Continuous Kubo–Greenwood formula: new approach to calculate transport and optical properties

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In this work, we develop a new method to compute the transport (static electrical σ_{1DC} and thermal K conductivity) and optical (real part of frequency–dependent $\sigma_1(\omega)$ conductivity) electron properties. We call it *the continuous Kubo–Greenwood* (KG) *formula*. It represents $\sigma_1(\omega)$ as an integral over the electron spectrum of the product of continuous functions. In contrast to the usual KG formula, it allows one to investigate contributions of different spectrum parts into the properties.

To make it possible, we propose a special smoothing technique that results in smooth squares of matrix elements (SSME). The relationship between SSME and $\sigma_1(\omega)$, σ_{1DC}, K is a continuous KG formula. This technique and the calculation algorithm of the properties are implemented in a parallel **C**ontinuous K**ubo**–**Gr**eenwood Prog**am** (CUboGrAm), which is compatible with the VASP code [1, 2].

Our method was verified by the comparison of σ_{1DC} and K for liquid aluminum obtained via continuous and the usual KG formulas by CUboGrAm and the GreeKuP code [3, 4], respectively. Also, we obtained and analyzed the density of electron states, SSME, the differential electrical and thermal conductivities of liquid aluminum.

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[1] Kresse G and Hafner J 1993 *Phys. Rev. B* **47** 558–561
[2] Kresse G and Hafner J 1994 *Phys. Rev. B* **49** 14251–14269
[3] Knyazev DV, Levashov PR 2013 *Comput. Mater. Sci.* **79** 817–829
[4] Knyazev DV, Levashov PR 2019 *Contr. to Plasma Phys.* **59** 345–353