Phonon DOS calculation for 3D-lattice
Manual

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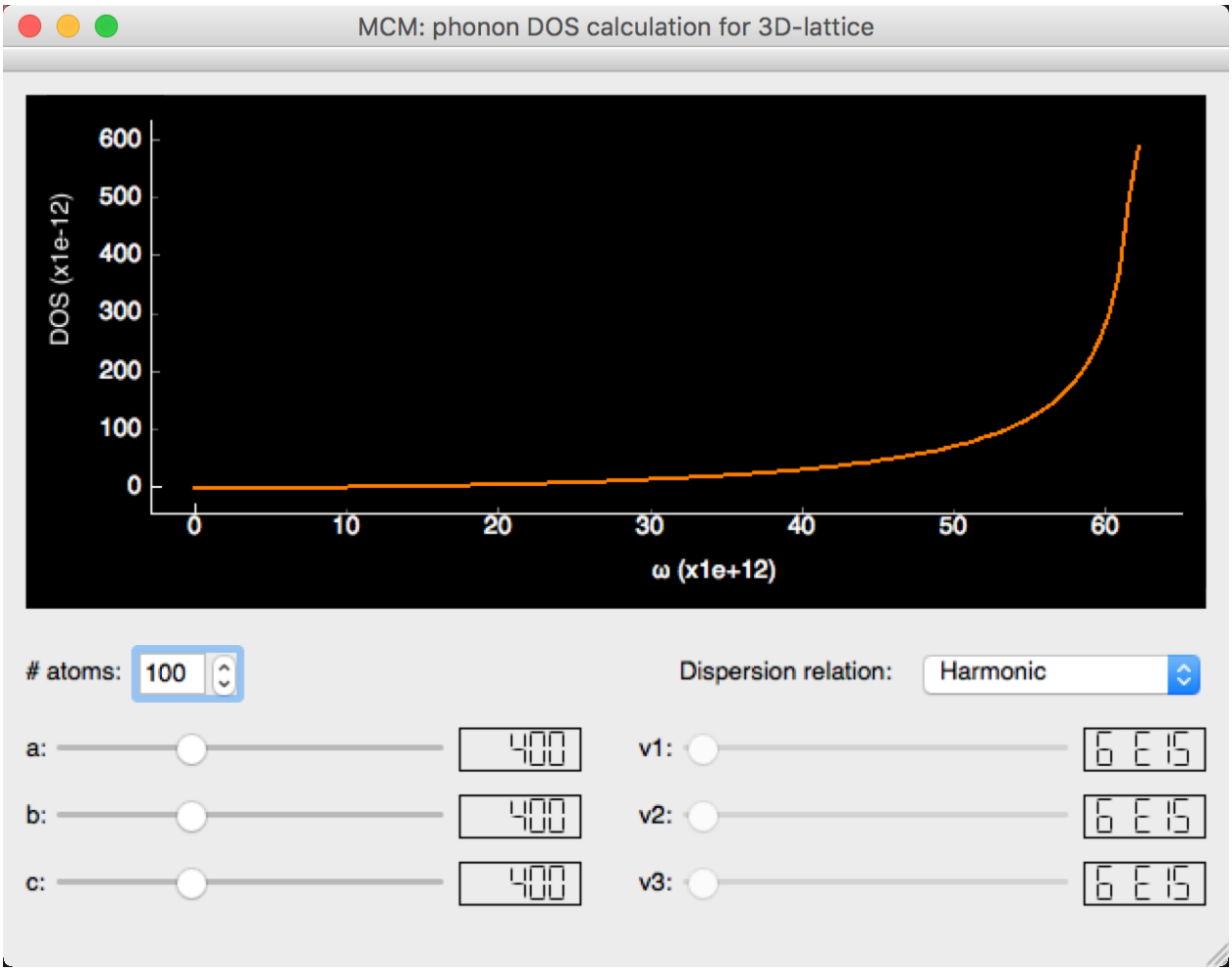
Packages required

- pyqtgraph
- numpy
- PyQt4

Instructions

Make sure you have all the packages mentioned above installed before running this program.
Start the program by running main.py with python3 (terminal: "python3 main.py").
The main window (see screenshot next page) will show you the DOS plot against angular frequency. You can manipulate the plot by using your mouse, for example zooming in and out and moving. After moving the plot you can re-enable automatic scaling by clicking the [A] in the bottom left corner of the plot. Below the plot are the controls for interacting with the simulation.
The integer-box labeled "# atoms" allows you to change the number of atoms used for the calculation. Increasing it will increase the resolution, but this will dramatically impact the performance. Note that this number is not really the number of atoms but it is half the number of atoms in one direction, the actual number of atoms is: $(2 \times \# - 1)^3$.
The combobox labeled "Dispersion relation" allows you to select the dispersion relation used for calculating the DOS (linear or harmonic).
The three sliders on the left allow you to change the lattice constants in the tree directions.
For simulations with the linear dispersion relation you can also change the propagation velocity for phonons with different polarisations with the sliders on the right side. Note: these sliders are disabled when using the harmonic dispersion relation.


MCM: phonon DOS calculation for 3D-lattice
DOS (x1e-12)
600
500
400
300
200
100
0
0
10
20
30
40
50
60
ω (x1e+12)
atoms:
100
Dispersion relation:
Harmonic
a:
400
b:
400
c:
400
v1:
6.15
v2:
6.15
v3:
6.15