Boundary Fluctuation Theory of Thermal Transport Coefficients

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In heterogeneous confined systems with coexisting layers of different phases, even the definitions of thermal transport coefficients (such as viscosity and thermal conductivity) present problems, and the conventional Green-Kubo correlation integrals of the corresponding expressions for fluxes give unphysical results.

In this work, we derive the exact linear response expressions for the shear viscosity and thermal conductivity across a system of arbitrary heterogeneity and finite extension in one Cartesian direction. The definitions of transport coefficients emerging directly from the derivations match an experimentalist's definitions; they are in terms of forces or gradients applied at the boundaries. In addition, our theory gives access to local values of viscosity and thermal conductivity in an arbitrarily thin layer of the system (which may contain an interface of different phases). It predicts a nonlinear velocity profile as a linear response to oscillatory shear stress applied at the boundaries and a non-uniform shear stress under oscillatory strain rate at the boundaries.

We apply our method to discuss linear and non-linear effects in the interfacial transport coefficients, such as the hydrodynamic friction coefficient and slip and Kapitza resistance, across solid-liquid interfaces characterized by different degrees of wetting. We discuss the consequences of spatially dependent viscosity and thermal conductivity on viscous heating of liquids and liquid mixtures confined between solid walls.