Simulations of nonideal plasmas by the method of molecular dynamics with wave packets

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Simulations by the method of molecular dynamics (MD) is a common practice to study equilibrium and nonequilibrium nonideal plasmas [1]. At the same time the applicability of MD is restricted to non-degenerate and fully ionized plasmas. Such a model is often too crude if applied to real experimental conditions. One of the possibilities to improve the method of MD without loosing its performance is to consider electrons as Gaussian wave packets. In this case the problem of choosing effective electron-ion interaction potential does not arise, and the precision of simulation of an individual particle collisions is increased. Furthermore when using antisymmetrized wave packets, the exchange interaction between electrons can be taken into accounts. This method was named Wave Packet Molecular Dynamics (WPMD).

At present the theoretical basis for WPMD has been developed [2], some MD simulations using WPMD without antisymmetrization [2] and Mote-Carlo simulations using WPMD with antisymmetrization [4] has been conducted. However, existing WPMD codes have two essential disadvantages: large simulations time when using antisymmetrization (it disallow to simulate dynamics of required number of particles) and broadening of the wave packets. In this report an experience of developing of effective WPMD algorithm is discussed, and different ways to solve the problem of wave packet broadening are proposed. Calculations of the dynamical conductivity of nonideal plasmas are also presented. It is expected that the new WPMD algorithm will allow to obtain more precise results compared to those obtained earlier by the standard MD. Moreover it will allow to consider higher electron densities (close to plasma degeneracy) where the standard MD is not applicable.

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