Modeling fine particle (dusty) plasmas and charge-stabilized colloidal suspensions as inhomogeneous Yukawa systems

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Abstract

In order to give a basis to the structure and correlation analysis of fine particle (dusty) plasma and colloidal suspensions, thermodynamic treatment of mixtures of macroscopic and microscopic charged particles within the adiabatic response of the latter is extended to include the case where the system is finite and weakly inhomogeneous. It is shown that the effective potential for macroscopic particles is composed of two elements: mutual Yukawa repulsion and a confining (attractive) Yukawa potential from their ‘shadow’ or the average charge density of macroscopic particles multiplied by the minus sign. The result clarifies the relation between two approaches hitherto taken where either a parabolic one-body potential is assumed or the average distribution is assumed to be flat with finite extension.

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I. INTRODUCTION

In many cases, we have systems composed of both macroscopic and microscopic particles where we can apply a theoretical treatment based on the adiabatic response of microscopic particles. Typical examples of charged particle systems are fine particle (dusty) plasmas and charge stabilized colloidal suspensions. For instantaneous positions of fine particles (in the former) or colloidal particles (in the latter), we take the statistical averages over the ambient plasma (electrons and ions) or positive and negative ions to have the screening of the charge of macroscopic particles. The effective interaction between them is then given approximately by the Yukawa (Debye-Hückel) or DLVO potential which accompanies the factor $\exp(-r/\lambda)$ characterized by the screening length $\lambda$.

In this article, we call macroscopic and microscopic particles simply ‘particles’ and ‘background’, respectively. The adiabatic response of background has been analyzed for the uniform system[1, 2]. It is shown that, in addition to the screening of Coulombic interactions between particles, we have to take the charge neutrality of the system into account as a confining potential due to the charge density of the background which cancels the average charge density of particles. Let us consider the case of one species of particles. If we consider only the effective interaction of Yukawa or DLVO type, the system would have a tendency to expand (explode) with the pressure which is a sum of the positive ideal gas pressure (of both particles and background) and the positive pressure coming from mutual Coulomb-like repulsion between particles. When the charge neutrality of the system as a whole is properly taken into account, however, the latter pressure is not positive definite: For example, when particles are randomly distributed without correlation, we have no average space charge and there should be no Coulombic contribution to the pressure. Moreover, from the result of weakly coupled plasmas described by the Debye-Hückle theory, we expect that, when the correlation develops between particles, the Coulombic contribution to the pressure becomes negative and the pressure is reduced from the ideal gas values.

In numerical simulations which have been useful in investigations of these systems[3–5], particles are usually regarded as interacting only via the Yukawa repulsion without any consideration on the charge neutrality of the system. The system of $N$ particles in a volume $V$ is regarded as a part of the infinite uniform system with the number density $N/V$ and the limit of $N, V \to \infty$ is taken within numerical possibilities. When the average density $N/V$...
is kept unchanged, for example by the periodic boundary conditions with the fixed volume, correct distribution functions between particles can be obtained: Since the change in $N/V$ is suppressed, we are implicitly confining repelling particles and the effect of the charge neutrality need not to be explicitly reflected in simulations. The consideration of the effect becomes necessary only in the expression of the correlation energy which is proportional to

$$\int d\mathbf{r}v(\mathbf{r})[g(\mathbf{r}) - 1].$$

The integrand is the interaction potential $v(\mathbf{r})$ multiplied by the pair correlation function $g(\mathbf{r}) - 1$ of particles, not by the pair distribution function $g(\mathbf{r})$. Since the difference $\int d\mathbf{r}v(\mathbf{r})$ is a finite (density-dependent) constant for the screened potential $v(\mathbf{r})$, the correction can be made separately, even if the effect of the charge neutrality is not taken into account explicitly in the simulation.

The Helmholtz free energy for a given configuration of particles can be calculated by taking the statistical average over microscopic particles. The effective interaction is related to terms in the Helmholtz free energy which includes the coordinates of particles. As far as the uniform system is concerned, other terms (not-including their coordinates) can be regarded as constants, even if their values depend on number density and other parameters. On the other hand, when one considers the system of finite extension (or of finite geometrical size), the latter terms also become important: They are directly related to the confinement (the size and the shape) of the system.

There have been two different approaches in treating finite systems. One is to assume that the system is locally charge neutral and apply the result of infinite uniform system \[6–8\] and the other is to assume some ad hoc confining potential \[9–11\]. In the latter, the parabolic potential of some sort has been usually adopted.

Both approaches have their own cases where they are applicable. They are, however, not complete. In the first approach, the geometrical size of the system is to be determined by some ad hoc external origin, for example, by the radius of tube containing discharges or colloidal suspensions. In the case of fine particle plasmas, we also have stationary generation and transport of plasma (electrons and ions) and there exists finite space charge which produces the electric field to maintain the ambipolar diffusion. Though the space charge density is small relative to electron or ion density (generally, proportional to the square of the ratio of the screening length to the system size), the local charge-neutrality is not
exactly satisfied. In the second approach, the geometrical size of the system is determined by the balance between the mutual repulsion of particles and the (often parabolic) confining potential. When the system is charge-neutral, the background neutralizing the system should have the effect which reinforces the confinement and this effect should also exist even when the system is not exactly charge-neutral. In order to rectify such incompleteness, it is necessary to construct a theory which includes both the non-uniformity of the system and the role of the background. In this article, we present some results in the case of weak non-uniformity.

We consider the system composed of particles (macroscopic charged particles) and background (microscopic charged particles). In the case of fine particle plasmas, the former is fine (dust) particles and the latter is electrons and ions. In the case of charge stabilized colloidal suspensions, they are colloid particles and positive or negative ions, respectively. Since the mass of macroscopic particles is much larger than those of microscopic ones, we regard the latter as adiabatically responding to the instantaneous configuration of the former and, after the statistical average with respect to the background, physical quantities become functions of the configuration of particles.

We assume that both particles and background of our system are described by component-dependent temperatures and we can apply usual thermodynamic treatment to our system. Since our system is often open in the sense that we have a flow of energy into and from our system, especially in the case of fine particle plasmas, the applicability of thermodynamics might be questionable. There exist, however, no other well-established frameworks and we may justify our assumptions as a realistic approach. In what follows, we describe the system in terms of fine particle plasmas. One may easily interpret the results into the case of colloidal suspensions.

As fine particle plasmas, we consider those generated by dc or rf discharge in inert gases such as Ar with the pressure $10 \sim 10^2$ Pa. Typical densities of neutral gas atoms, plasma (electrons and ions), and fine particles are of the order of $10^{15} \sim 10^{16}$ cm$^{-3}$, $10^8$ cm$^{-3}$, and $10^5$ cm$^{-3}$, respectively. As for neutral gas atoms, their distribution is considered to be uniform and stationary without flows throughout the system.

Here and in the following, suffixes $\alpha = e, i, p$ express electrons, ions, and (fine) particles, respectively. We consider the case where our system is in a stationary state and the distributions of electrons, ions, and particles are characterized by the temperatures $T_e$,
and $T_p$, respectively. In most experiments, $k_B T_e$ is of the order of a few eV, while $T_i$ and $T_p$ are much lower than $T_e$ and considered to be of the order of the room temperature. (In colloidal suspensions, both positive and negative ions are at the room temperature. In what follows, however, we do not use the fact $T_e \gg T_i$.) We denote the usually negative charge on a particle by $-Qe (Q, e > 0)$.

II. LOCAL AVERAGE AND FLUCTUATIONS

In our system there exist three different characteristic lengths, namely, the size of the system $L$, the mean distance between particles $a_p$, and the mean distances between electrons or ions $a_{e,i}$. Their typical values are $L \sim a$ few cm, $a_p \sim 10^{-2} \text{ cm}(= 10^2 \mu\text{m})$, and $a_{e,i} \sim 10^{-3} \text{ cm}(= 10 \mu\text{m})$ and holds the inequality

$$L \gg a_p \gg a_{e,i}.$$  \hspace{1cm} (2.1)

Taking a distance $\ell$ so that

$$L \gg \ell \gg a_p \gg a_{e,i},$$  \hspace{1cm} (2.2)

we define the local average of a quantity $A(r)$ at $r$, $\overline{A}(r)$, by the space average over the domain of volume $\ell^3$ (with linear dimension of the order $\ell$) centered at $r$;

$$\overline{A}(r) \equiv \frac{1}{\ell^3} \int_{\ell^3 \text{ centered at } r} A(r) dr.$$  \hspace{1cm} (2.3)

The $r$-dependence of $\overline{A}(r)$ is characterized by $L$. We also define the deviation (fluctuation) from the average $\delta A(r)$ by

$$\delta A(r) \equiv A(r) - \overline{A}(r).$$  \hspace{1cm} (2.4)

We denote the density of each component by $n_\alpha(r)$. The total charge density $\rho(r)$ is written as

$$\rho(r) = \rho_p(r) + \rho_{bg}(r),$$  \hspace{1cm} (2.5)

where $\rho_p(r)$ is the charge density of particles

$$\rho_p(r) = (-Qe)n_p(r) = (-Qe) \sum_{i=1}^{N} \delta(r - r_i)$$  \hspace{1cm} (2.6)

and $\rho_{bg}(r)$ the charge density of the background plasma composed of electrons and ions

$$\rho_{bg}(r) = (-e)n_e(r) + en_i(r).$$  \hspace{1cm} (2.7)
The electrostatic potential $\Psi(\mathbf{r})$ satisfies the Poisson’s equation

$$-\varepsilon_0 \Delta \Psi(\mathbf{r}) = \rho_p(\mathbf{r}) + \rho_{bg}(\mathbf{r}) = e[-Qn_p(\mathbf{r}) - n_e(\mathbf{r}) + n_i(\mathbf{r})], \quad (2.8)$$

or

$$-\varepsilon_0 \Delta \Psi(\mathbf{r}) = \overline{\rho}(\mathbf{r}) = \overline{\rho}_p(\mathbf{r}) + \overline{\rho}_{bg}(\mathbf{r}) \quad (2.9)$$

and

$$-\varepsilon_0 \Delta \delta \Psi(\mathbf{r}) = \delta \rho_p(\mathbf{r}) + \delta \rho_{bg}(\mathbf{r}), \quad (2.10)$$

separately. In (2.10), $\delta \rho_p(\mathbf{r})$ includes the coordinates of particles and determines the polarization of electrons and ions, $\delta n_e(\mathbf{r})$ and $\delta n_i(\mathbf{r})$, giving $\delta \rho_{bg}(\mathbf{r}) = e[-\delta n_e(\mathbf{r}) + \delta n_i(\mathbf{r})]$.

As for the polarization of electrons and ions, we adopt the approximation of the linear adiabatic response to the local potential fluctuation $\delta \Psi(\mathbf{r})$;

$$\delta n_e(\mathbf{r}) \sim \overline{n_e}(\mathbf{r})[\exp(e\delta \Psi(\mathbf{r})/k_B T_e) - 1] \sim \overline{n_e}(\mathbf{r}) \frac{e\delta \Psi(\mathbf{r})}{k_B T_e}, \quad (2.11)$$

$$\delta n_i(\mathbf{r}) \sim \overline{n_i}(\mathbf{r})[\exp(-e\delta \Psi(\mathbf{r})/k_B T_i) - 1] \sim -\overline{n_i}(\mathbf{r}) \frac{e\delta \Psi(\mathbf{r})}{k_B T_i}. \quad (2.12)$$

We then have

$$\delta \rho_{bg}(\mathbf{r}) = -\varepsilon_0 k_D^2(\mathbf{r}) \delta \Psi(\mathbf{r}) \quad (2.13)$$

and (2.10) reduces to

$$-\varepsilon_0 [\Delta - k_D^2(\mathbf{r})] \delta \Psi(\mathbf{r}) = \delta \rho_p(\mathbf{r}). \quad (2.14)$$

Here $k_D(\mathbf{r})$ is the (local) Debye wave number defined by

$$k_D^2(\mathbf{r}) = \frac{e^2 \overline{n_e}(\mathbf{r})}{\varepsilon_0 k_B T_e} + \frac{e^2 \overline{n_i}(\mathbf{r})}{\varepsilon_0 k_B T_i}. \quad (2.15)$$

Note that, since we have generation/loss of the plasma and its transport by the (ambipolar) diffusion, it is not assumed that $\overline{n_e}(\mathbf{r}) \propto \exp(e\Psi(\mathbf{r})/k_B T_e)$ nor $\overline{n_i}(\mathbf{r}) \propto \exp(-e\Psi(\mathbf{r})/k_B T_i)$ for averages. For typical electron and ion temperatures, $1/k_D$ is much smaller than the system size $L$;

$$L \sim 1 \text{cm} > \left(\frac{e^2 \overline{n_e}(\mathbf{r})}{\varepsilon_0 k_B T_e}\right)^{-1/2} \sim 10^{-1} \text{ cm} > \frac{1}{k_D} \sim \left(\frac{e^2 \overline{n_i}(\mathbf{r})}{\varepsilon_0 k_B T_i}\right)^{-1/2} \sim 10^{-2} \text{ cm}. \quad (2.16)$$

We can thus regard the length $\ell$ satisfying the inequality

$$L \gg \ell \gg \{1/k_D, \ a_p\} \gg a_{e,i}. \quad (2.17)$$
When $k_D$ is $r$-independent, the solution for (2.10) is given by

$$
\delta \Psi(r) = \int d\mathbf{r}' \exp\left(-k_D|\mathbf{r} - \mathbf{r}'|\right) \delta \rho_p(r')
$$

and $\delta \Psi(r)$ is determined by the values of $\delta \rho_p(r')$ within distances of the order of $1/k_D$ from $\mathbf{r}$. Since the position dependence of $1/k_D$ is characterized by $L$ and $L \gg 1/k_D$, we may write the approximate solution for (2.10) in the form (see Appendix)

$$
\delta \Psi(r) \sim \int d\mathbf{r}' u(r, \mathbf{r}') \delta \rho_p(r')
$$

where

$$
u(r, \mathbf{r}') = \frac{\exp(-k_D^+|\mathbf{r} - \mathbf{r}'|)}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}'|}$$

and

$$k_D^+ = k_D[(r + \mathbf{r}')/2].$$

III. EFFECTIVE INTERACTION

A. Helmholtz free energy for given configuration of particles

Under the conditions of fixed volume and fixed temperatures of electrons and ions, the work necessary to change the configuration of particles is given by the change in the Helmholtz free energy of the system of electrons and ions. The effective interaction energy for the system of fine particles is thus written as

$$U_{ex} = F_{id}^{(e)} + F_{id}^{(i)} + \left[\frac{1}{2} \int d\mathbf{r} \rho(\mathbf{r}) \Psi(\mathbf{r}) - U_s\right].$$

Here $F_{id}^{(e)} + F_{id}^{(i)}$ is the Helmholtz free energy of the background or the electron-ion plasma

$$F_{id}^{(e)} = k_B T_e \int d\mathbf{r} n_e(\mathbf{r}) \left[\ln[n_e(\mathbf{r})\Lambda_e^3] - 1\right],$$

$$F_{id}^{(i)} = k_B T_i \int d\mathbf{r} n_i(\mathbf{r}) \left[\ln[n_i(\mathbf{r})\Lambda_i^3] - 1\right],$$

$\Lambda_e$ and $\Lambda_i$ being the thermal de Broglie lengths. In the third term, the self-energy $U_s = (1/2) \sum_{i=j}^N (-Qe)^2/4\pi\varepsilon_0 r_{ij}$ included in the formal expression of the electrostatic energy is subtracted. We adopt the ideal gas value of the Helmholtz free energy for electrons and ions: Usually the coupling in the background plasma is very weak (the $\Gamma$ parameter is $10^{-3}$ to
and the non-ideal effects are negligible, while the coupling between fine particles can be very strong. (Thermal de Broglie lengths are introduced only to define the unit volume of the phase space and have no relations to statistical properties of our classical system.)

We expand $F_{id}^{(e)} + F_{id}^{(i)}$ with respect to fluctuations. Noting $\int d\mathbf{r} \delta n_{e,i} \ln[n_{e,i} \Lambda_{ei}^3] \sim \int d\mathbf{r} \delta n_{e,i} \sim 0$, we have, to the second order,

$$F_{id}^{(e)} + F_{id}^{(i)} \sim F_{id,0} + \frac{1}{2} \int d\mathbf{r} \left[ k_B T_e \frac{\delta n_e^2(r)}{\rho_e(r)} + k_B T_i \frac{\delta n_i^2(r)}{\rho_i(r)} \right] = F_{id,0} - \frac{1}{2} \int d\mathbf{r} \delta \rho_{bg}(\mathbf{r}) \delta \Psi(\mathbf{r}).$$

Here

$$F_{id,0} = k_B T_e \int d\mathbf{r} \ln[\rho_e(\mathbf{r}) \Lambda_{ei}^3] - 1 + k_B T_i \int d\mathbf{r} \ln[\rho_i(\mathbf{r}) \Lambda_{ei}^3] - 1$$

and (2.11), (2.12), and (2.13) are used. Since $\int d\mathbf{r} \delta \rho_p \overline{\Psi} \sim \int d\mathbf{r} \delta \rho_{bg} \overline{\Psi} \sim \int d\mathbf{r} \delta \rho_p \delta \Psi \sim \int d\mathbf{r} \overline{\rho_{bg}} \delta \Psi \sim 0$, the electrostatic energy is written as

$$\frac{1}{2} \int d\mathbf{r} \rho \Psi - U_s = \frac{1}{2} \int d\mathbf{r} [\overline{\rho}_p + \overline{\rho}_{bg}] \overline{\Psi} + \frac{1}{2} \int d\mathbf{r} [\delta \rho_p + \delta \rho_{bg}] \delta \Psi - U_s.$$  

From (3.4) and (3.6), we have

$$U_{ex} = F_{id,0} + \frac{1}{2} \int d\mathbf{r} [\overline{\rho}_p(\mathbf{r}) + \overline{\rho}_{bg}(\mathbf{r})] \overline{\Psi}(\mathbf{r}) + \left[ \frac{1}{2} \int d\mathbf{r} \delta \rho_p(\mathbf{r}) \delta \Psi(\mathbf{r}) - U_s \right].$$

By (2.19), the last term of (3.7) is rewritten as

$$\frac{(Qe)^2}{2} \sum_{i,j=1}^{N} u(r_i, r_j) - U_s - \frac{(Qe)^2}{2} \sum_{i=1}^{N} \int d\mathbf{r}' u(r_i, r') \overline{\rho}_p(r') + \frac{1}{2} \int \int d\mathbf{r} d\mathbf{r}' u(r, r') \overline{\rho}_p(r) \overline{\rho}_p(r').$$

The subtraction of self-interactions from the first term above gives the mutual Yukawa repulsion and the free energy stored in the sheath;

$$\frac{1}{2} \sum_{i,j=1}^{N} (Qe)^2 u(r_i, r_j) - U_s = \frac{(Qe)^2}{2} \sum_{i \neq j}^{N} u(r_i, r_j) - \frac{1}{2} \sum_{i=1}^{N} \frac{(Qe)^2 k_D(r_i)}{4\pi \varepsilon_0}.$$  

The Helmholtz free energy is finally given by

$$U_{ex} = F_{id,0} + \frac{1}{2} \int d\mathbf{r} \overline{\rho}_p(\mathbf{r}) \overline{\rho}_p(\mathbf{r})$$

$$+ \left[ \frac{1}{2} \sum_{i \neq j}^{N} (Qe)^2 u(r_i, r_j) + \sum_{i=1}^{N} (-Qe) \int d\mathbf{r}' u(r_i, r') \overline{\rho}_p(r') \right]$$

$$+ \frac{1}{2} \int \int d\mathbf{r} d\mathbf{r}' u(r, r') \overline{\rho}_p(r) \overline{\rho}_p(r') - \frac{1}{2} \sum_{i=1}^{N} \frac{(Qe)^2 k_D(r_i)}{4\pi \varepsilon_0}. \quad (3.8)$$
B. Potential for particles

The averages, $\overline{\rho_p}(r), \overline{\rho_{bg}}(r)$, and $\Psi(r)$, are to be determined so as to be consistent with the plasma generation and loss and the ambipolar diffusion in the system. Configuration-dependent terms in (3.8),

$$\frac{1}{2} \sum_{i \neq j}^N (Qe)^2 u(r_i, r_j) + \sum_{i=1}^N (-Qe) \int dr' [-\overline{\rho_p}(r')] u(r_i, r') - \frac{1}{2} \sum_{i=1}^N \frac{(Qe)^2 k_D(r_i)}{4\pi\varepsilon_0}, \quad (3.9)$$

describe the Helmholtz free energy for given distribution of particles $\{r_i\}_{i=1,...,N}$. The integral in the second term

$$\int dr' [-\overline{\rho_p}(r')] u(r_i, r') = \int dr' \frac{[-\overline{\rho_p}(r')]}{4\pi\varepsilon_0|r_i - r'|} \exp(-k_D^+|r_i - r'|) \quad (3.10)$$

can be regarded as the Yukawa potential at $r_i$ due to $[-\overline{\rho_p}(r')]$, the (imaginary) charge density which exactly cancels the average particle charge density $\overline{\rho_p}(r')$: We may call $[-\overline{\rho_p}(r')]$ the “shadow” to $\overline{\rho_p}(r')$ emphasizing its difference from the background plasma which really exists. The charge density of the shadow has the sign opposite to particles and the potential due to the shadow is attractive. Particles are thus mutually interacting via the Yukawa repulsion and, at the same time, confined by the attractive potential due to the shadow charge density $[-\overline{\rho_p}(r')][6–8].$

C. Infinite uniform system

In the limit where $V, N \to \infty$ with $N/V$ kept constant, we have

$$\delta \Psi(r) = \int dr' \frac{\exp(-k_D|r - r'|)}{4\pi\varepsilon_0|r - r'|} \delta \rho_p(r') = \sum_{i=1}^N \frac{(-Qe)}{4\pi\varepsilon_0|r - r_i|} \exp(-k_D|r - r_i|) - \overline{\rho_p} \quad (3.11)$$

and

$$\frac{1}{2} \int dr \delta \rho_p(r) \delta \Psi(r) - U_s = \frac{1}{2} \sum_{i \neq j}^N v(r_{ij}) - \frac{N (Qe)^2(N/V)}{2 \varepsilon_0 k_D^2} - \frac{N (Qe)^2 k_D}{2 \frac{4\pi\varepsilon_0}, \quad (3.12)$$

where

$$v(r) = \frac{(Qe)^2}{4\pi\varepsilon_0 r} \exp(-k_D r) \quad (3.13)$$

and $k_D$ is position-independent. In terms of the pair distribution function $g(|r - r'|)$, we have

$$U_{ex} = V n_e k_B T_e [\ln n_e \Lambda_e^3 - 1] + V n_i k_B T_i [\ln n_i \Lambda_i^3 - 1] + N \left[ \frac{n_p}{2} \int dr \psi(r) [g(r) - 1] - \frac{(Qe)^2 k_D}{8\pi\varepsilon_0} \right] \quad (3.14)$$

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The results thus reduce to the previous ones[].

In numerical simulations where the average density of particles is kept unchanged, the expression (3.12) is used and only the first term is computed in each step. Usually the number of particles is fixed and periodic boundary conditions are imposed. Though distribution functions are correctly evaluated directly from such simulations, we have to calculate the free energy based on the correlation energy (3.14).

D. Average with respect to particle distribution

Let us denote the statistical average with respect to the particles by $\langle \rangle$. Taking this average of (3.8) and noting that $\langle n_p(r) \rangle = n_p(r)$, we have

$$
\langle U_{ex} \rangle = F_{id,0} + \frac{1}{2} \int dr [\rho_p(r) + \rho_{bg}(r)] \Psi(r) + \frac{1}{2} (Qe)^2 \int \int dr dr' u(r, r') \left[ \sum_{i \neq j} \delta(r - r_i) \delta(r' - r_j) - \overline{n_p(r)} \overline{n_p(r')} \right] - \frac{1}{2} \sum_{i=1}^{N} \frac{(Qe)^2 k_D(r_i)}{4\pi \varepsilon_0} > .
$$

(3.15)

The statistical average $\langle \sum_{i \neq j} \delta(r - r_i) \delta(r' - r_j) \rangle$ is a function of both $r$ and $r'$. Since the average density changes with the scale length $L$ which is much larger than the mean distance between particles $a_p$, this function depends mainly on $r - r'$ and the dependence on $r$ or $r'$ is weak. We define a function $g(|r - r'|; (r + r')/2)$ with the arguments $r - r'$ and $(r + r')/2$, expecting the weak dependence on the latter:

$$
\langle \sum_{i \neq j} \delta(r - r_i) \delta(r' - r_j) \rangle \equiv \overline{n_p(r)} \overline{n_p(r')} g(|r - r'|; (r + r')/2).
$$

(3.16)

In the uniform system, $g(|r - r'|; (r + r')/2)$ reduces to the usual pair distribution function $g(|r - r'|)$. The third term on the right-hand side of (3.15) is expressed by this function as

$$
\frac{1}{2} \int \int dr dr' \rho_p(r) \overline{\rho_p(r')} [g(|r - r'|; (r + r')/2) - 1] u(r, r').
$$

(3.17)

The potential by the shadow (the second term of (3.9)) influences the distribution so that the average charge density approaches to $\overline{n_p(r)}$: The average force acting on the particles $i$ given by

$$
(-Qe)^2 < \sum_{j(\neq i)} [-\nabla_i u(r_i, r_j)] - \int dr' [-\nabla_i u(r_i, r')] \overline{n_p(r')} >
$$

(3.18)
reduces to zero since the average particle distribution is $\bar{\rho}_p(r)$. (In principle, there exists a possibility that, when particles are strongly correlated, the fluctuations have some effect on averages and averages and fluctuations need to be determined self-consistently. In this article, however, we assume that fluctuations are determined under given averages.)

IV. CONCLUSION AND DISCUSSIONS

In this article, the effective potential for particles is derived for given average distributions which are determined so as to be consistent with the generation/loss and the ambipolar diffusion of plasma. The result generalizes the analysis of the infinite uniform system\[^{[1, 2]}\] to finite weakly inhomogeneous systems.

Here we discuss the relation to previous approaches to finite systems, taking a typical example of particles in the cylindrical positive column discharges. In addition to facilitating simple geometry and symmetry, we assume the generation of plasma in the bulk and the loss to the outer boundary (wall of apparatus) by ambipolar diffusion. We expect similar discussions apply also to more complicated cases.

A. Case of negligible contribution to net charge density from particles

When the contribution of particles to the net charge density is negligible, the distribution of plasma and the electrostatic potential are determined independently of particles. Then the plasma distribution and the potential are approximately expressed respectively by

\[
\bar{n}_{e,i}(R) \sim \bar{n}_{e,i}(R = 0) J_0(R/R_a), \tag{4.1}
\]

and

\[
\bar{\Psi}(R) \sim \frac{k_B T_e}{e} \ln J_0(R/R_a) = -\frac{k_B T_e}{e} \left( \frac{R^2}{4R_a^2} + \ldots \right). \tag{4.2}
\]

Here $R$ is the distance from the symmetry axis, $J_0$, the 0-th order Bessel function, and $R_a$, a characteristic length of the order of (radial) system size which is determined by the ambipolar diffusion coefficient and the rate of plasma generation. The charge density around $R = 0$ is given by

\[
0 < -\varepsilon_0 \Delta \bar{\Psi}(R) \sim e\bar{n}_{e,i}(R = 0) \frac{1}{(k_D e R_a)^2} \ll e\bar{n}_{e,i}(R = 0), \tag{4.3}
\]
where \( k_{De} = [n_e(R = 0)e^2/\varepsilon_0k_B T_e]^{1/2} \) is the electron Debye wave number. Since usually \( 1/k_{De} \ll R_a \), the quasi-charge-neutrality holds and we have slightly positive net charge density. When the contribution of particles to the latter is negligible, particles are considered to be also in this electrostatic potential which is parabolic near the axis. We thus have a model where particles in a parabolic confining potential mutually interact via the Yukawa repulsion, corresponding to some of previous approaches to finite inhomogeneous system of particles\[9–11\].

The distribution of particles is analyzed in Appendix B. For the given value of the linear density of particles along the axis \( n_{p,z} \), particles are distributed within the radius \( R_0 \) such that

\[
\frac{R_0}{R_a} \sim 2 \left( \frac{T_i Q_n}{T_e n_e} \right)^{1/2},
\]

(4.4)

\( n_{p,z} \) being \( \pi n_p R_0^2 \). In order for the particle charges not to affect the potential, we have to have \( Q n_p / n_e \ll 1/(k_{De} R_a)^2 \ll 1 \) and therefore \( R_0/R_a \ll 1 \) (usually \( T_i/T_e \ll 1 \)).

B. Case of effective contribution to net charge density from particles

With the increase of \( n_{p,z} \), the radius \( R_0 \) and the charge density of particles \((-Qe)n_p\) increase and, when \((Q n_p)/n_e\) becomes not negligible compared with \(1/(k_{De} R_a)^2\), we have to couple the particle charge density with the potential and therefore with electron and ion distributions. Here, it is important to note the point that the potential and electron/ion distributions are related to the generation/loss and ambipolar diffusion of the plasma and their characteristic scale length cannot become much smaller than the system size, in our case, \( R_a \): The diffusion flux is controlled by the electric field and is almost continuous.

On the other hand, if the potential behaves as given by (4.2), the particle distribution is limited to the radius \( R_0 \) which is much smaller than \( R_a \), as given by (4.4); and, at the same time, the potential structure should reflect particle distribution with much smaller scale length: This apparently contradicts with the above point. The only possibility to avoid the contradiction is that the potential has the characteristic scale length which is much larger than the one given by (4.2) so that the particle distribution also has the scale length of the order of \( R_a \). In other words, the potential become almost flat (in the scale of the system size) where particles exist.

The simplest approximation in this case may be to assume that the potential is completely
flat where particles exist. In our previous analyses of structures and ordering of particles in finite systems, we have assumed the average particle distribution is uniform with finite extensions. This treatment may be justified as an approximate approach in the latter case.

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Appendix A

For the equation to be solved

\[ [\Delta - k_D^2(r)]\delta \Psi(r) = -\frac{\delta \rho_p(r)}{\varepsilon_0}, \]  

(4.5)

we first take the kernel \( u^{(1)}(r, r') \) defined by

\[ u^{(1)}(r, r') \equiv \frac{\exp(-k_D(r')|r - r'|)}{4\pi|r - r'|} \]

and consider an approximate solution

\[ \int d\mathbf{r}' u^{(1)}(\mathbf{r}, \mathbf{r}') \frac{\delta \rho(\mathbf{r}')}{\varepsilon_0}. \]  

(4.6)
Since

$$[\Delta - k_D^2(r)]u^{(1)}(r, r') = \frac{\exp(-k_D(r)|r - r'|)}{4\pi} \frac{1}{|r - r'|} \Delta \frac{1}{|r - r'|} + [k_D^2(r') - k_D^2(r)]u^{(1)}(r, r'),$$

we have

$$[\Delta - k_D^2(r)] \int dr' u^{(1)}(r, r') \frac{\delta \rho(r')}{\varepsilon_0}$$

$$= -\frac{\delta \rho_p(r)}{\varepsilon_0} + \int dr'[k_D^2(r') - k_D^2(r)]u^{(1)}(r, r') \frac{\delta \rho(r')}{\varepsilon_0}.$$

Noting that the characteristic scale of length for $k_D^2$ (or the density) is $L$ and the effective range of the kernel is of the order of $1/k_D$, the relative error is estimated to be of the order of $1/k_D L \ll 1$ or

$$[\Delta - k_D^2(r)] \int dr' u^{(1)}(r, r') \frac{\delta \rho(r')}{\varepsilon_0} \sim - \left( 1 + O\frac{1}{k_D L} \right) \frac{\delta \rho_p(r)}{\varepsilon_0}. \quad (4.7)$$

When we take the kernel

$$u^{(2)}(r, r') \equiv \frac{\exp(-k_D(r)|r - r'|)}{4\pi|r - r'|},$$

we have

$$[\Delta - k_D^2(r)]u^{(2)}(r, r')$$

$$= \frac{\exp(-k_D(r)|r - r'|)}{4\pi} \left[ \frac{1}{|r - r'|} \Delta \frac{1}{|r - r'|} + \frac{r - r'}{|r - r'|} \cdot \nabla k_D^2(r) - \Delta k_D(r) + |r - r'|(|\nabla k_D(r)|^2) \right],$$

$$[\Delta - k_D^2(r)] \int dr' u^{(2)}(r, r') \frac{\delta \rho(r')}{\varepsilon_0}$$

$$= -\frac{\delta \rho_p(r)}{\varepsilon_0} + \int dr' u^{(2)}(r, r') \frac{\delta \rho(r')}{\varepsilon_0} \cdot \nabla k_D^2(r)$$

$$+ \int dr' u^{(2)}(r, r')[-|r - r'|\Delta k_D(r) + |r - r'|^2(|\nabla k_D(r)|^2)] \frac{\delta \rho(r')}{\varepsilon_0},$$

and similarly

$$[\Delta - k_D^2(r)] \int dr' u^{(2)}(r, r') \frac{\delta \rho(r')}{\varepsilon_0} \sim - \left( 1 + O\frac{1}{k_D L} \right) \frac{\delta \rho_p(r)}{\varepsilon_0}. \quad (4.8)$$

The value of $k_D$ in the exponential function can thus be either taken at $r$ or $r'$ and therefore at $(r + r')/2$; In fact, $k_D(r) \sim k_D(r') \sim k_D[(r + r')/2] \sim [k_D(r) + k_D(r')]/2$ when $|r - r'| < 1/k_D$.

We note that, in order to have (4.7) or (4.8) at any point $r$ in the system, it is important to have $k_D(r)$ or $k_D(r')$ in the argument of the exponential function of the kernel. When
we fix the value of $k_D$ at some point $r_0$ and adopt $\exp(-k_D(r_0)|r - r'|)/4\pi|r - r'|$ instead of $u^{(1)}(r,r')$ or $u^{(2)}(r,r')$, 

$$\frac{k_D^2(r) - k_D^2(r_0)}{k_D^2(r_0)}$$

can be of the order of unity and, even if we have $k_D L \gg 1$, (4.5) is satisfied only around $r = r_0$.

**Appendix B**

We take the $z$-axis along the axis and express the coordinates in real space by $(R, z)$. The distribution of particles may be approximately estimated by assuming the uniform distribution with the radius $R_0$. The mutual interaction energy (per length along $z$) of uniformly distributed Yukawa particles is given by

$$\pi \frac{(-Qe)^2 n_p^2 R_0^2}{\varepsilon_0 k_D^2} \left[ \frac{1}{2} - K_1(k_D R_0) I_1(k_D R_0) \right],$$

where $K_1$ and $I_1$ are the modified Bessel functions. The energy due to the potential (4.2) is given by

$$\frac{\pi}{8} (Qe)n_p k_B T_e R_0^4 \frac{R_a}{R_0^2}.$$ 

When $k_D R_0 \gg 1$,

$$\left[ \frac{1}{2} - K_1(k_D R_0) I_1(k_D R_0) \right] \sim \frac{1}{2}$$

and, for given values of $n_{p,z} = n_p \pi R_0^2$, the total energy is minimum when

$$\left( \frac{R_0}{R_a} \right)^4 = \frac{4}{\pi \varepsilon_0} \frac{Qe^2 n_{p,z}}{k_B T_e R_0^2} \frac{1}{k_D^2 R_0^2}$$

or

$$\left( \frac{R_0}{R_a} \right)^2 = \frac{4}{\varepsilon_0} \frac{Qe^2 n_p}{k_B T_e} \frac{1}{k_D^2} = \frac{4 T_i Q n_p}{T_e n_{e,i}}.$$