Physics > Plasma Physics

Electronic transport coefficients from ab initio simulations and application to dense liquid hydrogen

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Using Kubo's linear response theory, we derive expressions for the frequency-dependent electrical conductivity (Kubo-Greenwood formula), thermopower, and thermal conductivity in a strongly correlated electron system. These are evaluated within ab initio molecular dynamics simulations in order to study the thermoelectric transport coefficients in dense liquid hydrogen, especially near the nonmetal-to-metal transition region. We also observe significant deviations from the widely used Wiedemann-Franz law which is strictly valid only for degenerate systems and give an estimate for its valid scope of application towards lower densities.

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