Quantum-mechanical simulations of strong-field phenomena using GPUs

Romanov A A[1,2,@], Silaev A A[1,2] and Vvedenskii N V[1,2]

[1] Institute of Applied Physics of the Russian Academy of Sciences, Ulyanova 46, Nizhny Novgorod 603950, Russia

[2] Lobachevsky State University of Nizhni Novgorod, Gagarin Avenue 23, Nizhniy Novgorod 603950, Russia

[@] romanoval@ipfran.ru

This work studies the prospects of using graphics processing units (GPUs) for quantum-mechanical simulation of computationally expensive problems in strong-field physics. The range of such phenomena includes various multielectron effects arising in the process of interaction of atoms, molecules, or atomic clusters with intense fields, as well as propagation effects during ionization-induced generation of low-frequency (terahertz or mid-infrared) radiation, high-order harmonic generation, etc. Using the developed algorithm for solving the three-dimensional time-dependent Schrödinger equation in a spherical coordinate system on GPUs, we compare the performance of numerical modeling of various ionization-stimulated phenomena using different computational configurations with modern central processors and graphic accelerators. A range of problems is determined where graphics accelerators provide a significant performance advantage in the numerical simulation of strong-field phenomena compared with central processors. The work was supported by the Russian Science Foundation (Grant No. 18-11-00210).