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Phonon interference and emergence of energy wave packets

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Energy transport in low dimensional systems has been of interest for over 60 years, since the seminal paper by Fermi, Pasta, and Ulam on the vibrational modes of a one-dimensional non-linear string, popularly known as the FPU problem. Several studies have demonstrated that unlike bulk three-dimensional systems, the energy transport in low dimensional systems does not follow Fourier's law of heat conduction. The thermal conductivity for these systems is ill-defined and is reported to diverge, scaling with the size of the system. Such divergence is also observed in realistic polymer chains as well as in two dimensional materials such as graphene. More recently, this anomalous behavior has been linked to the presence of cross-correlation between different phonon modes arising from collective phonon excitations. To elucidate the relationship between the phonon modes and energy transport more deeply, we analyze the local energy fluctuations of a linear mono-atomic chain and relate them to the phonon modes. We demonstrate theoretically that normal modes of the displacements interfere to produce energy wave packets. We further derive the condition that pairs of phonon modes interfere to produce waves of energy if and only if three-phonon scattering law is satisfied by the trio, even in the absence of phonon-phonon scattering. In general, for n^{th} order in the interaction potential, n displacement normal modes combine to form energy waves if and only if $(n+1)^{th}$ order phonon scattering law is satisfied between them. Further, we show that the frequency and decay of the energy normal modes are directly associated with the collective excitation of phonon modes. Our theoretical findings link the established theory of phonon excitation modes to the normal modes of energy in crystal lattices from statistical-mechanical first principles.

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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