

1D vibrational density of states

Consider a mass-and-spring chain with N masses M and spring constant K and length $L = Na$ in one dimension. The exact dispersion relation is

$$\omega(k) = 2\sqrt{\frac{K}{M}}|\sin(ka/2)|$$

while the Debye approximation is simply

$$\omega(k) = \sqrt{\frac{K}{M}}ka$$

Recall that the allowed wavenumbers for periodic boundary conditions are

$$k = \frac{2\pi n}{Na}, \quad n = 0, \pm 1, \pm 2, \dots, N/2$$

Write a computer program to create histograms of ω values using the exact dispersion relation and using the Debye model. Plot your results on the same axes and discuss the similarities and differences. *Hint:* You should choose enough histogram bins to reveal noteworthy details. However, you need enough k -points to be able to fill in the histogram.