SKIES: THE PROGRAM FOR SOLUTION OF KINETIC EQUATION FOR SOLIDS FROM FIRST PRINCIPLES USING ALLEN'S VARIATIONAL APPROXIMATION METHOD

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The study of transport properties in metals is crucial for the requirements of both the extreme states of matter physics and basic issues in the solid state physics like the description of electron-phonon interaction. Methods based on the solution of the Boltzmann kinetic equation are among the most widely used theoretical approaches to the analysis of the transport properties of conductors. Based on a generalization of the least order variational approximation (LOVA) approach, Allen suggested a technique [1, 2] for solving the kinetic equation.

We present the new implementation of Allen's LOVA method in our program code `SKiES` (**S**olver of **Ki**netic **E**quation for **S**olids). The program serves for first principles calculations of electronic transport and allows one to obtain temperature dependence of transport properties in a wide temperature range in solid state. Wannier interpolation procedure [3,4] is used for an accurate Brillouin zone sampling. Description of the computational wokflow and main code's functionalities are provided. The examples for electrical resistivity and thermal conductivity of Al and Ag are given and the comparison with some known experiments is made. Special attention is devoted to final results' convergence issues, especially connected with Wannier interpolation.

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