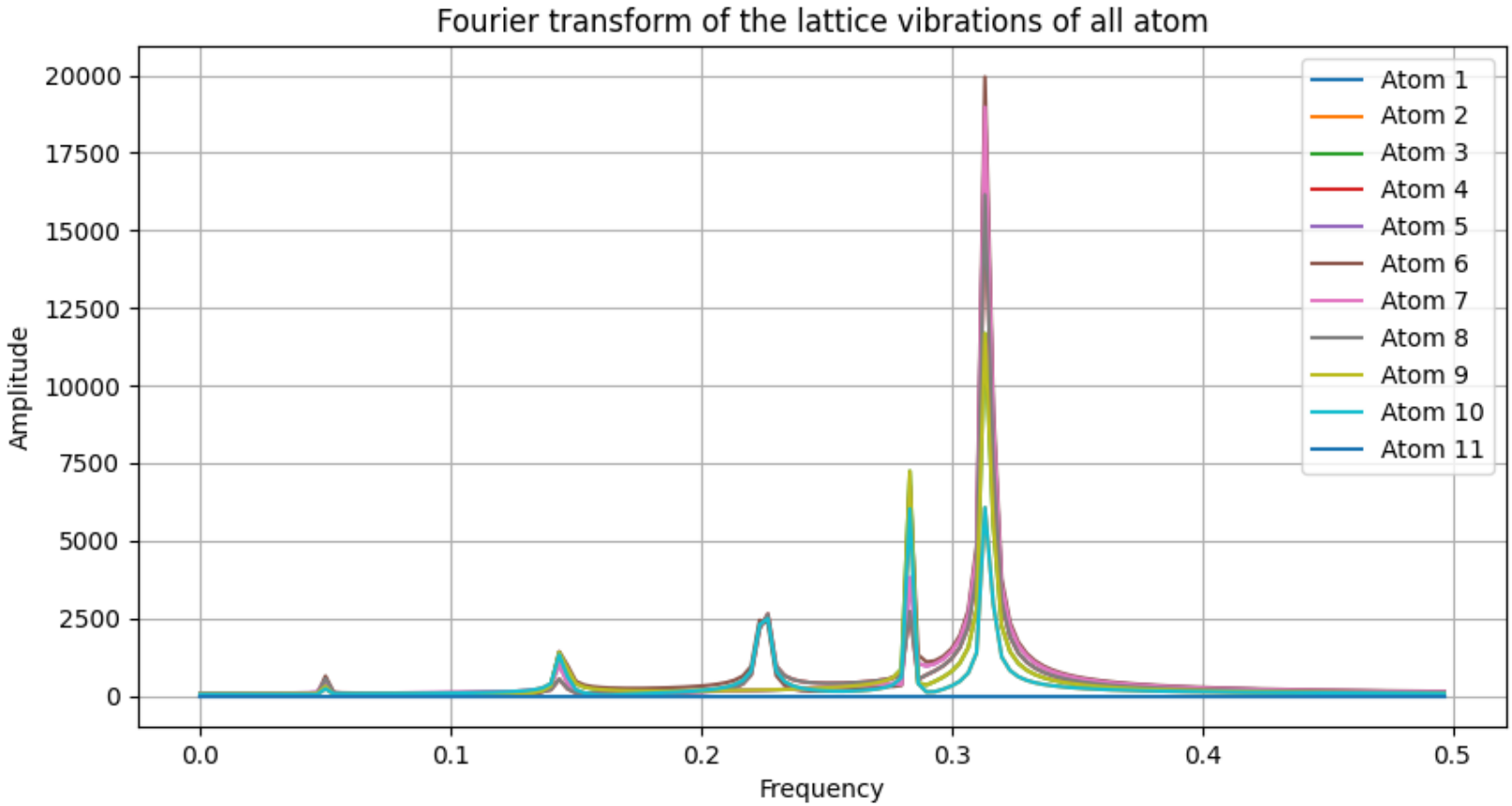

Figure: FFT obtained from simulating a normal mode

Normal mode

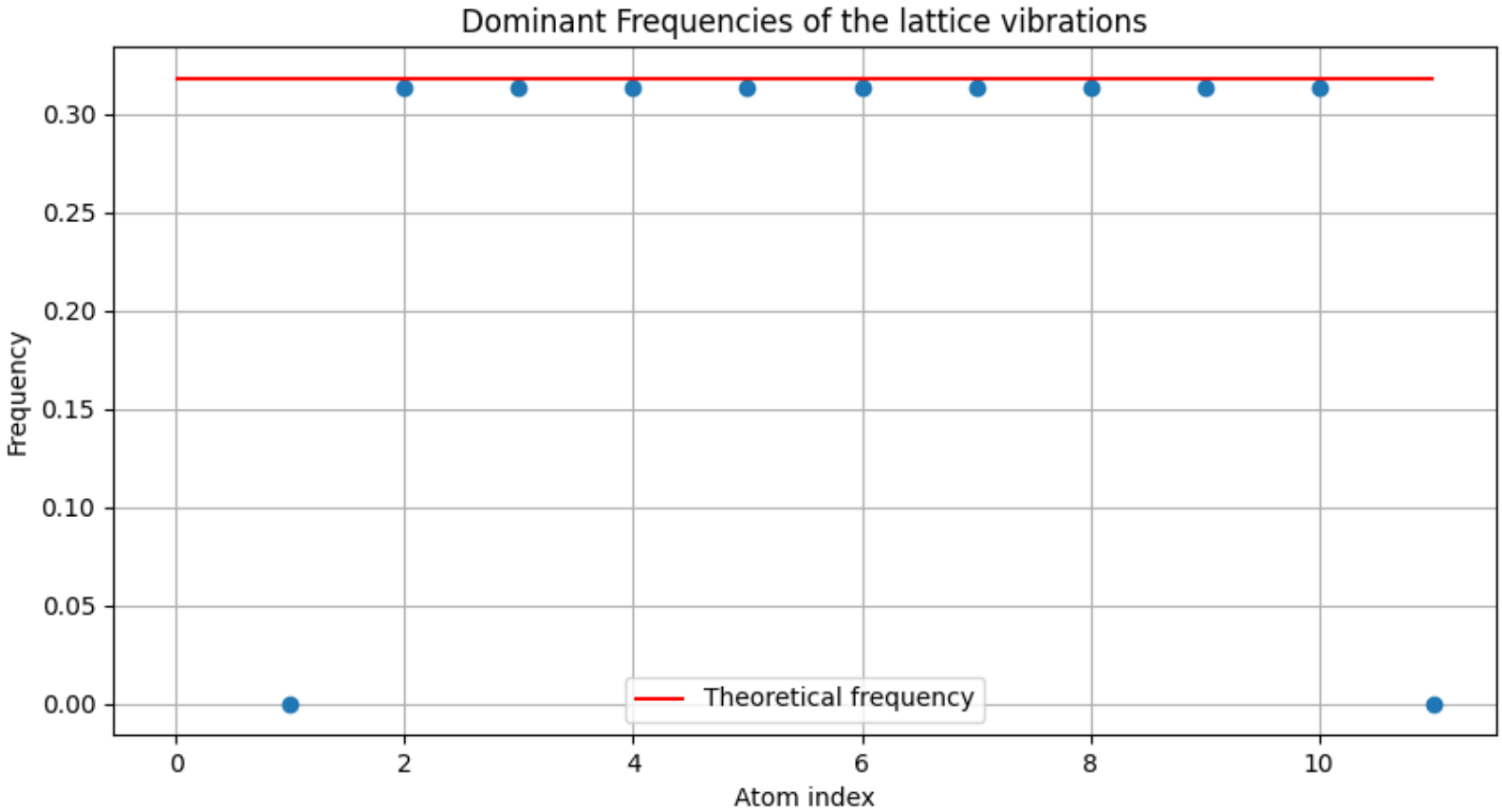

Figure: Frequency of each atom compared with theoretical

Symmetric perturbation

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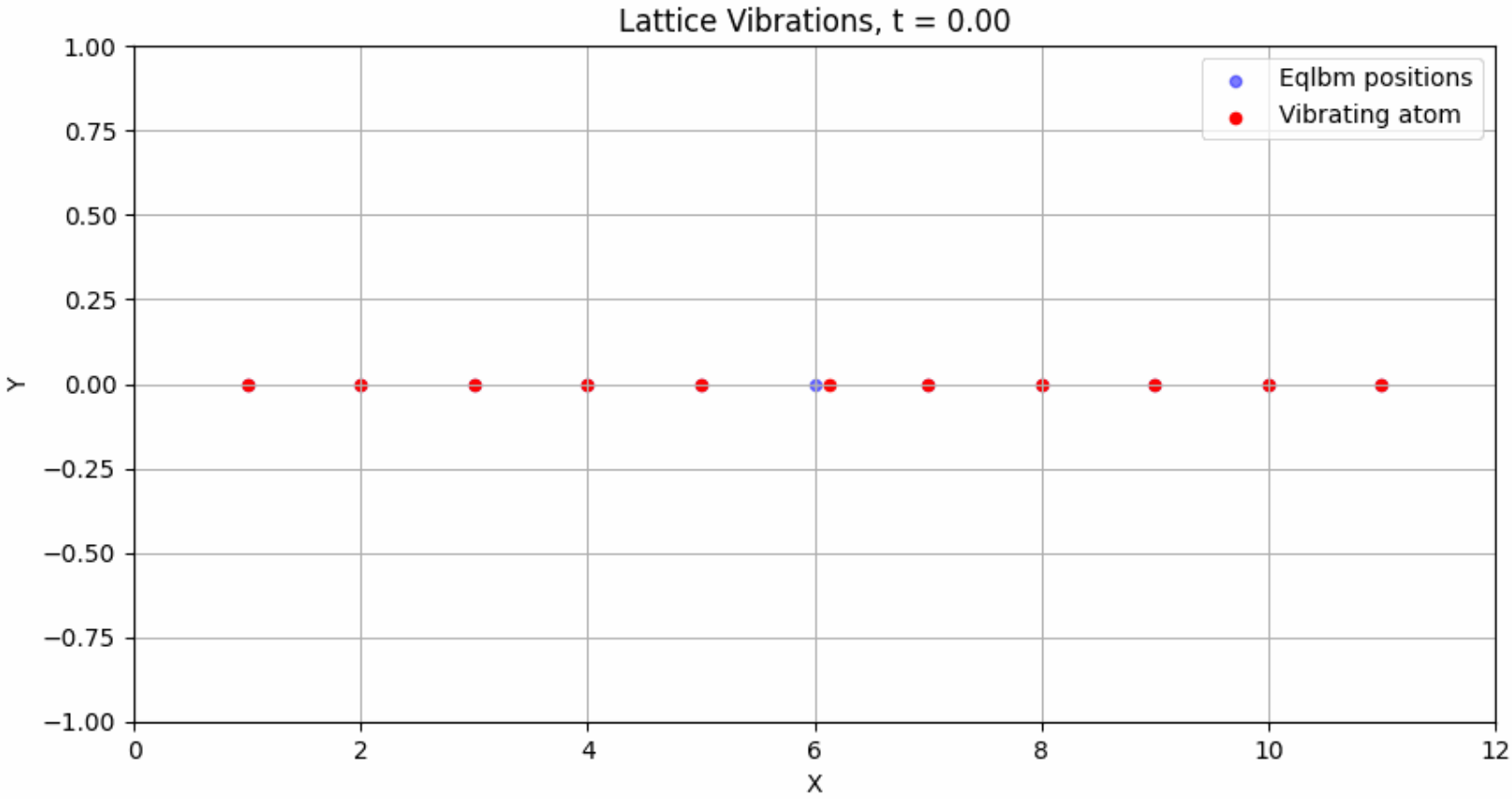

Figure: Symmetric perturbation animation (gif unavailable in pdf)

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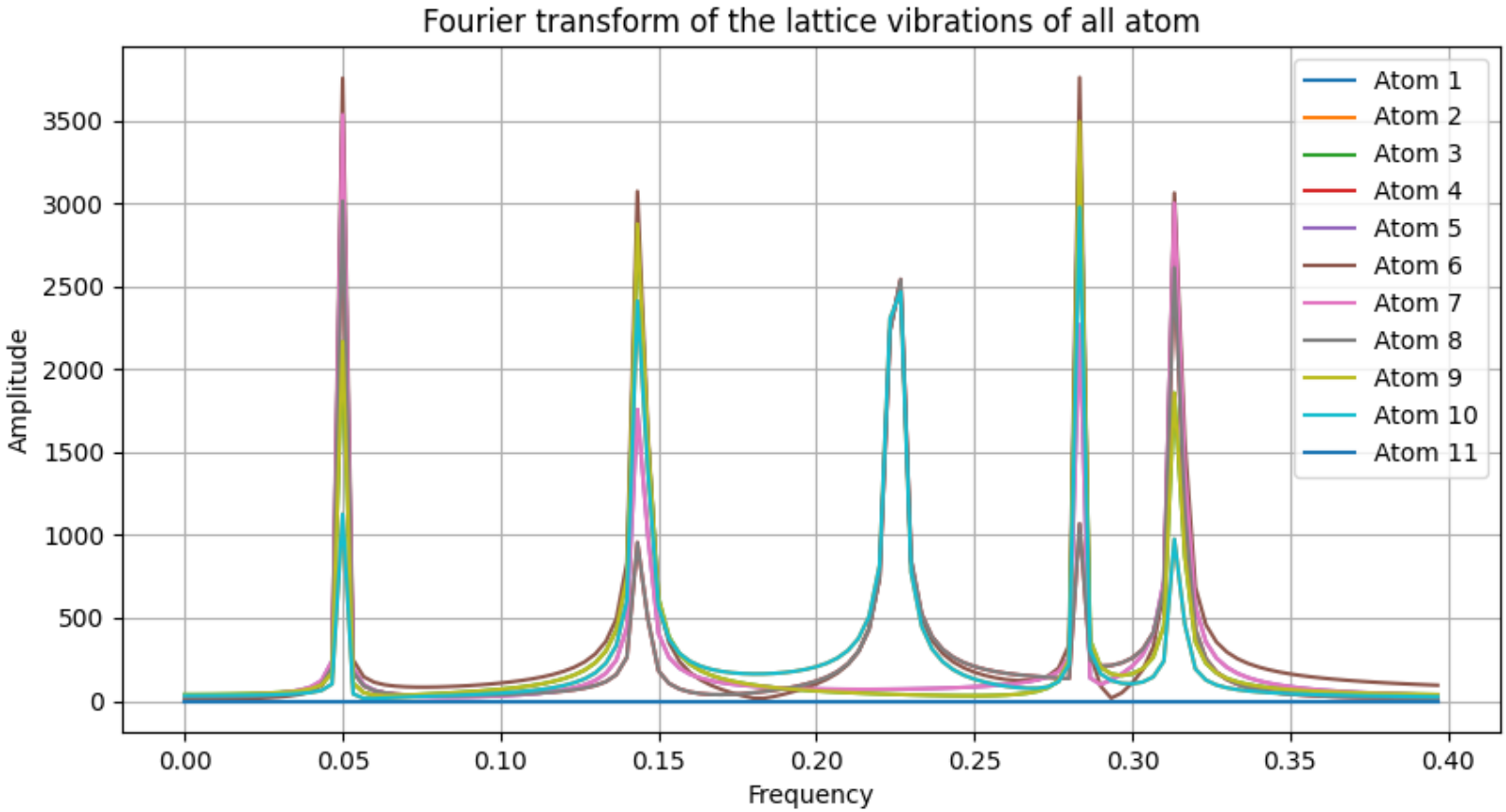

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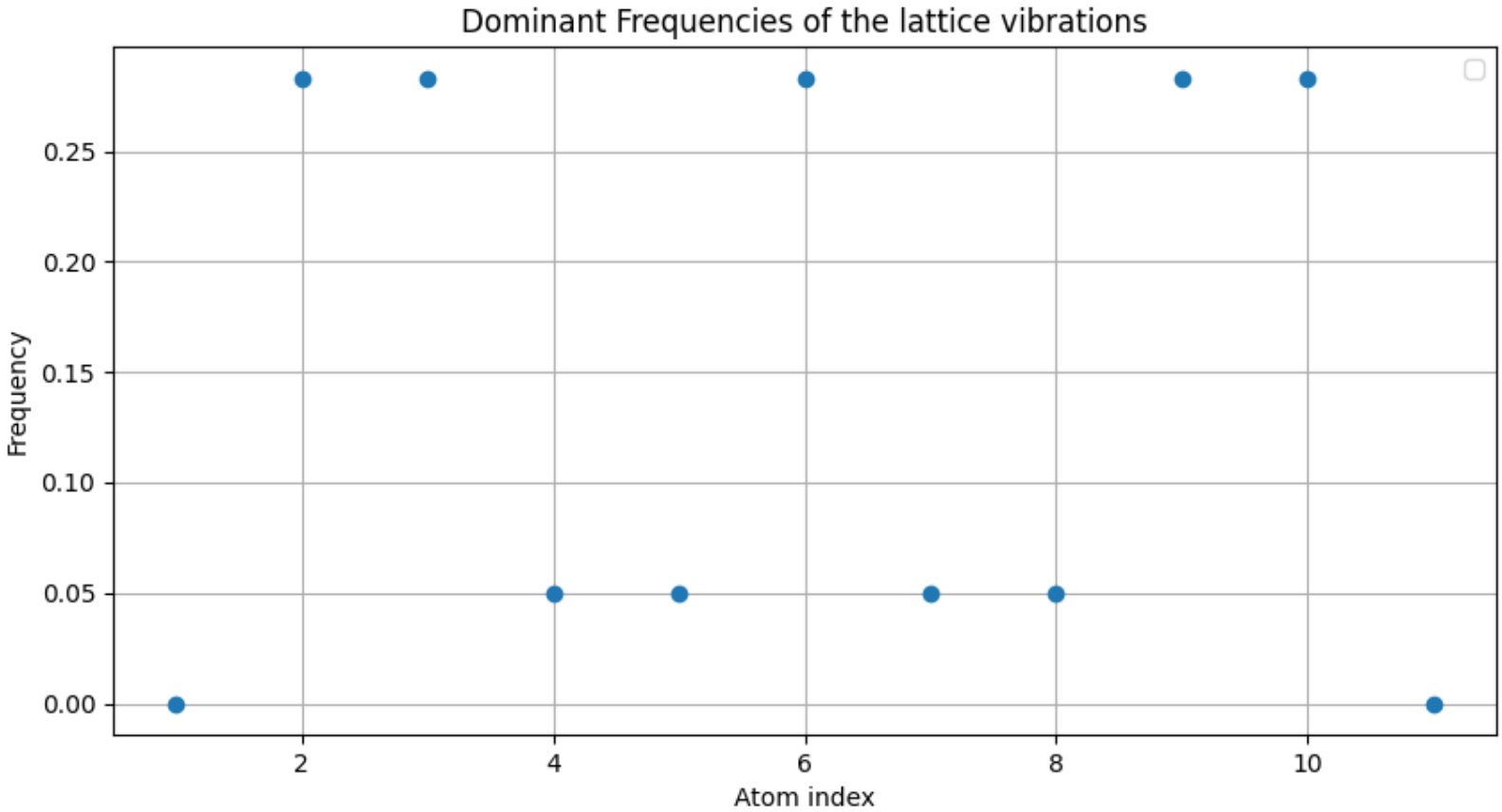

Figure: Frequency of each atom compared in symmetric perturbation

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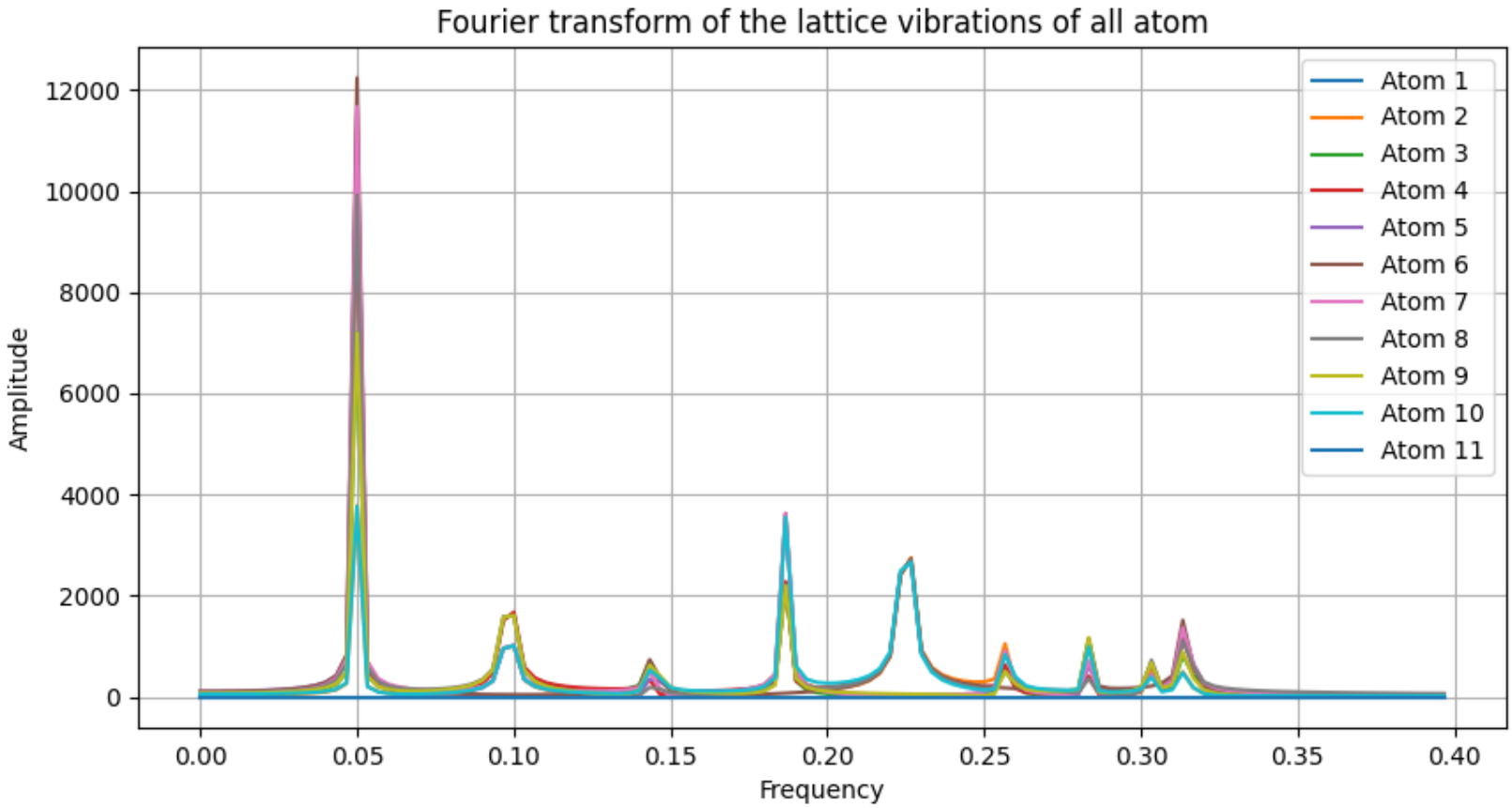

Figure: FFT obtained from simulating random perturbation - trial1

Random perturbation

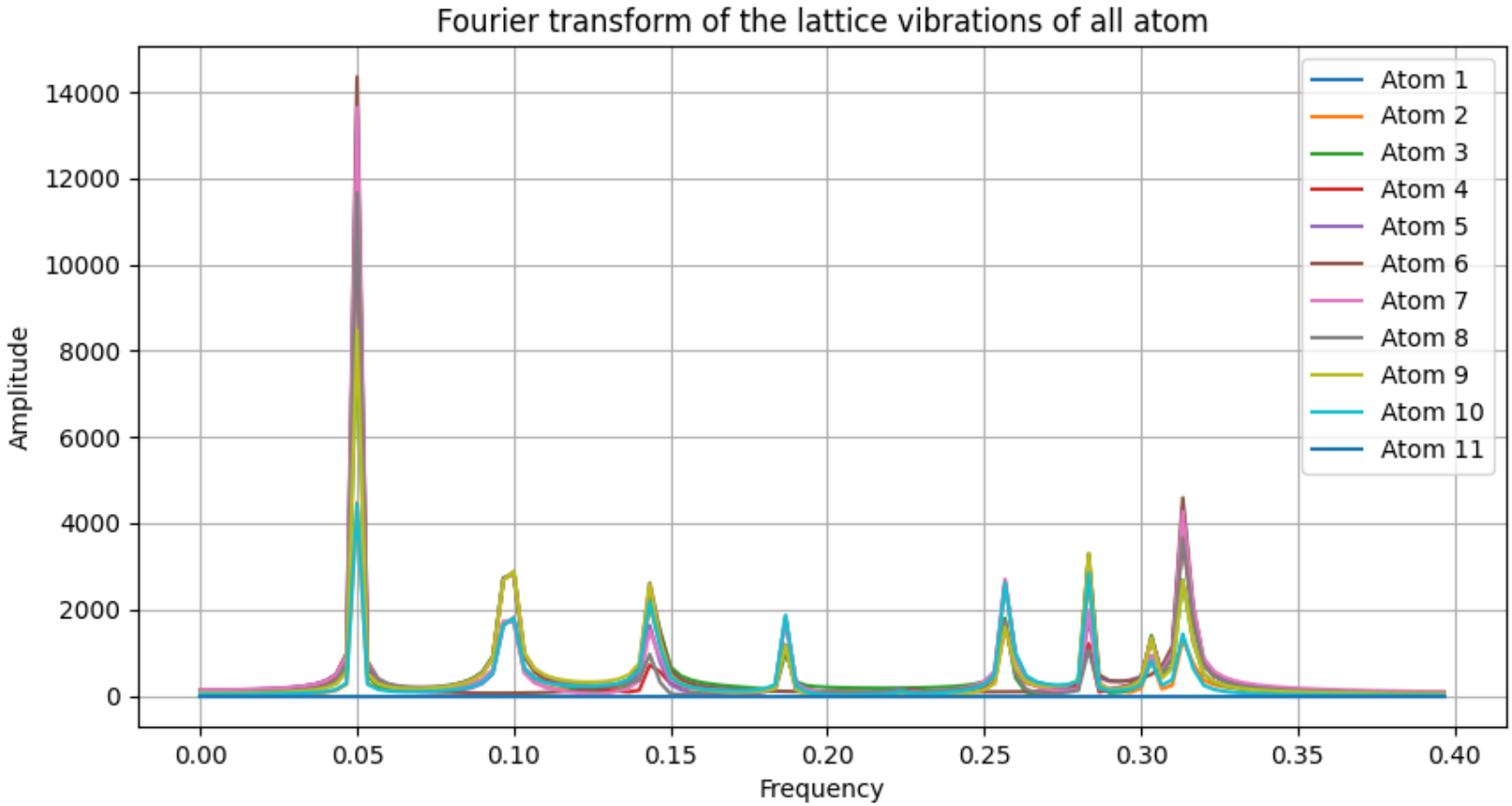

Figure: FFT obtained from simulating random perturbation - trial2

Random perturbation

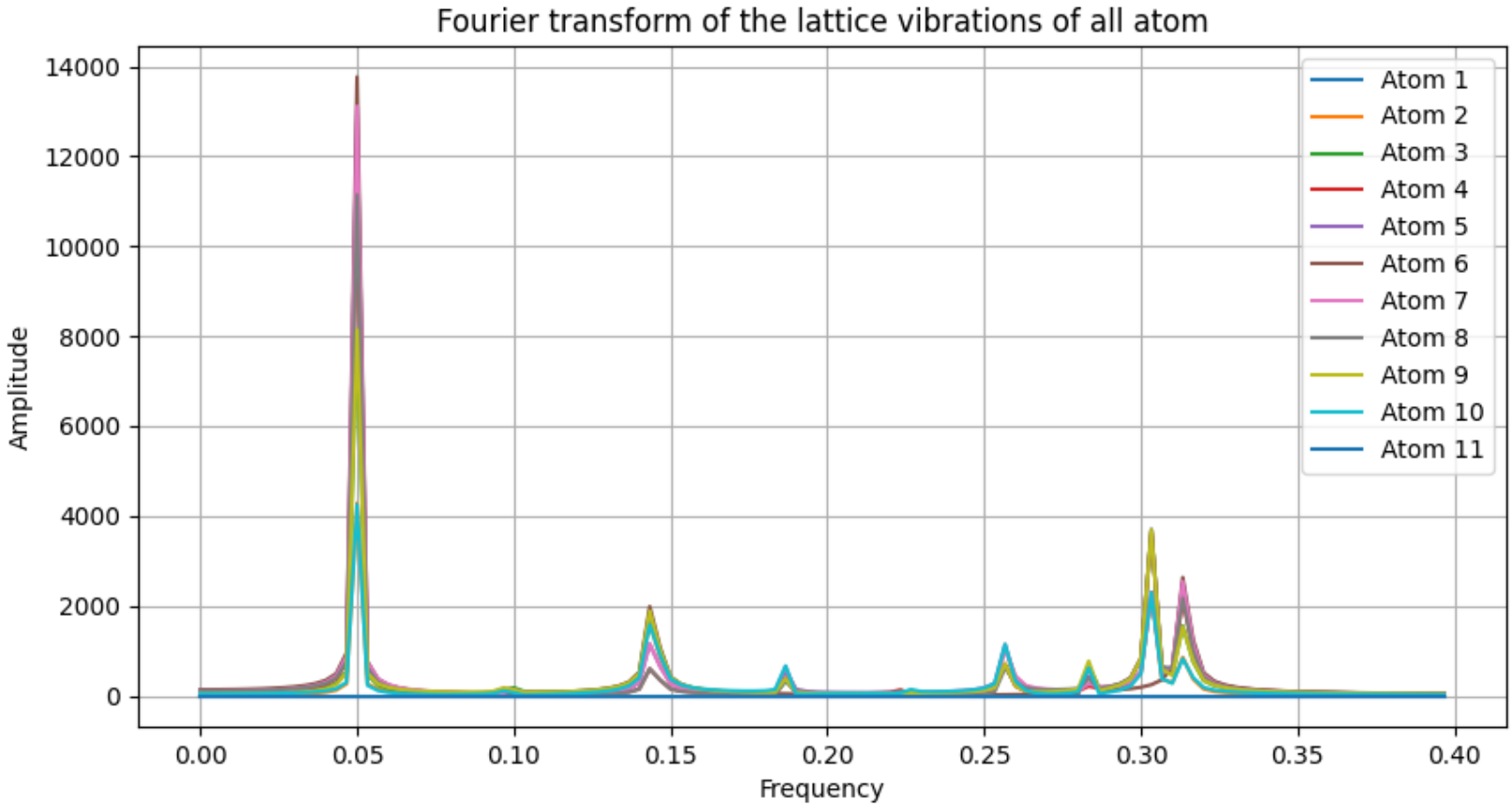

Figure: FFT obtained from simulating random perturbation - trial3

Random perturbation

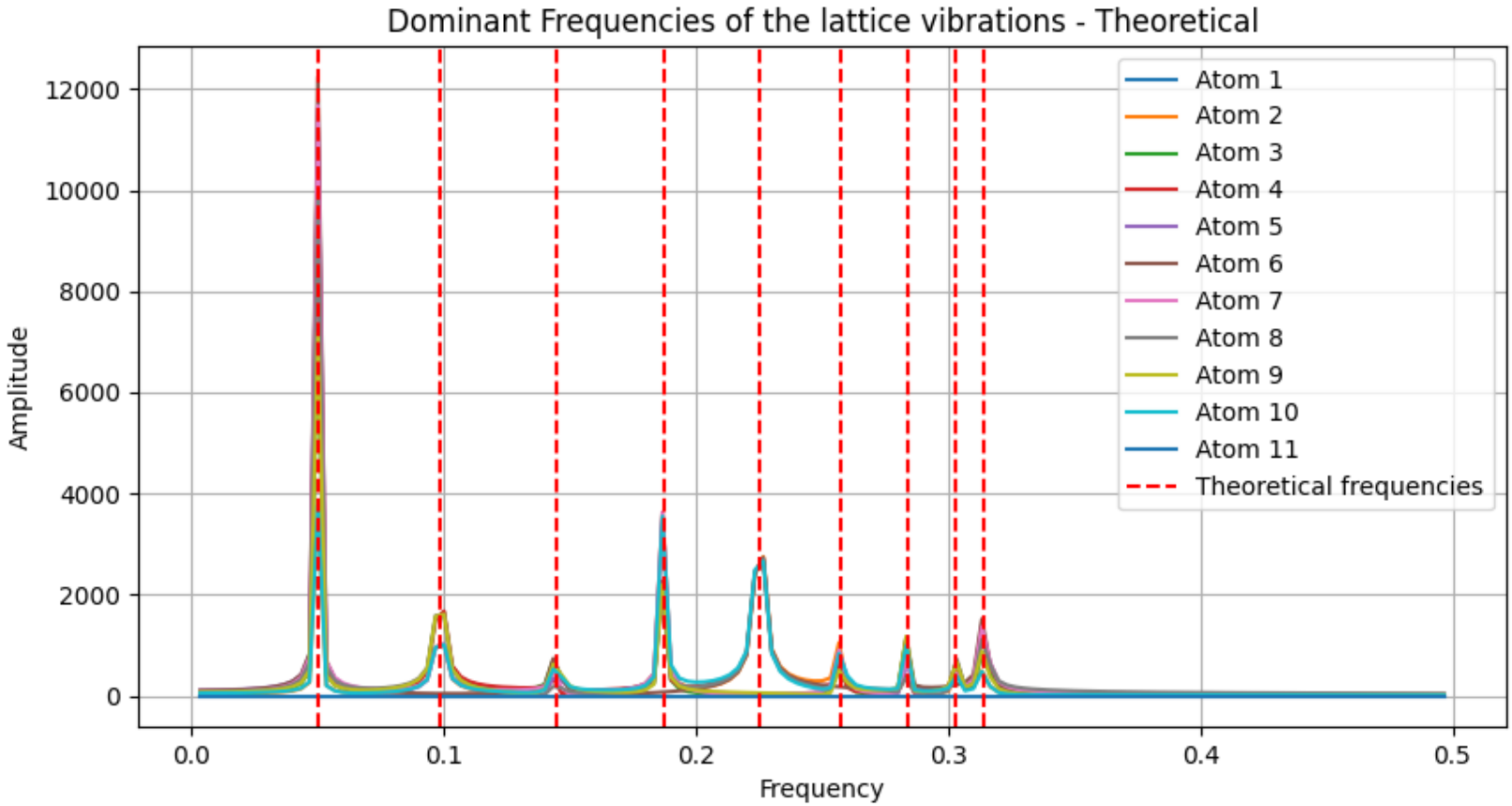

Figure: Vibrational modes compared with theoretical frequencies

Dispersion Law

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

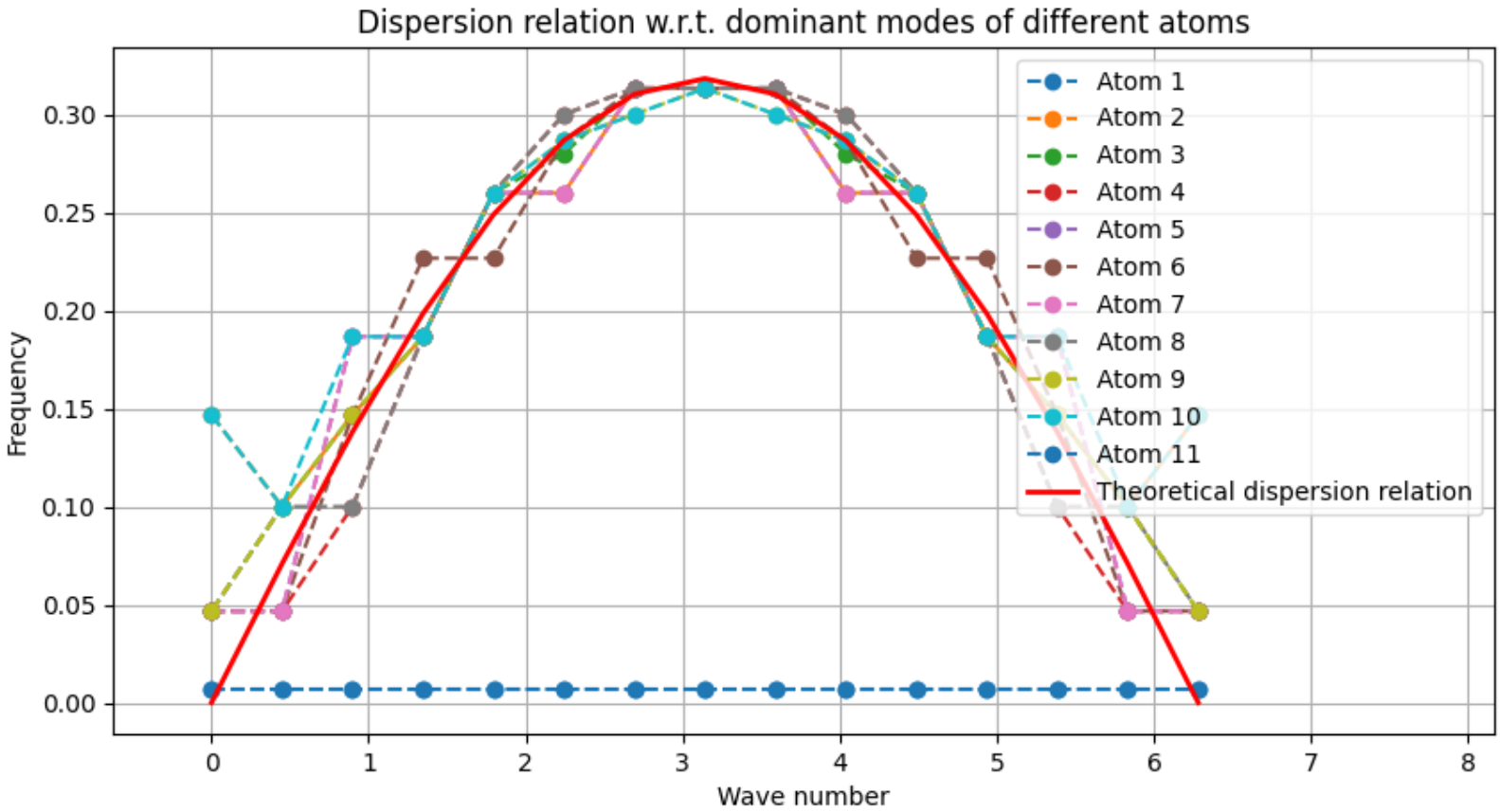

Figure: Dispersion law - 9 vibrating atoms

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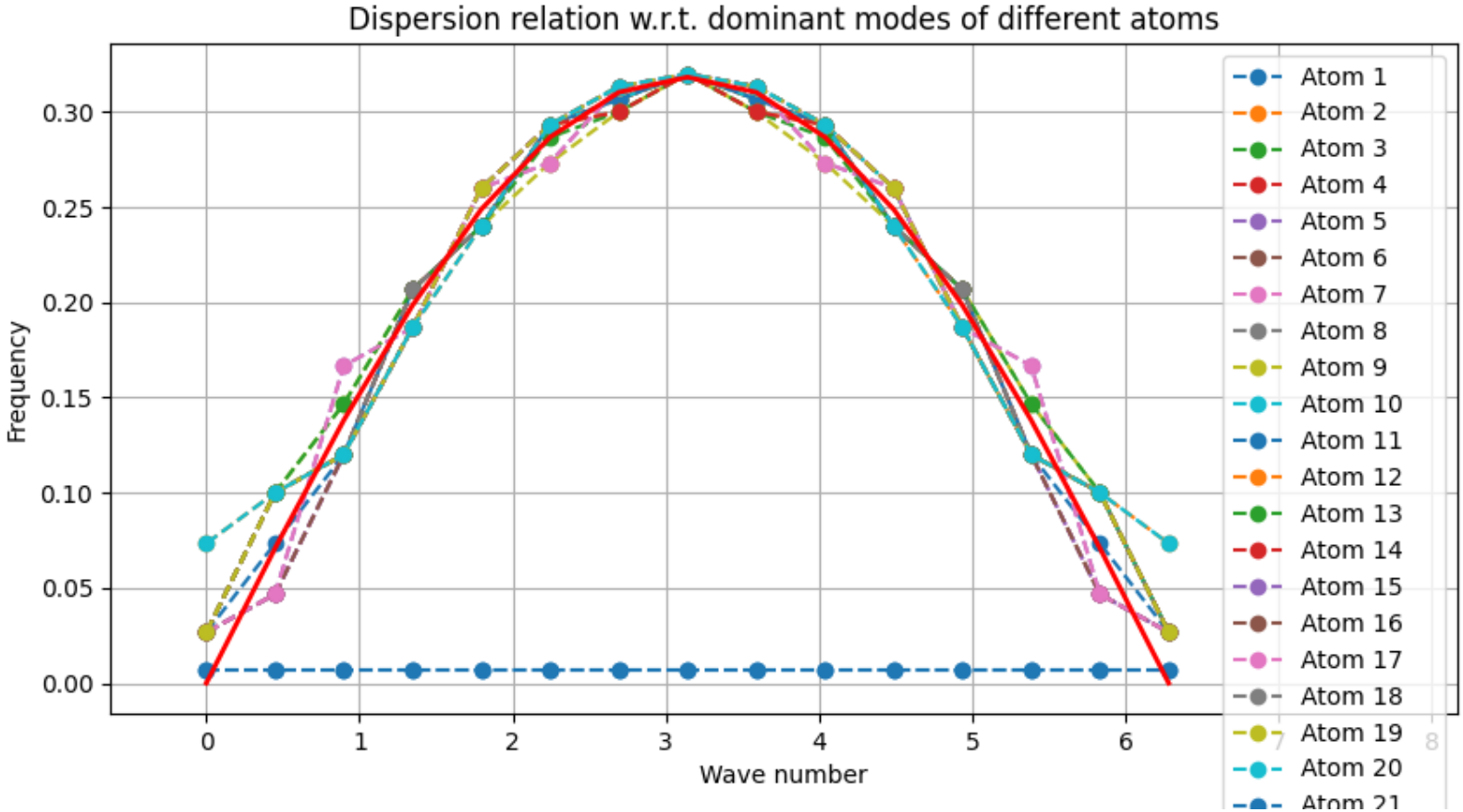
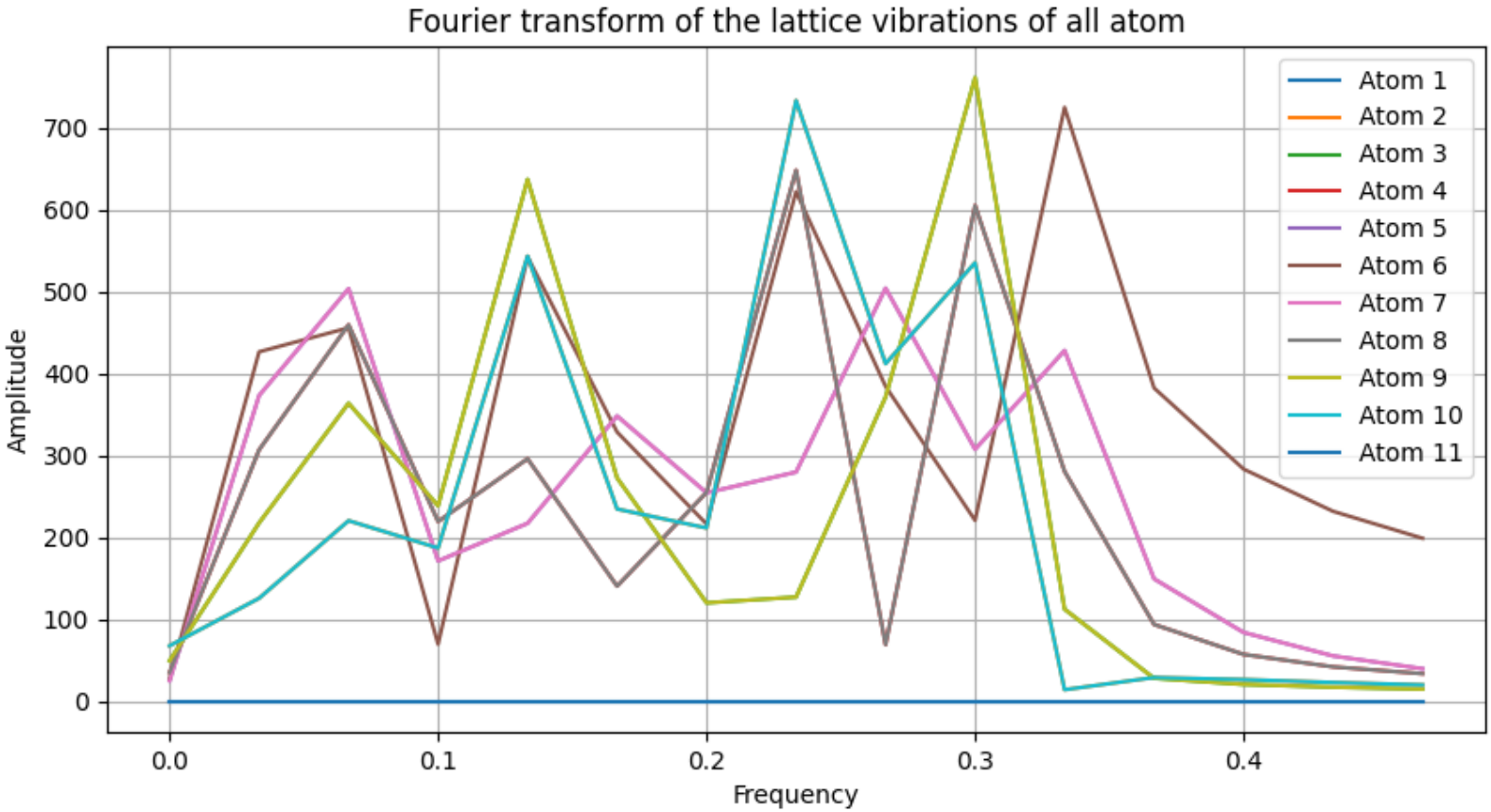


Figure: Dispersion law - 19 vibrating atoms

Impact of time



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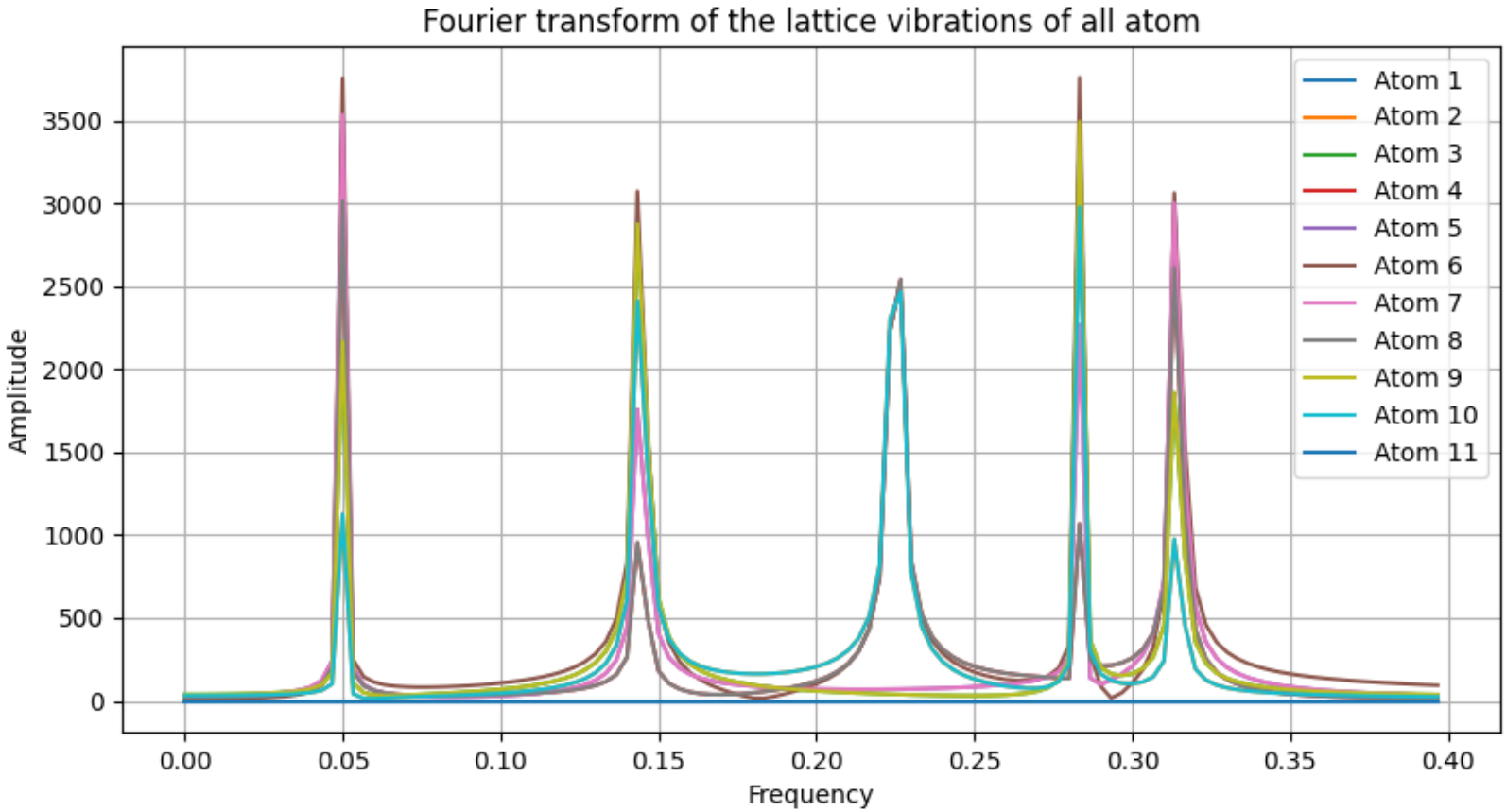

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Boundary conditions

Why it is essential for this implementation?

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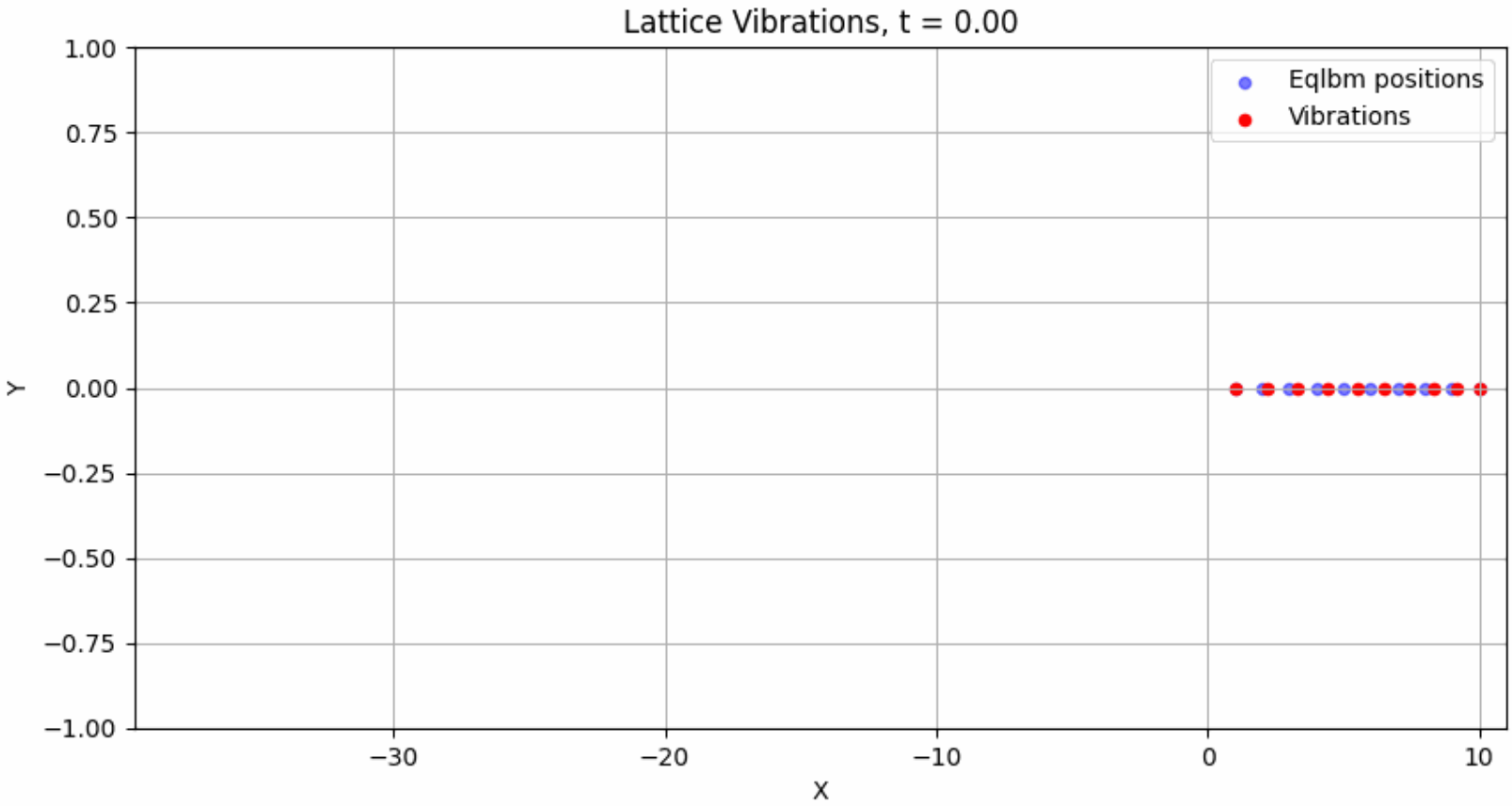

Figure: Failed Lattice vibration animation (gif not available in pdf)

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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- Random perturbations lead to the emergence of all possible vibrational modes.
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- Observing the system for a longer period of time separates the modes.
- Model versatile to different perturbations as well as different size of systems.

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- 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

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