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A New Formalism for Quantifying Character of Vibrational Modes in Solids: Distinguishing Between Propagons, Diffusons and Locons HAMID REZA SEYF, ASEGUN HENRY, Georgia Institute of Technology — The solutions to the equations of motions for the atoms in homogenous crystalline solids result in plane wave modulated velocity fields for the normal modes of vibration. However, when a system lacks periodicity, either compositional or structural, the normal modes of vibration can still be determined, but the solutions take on different characters and many modes may be non-plane wave modulated. Previous work has classified the types of vibrations into three primary categories, namely propagons, diffusons and locons. Localized modes can be distinguished by calculation of participation ratio while distinguishing between propagons and diffusons is challenging because both are spatially delocalized. We present a new method that quantifies the extent to which a mode's character corresponds to a propagating mode, e.g., with a plane wave modulation. This then allows for clear and quantitative distinctions between propagons and diffusons. By resolving this issue quantitatively, one can now automate the classification of modes for any arbitrary structure subject to a single constraint that the atoms must vibrate stably around their respective equilibrium sites.

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