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Fast zero-point family of methods for computing phonon dispersion

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Phonon dispersion curves are important to the analysis of energy transport in semiconductor and insulator materials. Experimentally, they can be determined using neutron/x-ray scattering or Raman spectroscopy techniques that involve the interaction of phonons with different forms of radiation. Theoretically, under harmonic approximation, they can be computed from the dynamical matrix extracted from force constants. Time correlations of dynamic variables in the reciprocal space offer a rich theoretical setting for computing the phonon dispersion curves, particularly for systems with marked anharmonic interactions. Currently, there are two general methods using the time correlation approach. In the first, the phonon dispersion is calculated using the frequencies extracted from the zero time expectation value of the correlation of displacements in the reciprocal space; equipartition of energy between the phonon modes is implicitly assumed. In the second method, the frequencies obtained from the Fourier transform of the time correlation of velocities are used to compute the dispersion of phonon modes. While the equipartition approach is computationally fast, since it requires only the zero time correlations, the assumption of equipartition of energy between the modes can result in tangible errors, especially at lower temperatures. In contrast, the Fourier method is more accurate but requires long correlation times for resolving the frequencies, making this approach computationally expensive. In this work, we present a family of methods to compute the normal mode frequencies from the ratio of the expectation value of the correlation of conjugate variables at zero time. This approach is computationally as fast as the equipartition methods, but is also robust and works even in the absence of equipartition. We present two variants of this approach that are appropriate for use in atomistic simulations. In the first, the phonon dispersion curves are calculated using the ratio of the normal mode amplitudes for velocity and displacement while in the second they are computed analogously from velocity and acceleration. We further elucidate the attractiveness of the second approach entailing velocity and acceleration for systems exhibiting anisotropic and highly anharmonic vibrations. Although the approach involving velocity and displacement is known before, we derive a family of zero-point methods from statistical-mechanical first principles. Finally, we demonstrate the accuracy, efficiency, and robustness of the zero-point methods on model linear chains and graphene using atomistic simulations.

Biography

Anant Raj received his Undergraduate Degree in Mechanical Engineering from the Indian Institute of Technology, Kanpur in 2010. He received a Master's degree in Nuclear Engineering from the North Carolina State University, Raleigh in 2013 and continued to pursue a PhD degree under the guidance of Prof Jacob Eapen. During his graduate studies, he was introduced to the fascinating field of materials science and the intricacies of probing materials behavior using statistical mechanics and atomistic simulations. He received his PhD on phonon dynamics and beyond-phonon descriptors for energy transport in materials. He is currently working as a Post-doctoral Research Scholar at the North Carolina State University.

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