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Nonlinear Transport and Noise Properties of Acoustic Phonons.[1]
KAMIL WALCZAK, Pace University — We examine heat transport carried by acoustic phonons in molecular junctions composed of organic molecules coupled to two thermal baths of different temperatures. The phononic heat flux and its dynamical noise properties are analyzed within the scattering (Landauer) formalism with transmission probability function for acoustic phonons calculated within the method of atomistic Green's functions (AGF technique). The perturbative computational scheme is used to determine nonlinear corrections to phononic heat flux and its noise power spectral density with up to the second order terms with respect to temperature difference. Our results show the limited applicability of ballistic Fourier's law and fluctuation-dissipation theorem to heat transport in quantum systems. We also derive several noise-signal relations applicable to nanoscale heat flow carried by phonons, but valid for electrons as well. We also discuss the extension of the perturbative transport theory to higher order terms in order to address a huge variety of problems related to nonlinear thermal effects which may occur at nanoscale and at strongly non-equilibrium conditions with high-intensity heat fluxes.

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Kamil Walczak
Department of Chemistry and Physical Sciences, Pace University, 1 Pace Plaza, New York, NY 10038, USA

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