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Improved method of calculation of mode lifetime in low dimension[1] YANG GAO, MURRAY DAW, Dept. of Physics & Astronomy, Clemson University, Clemson, SC 29634 — While vibrational mode lifetimes is an important property of materials, the method of calculation is surprisingly undeveloped. Recently, Dickel and Daw [1,2] proposed a theory to do the calculation efficiently. It is developed based on the Liouvillan and the recursion method. The mode lifetime can be represented in terms of moments of the power spectrum of Liouvillan. To verify the theory numerically, we applied this method and molecular dynamics to three different models of low dimension. Calculations are done by molecular dynamics(MD) and Monte Carlo(MC), and the result shows that the relation between mode lifetime τ and moments can be found,

$$\tau = F(\mu_2, \mu_4, \mu_6, ...)$$

and also lifetime can be approximated nicely with some low order moments:

$$\tau = \tau_2 \tilde{F}(\gamma_4, \gamma_6, ...), \tau_2 = \sqrt{\frac{1}{\mu_2}}, \gamma_n = \frac{\mu_n}{\mu_2^{\frac{n}{2}}}$$

[1] D. Dickel & M. S. Daw. Improved calculation of mode lifetimes, part i: Theory. *Comp. Mat. Sci.*, 47:698, 2009.
[2] D. Dickel & M. S. Daw. Improved calculation of mode lifetimes, part ii: Numerical Result *Comp. Mat. Sci.*, 2010.

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