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Quantum dynamics of charged fermions in the Wigner formulation of quantum mechanics

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Plasma media is quantum mechanical even at high temperature and low density since the Heisenberg uncertainty principle is necessary to keep the electrons from collapsing into the ions, thus it cannot be described in the framework of classical mechanics. Nevertheless the classical molecular dynamics and Monte Carlo simulations became a traditional way of calculation of thermodynamic and transport properties of non-ideal plasmas. The main difficulty of these methods remains the treatment of bound states and 'sign'problem of electrons in dense plasma. As this is a quantum-mechanical or quantum-statistical problem more complex simulation approaches should be used [1]. In this work we combine the Wigner and Feynman formulations of quantum mechanics with path integral Monte Carlo and molecular dynamics methods for construction of the quantum dynamics method in the phase space. An explicit analytical expression of the Wigner function in path integral form has been derived, accounting for Fermi statistical effects by an effective pair pseudopotential in phase space allowing to avoid 'sign'problem of fermions. Pseudopotential depends on coordinates, momenta and the degeneracy parameter of fermions and takes into account Pauli blocking of fermions in phase space. A new quantum Path Integral Monte Carlo method has been developed to calculate average values of arbitrary quantum operators in phase space. Calculations of the momentum distribution functions and the pair correlation functions of degenerate ideal Fermi gas have been carried out in good agreement with the analytical expressions for testing the developed approach over a wide range of momentum and degeneracy parameter. Comparison of the obtained momentum distribution functions of strongly correlated Coulomb systems with the Maxwell–Boltzmann and the Fermi distributions shows the significant influence of the strong interparticle interaction both at small momenta and in high energy quantum 'tails'.

We have also developed the new method for calculation of the kinetic coefficients of dense plasma. To calculate kinetic properties we use quantum dynamics in the Wigner representation of quantum mechanics. The Wigner-Liouville equation is solved by a combination of molecular dynamics and path integral methods. The initial conditions of the Wigner-Liouville equation are sampled by path integral Monte Carlo method which allow to calculate also such thermodynamic quantities as the internal energy, pressure and pair distribution functions in a wide range of density and temperature. To study the influence of the interparticle interaction on the dynamic properties of dense plasmas we apply the quantum dynamics in the canonical ensemble at finite temperature and compute temporal momentum-momentum correlation functions and electrical conductivity according to the quantum Kubo formulas. Our numerical results agree well with available theoretical and experimental results. This work has been supported by the Russian Science Foundation via grant 14-50-00124.

1. Ebeling W, Fortov V and Filinov V 2017 Quantum Statistics of Dense Gases and Nonideal Plasmas (Berlin: Springer)

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