Modal discontinuous Galerkin scheme for three-dimensional electron Boltzmann transport equation under far-from-equilibrium conditions

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The Boltzmann transport equation describes the incoherent time evolution of a quantum system consisting of a substantial number of quasiparticles (for instance electrons, phonons, excitons) and their interactions, subject to electrostatic effects in terms of the corresponding distribution function in phase space. Due to the high number of dimensions (six dimensions in phase space and one dimension in time) and their intrinsic physical properties (in particular, the non-parabolicity of the momentum-energy dispersion), the construction of efficient numerical method represents a challenge and requires a careful balance between accuracy and computational complexity.

In the current research, the development of a numerical method for solving the three-dimensional electron Boltzmann transport equation (BTE) under far-from-equilibrium conditions is demonstrated. A modal discontinuous Galerkin (DG) scheme based on hexahedral meshes is employed for the numerical solution of the three-dimensional electron BTE. A simple collisional model so-called the relaxation time approximation is used to handle the complex collisional integral operator. For the spatial discretization, the polynomial solutions are represented by scaled Legendre basis functions, and the numerical flux based on an upwind scheme is used for the solution stability. All the integrals appearing in the DG formulation are approximated with the Gauss-Legendre quadrature rule. A third-order explicit SSP-RK based temporal discretization scheme is used to the resulting semi-discrete ordinary differential equation. We study numerically the verification of the theoretical and convergence analysis. The performance of the proposed scheme is assessed by solving some benchmarks in the simulations of quantum physics.

Keywords: Modal Discontinuous Galerkin, Electron Boltzmann transport equation, far-from-equilibrium conditions

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