Thermodynamic functions for Coulomb system in Paul trap

D S Lapitsky, V S Filinov, R A Syrovatka, L V Deputatova, L M Vasilyak, V I Vladimirov and V Ya Pecherkin
Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
E-mail: dmitrucho@yandex.ru

Abstract. The virial equations for Coulomb system were theoretically studied. The system was captured by the linear Paul trap. The dependence of virial equations on parameters of particles and trap were found. The dynamics of pair correlation functions of Coulomb systems in electrodynamic trap have been obtained. The considered system showed to be highly nonideal with coupling parameter $\Gamma = 10^{10}$.

1. Introduction
The possibility of charged particle capturing by alternating electric fields of the Paul trap was theoretically and experimentally shown in [1,2]. The method of particle capturing and removal from gas flows by electrodynamic traps has been suggested in [3–5]. Trap examples, their modifications and the physical parameters needed for particle capturing have been obtained in [1,6–9]. Similarly charged microparticles in the trap can form strongly correlated nonlinear Coulomb systems with such effects as: system self-locking near the ends of the linear Paul trap [4,10], self-organizing in layers [11] which can be harmful for particle filtering. The average potential energy of interparticle interaction can be much higher than their average kinetic energy and affects the behavior in Coulomb system. The aim of this work is theoretical study of virial equations for strongly coupled Coulomb systems of charged particles in electrodynamic traps, its time evolution and the influence of trap parameters on it.

The equations of state of nonideal dissipative flat and 3-d systems of particles in dusty plasmas were studied in [12,13]. For the analysis of the equations of state the spatial correlation functions are usually used [14].

This paper presents time evolution of pair correlation functions of the Coulomb systems of microparticles without Debye screening inside the Paul trap. Using the statistical theory of liquid state [15] thermodynamic properties of strongly nonideal Coulomb system have been calculated: full energy of the system, its internal pressure and Coulomb coupling parameter $\Gamma$ [16,17]. The considered system is highly nonideal with coupling parameter of order $10^{10}$.

2. Mathematical simulation
In simulations, 4 electrode trap was used [1]. The trap in simulations consisted of four cylindrical electrodes with radii $r = 1.5$ mm and length $L = 10$ cm, located along central axis $y$. Interelectrode distances were $h = 1.6$ and 2 cm. Alternating voltage $U_0 \sin(\omega t)$ with phase
Figure 1. Coulomb system of 10 000 microparticles captured inside the trap at 7.5 s after injection. Black lines in left figure and black dots at the right one are trap electrodes. Grey dot and ring indicate the central particle and sphere inside which pair correlation function $g(r)$ was calculated.

shift equal to $\pi$ between neighboring electrodes was applied to the trap. The alternating-voltage amplitude was $U_\omega = 5$ kV and frequency of alternating voltage was 50 Hz.

Particles motion was simulated by Brownian dynamic method and was described by the system of Langevin equations:

$$m_p \frac{d^2 r_i}{dt^2} = F_t(r_i) + F_{\text{int}}(r_i) - 6\pi \eta r_p \frac{dr_i}{dt} + F_g + F_b,$$

where $m_p$ and $r_p$ are particle mass and radius respectively in assumption of spherical particles, $r_i$ is radius vector of particle $i$, $\eta$ is the dynamic viscosity of the gas medium ($\eta = 18.2 \ \mu\text{Pa s}$ [18]), $F_t(r_i)$ is the force of the trap electrodes, $F_b$ are stochastic delta-correlated forces accounting for stochastic collisions with neutral particles (the temperature of medium was $T = 300 \ \text{K}$), $F_g$ is the gravitational force. To simulate dynamics of charged particles, system (1) was solved by the numerical method [19].

In simulations, 10 000 particles were injected in the center of the trap. Parameters of the simulations were taken close to experimental data [1, 3]. Particle density was 3990 kg/m$^3$. The number of independent numerical experiments was carried out for particles with radii $r_p = 1–2 \ \mu\text{m}$ and charges $q_p/e = 2500$ to 10 000, where $e$ is the elementary electron charge.

Figure 1 presents Coulomb system of 10 000 microparticles captured inside the trap at 7.5 s after injection. Black lines in left figures and black dots in the right ones are trap electrodes.
Figure 2. Time evolution of pair correlation function $g(r)$ for 1 $\mu$m particles with $g_p/e = 2500$. Black solid line corresponds to start time and dash line corresponds to 10 s after injection.

Grey dot in the center of the Coulomb system and ring indicate the central particle and sphere inside which pair correlation functions $g(r)$ were calculated. The diameter of the sphere in simulations was equal to $r_g = h/2$ (in figure 1) that was enough to cover sufficient amount of particles, to calculate the $g(r)$ the sphere was divided into 20 concentric spheres and the number of particles inside each of these spheres as well as spheres volumes were calculated. Figure 2 presents time evolution of pair correlation function at the first moment after injection and at 10 s after injection. Figure 2 presents b-spline approximation of the $g(r)$ that can be harmful for the first peak for $g(r)$ at the first moment after injection but this Coulomb system state was not analyzed in the work. First peaks of $g(r)$ in figure 2 was shifted because of interparticle Coulomb repulsion.

For calculations of Coulomb system energy $U$ and inner pressure $P$, we have used the following modifications of the related formulas of statistical theory of liquid state [15]:

$$U = \sum_N \left( \frac{m_pv_i^2}{2} + m_p g h_i \right) + \frac{3}{2} kT + \frac{2\pi}{v} \int_0^\infty \Phi(r) g(r) r^2 dr \approx \frac{2\pi}{v} \int_0^{r_g} \Phi(r) g(r) r^2 dr,$$

$$P = \frac{2}{3v} \left[ 1 - \frac{\pi}{v(m_pv_i^2)} \int_0^\infty \frac{d\Phi(r)}{dr} g(r) r^3 dr \right] \approx \frac{2\pi}{3v^2} \int_0^{r_g} \frac{d\Phi(r)}{dr} g(r) r^3 dr,$$

where $\Phi(r)$ is the Coulomb potential of interparticle interaction, $N$ is the number of particles inside the grey sphere of volume $V$ in figure 1, $v = V/N$ is the volume occupied by one particle, $v_i$ and $h_i$ are speed and height of the particle number $i$ above the bottom electrode respectively, $g$ is the free fall acceleration and $\langle m_pv_i^2 \rangle/2$ is the average kinetic energy of particles. The trap limited the considered system of particles and pair correlation function $g(r)$ was taken in the sphere of fixed radius $r_g$, so integrals in equations (2) converged. In the equations for $U$ and $P$ terms accounting for average kinetic, gravitational and thermal energies were neglected because they were of two or four orders of magnitude smaller than terms accounting for potential energy.
Figure 3. Time evolution of energy of Coulomb system for different interelectrode distances.

Figure 4. Time evolution of pressure of Coulomb system for different interelectrode distances.

of interparticle interaction. For an example in case of 1 \( \mu \)m particles type,

\[
\left[ \sum (m_p v^2 / 2 + m_p g h) \right] (kT)^{-1} \sim 10^9
\]

while

\[
\left[ \frac{2\pi}{\nu} \int_0^{r_\infty} \Phi(r)g(r)r^2 dr \right] (kT)^{-1} \sim 10^{11}.
\]
Figure 5. Time evolution of virial equations for different interelectrode distances and particle charges: from $q_p/e = 2500$ for 1 µm particles to $q_p/e = 10000$ for 2 µm particles.

The evolution of energy and pressure of the Coulomb systems for different interelectrode distances of the trap are presented in figures 3 and 4. The Coulomb coupling parameter related to figures 3 and 4 was of order [16, 17]

$$\Gamma = \left[ \frac{2\pi}{\nu} \int_0^{r_s} \Phi(r)g(r)r^2dr \right](kT)^{-1} \sim 10^{10} - 10^{11}$$

indicating highly nonideal state of Coulomb system. After particles injection the average distance between particles increases and the energy of interparticle interaction decreases. This causes the energy and pressure decay. The Coulomb systems tend to stabilize and energy and pressure tend to an asymptotic value.

As the kinetic energy of particles is much bigger than thermal energy the virial equation for Coulomb system is presented by the equation $PV/(\langle m_p v^2 \rangle/2)$.

The dependencies of virial equations on the trap and particle parameters are presented in figure 5. The dependence $PV/(\langle m_p v^2 \rangle/2)$ decreases with the growth $q_p$ and with decreasing of interelectrode distance.

3. Conclusion

The thermodynamic functions of Coulomb system were studied. Using the statistical theory of liquid state time evolution of pair correlation functions, energy, pressure and virial equations of Coulomb systems has been studied for different sizes of electrodynamic traps.

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