pynamic-structure-factor validation

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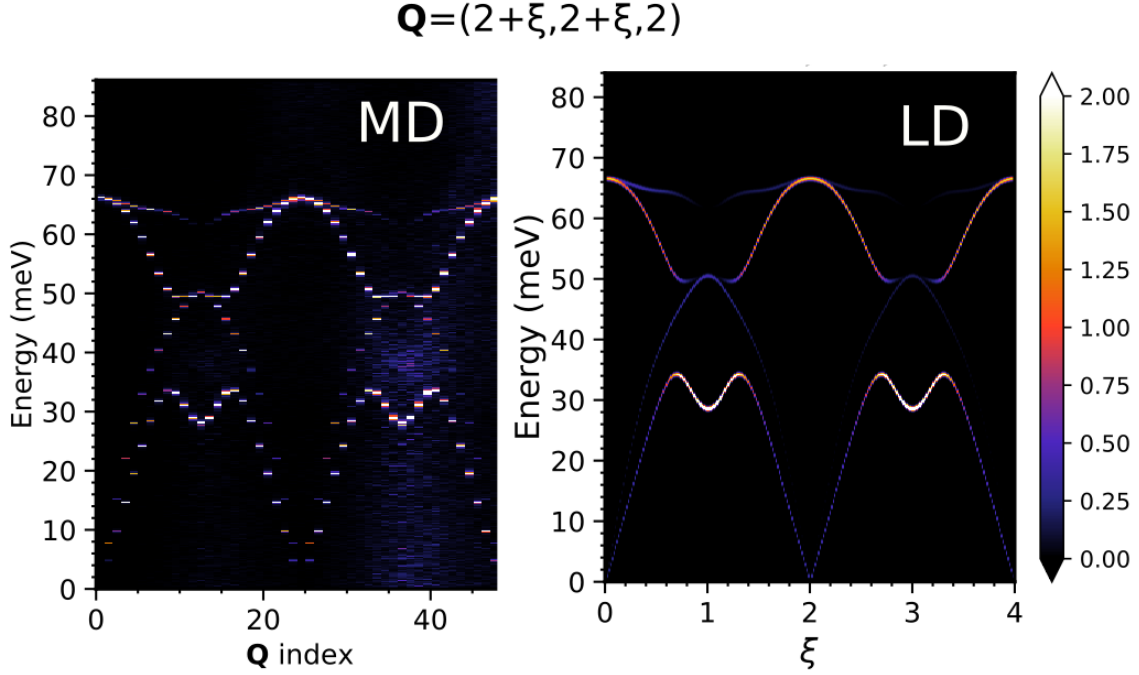(Dated: June 11, 2021)

Q=(2+ξ,2+ξ,2)

FIG. 1.

Abstract

In this document, I compare some (rather underconverged) results from my pynamic-structure-factor (PSF) code to other high-quality results.

VALIDATION

The results in the following figures compare inelastic neutron dynamic structure factors $S(\mathbf{Q}, \omega)$ computed with my PSF code from molecular dynamics (MD) to those computed from harmonic lattice dynamics (LD) using PHONOPY [1] and SNAXS [2]. The inputs to $S(\mathbf{Q}, \omega)$ from the harmonic expansions are phonon eigenvectors and energies [3] (and scattering lengths, masses etc), but the structure factors are a δ function in energy. Anharmonicity is entirely neglected. To ease comparison to the MD results, where the linewidths are real, physical anharomic broadening, the LD results are broadened with a gaussian function using $\sigma = 0.5$ meV. The force constants from PHONOPY were calculated using the same
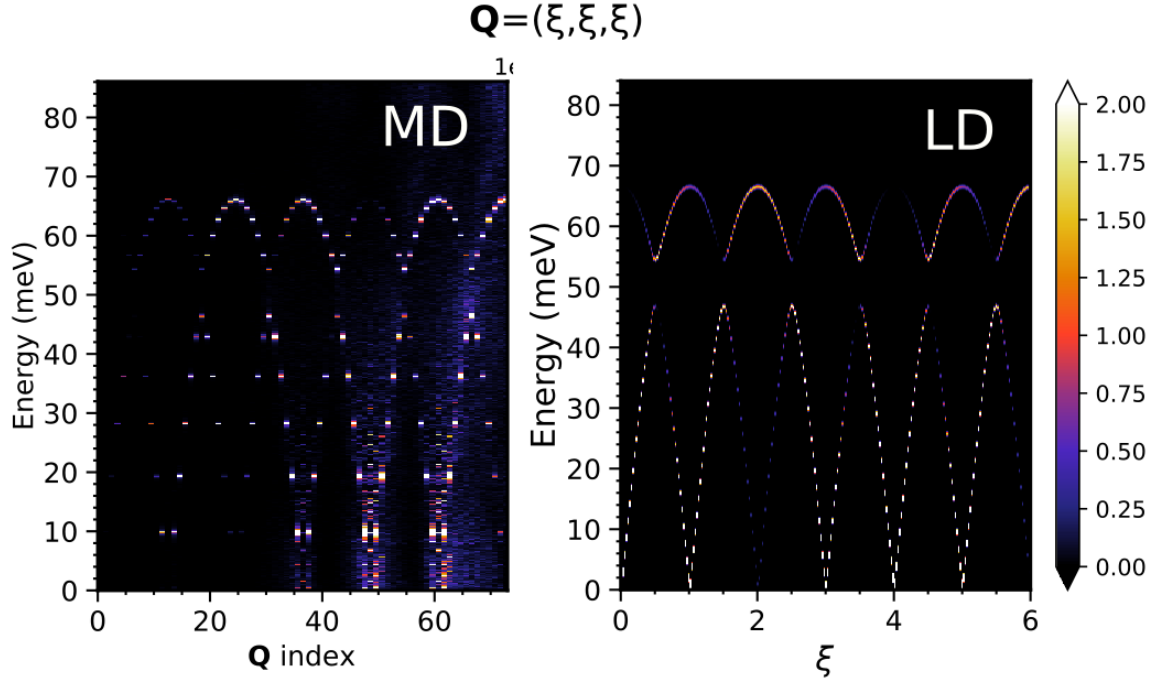
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FIG. 2.

empirical potential (i.e. Tersoff) as the MD simulation and a 4x4x4 supercell (using the 8-atom conventional cell as the "primitive" cell). The FORCESETS and POSCAR files are in the 'phonopy' directory in the 'example' directory. The MD trajectories and plots were generated using the scripts in the 'example' directory.

I picked 2 different high-symmetry directions and an off-high-symmetry path to sample different parts of reciprocal space. I also compare a constant-Q scan to more easily compare the relative intensities of phonon peaks. The agreement is very good everywhere. The crappy look to the MD figures is the 'coarseness' of the **Q**-point grid (i.e. the small supercell size in the MD calculation).

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[1] A. Togo and I. Tanaka, Scr. Mater. **108**, 1 (2015).
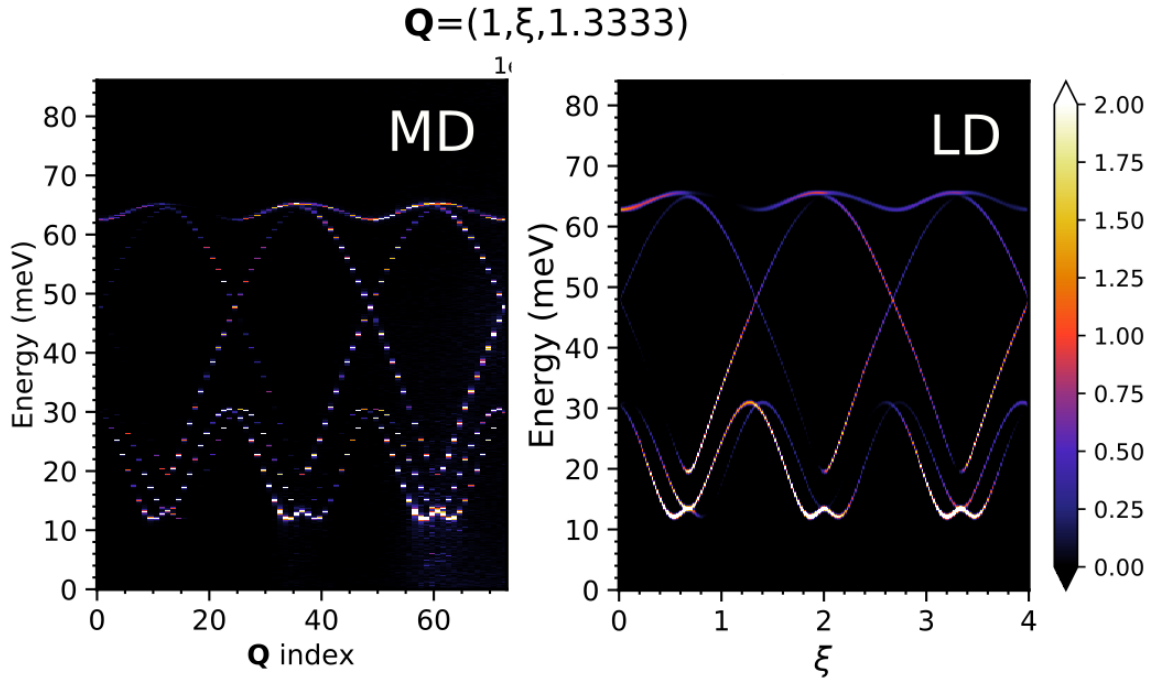
[2] D. Parshall, Simulating neutron and x-ray scans.

FIG. 3.

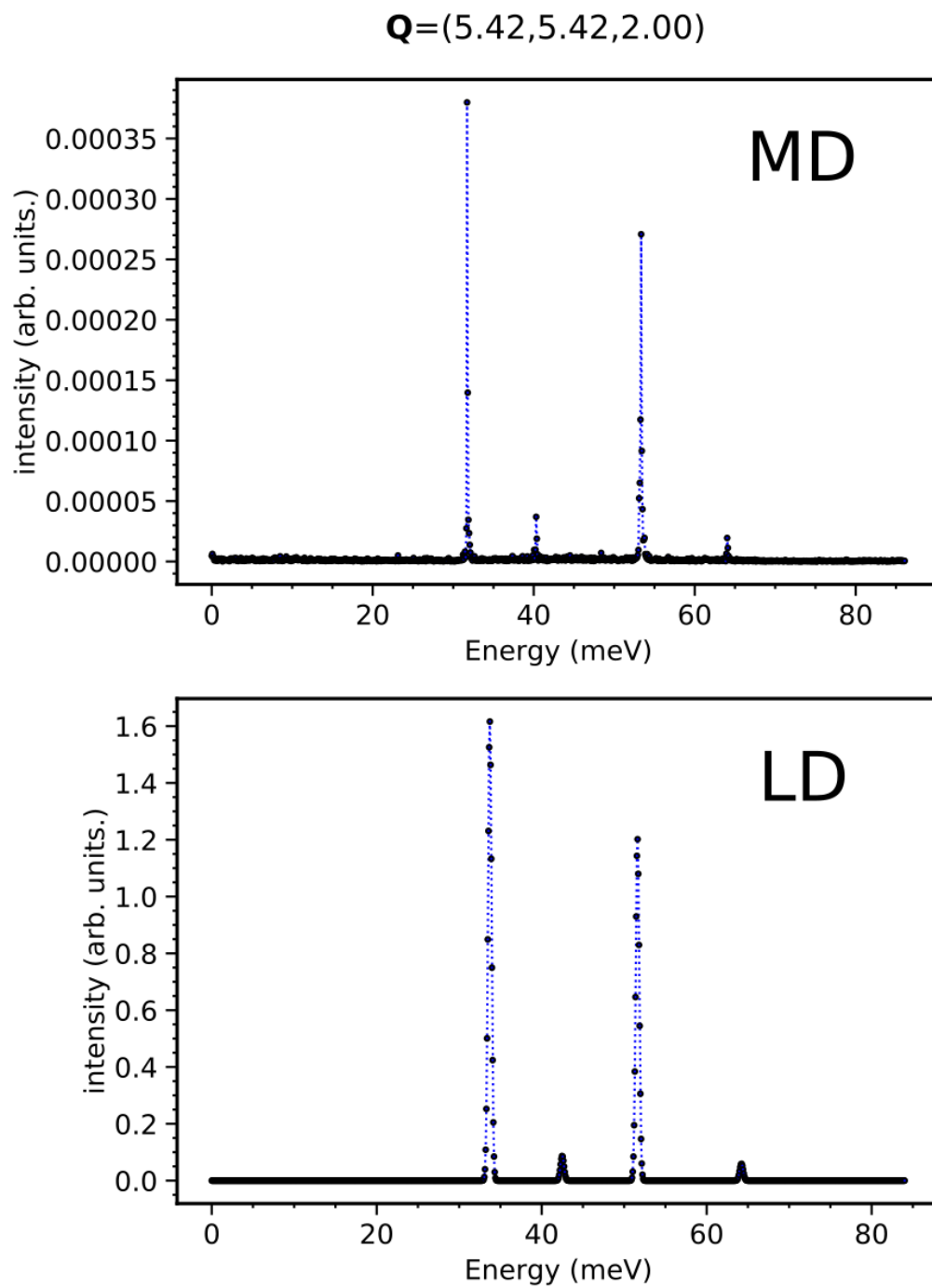[3] G. L. Squires, *Introduction to the theory of thermal neutron scattering* (Courier Corporation, 1996).

Q=(5.42,5.42,2.00)

FIG. 4.