PHYS416- Computer Applications in Physics

Homework 3 - Vibrations of Atoms in a Solid

Name: Süleyman Ertekin

Student Number: 200218018019

Date of Submission: 3.11.2024

I pledge that I worked entirely alone on this homework and will not share information about any aspect of this homework with any other persons.

```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
```

Parameters

N = 26 # Number of masses
 m = 1.0 # Mass of each object
 k = 6.0 # Spring constant
 C = 1.0 # External force
 omega = 2.0 # Angular frequency

Calculating alpha (main diagonal element)

alpha = 2 * k - m * omega**2

Constructing the main diagonal (alpha) and the off-diagonals (-k)
main_diagonal = [alpha] * N
main_diagonal[0] = alpha - k # Adjusting the first element
main_diagonal[-1] = alpha - k # Adjusting the last element
off_diagonal = [-k] * (N - 1)

Creating the tridiagonal matrix
matrix = np.diag(main_diagonal) + np.diag(off_diagonal, k=1) +
np.diag(off_diagonal, k=-1)

Convert matrix to DataFrame for better display

```
matrix_df = pd.DataFrame(matrix)
print("26x26 Matrix:")
print(matrix_df)
# Constructing the right-hand side vector with external force applied to the first
mass
rhs = np.zeros(N)
rhs[0] = C # External force applied to the first mass
# Solving for the displacement amplitudes Ui
U = np.linalg.solve(matrix, rhs)
# Calculating the amplitudes of each mass
amplitudes = np.abs(U)
# Plotting the amplitudes of the vibrations for each mass
plt.figure(figsize=(12, 8))
plt.plot(range(1, N + 1), amplitudes, marker='o', color='b', linestyle='-',
markersize=6)
plt.xlabel("Mass index (i)")
plt.ylabel("Amplitude | U$ i$|")
plt.title("Amplitudes of Vibrations of Masses")
plt.xticks(range(1, N + 1)) # Ensures all mass indices are visible on the x-axis
plt.grid(True)
plt.show()
26x26 Matrix:
```

0 1 2 3 4 5 6 7 8 9 ... 16 17 18 19 \ 0 2.0 -6.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ... 0.0 0.0 0.0 0.0 1 -6.0 8.0 -6.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ... 0.0 0.0 0.0 0.0 4 0.0 0.0 0.0 -6.0 8.0 -6.0 0.0 0.0 0.0 0.0 ... 0.0 0.0 0.0 0.0 5 0.0 0.0 0.0 0.0 -6.0 8.0 -6.0 0.0 0.0 0.0 ... 0.0 0.0 0.0 0.0 6 0.0 0.0 0.0 0.0 0.0 -6.0 8.0 -6.0 0.0 0.0 ... 0.0 0.0 0.0 0.0 7 0.0 0.0 0.0 0.0 0.0 0.0 -6.0 8.0 -6.0 0.0 ... 0.0 0.0 0.0 0.0 8 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -6.0 8.0 -6.0 ... 0.0 0.0 0.0 0.0 9 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -6.0 8.0 ... 0.0 0.0 0.0 0.0 10 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -6.0 ... 0.0 0.0 0.0 0.0 15 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ... -6.0 0.0 0.0 0.0 16 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ... 8.0 -6.0 0.0 0.0 20 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ... 0.0 0.0 0.0 -6.0

20 21 22 23 24 25

- 0 0.0 0.0 0.0 0.0 0.0 0.0
- 1 0.0 0.0 0.0 0.0 0.0 0.0
- 2 0.0 0.0 0.0 0.0 0.0 0.0
- 3 0.0 0.0 0.0 0.0 0.0 0.0
- 4 0.0 0.0 0.0 0.0 0.0 0.0
- 5 0.0 0.0 0.0 0.0 0.0 0.0
- 6 0.0 0.0 0.0 0.0 0.0 0.0
- 7 0.0 0.0 0.0 0.0 0.0 0.0
- 8 0.0 0.0 0.0 0.0 0.0 0.0
- 9 0.0 0.0 0.0 0.0 0.0 0.0
- 10 0.0 0.0 0.0 0.0 0.0 0.0
- 11 0.0 0.0 0.0 0.0 0.0 0.0
- 12 0.0 0.0 0.0 0.0 0.0 0.0
- 13 0.0 0.0 0.0 0.0 0.0 0.0
- 14 0.0 0.0 0.0 0.0 0.0 0.0
- 15 0.0 0.0 0.0 0.0 0.0 0.0
- 16 0.0 0.0 0.0 0.0 0.0 0.0
- 17 0.0 0.0 0.0 0.0 0.0 0.0
- 18 0.0 0.0 0.0 0.0 0.0 0.0
- 19 -6.0 0.0 0.0 0.0 0.0 0.0
- 20 8.0 -6.0 0.0 0.0 0.0 0.0
- 21 -6.0 8.0 -6.0 0.0 0.0 0.0
- 22 0.0 -6.0 8.0 -6.0 0.0 0.0
- 23 0.0 0.0 -6.0 8.0 -6.0 0.0
- 24 0.0 0.0 0.0 -6.0 8.0 -6.0
- 25 0.0 0.0 0.0 0.0 -6.0 2.0

