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Improved Calculation of Vibrational Mode Lifetimes in Anharmonic Solids[1] MURRAY DAW, YANG GAO, Clemson U, DOYL DICKEL, Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany, DAVID HARRISON, Clemson U — We propose and evaluate a formal foundation for practical calculations of vibrational mode lifetimes in solids. The approach is based on a recursion method analysis of the Liouvillian. From this we derive the lifetime of a vibrational mode in terms of moments of the power spectrum of the Liouvillian as projected onto the relevant subspace of phase space. In practical terms, the moments are evaluated as ensemble averages of well-defined operators, meaning that the entire calculation is to be done with Monte Carlo. These insights should lead to significantly shorter calculations and improved understanding of mode lifetimes and lattice thermal conductivity. Evaluation performed on model systems have been encouraging. [See Dickel & Daw, Comp Mat Sci, v47 p698 and v49 p445 (2010)].

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