IMPLEMENTATION OF THE CONTINUOUS KUBO–GREENWOOD FORMULA TO CALCULATE TRANSPORT PROPERTIES OF QUANTUM PLASMA

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Nowadays, many papers are devoted to the study of materials under the influence of laser radiation. Numerical simulations can be used to interpret such experiments. Transport and optical properties are required in simulations; they can be obtained by performing quantum calculations.

Our work is devoted to the *ab initio* computation of the transport properties of aluminum, widely used in experiments. The quantum molecular dynamics is used to simulate ions motion; the electronic structure is calculated by the density functional theory. These calculation stages are carried out via the Vienna *Ab initio* Simulation Package (VASP) [1]. We calculate the transport properties by the Kubo–Greenwood (KG) formula using the parallel program implemented by the authors of this paper. One can find more details in [2, 3].

The purpose of our work is also to understand how the transport properties are formed. Therefore, the calculation of static electrical σ_{1DC} and thermal K conductivity is done by the *continuous Kubo–Greenwood formula*. It expresses σ_{1DC} and K as an integral over the electron energy spectrum of the product of continuous functions. In this way, one can study the contributions of different spectrum parts to the values of the properties.

To implement the continuous KG formula, we developed a special technique that results in *smooth squares of matrix elements* (SSME) $D(\varepsilon_1, \varepsilon_2)$. They show the intensity of the electron transition between levels with energies ε_1 and ε_2. Using $D(\varepsilon_1, \varepsilon_2)$, we not only can obtain the values of σ_{1DC} and K but also analyze the contributions of electronic transitions to the properties. For calculations via the continuous KG formula, we developed a VASP–compatible parallel **C**ontinuous K**ubo**–**Gr**eenwood Progr**am** (CUboGrAm).

The transport properties of liquid aluminum were calculated at temperature $T = 3000$ K and density $\rho = 2.7$ g/cm^3 using the CUboGrAm code. We obtained and analyzed the density of states, SSME, the differential electrical and thermal conductivity for this system. The work is supported by the Russian Science Foundation, grant No. 20-42-04421.

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