Simulation of a Coulomb Plasma by the Many-Particle Method

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This paper is review of *ab initio* simulation of classical Coulomb plasma. A system of charged classically moving particles interacting by Coulomb's law was investigated. This particle system represents a plasma model. Such a model is known in plasma physics as a classical (particle dynamics is classical) Coulomb (only electrostatic interaction is accounted) plasma.

A numerical model presented in this paper use PLASMIC-Code, which has been described in detail [1]. Some progress in numerical solution technique is presented now.

The method of particles [2] consists of a numerical solution of Newton's equations of motion for all particles of the system under consideration. The method of particles combined with the ideology of an *ab initio* simulation is very fruitful for studying the fundamental properties of many-charged-particles systems and classical Coulomb plasma.

An original algorithm of the equations numerical solution is proposed. The basic idea was to improve the accuracy of closest neighbour-particle interaction time-variation calculation. The time-evolution of a fully ionized plasma, confined within a cubic volume with walls impenetrable for particles was considered. The trajectories of n positively charged particles (ions) and zn negatively charged particles (electrons) were calculated by solving numerically the Newton equations.

Particles were considered uniformly charged mutually penetrable small diameter spheres [2]. The value of sphere diameter must be chosen sufficiently small in order not to influence the calculation results. The validity of this condition was verified by diameter variation. At the initial moment, $t=0$, the coordinates and velocities of all particles were assigned by a random number generator. In most cases the coordinates corresponded to a uniform distribution; the velocities corresponded to the Maxwell velocity distribution function with a certain initial temperature.

The cube walls were regarded as mirror-reflecting ones. The corresponding boundary conditions were is follows. If at some time step a particle falls out of the cube volume, then the component of its velocity normal to the wall changes its sign. In other studies we use a variety of initial and boundary conditions versions.

A substantial progress in the carrying out of an enormous calculation size was achieved due to the creation of an original method. Assume that at a certain time moment, t_0, all the particles coordinates $r_k(t_0)$ and velocities $v_k(t_0)$ are known. The procedure of the $r_k(t_0+\Delta t)$ and $v_k(t_0+\Delta t)$ values determination, for the external (large) time step Δt, is the following. The calculation was conducted in two stages - predictor and correction stages. At the predictor stage integration with low accuracy was made by Runge-Kutta method. The average values of the coordinates and error of step are calculated. After that, one finds for each particle full force and four nearest particles at average coordinates. At the correction stage the Newton equations are integrated over time interval Δt using a Runge-Kutta fourth order of accuracy procedure with internal (small) time step $\delta t = \Delta t/N_t$, where N_t represents the number of internal steps.

At Runge-Kutta procedure the force acting on each particle is calculated in the form of a sum of two forces. The first force is due to the given particle interaction with its nearest neighbours, and with the particles for which the given particle is the nearest neighbour. The second force is due to the interaction with all rest of the particles and approximates by linear function of time. Time steps in the range $0.05<\Delta t/t_{ei}<1$ and $20<N_t<300$ were usually used in the calculations (here t_{ei} is average electron time of flight over a mean distance between ions).

The algorithm makes it possible to simulate with the *IBM PC 586 200 MHz* a systems up to 10^4 charged particles in a reasonable time. Time evolution of systems were traced over the time interval $t=(100\text{-}1000)\,t_{ei}$. The total energy conservation law was fulfilled in this conditions with an accuracy better then 1%. PLASMIC-Code has the big diagnostic part - the particle energy distribution functions, the mean values of potential energy, pressure, the kinetic coefficients and etc.

The research of classical Coulomb plasma (see review [3]) by computer simulation showed that recombination process is suppressed. The electron total energy distribution function was stationary and differed drastically both from the Boltzmann distribution law, which electrons must obey at equilibrium, and from distribution derived in the theory of three-body recombination. Analytical considerations show that the electron total energy distribution function may be obtained if one excludes the detailed balancing principle [3]. The three-body recombination at this state is suppressed by anomalously high and anomalously directed microfield caused drift.

In this paper (see also [4-5]) on the basis of the more exact and long many-particles-dynamics calculations the conclusion is made that slowing down of three-body recombination takes place, but for its explanation there is no necessity in the so radical assumptions. The observable effect of metastable state of supercooled plasma can be explained by adiabatic character of collisions between free and coupled electrons at far flights. On the example of a problem of two bodies, moving in central field, research of the characteristics of collisions coupled and free electrons carried out. Study of influence of features of Coulomb collisions on the electron drift coefficient and the electron diffusion coefficient along energy axis carried out. On the basis of the analysis of a problem of interaction free and coupled electrons in a field of ion it is possible to generalize about a significant deviation from the law of Coulomb collision cross-section. It is possible to speak about adiabatic character collisions in a plasma at far flights. Significant transfer of energy occurs or in case aiming parameter near radius of a orbit coupled electron, or at case very small energy of free electron, when its grab and fall on attracting dipole occurs. In these cases collision with transfer free electron of energy about coupled electron binding en-

ergy occurs. Such character of collisions does not permit to use for the description of process three-body recombination Fokker-Planck equation because of large size of energy microjumps.

The carried out many-particles-dynamics calculations of a system from 4000 particles demonstrate slowing down recombination about in ten times for a plasma with parameter characterizing the degree of plasma coupling $\delta=2e^6N_e/T_e^3\approx0{,}02$. Parameters of plasma of hydrogen are $N_e=10^{14}$ cm^{-3}, T_e=0,03 eV. The time of calculation is $850\ t_{ei}$. There are the numbers of "bounded" electrons N_e on the figure. Curves 1, 2, 3 represent the number of electrons N_e with full energy $\varepsilon < -2T_e, -4T_e, -6T_e$. At the time $t\approx50t_{ei}$ appears observable number of bounded electrons. The number of bounded electrons with full energy $\varepsilon < -4T_e, -6T_e$ depends linear from the time $t\approx100t_{ei}$. The computer experimental time of recombination is equal $t_{rec}\approx13000t_{ei}$, Thompson theory of three-body recombination time is equal $t_{rec}\approx2000t_{ei}$ [4].

The electron energy distribution function at the end of computation has not reached yet equilibrium distribution. The computation of 2-dimensional system was carried out for demonstration of achievement of the equilibrium state. Relaxation to the equilibrium state in the 2-dimensional system is faster as the close collisions occur more often. For the 2-dimensional system influence of the walls because of other ratio of volume and surface is loosed. Distribution, close to the equilibrium state, taking into account cut of potential of interaction on close distances is received.

Important aspect at simulation by a particles method is the account of influence of surface effects - boundary conditions. The study of the influence of different type boundary conditions to process recombination in a finite system of particles is carried out [5]. Is shown, that the mirror-reflecting walls can result to insignificant stimulate of recombination process. Specular walls do not have pronounced effect on the recombination relaxation rate. The walls introduce some mixing over different degrees of freedom of particles. In consequence of this mixing, the parameters of collisions in the volume change and, in perfect agreement with the principle of equilibrium-directed relaxation, the recombination flux somewhat increases.

It is possible to generalize that the known formulas of three-body recombination [6] describe filling of a coupled states up to binding energy about two - three temperatures. Further downward relaxation of electrons along the energy axis in a classical system slows drastically owing to the adiabatic nature of collisions of free and coupled electrons.

References

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