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Simulating ionic thermal trasport by equilibrium ab-initio molecular dynamics ARIS MARCOLONGO, SISSA, Trieste, Italy, PAOLO UMARI, Università di Padova, Padua, Italy, STEFANO BARONI, SISSA, Trieste, Italy — The Green-Kubo approach to thermal transport is often considered to be incompatible with ab-initio molecular dynamics (AIMD) because a suitable quantum-mechanical definition of the heat current is not readily available, due to the ill-definedness of the microscopic energy density to which it is related by the continuity equation. We argue that a similar difficulty actually exists in classical mechanics as well, and we address the conditions that have to be fulfilled in order for the physically well defined transport coefficients to be independent of the ill defined microscopic energy density from which they derive. We then provide two alternative approaches to calculating thermal conductivites from equilibrium AIMD. The first is based on the Green-Kubo formula, supplemented with an expression for the energy current, which is a generalization of Thouless' expression for the adiabatic charge current. The second approach, which avoids the recourse to an energy current altogether, rests on an efficient and accurate extrapolation to infinite wavelengths of the energy-density time correlation functions. The two methods are compared on a simple classical test bed, and their implementation in AIMD is demonstrated with the calculation of the thermal conductivity of simple fluids.

Stefano Baroni
SISSA, Trieste, Italy

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