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On the interpretation of computer simulation of classical Coulomb plasma

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Contents

Abstract. The conclusions on the violation of some of the basic principles of statistical mechanics and physical kinetics reported by Mayorov, Tkachev, and Yakovlenko [Usp. Fiz. Nauk **164** (3) 297 (1994); Phys. – Uspekhi **62** (3) 276 (1994)] are shown to be insufficiently substantiated. These conclusions have been drawn from the results of a computer simulation of classical Coulomb plasma, but it is suggested here that these results admit an alternative interpretation. Rejection of the principle of detailed balancing is not an inevitable consequence of the computer simulation results; that this is so also follows from an analysis of microscopic processes reported in the present study. In fact, the behaviour of this type of plasma can substantially depend on near-wall phenomena. A limiting case of the system under consideration (two particles with opposite charges in a closed space) is analysed: collisions of the particles with perfectly reflecting walls are found to make the system behaviour ergodic and to lead to a distribution function that decreases in the domain of negative centre-of-mass energies.

... "*The site of devil's dislocation has not yet been found*" ...
S I Yakovlenko "How we found the devil" [2]

1. Introduction

In the March 1994 issue of *Physics – Uspekhi* there appeared under the heading 'From the current literature' an article by Mayorov, Tkachev, and Yakovlenko (hereafter referred to as MTY) "Metastable supercooled plasma" [1]. The authors overviewed the results of their computer simulation of the behaviour of a classical Coulomb plasma within a closed space [3, 4]. We think that some assertions and conclusions in Ref. [1] are not sufficiently substantiated and deserve comments.

MTY have studied plasma behaviour using the many-particle dynamics (MPD) computation method. The MPD method consists in the numerical solution of Newton's equations of motion for an ensemble of point electric charges enclosed in a finite space and obeying the Coulomb law. According to Ref. [1], in a plasma, supercooled relative to the ionisation equilibrium and confined by perfectly reflecting (elastic) walls, the recombination process rapidly slows down and a steady state is established that is different from the one expected for bulk-ionisation equilibrium.

On the basis of the results of their simulation, MTY came to the conclusion that one should abandon the "long-held views on the statistics of isolated (microcanonical) systems" [1] and predicted the feasibility of the eventual formation of long-lived plasmoids of the ball lightning type.†

MTY state [1] that they were able to derive an analytical expression for the energy distribution function in an isolated plasma (free from any "external stochastic action") only "at the price of rejecting the principle of detailed balancing" and, further, that "the computer simulation results showed the need to reconsider one of the fundamental principles of statistical mechanics and physical kinetics: namely the law of entropy rise in its present formulation"‡.

† We apologise in advance for the abundance of quotations from Ref. [1]: this is unavoidable in this type of communication.

‡ A relaxation towards thermodynamic equilibrium needs an intervention from outside that would make the system partly 'forget' its previous state. At this point one should pluck up courage and implicitly formulate the principal conclusion: given that the fulfilment of the laws of statistical mechanics requires a stochastic action from outside and that these laws correspond sufficiently well to what we observe in real life, there should exist an external source of stochastic action. We call it *external stochastiser* — its other name is devil" [2].

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Strictly speaking, such radical conclusions on the infringement of fundamental principles do not follow from the simulation data [1]. In our opinion, these data admit an alternative interpretation that does not require either the rejection of the principle of detailed balancing or a revision of the basic concepts of physical kinetics and statistical mechanics. Figuratively speaking, if the roof leaks, this is not a sound reason for breaking down the foundation.

2. The principle of detailed balancing: for an against

This is a fundamental principle of statistical physics, which states that in an equilibrium system every microscopic process proceeds at the same rate as the corresponding reverse process [5]. The principle of detailed balancing does not make it necessary to specify explicitly the kind of the equilibrium; different microscopic processes can have differing rates depending on the conditions prevailing in the system. An apparent violation of this principle might be due either to the lack of an actual equilibrium in the system or to an inadequate account of all the channels bringing the system to or removing it from a given state.

MTY believe that the recombination 'freezing' is related to the conservation of dynamic memory in a plasma isolated from any external action by perfectly reflecting walls. However, one can notice, on one hand, that there was no analysis of the correlation functions, although the latter might afford evidence on the dynamic memory conservation. On the other hand, there are no data whatsoever on the elementary recombination – ionisation processes that might reveal the dynamics of microscopic processes in the observed behaviour of the plasma. Evidently, the observed retardation of the recombination process may be explained either by the relative drop in the rate of recombination or by an increase in the rate of ionisation.

The lack of detailed information on the spatiotemporal evolution of the elementary processes (in particular, on the lifetimes of the bound states of the particles and specific decay mechanisms) makes it difficult to establish the origin of the so-called unexpected properties of the simulated plasma confined by perfectly reflecting walls in the MTY paper [1]. Moreover, it seems to us, to say the least, unjustified to draw radical conclusions on the basis of indirect evidence.

At this point, one should recall that the Boltzmann distribution does, in fact, follow from the principle of detailed balancing only under some additional assumptions (cf. Ref. [6]); in general, these assumptions are not valid under the conditions of computer simulation [1]. Therefore, one is not entitled to infer a violation of the principle of detailed balancing from the mere fact that the derived distribution function differs from the Boltzmann distribution.

3. Analysis of microscopic processes

In Ref. [1], the interpretation of the simulation results is based on the implicit assumption that the 'unexpected properties' of the simulated classical Coulomb plasma are due to bulk phenomena in the plasma; the perfectly reflecting walls are assumed to play only one role, namely isolate the plasma from the 'outside stochastic actions' (MTY regard this isolation as indispensable for the establishment of the presumed equilibrium state). Actually, these assumptions are far from being evident; they need justification, which is not provided in Ref. [1].†

When the total number of particles in the system under consideration is $N_0 \leqslant 10^3$, a significant part of them is located in the layer adjoining the walls, where the behaviour of the particles substantially differs from the bulk behaviour. Consequently, there are no reasons to regard the system considered in Ref. [1] as adequately representing the bulk properties of classical Coulomb plasma. Moreover, the characteristic particle time of flight from wall to wall $\tau_{\text{wall}} = L/V_{\text{T}}$ turns out to be comparable with (or a little longer than) the fastest characteristic times of particle bulk phenomena (here L and V_{T} represent the system size and particle thermal velocity, respectively), and is much shorter than the three-body recombination time: $\tau_{\text{wall}} \ll \tau_{\text{r}}$.

Table 1 presents the characteristic time scales for the three plasma simulation versions discussed in Ref. [1]. Here N, T, δ, and t represent the plasma number density, temperature, and the nonideality parameter, along with the actual time of simulation-system observation, respectively. The listed values of the three-body recombination time τ_{r} and the Coulomb collision time τ_0 were calculated with the use of the well-known formulas given in Ref. [1]. We have normalised all these times to $\tau_{\text{ei}} = N^{-1/3}/V_{\text{T}}$, which represents the characteristic time of flight of an electron over a mean inter-ion distance.

Table 1. Real parameters of three versions of simulation [1].

N/cm^{-3}	T/eV	δ	t/τ_{ei}	$\tau_{\text{r}}/\tau_{\text{ei}}$	τ_0/τ_{ei}	$\tau_{\text{wall}}/\tau_{\text{ei}}$
10^{20}	1.7	0.12	46	4.6×10^1	1.4	8
10^{17}	0.28	0.28	59	3.2×10^2	3.3	8
10^{14}	0.1	0.0006	50	8.5×10^4	13.5	8

The physical meaning of the aforementioned time deserves special consideration: this time plays an important role in the MTY concepts. Nevertheless, in their opinion, "this characteristic time does not appear in the traditional approach to kinetic problems based on a cut-off Bogolyubov chain" [1]. First of all, τ_{ei} does not depend on the mutual interaction between particles and makes sense even in the ideal gas. In reality, this is a purely kinematic characteristic time. Imagine a very sharp perturbation of plasma density (or of some other integral property of the medium). Let its initial spatial scale be very small (of the order of $N^{-1/3}$): the original conditions will be restored in time τ_{ei}. Of course, such a process could be called relaxation, but this would not relieve one from the necessity to analyse the corresponding correlation functions and to determine the correlation decay time. In a nonideal plasma the latter may turn out to be of the order of τ_{ei}, its precise value being determined by the mechanism of particle mutual interaction — what an occasion for recalling the well known effects of the spin echo and plasma echo type!

It follows from Table 1 that the statistical and kinetic properties of the system we are considering here depend to

† It is noteworthy that MTY do not discuss the physical nature of the so-called outside stochastic action: the demonological [2] and philosophical [3] aspects of the problem have been considered by Yakovlenko in separate publications.

a large extent on the near-wall rather than on bulk phenomena. This is especially so in the Knudsen gas case (see the third simulation version in Table 1). In Ref. [1] the choice of the boundary condition type described as a box with mirror walls is motivated as follows: the often used periodic boundary conditions bring the simulation far away from the initial dynamic equations; hence, they ''are inadmissible in studies of the fundamental properties of plasmas''. In our opinion, however, the model with perfectly reflecting walls, although very interesting in itself, may move the simulation even further away from reality: this is due to limitations in parameters available for use in computer simulation.

In this connection, it would be helpful to compare the existing bulk recombination theory with computer simulations employing periodic boundary conditions. A detailed comparative analysis of the two computation schemes (with either mirror-wall type or periodic boundary conditions) would also be very interesting.

4. The role of perfectly reflecting walls

In Section 4.2 of Ref. [1] entitled ''Anomalous drift towards positive energies'' one reads, ''In order to interpret reasonably the results of the *ab initio* simulation we had to postulate a strong drift along the energy axis from the zone of negative to the zone of positive electron energies. This drift is due to the microfields produced by all the charged particles''.

The hypothesis of the microfield origin of the anomalous drift finds in Ref. [1] no convincing confirmation. Instead, one learns from the final summary that ''it is also necessary to investigate the mechanism of the drift along the energy axis caused by the microfield discovered during MPD computer simulation''. The possible influence of perfectly reflecting walls on the formation of this drift is neither discussed, nor even mentioned†.

The confinement of the plasma-filled space imposes some obvious limitations on the behaviour of two kinds of particle bound states (particle aggregates), namely large bound states with sizes exceeding the wall-to-wall spacing and small-size aggregates with nonzero centre-of-mass velocities relative to the walls. In fact, the elastic reflection of particles from the wall does not exclude the energy exchange between the centre-of-mass and orbital motions. Therefore, the inter-action of a bound-particle aggregate with a perfectly reflecting wall turns out to be, generally speaking, an inelastic collision. It yields a nonzero contribution to the redistribution of particles between the free and bound states.

Consider now a particle bound state (aggregate) comprising two particles with opposite charge signs. A collision of such an aggregate with a perfectly reflecting wall may result in its 'ionisation' (a 'recombination' is also possible). In order to shed some light on the influence of the wall upon the ergodic properties of Coulomb systems, it is appropriate to consider the simplest case of a 'plasma' consisting of only two particles confined in a closed space.

† This is rather strange because in the same article MTY emphasised the important role of walls obeying all kinds of reflection laws but this one. In particular, it is noted in Ref. [5] that in the case of thermostated walls, the relation between the temperature of the gas T and the wall T_{wall} in equilibrium is given by $T = 3T_{\text{wall}}/4$(!?).

According to the ergodic hypothesis, the time-averaged value of any dynamic variable should coincide with its value averaged over the phase space with the $\delta[H(\boldsymbol{p}_i, \boldsymbol{q}_i) - H_0]$ measure. Here H_0 represents the total energy, while the Hamiltonian H has the form

$$H(\boldsymbol{p}_i, \boldsymbol{q}_i) = \frac{\boldsymbol{p}_1^2}{2m_1} + \frac{\boldsymbol{p}_2^2}{2m_2} - \frac{e^2}{|\boldsymbol{q}_1 - \boldsymbol{q}_2|} . \quad (1)$$

Thus, on the assumption of the validity of ergodicity, the distribution over the binding energy of the aggregates should satisfy the equation:

$$f(\varepsilon, H_0) = \int\limits_{\boldsymbol{q}_i \in V} \mathrm{d}\boldsymbol{p}_i \, \mathrm{d}\boldsymbol{q}_i \, \delta[H(\boldsymbol{p}_i, \boldsymbol{q}_i) - H_0] \delta[E(\boldsymbol{p}_i, \boldsymbol{q}_i) - \varepsilon] , \quad (2)$$

where

$$E(\boldsymbol{p}_i, \boldsymbol{q}_i) = H(\boldsymbol{p}_i, \boldsymbol{q}_i) - \frac{(\boldsymbol{p}_1 + \boldsymbol{p}_2)^2}{2(m_1 + m_2)} \quad (3)$$

represents the total energy of the particle pair in the centre-of-mass reference frame. The integration in formula (2) should be performed over all momenta and a certain domain V of the configuration space. Should this domain be invariant with respect to some translations and rotations, one would have to take into account the corresponding integrals of motion in Eqn (2).

We note that in Ref. [1] MTY use a distribution function $f(\varepsilon)$ over particle total energy in the laboratory reference frame, and their criterion for the existence of a bound state amounts to the negative sign of this energy. Such a restriction does not correspond to a more adequate criterion involving pair correlation functions. In particular, this approach is unable to distinguish two-particle aggregates from many-particle ones. It is also evident that in weakly nonideal plasmas the criterion based on the $f(\varepsilon)$ function would underrate the number of two-particle bound states: for instance, a two-particle aggregate with a sufficiently high centre-of-mass velocity may, indeed, have a positive total energy. In our analysis we use a different criterion: the particle aggregate is regarded to be in a bound state if $E(\boldsymbol{p}_i, \boldsymbol{q}_i) < 0$ (which means that the particle orbits are elliptical in the centre-of-mass reference frame).

Consider now two rather evident properties of integral (2). First, one has $f(\varepsilon, H_0) \neq 0$ only if $\varepsilon < H_0$; in this case $f(\varepsilon, H_0) \simeq (H_0 - \varepsilon)^{d/2-1}$ with $\varepsilon \to H_0$, where d is the dimension of the region V. Second, it is easy to derive an asymptotic expression for $f(\varepsilon, H_0)$ when $\varepsilon < 0$ and $|\varepsilon| \gg e^2/L$, where L is the minimal characteristic length of the region V. We have:

$$f(\varepsilon, H_0) \simeq \begin{cases} \varepsilon^{-2} , & d = 2 , \\ \varepsilon^{-5/2} , & d = 3 . \end{cases} \quad (4)$$

There are certain domains V, for which the integral (2) can be calculated analytically, but the corresponding analytical expressions are too cumbersome to be reproduced here.

We have used our computer to test the ergodicity of the system; the computer simulation was performed as follows. We assigned two unit-mass particles with unit electrical charges of opposite sign to move within a square with perfectly reflecting sides (mirrors). The square-shaped boundary ($d = 2$) was set up to have unit length sides. Explicit expressions for particle trajectories are readily derived from the appropriate formulas of mechanics. The computations are thus reduced to finding out which of the particles had a collision with a wall, and when and where did this event (particle reflection from the wall) occur. This makes numerical solution of differential equations unnecessary. By finding the roots of algebraic equations much higher accuracy can be achieved. For instance, after several thousands of collisions, the relative change in the particle total energy was of the order of 10^{-7}.

We plotted the distribution function $f(\varepsilon, H_0)$ thus obtained in the form of a histogram representing the residence time of the system in states with binding energies in the $(\varepsilon, \varepsilon + \Delta\varepsilon)$ interval. The results of a typical computation of the function $f(\varepsilon, H_0)$ with $H_0 = 0.3$ obtained after about 10^{-4} collisions with the wall are shown by the broken line in Fig. 1. The tail of the distribution was cut off at $\varepsilon = -10$. The maximal binding energy modulus $|\varepsilon|$ in our simulation was 10^3. The solid curve represents the analytically calculated dependence (2). The two curves were normalised to make the integrals of both functions coincide.

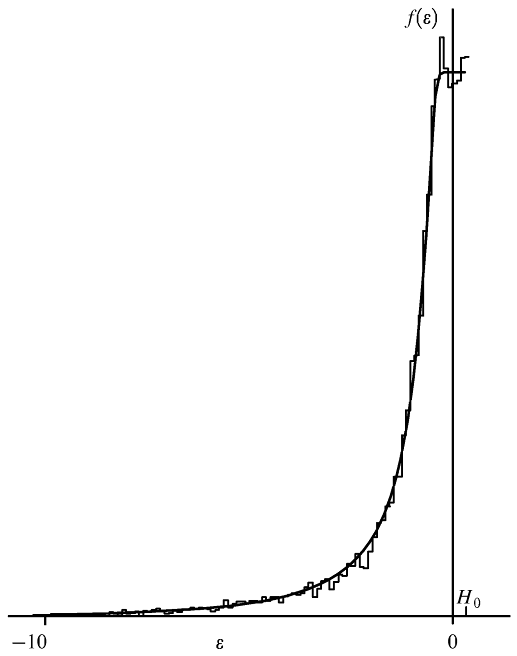

Figure 1. Energy distribution function in the centre-of-mass system for the case of two particles in a closed space. The solid line represents formula (2); the broken line shows the results of computer simulation.

The evident agreement between the analytical formula and the computer simulation results confirms the ergodicity of our two-particle classical 'plasma' model. One should make it clear that such a large number of particle–wall collisions was needed only to scan the largest possible part of the isoenergetic surface and to accumulate data for statisitical evaluation. We obtained similar results for a large ensemble of equal-total-energy particle pairs not interacting with each other. In this case a few collisions with the wall yield reliable simulation data. The distribution function (2) is here different from the Boltzmann distribution but this can be explained without rejecting either the principle of detailed balancing (contrary to Ref. [1]) or the ergodic hypothesis for our system. Thus, the difference between the distribution function $f(\varepsilon)$ reported in Ref. [1] and the one expected for a bulk-recombination plasma may be due to the influence of perfectly reflecting walls. Indeed, it follows from the characteristic times listed in Table 1 that this influence cannot be neglected.

In Ref. [1] the recombination retardation was attributed to incomplete system intermixing (that is, retention of the dynamic memory). Zhidkov and Galeev [7] arrived at a similar conclusion with regard to the retention of the dynamic memory for the conditions of computer simulation [1] for an unbounded plasma by calculating the Lyapunov exponents. In Ref. [7], retention of the dynamic memory was attributed to the presence of invariant tori in the Coulomb system phase space, which would naturally lead to ergodicity violation.

The existence in unbounded plasma of fairly small particle aggregates, weakly interacting with the rest of the system, and of the corresponding invariant tori is beyond any doubt. However, it follows from the agreement of the analytical and computed curves in Fig. 1 that perfectly reflecting walls bring about complete destruction of the invariant tori and formation of a distribution function that decreases in the negative energy range. Thus, it is possible to draw another conclusion from the results of the computer simulation [1], namely that the ergodicity of Coulomb plasma improves instead of being violated.

5. Conclusion

The main results of the present work are as follows.

The need to reject the principle of detailed balancing does not inevitably follow from the computer simulation data reported in Ref. [1]. This need is not confirmed by our analysis of the dynamics of microscopic processes.

The relations between the characteristic times in the computer simulation [1] indicate that near-wall processes can significantly affect the behaviour of the plasma.

An analysis of the limiting case of the system under consideration (two oppositely charged particles in an enclosed volume) shows that collisions of particles with perfectly reflecting walls lead to an ergodic plasma behaviour with a distribution function that decreases in the domain of negative centre-of-mass energies.

Various interpretations of the computer simulation [1] that do not take into account the wall effect to which we have drawn attention are in our opinion unfounded.

Of course, we could not dwell here on all the aspects of the discussed study. Let us just mention that the rather hypothetical analogy between plasma ionisation and metastable states occurring in phase transitions of the first kind, mentioned in the title of Ref. [1] and the abstract, but practically not elaborated in the text of the article, leaves more questions than answers.

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Comment on the article

'On the interpretation of computer simulation of classical Coulomb plasma' by A M Ignatov, A I Korotchenko, V P Makarov, A A Rukhadze, A A Samokhin

S A Mayorov, A N Tkachev, S I Yakovlenko

Fallacy of the new interpretation. The main content of the article by Ignatov et al. consists in a new interpretation of those results of our computer simulation that have been reported fully in Ref. [1] and briefly described in our review article [2]. We found a retardation of the recombination relaxation in a system comprising a large number (~ 1000) of Coulomb particles enclosed in a three-dimensional box with perfectly reflecting (perfectly elastic) walls. Ignatov et al. attribute this effect to the 'ionisation' of the bound-particle aggregates at the walls. They believe that ionisation of a bound pair of particles occurs upon collision with the wall: total energy of the particle pair is then redistributed between the energy of motion of the two-particle aggregate as a whole, and the binding energy of the pair of particles.

This interpretation is wrong:

1. Under the conditions of our computer simulation the aforementioned effect is very weak. Actually, the non-inertial effects in the course of the particle-pair reflection from the wall are negligibly small because of the great disparity between the electron and proton masses (please note that in our computer simulation of particle dynamics we attributed to the particles their true masses). Even simple estimates show that the effects considered here are weak, and this was confirmed by direct computer simulations. In the case of an infinite ion mass these effects are altogether absent, but, as expected, simulations with infinite ion mass yielded an electron distribution function practically indistinguishable from that for the case of the ion mass equal to the mass of a proton.

2. In the supercooled plasma we are cosidering here (the initial conditions conform to full ionisation of the plasma at a low temperature) any energy exchange between the translational and ionisation degrees of freedom that is reversible in microscopic terms would be expected, according to generally accepted concepts, to favour recombination rather than ionisation, in contrast to the views of Ignatov et al. We have also verified this directly in our computer simulations. In the case of particles of equal mass the distribution function over the total energy was found to approach the recombination distribution. As expected, the number of bound electrons exceeded that observed in an electron – ion plasma under similar conditions. We reported elsewhere [3] the results of our many-particle dynamics simulations for particles of equal masses with an analysis of the effects of noninertial behaviour of the centre-of-mass system on reflection from the wall.

Thus, the retardation of recombination relaxation under the conditions of our computer simulation cannot be attributed to the deformation of the bound-electron distribution produced by particle reflection from perfectly elastic walls, as has been suggested by Ignatov et al.

Other erroneous statements. The article by Ignatov et al. contains a number of further substantial misconceptions in the understanding of the three-body recombination process and misrepresentations of the results obtained by other authors. In particular, one has the impression that Ignatov et al. have restricted their study of our research to reading the popular science literature they refer to, instead of our original scientific publications listed in the references to our review article [2]. Let us dwell here only on a few examples.

1. It follows from Section 3 of the article by Ignatov et al. that these authors have not understood that the time of the establishment of recombination relaxation (i.e., the time for the establishment of the distribution at the 'throat of the sink') is much shorter than the recombination time (the time required for the bulk of the electrons to pass through the 'throat of the sink'). After an unsound juxtaposition of various characteristic times in Table 1, the authors came to the misguided conclusion that the total system observation time in our computer simulation was too short. This is particularly surprising, since this problem has been analysed in detail in our study [1] (cited in our review [2] also as Ref. [1]). One can also find there a comparison of the characteristic recombination relaxation times with the total system observation times; all these times together with the calculation parameters are tabulated in Ref. [1]. It is noteworthy that in our review [2], discussed by Ignatov et al., we reproduced Fig. 1 from the original work [4]; this figure illustrates the incompatibility of relaxation times derived from simulation and from traditional theory.

2. In the aforementioned Section 3 of the article its authors correctly state that for the determination of the physical nature of τ_{ei} it is necessary to find the correlation decay time. This is exactly what we have done in Ref. [5], by analysing, in particular, the correlation functions of plasma microfields together with the electron and ion potential energies. The definition of this time is to be found on page 281 of our review [2], where there is a direct reference to this research.

3. In Section 4 of the article its authors use the results of their analysis of a two-dimensional system of two particles with equal mass in order to interpret our results. We find this puzzling: even without any calculations it is obvious that for two energy-isolated particles the equilibrium distribution will not be Boltzmannian. It does not matter what kind of mechanism (a wall-dependent or some other one) drives the relaxation towards equilibrium. The dis-

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tribution for ''a large ensemble of particle pairs not interacting with each other'' discussed by Ignatov et al., is indeed radically different from the equilibrium distribution for an ensemble consisting of as few as ten particles.

The question how many particles are required for a distribution approaching to the Boltzmann distribution was quite thoroughly analysed in the Appendix to our article [1]. Let us recall that we compared in greatest detail the results of our simulation not with the Boltzmann formula but with the recombination distribution derived from the traditional theory based upon the principle of detailed balancing in its traditional formulation.

4. In the final part of Section 4, Ignatov et al. assert that Zhidkov and Galeev [6] reached a conclusion similar to ours concerning the retention of dynamic memory in a system comprising many Coulomb particles. In reality, these authors have come to a diametrically opposite conclusion: namely that the ''motion is Lyapunov-unstable and, consequently, stochastic''. Incidentally, this result was obtained in Ref. [6] because of fallacious analysis of the nature of motion of the dynamical system (see Ref. [7] for further details).

5. In the footnote to Section 4 Ignatov et al. ascribe to us an evidently erroneous assertion that gas–wall equilibrium occurs with the temperatures of the gas and the wall not being the same. What we have stated in our papers was different [1, 8]. When the reflections of the particles from the walls are inelastic (a case also simulated in our computer) the equilibrium is violated; therefore, one has to independently verify whether the particle distribution is Maxwellian (which we have done in our simulations). The equilibrium violation under the reflection law we have selected manifests itself in the requirement of different gas and wall temperatures at equal heat fluxes to and from the wall.

Since lack of space prevents us from dealing with other misconceptions in the article by Ignatov et al., we leave it to the readers to find out for themselves the real state of affairs by becoming acquainted with our original publications.

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