First-Principles Calculation of Resistivity for Neon at High Pressure and High Temperature

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We investigate the electrical conductivity of neon under various thermodynamic conditions using the Kubo–Greenwood formula (KGF), which helps us to understand the process of neon metallization at high pressures.

A new mathematically rigorous criterion for selecting the optimal broadening parameter of the finite-width δ-function approximation in KGF is presented. The proposed criterion is based on an analysis of the stability of the dynamic conductivity curve and minimizing the root mean square deviation between curves obtained by sequentially varying the broadening parameter value.

The method is applied to calculate the electrical conductivity of neon in the temperature range up to 100 kK and densities up to 14 g/cm^3. It is shown that the choice of broadening significantly affects the accuracy of the static conductivity calculation. The method provides the reproducibility and physical stability of the results and can be applied to a wide range of problems requiring the calculation of transport and optical properties of materials.