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Electronic transport properties of matter under extreme conditions from density functional theory

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The determination of thermoelectric transport coefficients of dense, partially ionized matter is a great challenge for both experiment and theory. In the past two decades, density functional theory (DFT) has evolved to an efficient tool for making theoretical predictions of properties of matter under extreme conditions. Many of these are of high relevance for modelling the interior states, evolution, and magnetic field dynamics of stellar and planetary objects. Here I will give an overview on the generalized Kubo-Greenwood (KG) formalism [1] that is frequently used in calculations of electronic transport properties using the Kohn-Sham states from DFT. Several examples of successful application of this technique to various solid and fluid metals will be presented. Furthermore, a comparison of optical reflectivities of molecular fluids observed in dynamic compression experiments [2] will be made, including a discussion of the influence of the exchange-correlation functional on the DFT results. Finally, the limitations of the KG formalism with respect to its capability of describing electron-electron collisions will be discussed by examining the thermopower and Lorenz number of weakly degenerate hydrogen plasmas. It is shown [3] that the DFT results approach the limiting values for a Lorentz plasma, which is a model system that only considers electron-ion collisions, instead of agreeing with the Spitzer results [4], which were derived taking both electron-ion and electron-electron scattering into account. These recent findings [3] are of substantial importance for future methodical developments to calculate transport properties of matter under extreme conditions and, especially, for correctly assessing the results obtained via the Kubo-Greenwood formalism in relation to experiments and other theoretical approaches. This work is supported by the DFG within the FOR 2440 "Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics."

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