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Molecular dynamic study of pressure fluctuations spectrum in plasma

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Abstract. Pressure of plasma is calculated by using classical molecular dynamics method. The formula based on virial theorem was used. Spectrum pressure's fluctuations of singly ionized non-ideal plasma are studied. $1/f$-like spectrum behavior is observed. In other words, flicker noise is observed in fluctuations of pressure equilibrium non-ideal plasma. Relations between the obtained result and pressure fluctuations within the Gibbs and Einstein approaches are discussed. Special attention is paid to features of calculating the pressure in strongly coupled systems.

1. Introduction

It is well known that fluctuations of thermodynamic quantities are characterized by a Gaussian distribution function. According to Einstein approach the probability of thermodynamic fluctuations near the equilibrium point is described by the relation [1]:

$$w(\Delta x) \sim \exp^{\Delta S(\Delta x)}, \tag{1}$$

where Δx is deviation of thermodynamic quantity from equilibrium value, $\Delta S(\Delta x)$ is the deviation of entropy from its equilibrium value, which depends on the value of the fluctuations. Assuming that the entropy is analytic function, and considering that the equilibrium point corresponds to the point of its maximum it can be represented as a power series: $\Delta S(\Delta x) = a_2\Delta x^2 + a_3\Delta x^3 + ...$ The first member of this series gives a Gaussian distribution for (1) at negligibly small deviation of x from the equilibrium value.

The article [2] presents non Gaussian fluctuations of pressure in plasma. Resolving of this paradox was general motivation of this work.

In this paper spectrum pressure fluctuations was determined by MD simulation. The first three sections are devoted to the description of the model, discussion of the simulation accuracy and validity of the model for studying pressure fluctuations. The final section presents the results and their discussion.

2. Simulation model

The model is exactly the same as in the [2]. It considers a system of non-degenerate electrons and singly charged ions with masses m and M respectively . The mass ratio is chosen to be equal

$M/m = 100$, since the values of $M/m \geq 100$, this parameter has little effect on the dynamics of electrons [3]. For the integration of the equations of motion used Leap-Frog scheme second-order accuracy with time step $\Delta t = 1.66$ as. The Langevin thermostat is applied for equilibration system. Presented in this paper results obtained from analysis of the equilibrium MD trajectory without using any thermostat, the total duration of which was 8.3 ps, which corresponds to the 5×10^6 steps in time. The temperature of ions and electrons are equal $T = 11600$ K. The number of ions and electrons in the system is $N = 1000$. The periodic boundary conditions are used.

To eliminate the Coulomb singularity and to account for quantum effects the electron-ion interaction potentials are usually corrected at short distances [4]. A simple shell-like potential was used:

$$\begin{cases} U(r_{ij}) = -\frac{e^2}{4\pi\varepsilon_0 r_{ij}}, & r_{ij} \geq r_{\text{cut}}, \\ U(r_{ij}) = -\frac{e^2}{4\pi\varepsilon_0 r_{\text{cut}}} = E_0 = -5.0 \quad \text{eV}, & r_{ij} < r_{\text{cut}}. \end{cases} \tag{2}$$

The electron-electron interaction and ion-ion interactions are the simple Coulomb. The potential energy of system is pair-additive. It means that total potential energy of system is the potential energies of all particles pairs in sum.

3. Pressure calculations

The technique of pressure calculations used in this article is conventional for this class of problems [5–8]. The pressure P can be calculated by a mechanistic prescription equating the exterior and interior forces on the container [5, 9]. This leads to the virial expression for the pressure in an atomic system:

$$P = \frac{k_B T N}{V} - \frac{1}{3V}\overline{\sum_i \mathbf{f}_i \mathbf{r}_i}. \tag{3}$$

It should be noted that this method of obtaining the equation (3) is not really valid for the infinite periodic systems used in computer simulations: there are no container walls and external forces. This article do not discuss the problem of finding limits applicability of virial expression here. It considers only the applicability of formula (3) for the potential (2) with periodic boundary conditions. The equation (3) is proved for the case when the potential energy of the system is a homogeneous function (if the argument is multiplied by a coefficient, then the result is multiplied by some power of this coefficient $E_{\text{p}}(\alpha\mathbf{r}) = \alpha^k E_{\text{p}}(\mathbf{r})$) [10]. The proof is based on Bogolyubov-Zubarev theorem. The main advantages of this evidence is independence on any suggestions about container walls and any separation of internal and external forces. The potential (2) is homogenous function ($k = -1$). Thats why according to [10] equation (3) is the exact expression for calculating the instantaneous pressure of an infinite system.

Well known that MD simulations with periodic boundary conditions is only approximation of continues infinite media. The so-called long-range corrections of equation (3) usually are used to account the difference between the infinite system and the system with periodic boundary conditions [11, 12]. The potential (2) is pair-additive. The article [7] shows that in this case any long-range correction is not needed.

For further discussion, it is important to emphasize that all the evidence of the formula (3) explicitly or implicitly use the Gibbs approach.

4. Numerical noise and pressure fluctuations

The fluctuation of any quantity determined from MD simulations consists of physical fluctuation and numerical errors. The important task in the study of pressure fluctuations is to evaluate last one. There are three general sources of numerical mistakes in MD—errors computing force acting between two particles, summation of forces acting on the particle and integration equations of

motion. The contribution of these errors can be estimated by the change in pressure when increasing of accuracy of computing forces or decreasing of the time step. It was established that the relative error of three sources outlined above does not exceed 10^{-8}.

It was found that increasing amounts of particles N in the system leads to the fast increasing computational error. But the dispersion of pressure behaves like N^{-1} in full agreement with the generally accepted theory. So increasing number of particles in the system leads to the fast increasing of the ratio between numerical and physical fluctuations of pressure. The source of it is a summation on the right hand side of equation (3). Let approve it analytically.

Replace the summation over the particles on the summation in pairs:

$$\sum_{i}^{N} f_i r_i = \sum_{i}^{N} \sum_{j>i}^{N} f_{ij} r_{ij} = W. \tag{4}$$

Let's present the virial of a system W as the sum of three variables. Where W_{ee}, W_{ii} and W_{ie} is the virial of all electron-electron, ion-ion and electron-ion interactions respectively:

$$W = W_{ee} + W_{ii} + W_{ei}. \tag{5}$$

According to the [13], you can replace the summation over pairs of particles to integration at an average density n including the pair correlation function $g(r)$. Without loss of generality we can assume molecular cell a spherical with radius R:

$$W_{ee} = \sum_{i}^{N_e} \sum_{j>i}^{N_e} f_{ij}^{ee} r_{ij} = \sum_{i}^{N_e} w_i^{ee}, \tag{6}$$

$$w_i^{ee} = \sum_{j>i}^{N_e} r_{ij}^{ee} f_{ij} = \int_0^R [r f(r)] \, (n_e g_{ee}(r))(4\pi r^2 \, dr) =$$

$$= 4\pi n_e \int_0^R g_{ee}(r) \left(-\frac{1}{r^2} \right) r^3 \, dr = -4\pi n_e \int_0^R g_{ee}(r) r \, dr. \tag{7}$$

To simplify the equations coefficient $\frac{e^2}{4\pi\varepsilon_0}$ omitted. The well-known property of the pair correlation function is $\lim\limits_{r\to\infty} (g(r)) = 1$. Assume that $g(r) = 1$ for sufficiently big r:

$$w_i^{ee} \approx -4\pi n_e \left[\int_0^{\varepsilon} g_{ee}(r) r \, dr + \int_{\varepsilon}^{R} r \, dr \right] =$$

$$= \varphi_{ee}(\varepsilon) + 2\pi n_e R^2 \sim R^2 \sim N^{\frac{2}{3}},$$

$$W_{ee} = N_e(\varphi_{ee}(\varepsilon) + 2\pi n_e R^2) \sim N^{\frac{5}{3}}. \tag{8}$$

Similarly we can prove the following assertions:

$$W_{ii} \approx N_i(\varphi_{ii}(\varepsilon) + 2\pi N_i n_i R^2) \sim N^{\frac{5}{3}}, \tag{9}$$

$$W_{ei} \approx (N_i + N_e)\varphi_{ei}(\varepsilon) - 2\pi R^2(N_i n_e + N_e n_i) \sim N^{\frac{5}{3}}. \tag{10}$$

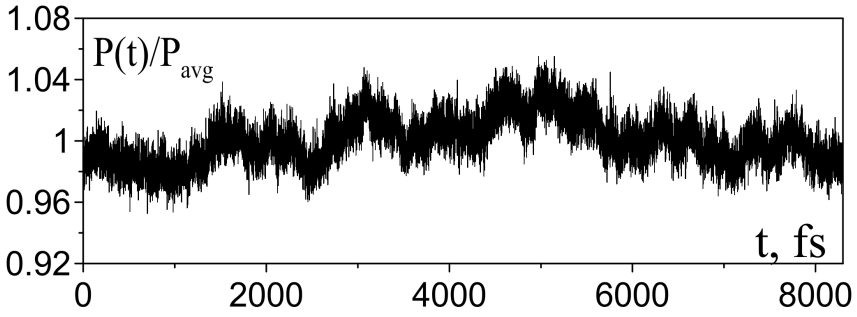

Figure 1. Dependence of normalized pressure on time.

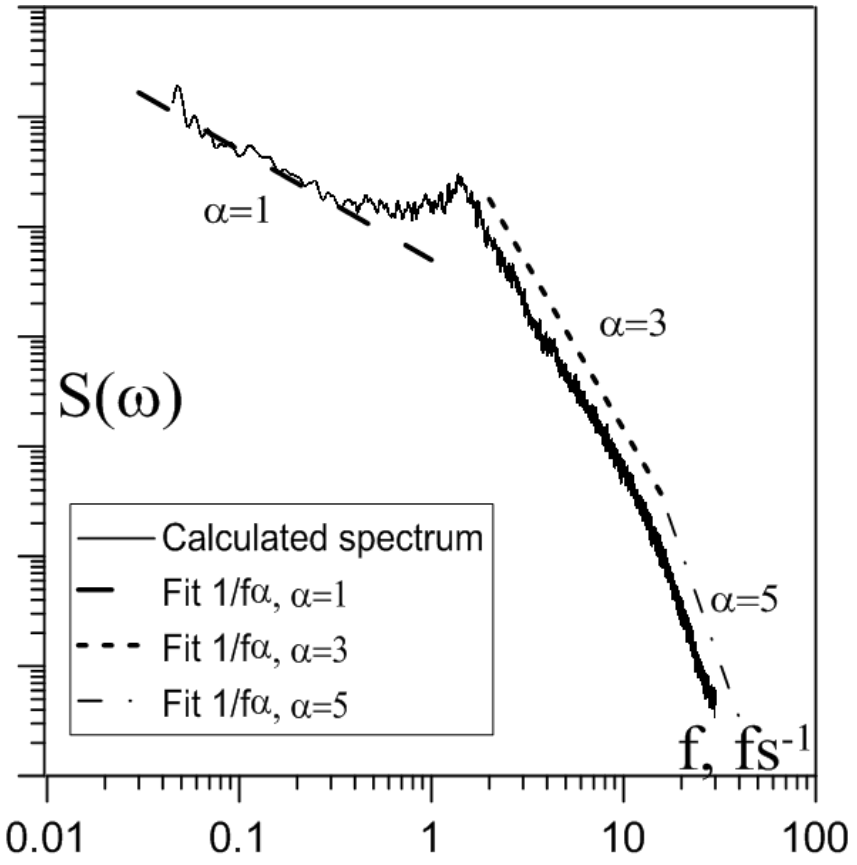

Figure 2. Pressure fluctuations spectrum $S(\omega)$, $f = \omega/2\pi$. The solid line represents the MD result. Other lines are fits of it.

It appears from this that the virial W is little difference between the two fast-growing and very close quantities W_{ei} and $W_{ee} + W_{ii}$. This conclusion and equation (8,9,10) are perfectly confirmed by the MD results. Note that the numerical problem in formula (3) exists only in systems with a long-range potentials because $\lim\limits_{R\to\infty} w_i^{ee}(R) = const$ for short-range force fields.

After analyzing all sources of numerical errors can conclude that the ratio of amplitudes of numerical noise and thermodynamic fluctuations is less 10^{-3}.

5. Spectrum pressure fluctuations

Consider a system with temperature $T = 11600$ K and density $n_e = n_i = 5 \times 10^{18}$ cm^{-3}. According to the article [2] at these parameters difference between Gaussian distribution and distribution of pressure fluctuations are most evident. Electron plasma period in this system is $\tau_e = 1/f_e = 2\pi/\omega_e = \sqrt{\epsilon_0 m_e/(e^2 n_e)} = 49$ fs. The MD trajectory length is 8.3 ps. or 169 electron plasma periods. The coupling parameter is:

$$\Gamma = \left(\frac{4\pi n_e}{3}\right)^{1/3} \frac{e^2}{4\pi\epsilon_0 k_B T} = 0.4. \tag{11}$$

The average of the pressure P_{avg} and its variance were calculated according to generally accepted formulas. Figure 1 shows the dependence of the normalized equilibrium pressure in the electron-ion system on time. Without any analysis it is obvious that $P(t)$ is not Gaussian process. To analyze properties of this process we estimate spectrum of pressure as function of time. There is an conventional way of calculating the spectrum $S(\omega) = |\mathcal{F}\{P(t)\}|^2$, where $\mathcal{F}$ the Fourier transform. But Welch method is used here. Although mathematically this method is equivalent to Fourier transform based one, they differ from the numerical point of view. The Welch method is more precisely (see [14] for the details).

The spectra pressure fluctuations are given in figure 2. According to the Einstein approach [1], this spectrum should be white noise spectrum ($S(\omega) = const$). But it is clear that the graph can be approximated by superposition of three lines:

$$\begin{cases} S(\omega) = c_1/f, & 0.03 < f < 0.3 \quad \text{fs}^{-1}, \\ S(\omega) = c_2/f^3, & 2 < f < 20 \quad \text{fs}^{-1}, \\ S(\omega) = c_3/f^5, & f > 20 \quad \text{fs}^{-1}, \end{cases} \tag{12}$$

where c_1, c_2 and c_3 some constants, $f = \omega/2\pi$. Maximum of spectrum is reached at the minimum resolvable frequency. Maximum of spectrum is reached at the minimum resolvable frequency and depends on the time observation (length of MD trajectory). Last property and shape of the spectrum allowed to assert that the flicker noise are observed in pressure fluctuations of equilibrium plasma [15–19].

For Coulomb systems pressure and potential energy are strongly correlated values [10, 20]. There are articles [21–24] which reported flicker noise in potential energy of their system. In all cases it is different biophysical MD system with a strong Coulomb interaction. This demonstrates that the flicker noise is observed for a fairly wide range of different Coulomb systems.

6. Conclusions

The spectrum of equilibrium plasma pressure are investigated. Confirmed result of the article [2]: fluctuation of plasma with temperature $T = 11600$ K and density $n_e = n_i = 5 \times 10^{18}$ cm^{-3} are non Gaussian. On the basis of the obtained spectrum concluded that the flicker noise are found in the pressure fluctuations.

It is shown that the accuracy of calculations by formula (3) requires special attention in the case of long-range potentials. A physical explanation of the reasons for this are given.

The article [10] shows that the pressure fluctuations in the Gibbs and Einstein approach are not equal. Moreover their physical meaning is generally not equivalent. Any conclusions about Gauss distribution of pressure fluctuations are obtained using Einstein's approach. At the same time all results based on the virial equation obtained in the Gibbs approach. This is the reason of paradox, which is announced in the introduction.

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