Institute of Physics Publishing Journal of Physics: Conference Series **35** (2006) 78–93
doi:10.1088/1742-6596/35/1/007 Progress in Nonequilibrium Green's Functions III

Thermodynamics of a Correlated Confined Plasma.
I. Macroscopic System

Wolf Dietrich Kraeft[1,2] **and Michael Bonitz**[2]

[1] Institut für Physik, Universiät Greifswald, Domstr. 10a, D-17489 Greifswald
[2] Institut für Theoretische Physik und Astrophysik, Universität Kiel, Leibnizstr.15, D-24098 Kiel

E-mail: `wolf-dietrich.kraeft@uni-rostock.de`

Abstract. We consider classical and quantum systems of charge carriers which are confined by a three-dimensional harmonic potential. Thermodynamic functions are determined, and the transition to an unconfined system is discussed.

1. Introduction

The investigation of spatially confined particles in a trap, is of current interest. Especially the formation of lattice structures of charge carriers, such as ions in Penning traps, e.g. [1], electrons in quantum dots [2] and of dust particles is investigated both experimentally and theoretically in various laboratories [1]-[9]. The formation of *different* types of clusters was investigated, e.g., in [10]. The goal of this paper is to give some survey over the existing theoretical and thermodynamical concepts to be applied in in further investigations.

We will, in particular, consider the total energy of systems of charged particles in a trap. The latter is assumed to be realized by a parabolic potential and confines the particles and replaces the role of a neutralizing background which otherwise is necessary to compensate the repulsive forces between the charged particles. We consider, e.g., a one component plasma (OCP). The consideration of effective potentials and the transition to macroscopic systems, i.e., to homogeneous systems, is of interest. In [11], a two–dimensional Yukawa fluid was investigated. For theoretical concepts such as improved screening see [3] and [12].

2. Total Energy

In contrast to [6], where there are considered classical plasmas only, we deal also with quantum statistical expressions for the total energy of a system of charge carriers. In particular, we have an ideal part E^0, containing the kinetic energy and the potential energy due to an external field Φ_R (first line of Eq.(1)), a contribution which corresponds to the self–consistent field and the corresponding exchange part (second line of (1), there, however without exchange). The latter contributions are referred to as Hartree and Hartree–Fock terms E^H and E^{HF}, respectively. The most interesting contribution is the correlation energy E^{corr} (third line of (1)) mediated by the Coulomb interaction between the charged particles. Then, the total (classical) energy of the system is given by (see [6])

$$E_R = \frac{3}{2} N k_B T + \int d\mathbf{r}_1 n(\mathbf{r}_1) e \Phi_R(\mathbf{r}_1)$$

$$
\begin{aligned}
&+ \frac{1}{2}\int d\mathbf{r}_1 d\mathbf{r}_2 n(\mathbf{r}_1)n(\mathbf{r}_2)e^2 G(\mathbf{r}_1|\mathbf{r}_2) \\
&+ \frac{1}{2}\int d\mathbf{r}_1 d\mathbf{r}_2 n(\mathbf{r}_1)n(\mathbf{r}_2)g(\mathbf{r}_1,\mathbf{r}_2)e^2 G(\mathbf{r}_1|\mathbf{r}_2)\,. \qquad (1)
\end{aligned}
$$

In general, the Green's function $G(\mathbf{r}_1|\mathbf{r}_2)$ may account for boundary conditions[6]; in the following, it is replaced by $\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}$. A shorthand notation of Eq. (1) reads

$$
E_R = E^0 + E^H + E^{HF} + E^{corr}\,. \qquad (2)
$$

Each of the terms of (2) depends on the trap potential. We assume the trap potential to be given by

$$
U = e\Phi_R(\mathbf{r}) = cr^2\,. \qquad (3)
$$

The inhomogeneity caused by the trap is assumed to be represented by the single-particle distribution. This is the case, if the correlation function g changes at smaller scales in space than the single particle distribution $n(\mathbf{r})$ does, see the (classical) discussion near Eq. (4.61) in Ref.[6]. Eventually, a gradient expansion with respect to the coordinates has to be performed $\mathbf{r}_1, \mathbf{r}_2 \to \mathbf{r}_1-\mathbf{r}_2,\ \frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$. In a first step, the two–particle distribution function F is represented by

$$
F_{12}(\mathbf{r}_1,\mathbf{r}_2) = n(\mathbf{r}_1)n(\mathbf{r}_2)[1+g_{12}(\mathbf{r}_1-\mathbf{r}_2)]\,,
$$

where the correlation function g depends on the difference variables only. Otherwise one has to solve the equation for g more rigorously; see [6], p.131, and [13] for discussion. It is necessary to consider the *second* equation of the BBGKY hierarchy; see the first equation of the hierarchy Eq. (4.54) in [6].

The total energy of interacting particles in an external potential was given in a quantum statistical formulation in several monographs, see, e.g., [14], [15]- [16]. The contributions determined essentially by the Coulomb potential are represented in terms of Feynman diagrams which are given in Fig. 1. Here, the full lines mean propagators of single particles in an external potential, the dashed lines are the bare two particle interaction, e.g., the Coulomb potential, and the wavy lines are screened potentials, which are, e.g., of Debye or of Yukawa type.

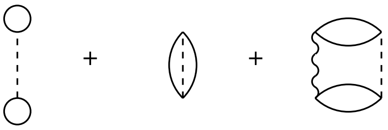

Figure 1. Lowest order terms

2.1. Noninteracting particles in a trap

To start, we consider the energy of particles in the trap without Coulomb interaction between the particles ([16], Eq.(3.222)).

In this case, the mean potential energy reads

$$
\langle V(\mathbf{R})\rangle = \pm i \sum_a \sum_\sigma \int \frac{d\mathbf{p}}{(2\pi)^3}\frac{d\omega}{2\pi}\frac{\omega - \frac{p^2}{2m_a}}{2} G_a^<(\mathbf{p}\sigma\omega,\mathbf{R})\,. \qquad (4)
$$

In the following we will drop the spin variable σ. We use the relevant correlation function which is given by the Kadanoff-Baym ansatz ([14], Eq.(9.12))

$$
G_a^<(\mathbf{p}\omega,\mathbf{R}) = 2\pi\delta\left(\omega - \frac{\mathbf{p}^2}{2m_a} - c\mathbf{R}^2\right) f_a(\mathbf{p},\mathbf{R})\,. \qquad (5)
$$

The integration over $\mathbf{p}$ may be performed in the *non-degenerate* case with

$$f_a(\mathbf{p}, \mathbf{R}) = \exp\left[-\beta\left(\frac{p^2}{2m_a} - \mu_a + c\mathbf{R}^2\right)\right] , \tag{6}$$

where $\beta = 1/k_BT$. We get for the potential energy of particles located at $\mathbf{R}$

$$\langle V(\mathbf{R})\rangle = \sum_a n_a \frac{cR^2}{2} e^{-\beta c R^2} .$$

Taking the average over $\mathbf{R}$, we arrive at

$$\langle V\rangle = \int d\mathbf{R}\, \langle V(\mathbf{R})\rangle = \sum_a \frac{3}{4}\left(\frac{\pi}{c}\right)^{3/2} n_a \beta^{-5/2} . \tag{7}$$

Instead of the constant c, we will now introduce the *volume of the trap.* We introduce the effective extension R_{trap} of the trap

$$R_{trap} = \frac{\int d\mathbf{r}\, r e^{-\beta c r^2}}{\int d\mathbf{r}\, e^{-\beta c r^2}} = 2\left(\frac{1}{\pi c \beta}\right)^{1/2} , \tag{8}$$

yielding the effective *volume of the trap*

$$V_{trap} = \frac{4\pi}{3} R_{trap}^3 = \frac{32}{3}\left(\frac{1}{\pi c \beta}\right)^{3/2} , \tag{9}$$

with the result for the potential energy

$$\frac{\langle V\rangle}{N} = \frac{9\pi^2}{128} k_BT . \tag{10}$$

We now consider the quantum case. N noninteracting particles correspond to N three-dimensional quantum-mechanical harmonic oscillators in the potential $\frac{m}{2}\omega^2 r^2$ which is related to the above trap potential U (3) by $c = \frac{m}{2}\omega^2$ ([17], Example 8.1, [18]). For such a system, we write the sum of states for one three-dimensional harmonic oscillator

$$Z(T, V, 1) = \sum_{n_x, n_y, n_z} \exp\left[-\beta\hbar\omega\left(\frac{3}{2} + n_x + n_y + n_z\right)\right] = \sum_\nu \frac{1}{2}(\nu{+}1)(\nu{+}2) \exp\left[-\beta\hbar\omega\left(\frac{3}{2} + \nu\right)\right] .$$

Here the latter expression accounts for the degeneracy of the eigen values. With $\sum_{\nu=0}^{\infty} e^{\alpha\nu} = 1/(1 - e^{\alpha})$ and $\sum_{\nu=0}^{\infty} \nu^{\tau} e^{\alpha\nu} = \frac{\partial^{\tau}}{\partial\alpha^{\tau}} \sum_{\nu=0}^{\infty} e^{\alpha\nu}$ we get

$$Z(T, V, 1) = \frac{e^{-\frac{3}{2}\beta\hbar\omega}}{(1 - e^{-\beta\hbar\omega})^3} .$$

For N non-interacting three–dimensional oscillators we arrive at

$$Z(T, V, 1) = \frac{e^{-\frac{3N}{2}\beta\hbar\omega}}{(1 - e^{-\beta\hbar\omega})^{3N}} ,$$

from which the free energy follows as

$$F = -k_BT \ln Z = \frac{3N}{2}\hbar\omega + 3Nk_BT \ln\left[1 - e^{-\beta\hbar\omega}\right] .$$

With the entropy given by $S = -\frac{\partial F}{\partial T}|_{V,T}$, the internal energy follows according to $U = F - TS$

$$U = N\hbar\omega \left[\frac{3}{2} + \frac{3}{e^{\beta\hbar\omega} - 1} \right] . \tag{11}$$

At high temperatures, i.e. for $\beta\hbar\omega \to 0$, we have

$$U = 3Nk_B T \, , \tag{12}$$

whereas for low temperatures, i.e. for $\beta\hbar\omega \to \infty$, we get the zero point energies

$$U = \frac{3N}{2}\hbar\omega \, . \tag{13}$$

A detailed discussion shows that, for $T = 0$, the energy per particle (11) scales with the density like

$$\frac{U}{N} = \frac{3\hbar\omega}{2} = \frac{3\hbar}{2} A n^{2/3} \, , \tag{14}$$

where A is a constant.

2.2. Self consistent field and exchange
Next we consider the Hartree (mean field) and the Hartree–Fock (exchange) terms.

2.2.1. Hartree energy We restrict ourselves to the equilibrium case. For the discussion of non-equilibrium properties, we refer to [19]. The Hartree term is written in terms of Green's functions

$$\langle V \rangle_H = -\frac{1}{2} \sum_{ab} \sum_{\sigma} \int \delta(t_1, t_{1'}) V_{ab}(12) G_a(1'1^+) G_b(22^+) d1' d2 \, . \tag{15}$$

Fourier transformation or Fourier series, respectively, with respect to the difference variables leads to

$$\langle V \rangle_H = -\frac{1}{2} \sum_{ab} \sum_{\sigma} \int d\mathbf{r}_1 d\mathbf{r}_2 V_{ab}(\mathbf{r}_1 - \mathbf{r}_2) \frac{1}{(-i\beta)^2} \sum_{\nu'} \sum_{\nu''} \int \frac{d\mathbf{k}' d\mathbf{k}''}{(2\pi)^6} G_a(k' z_{\nu'}, \mathbf{r}_1) G_b(k'' z_{\nu''}, \mathbf{r}_2) \, . \tag{16}$$

For the Fourier coefficients $G_a(k z_\nu, \mathbf{r})$ we use Eq. (9-31) of [14] and assume a spatial gradient approximation to be applicable

$$G(p, z; R) = [z - (p^2/2m) - U(R) - \Sigma(p, z; R)]^{-1} \, . \tag{17}$$

In our approximation, we consider the first order with respect to the potential, i.e., the Hartree self energy Σ is taken to be independent of U, and thus equals zero, where a neutralizing background is assumed, see below. The summation over ν is carried out using the residuum theorem and gives

$$\langle V \rangle_H = \frac{1}{2} \sum_{ab} (2s_a + 1)(2s_b + 1) \int d\mathbf{r}_1 d\mathbf{r}_2 \int \frac{dk' dk''}{(2\pi^6} V_{ab}(\mathbf{r}_1 - \mathbf{r}_2) f_a(k', \mathbf{r}_1) f_b(k'', \mathbf{r}_2) \, . \tag{18}$$

In the non-degenerate case, we use (6) instead of the Fermi functions. Now the momentum integration may be carried out, and we apply

$$n_a = \frac{(2s_a + 1)}{\Lambda_a^3} e^{\beta\mu_a} \, , \quad \Lambda_a = \frac{h}{(2\pi m_a k_B T)^{1/2}} \, .$$

In this approximation, we may as well start from the classical level, i.e., from the second integral of formula (1)

$$\langle V\rangle_H = \frac{(AN)^2}{2} e^2 \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{e^{-\beta c(r_1^2+r_2^2)}}{|\mathbf{r}_1-\mathbf{r}_2|}\,, \tag{19}$$

with the result

$$\frac{\langle V\rangle_H}{N} = \frac{\sqrt{2}}{32}\pi^3 \frac{ne^2}{2}\frac{k_B T}{c}\,. \tag{20}$$

The trap parameter c is of the dimension *energy/length*^{2}. The result (20) confirms the fact that the Hartree energy diverges for $c \to 0$. In the homogeneous case, this divergence has to be removed by a compensating background.

2.2.2. Exchange For electrons at low temperatures, the exchange energy

$$\langle V\rangle_{HF} = \frac{1}{2}\sum_{ab}\delta_{ab}\sum_{\sigma}\int d1 d\bar{1} V_{ab}(1\bar{1}) G_a(1\bar{1}) G_b(\bar{1}1^+) \tag{21}$$

is of the same order as the direct term. One has to be careful in performing the time integrations; according to Eq. (12-25) in [14] we have, after taking the non-degenerate limit,

$$\langle V\rangle_{HF} = -\frac{1}{2}\sum_a (2s_a+1)\int d\mathbf{R}_a \int \frac{d\mathbf{k}d\mathbf{l}}{(2\pi)^6}\frac{4\pi e^2}{l^2}$$
$$\times \exp\left(-\frac{\beta k^2}{2m_a} + \beta\mu_a - \beta c R_a^2\right) \exp\left(-\frac{\beta(\mathbf{k}-\mathbf{l})^2}{2m_a} + \beta\mu_a - \beta c R_a^2\right)\,, \tag{22}$$

where the integrations over the momenta can be carried out yielding

$$\langle V\rangle_{HF} = -\frac{1}{2}\sum_a \frac{2\pi z_a^2 e^2 \lambda_{aa}^2}{2s_a+1}\int d\mathbf{R}_a e^{-2\beta c R_a^2}\,, \tag{23}$$

and the integral over $\mathbf{R}_a$ gives $(\frac{\pi}{2\beta c})^{3/2}$. If one again introduces the *volume of the system* (9), one gets a *non–diverging* result, in particular also for $c \to 0$, in agreement with earlier work [15].

2.3. Correlation Energy

2.3.1. Born approximation for a confined system We restrict ourselves to the Born approximation, i.e., only the terms up to the order V_{coul}^2 are taken into account. In order to avoid divergencies, one of the potentials has to be a screened one (see e.g., [15]). Exchange contributions of this order are not considered, and the direct (D) contribution of the order e^4, $D4$, reads

$$\langle V\rangle_{D4} = -\frac{i}{2}\sum_{ab}\sum_{\sigma}\int V_{ab}^s(12) V_{ba}(\bar{2}\bar{1}) G_b^0(\bar{2}2) G_b^0(2\bar{2}) G_a^0(1\bar{1}) G_a^0(\bar{1}1) d1d2d\bar{1}d\bar{2}\,. \tag{24}$$

The analytical evaluation of Eq.(24) is possible in the non-degenerate case [15] for particles in an infinite volume (i.e., without trap). The degenerate case without trap has to be dealt with numerically [20], only the case $T = 0$ is known analytically (Gell-Mann & Brueckner, see, e.g., [20]). The quantum case for particles in a trap cannot be evaluated analytically.

Here we consider the classical limit of the correlation energy in Born approximation (24) in the presence of the trap. Manipulations along the lines given above, e.g., for the Hartree case, lead to the classical expression for an OCP (after spin summation)

$$\langle V\rangle_{D4} = \frac{\beta}{2}\int d\mathbf{r}_1 d\mathbf{r}_2 n(\mathbf{r}_1)n(\mathbf{r}_2)\frac{e^2}{\mathbf{r}_1-\mathbf{r}_2}e^{-\kappa(\mathbf{r}_1-\mathbf{r}_2)}\frac{e^2}{\mathbf{r}_1-\mathbf{r}_2}\,. \tag{25}$$

This is the third integral of Eq. (1) in the lowest order in the interaction. It becomes, using the convolution theorem,

$$\langle V\rangle_{D4} = -\frac{N^2A^2e^4}{2k_BT}\int\frac{d\mathbf{k}_3}{(2\pi)^3}\left(\frac{\pi}{\beta c}\right)^3\exp\left(-\frac{k_3^2}{2\beta c}\right)\frac{8\pi}{k_3}\arctan\frac{k_3}{\kappa}\,, \tag{26}$$

where we used the Fourier transform

$$\frac{1}{r^2}\exp(-\kappa r)|_{FT}\rightarrow\frac{8\pi}{k}\arctan\frac{k}{\kappa}$$

and obtain the final result

$$\langle V\rangle_{D4} = -2\beta N^2A^2e^4\frac{\pi^3}{(\beta c)^2}\left[1-\Phi\left(\frac{\kappa}{\sqrt{2\beta c}}\right)\right]\exp\left(\frac{\kappa^2}{2\beta c}\right)\,. \tag{27}$$

The expression (27) is of the dimension *energy* as it should: A has the dimension 1/ *Volume*, and βc has the dimension *length*$^{-2}$.
The main ingredient of this equation is the function $\Phi_c(\kappa R_{trap})$ (34) which is discussed below and displayed in Fig. 2. We underline that this result is finite even for an unscreened plasma, $\kappa\rightarrow 0$, however *only* in the presence of the trap. The limit of an unconfined system, $c\rightarrow 0$, is more difficult to discuss. We may introduce the *volume of the trap* (9) into (27) and arrive at

$$\frac{\langle V\rangle_{D4}}{N} = -2\beta ne^4\times\left(\frac{3}{32}\sqrt{\pi}(\beta c)^{3/2}\right)\times\frac{\pi^3}{(\beta c)^2}\left[1-\Phi\left(\frac{\kappa}{\sqrt{2\beta c}}\right)\right]\exp\left(\frac{\kappa^2}{2\beta c}\right)\,. \tag{28}$$

For large c (narrow trap), we find

$$\frac{\langle V\rangle_{D4}}{N} = -\frac{3\pi^{7/2}}{16}\frac{ne^4}{k_BT}\left(\frac{k_BT}{c}\right)^{1/2}\,. \tag{29}$$

Besides the case of finite c, also the limiting case $c=0$ is of interest. The numerical discussion of the relevant function is displayed in Fig. 2.

2.3.2. Transition to a Homogeneous System ($c=0$) Starting from Eq. (25) *with screening*, we obtain

$$\langle V\rangle_{D4}|_{c=0} = -\frac{N^2A^2e^4}{2k_BT}\int d\mathbf{r}_1 d\mathbf{r}_2\frac{e^{-\kappa|\mathbf{r}_1-\mathbf{r}_2|}}{|\mathbf{r}_1-\mathbf{r}_2|^2}\,. \tag{30}$$

A coordinate transformation leads to (V denotes the Volume)

$$= -\frac{VN^2A^2e^4}{2k_BT}\int_0^\infty 4\pi e^{-\kappa r}dr = -\frac{VN^2A^2e^4}{2k_BT}\frac{4\pi}{\kappa}\,, \tag{31}$$

where $\kappa^2=\frac{4\pi ne^2}{k_BT}$ and

$$\langle V\rangle_{D4}|_{c=0} = -k_BTV\frac{\kappa^3}{8\pi}\frac{N^2A^2}{n^2}\,, \tag{32}$$

i.e. we recover the well-known result for the potential energy with $\frac{N^2A^2}{n^2} = 1$.

If we try to linearize in c, we expect to obtain a correction to (30)

$$\langle V \rangle_{D4} |_{c=0} = \frac{N^2 A^2 e^4 \beta c}{2 k_B T} \int d\mathbf{r}_1 d\mathbf{r}_2 (\mathbf{r}_1^2 + \mathbf{r}_2^2) \frac{\exp[-\kappa |\mathbf{r}_1 - \mathbf{r}_2|]}{|\mathbf{r}_1 - \mathbf{r}_2|^2} , \tag{33}$$

which, however, is a divergent result. As a consequence, an expansion with respect to c is not possible. On the other hand, of course the homogeneous limit of Eq. (27) should exist and give (32) for small c. To discuss the small c case analytically, we use the *asymptotic representation* for the error function Φ which reads

$$\Phi(x) = 1 - \frac{e^{-x^2}}{x\sqrt{\pi}} \left(1 - \frac{1}{2x^2} + \frac{3}{4x^4} \mp \cdots \right) .$$

The asymptotic expression

$$x\sqrt{\pi} e^{x^2} [1 - \Phi(x)] = 1 - \frac{1}{2x^2} + \frac{3}{4x^4} \mp \cdots$$

tends to unity for $x \to \infty$. From (27), we then get the expected $1/\kappa$ dependence like in (32) if we numerically discuss the function

$$\Phi_c(\kappa R_{trap}) = \kappa \left(\frac{\pi}{2\beta c} \right)^{1/2} \left[1 - \Phi \left(\frac{\kappa}{\sqrt{2\beta c}} \right) \right] \exp \left(\frac{\kappa^2}{2\beta c} \right) , \tag{34}$$

which approaches unity for small c, see Fig. 2. For small βc or large R, one should use the asymptotic expression.

Therefore the quantity

$$x^2 = \frac{3}{2} \frac{V_{coul}(\bar{r})}{\bar{\Phi}_R} = \frac{\kappa^2}{2\beta c}$$

is an additional parameter for inhomogeneous systems.

The remaining pre-factor is then essentially $1/[\kappa(\beta c)^{3/2}]$. $(\beta c)^{-3/2}$ plays the role of the volume V occurring in (31); there we have V/κ. The quantity $(\beta c)^{-3/2}$ has to be connected to $(4\pi/3)R_{trap}^3$.

2.3.3. Debye limiting law and nonlinear effects The case of high temperatures and low densities leads to the Debye limiting law. The case of low densities and low temperatures is of interest, too. (Low temperatures and high densities correspond to the Gell-Mann Brueckner case).

Here, we consider the classical case. Then an appropriate approximation for the two–particle distribution function reads

$$f_{ab}(r) = \exp \left[- \frac{e^2}{k_B T} \frac{e^{-\kappa r}}{r} \right] , \tag{35}$$

and the correlation energy becomes

$$V = \frac{1}{2} \sum_{ab} N_a n_b \int V_{ab}(r) \left[f_{ab}(r) - 1 \right] d\mathbf{r} . \tag{36}$$

On the other hand, the familiar Debye limiting law expression follows from (36) with the linearized exponential of (35)

$$V_{lim} = - \frac{1}{2} \sum_{ab} N_a n_b \int V_{ab}(r) \frac{e^2}{k_B T r} e^{-\kappa r} d\mathbf{r} , \tag{37}$$

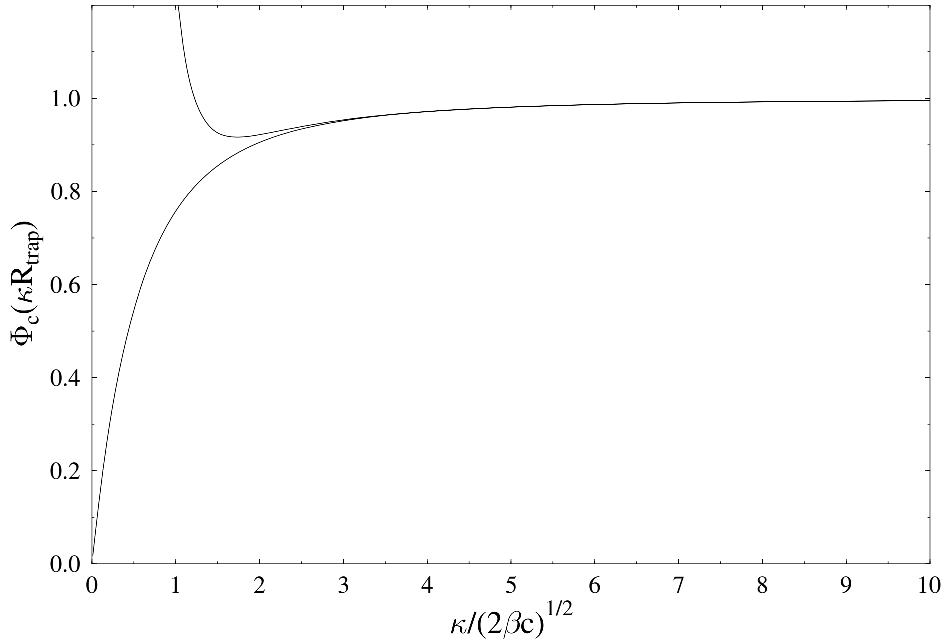

Figure 2. Trap function (34) and asymptote (diverging for small abscissa). $R_{trap} = 2/(\pi c\beta)^{1/2}$

with the known result

$$V_{lim} = -k_B T V \frac{\kappa^3}{8\pi} . \tag{38}$$

The ratio V/V_{lim} ((36) vs. (38)) is displayed in Fig. 3. Furthermore, to extend this to particles in a trap, one would additionally need to include macroscopic space dependence via the single particle distributions like in (25).

The above result is closely connected to the question of nonlinear screening [12], [21], [22] which is expected to be of relevance in particular in dusty plasmas containing highly charged particles. This will be discussed elsewhere.

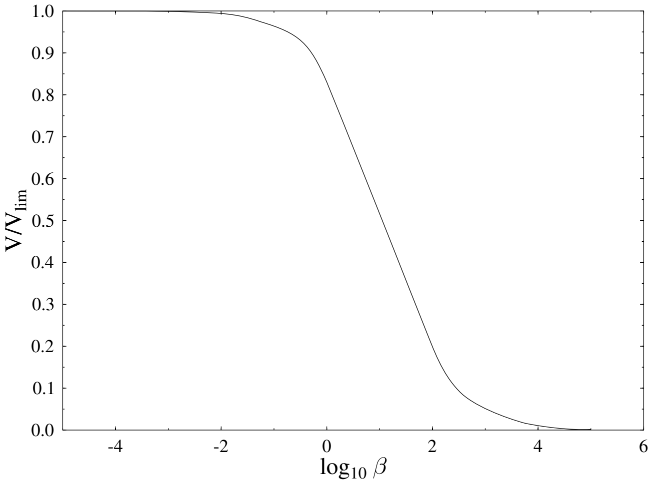

Figure 3. Ratio of the low–density/low–temperature correlation energy (36) to the Debye limit (38) as a function of the dimensionless parameter $\beta = ryd/k_BT$, $\kappa = 0.1$

3. Effects of Strong Correlations. Improved pair distribution function

So far, correlation effects were discussed only in the Born approximation which is valid for weak coupling, i.e. $\Gamma = \left(\frac{4\pi n}{3}\right)^{1/3} l$, where l is the Landau length, $l = e^2/k_BT$. A more rigorous inclusion of higher order correlations is possible via HNC schemes which will be considered in this section.

Up to now, the macroscopic inhomogeneity is only accounted for by the single particle distribution function. In this section, we will only consider two–particle quantities. Macroscopic and microscopic space dependence enter the binary density operator F_{12} via the expression [13] $F_{12}(R, r) = f_1(R)f_2(R)[1 + g_{12}(R, r)]$ with g_{12} denoting the pair correlation function which is related to the pair distribution function by $f_{12} = 1 + g_{12}$. We assume in the following that there are two well separated length scales such that g_{12} does not depend on the center of mass coordinate $R = (r_1 + r_2)/2$, i.e. $g_{12} = g_{12}(r)$. This means we separate the spatial dependencies corresponding to the macro scale [$\mathbf{R}$ which is set by the external potential $U(\mathbf{R})$] and a micro scale [relative coordinates $\mathbf{r}$; this scale is determined by the range of the interaction potential and enters the pair correlation $g_{12}(\mathbf{r})$]. This is, in particular, justified in the frequently encountered situation where the trap dimension is large compared to the correlation or screening lengths, $R_{trap} \gg r_{corr}$, see also [19].

Another important quantity characterizing the binary correlations is the static structure factor $S(\mathbf{k})$ (n is the density) which follows from the pair correlation function by

$$S(\mathbf{k}) = 1 + n \int d\mathbf{r} g(\mathbf{r}) e^{-i\mathbf{kr}} .$$

We go beyond the Born (Debye) approximation by calculating the binary distribution function using HNC (hyper netted chain) techniques which is expected to be valid up to about $\Gamma = 100$. In the HNC, screening is produced automatically, and quantum effects may also be accounted for in lowest order, see discussion below.

3.1. Thermodynamics

For the determination of thermodynamic functions, we follow the idea outlined in [23]. If the pair distribution function f_{ab} is known the mean value of the correlation energy $E_{\rm corr}$ is given by

$$E_{\rm corr} = \frac{1}{2} \sum_{ab} n_a N_b \int V_{ab} g_{ab} d\mathbf{r} . \qquad (39)$$

Note that in quantum system, there is a (small) difference between potential and correlation energy due to correlation effects in the quantum kinetic energy, see [24].

In (39), V_{ab} has to be the bare Coulomb potential. Screening effects enter only via f_{ab}, e.g. [25]. Thermodynamic functions such as the free energy may then be determined by a charging procedure.

3.2. Pair Distribution of an OCP via HNC

Now we determine the pair distribution for the case of an OCP, generalizations to multi-component systems are straightforward. We will discuss the two–particle correlations in the approximation of a homogeneous system. For such a system, the binary distribution function $f(\mathbf{r}_{12})$ is determined by the following scheme:

$$\begin{aligned} &g(\mathbf{r}_{12}) = f(\mathbf{r}_{12}) - 1 \\ &f(\mathbf{r}_{12}) = \exp\left[-\beta\phi(\mathbf{r}_{12}) + S(\mathbf{r}_{12})\right] \\ &S = N + E \rightarrow N \end{aligned}$$

$$
\begin{aligned}
g(\mathbf{r}_{12}) &= X(\mathbf{r}_{12}) + N(\mathbf{r}_{12}) \\
N(\mathbf{r}_{12}) &= n\int X(\mathbf{r}_{13})g(\mathbf{r}_{23})d\mathbf{r}_3 \\
g(\mathbf{r}_{12}) &= X(\mathbf{r}_{12}) + n\int X(\mathbf{r}_{13})g(\mathbf{r}_{23})d\mathbf{r}_3\,. \qquad (40)
\end{aligned}
$$

Here, $X(r_{12})$ is the direct correlation function, $N(r_{12})$ represents node diagrams, whereas bridge diagrams $E(r_{12})$ are neglected in HNC. As the system is isotropic and assumed to be locally homogeneous (the dependence on the center of mass coordinate was neglected), we use $\mathbf{r}_{12} \to r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$.

The equations may be rearranged to give

$$N(r_{12}) = n\int [g(r_{13}) - N(r_3)]g(r_{32})d\mathbf{r}_3\,. \qquad (41)$$

This integral is of convolution type and is thus, after Fourier transformation, written in algebraic shape

$$N(k) = \frac{ng^2(k)}{1+ng(k)}\,. \qquad (42)$$

The relation (42) can be taken as the starting point of an iteration scheme, beginning with $f^0_{12}(r) = \exp[-\beta\Phi_{12}(r)] = g^0_{12}(r) + 1$, which is Fourier transformed and used in (42). Then $N(k)$ is determined, after Fourier transformation, yielding an improved g, etc.

There exists another iteration scheme which starts from the version

$$g(r_{12}) = X(r_{12}) + n\int X(r_{13})g(r_{32})d\mathbf{r}_3\,, \qquad (43)$$

and Fourier transformation leads to

$$N(k) = \frac{nX^2(k)}{1-nX(k)}\,. \qquad (44)$$

In this case, the iteration scheme starts with $X^0(r) = \exp[-\beta\Phi(r)] - 1$. Then again a Fourier transformation is performed and the result is inserted into Eq. (44). Back transformation gives the next iteration step. According to some experience, the convergence of the scheme (43, 44) is better than that of (41, 42).

We give an example for a Yukawa–type potential and show the binary distribution function for two sets of parameters in Fig. 4 whereas the corresponding structure factors are shown in Fig. 5. Finally, in our approximation, the result for the binary density operator F_{12} depends also on the macroscopic inhomogeneity which is accounted for by multiplying the pair distribution function f_{12} by the single particle distributions, i.e. by the factor $exp(-const[|\mathbf{r}_2 + \mathbf{r}_1|^2])$.

3.3. Generalization to Quantum Systems

We discuss the possibility to include quantum effects via effective potentials. Now one has to choose the potential Φ to be used in the HNC procedure such that it includes, at short distances, quantum effects. A suitable approximation is to use the sum of the direct Kelbg potential [26] and an exchange term (46).

Quantum effects produce short range corrections to the (binary) distribution function which may be expressed in terms of an additional short range correction $V'_{ab}(\mathbf{r})$ to the Coulomb potential $V_{ab}(\mathbf{r})$ and may be written using the (two–particle) *Slater sum* $S_{ab}(\mathbf{r})$ which was computed in

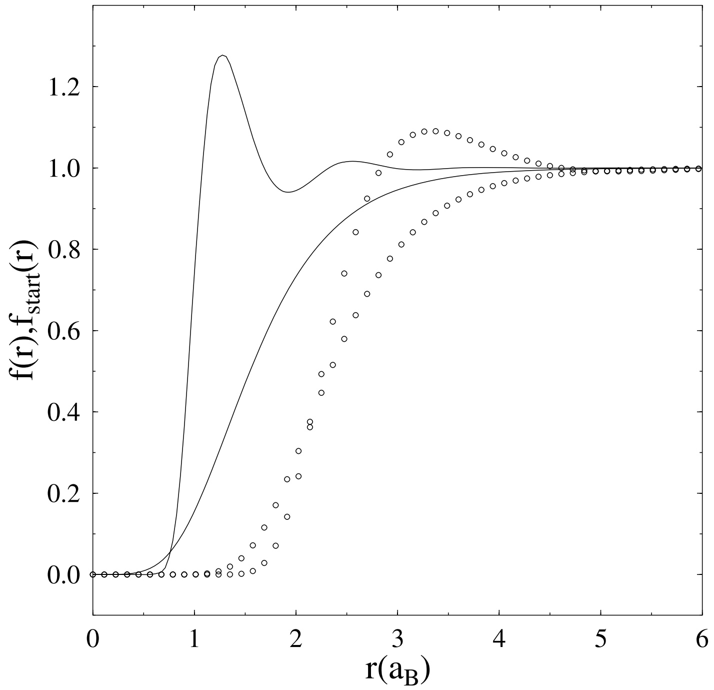

Figure 4. Radial distributions for a repulsive Yukawa potential with $\kappa = 1.5$: curves with maxima correspond to $f_{12}(r)$, the monotonic curves are the start solutions of the iteration. Full line: $1/(k_BT) = 25$, and density $n = 0.5$; circles: $1/(k_BT) = 100$, $n = 0.02$. Atomic units are used.

Refs. [26]–[27] to give results for the effective potential. The direct potential was determined in [26]. The screened version of the direct potential reads [28, 29]

$$\begin{aligned} V_{ab}^{\text{Kelbg,sc}}(r) &= \frac{e_a e_b \pi^{1/2} r_D}{2\lambda_{ab}} \frac{1}{r} \Bigg[\exp\left(-\frac{r}{r_D} + \frac{\lambda_{ab}^2}{4r_D^2}\right) \left\{ \Phi\left(\frac{r}{\lambda_{ab}} - \frac{\lambda_{ab}}{2r_D}\right) + 2\Phi\left(\frac{\lambda_{ab}}{2r_D}\right) - 1 \right\} \\ &+ \exp\left(\frac{r}{r_D} + \frac{\lambda_{ab}^2}{4r_D^2}\right) \left\{ 1 - \Phi\left(\frac{r}{\lambda_{ab}} + \frac{\lambda_{ab}}{2r_D}\right) \right\} \Bigg] \end{aligned} \tag{45}$$

where $\lambda_{ab} = \hbar/(2m_{ab}k_BT)^{1/2}$, $m_{ab} = m_a m_b/(m_a + m_b)$. A simple exchange approximation is the term without interaction only, namely

$$V_{ab}^{\text{exch}}(r) = \frac{\delta_{ab}}{2s_a + 1} k_BT \exp\left(-r^2/\lambda_{ab}^2\right). \tag{46}$$

Alternatively, one can treat strongly correlated Coulomb systems via first principle numerical simulations such as Molecular Dynamics or Monte Carlo. This has been done also for quantum systems using effective quantum potentials. Here also *improved* Kelbg potentials are available which are applicable to situations of strong coupling, see e.g. [30, 31, 32, 33] and references therein.

4. Equilibrium BBGKY-Hierarchy and Simple Solutions

The first two equations of the equilibrium BBGKY-hierarchy read, for the single particle distribution unction ($\mathbf{q_i}$ denote particle coordinates),

$$k_BT\frac{\partial F_1}{\partial \mathbf{q}_1} + F_1\frac{\partial U_1}{\partial \mathbf{q}_1} + n\int d\mathbf{q}_2\, \frac{\partial U_{12}}{\partial \mathbf{q}_1} F_{12}(\mathbf{q}_1\mathbf{q}_2) = 0 \tag{47}$$

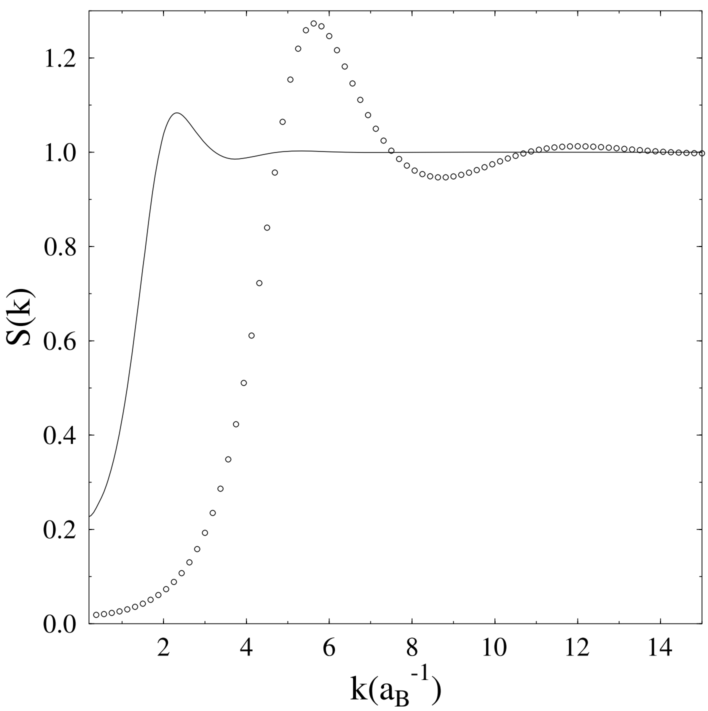

Figure 5. Static structure factor for the same system as in Fig. 4. Full line: $1/(k_BT) = 100$, density $n = 0.02$; circles: $1/(k_BT) = 25$, $n = 0.5$.

and for the two–particle distribution function

$$k_BT\frac{\partial}{\partial \mathbf{q}_1}F_{12}(\mathbf{q}_1\mathbf{q}_2) + F_{12}\frac{\partial}{\partial \mathbf{q}_1}(U_{12}+U_1+U_2) + n\int \frac{\partial}{\partial \mathbf{q}_1}U_{13}(\mathbf{q}_1\mathbf{q}_3)F_{123}(\mathbf{q}_1\cdots\mathbf{q}_3)d\mathbf{q}_3 = 0\,. \quad (48)$$

Correlation functions are defined as

$$\begin{aligned} F_{12} &= F_1F_2 + g_{12}\,, \\ F_{123} &= F_1F_2F_3 + F_1g_{23} + F_2g_{31} + F_3g_{12} + g_{123}\,. \end{aligned} \quad (49)$$

4.1. Approximate solutions of the hierarchy.
Now we discuss a number of important approximations.

1) From (47), we get the simplest approximation by neglecting the integral term

$$F_1(\mathbf{q}_1) = const_1 \exp\left\{-\beta U_1(\mathbf{q}_1)\right\}\,. \quad (50)$$

So far, interactions were completely neglected, and (50) gives the spatial distribution of noninteracting particles in the trap.

2) In a next approximation, we simplify the integral term of (47) according to the first line of Eq. (49) and neglect correlations, g_{12},

$$n\int d\mathbf{q}_2\,\frac{\partial U_{12}}{\partial \mathbf{q}_1}F_1F_2 = nF_1\frac{\partial}{\partial \mathbf{q}_1}\int d\mathbf{q}_2\,F_2U_{12},$$

resulting in the Hartree (mean field) approximation,

$$F_1 = const_2 \exp\left\{-\beta\left(U_1 + n\int U_{12}F_2 d\mathbf{q}_2\right)\right\}\,, \quad (51)$$

where the particles move in an effective potential. This equation may be solved by successive iterations starting with (50) for F_2 under the integral.

3) We now consider Eq. (48). Neglecting the integral term, we get

$$F_{12} = const_3 \exp\left\{-\beta\left(U_{12} + U_1 + U_2\right)\right\} \;, \tag{52}$$

which describes the two-particle distribution in binary collision approximation, however, screening is not included.

4) Further we consider Eq. (48) including the integral term, but omitting the three-particle correlations, $g_{123} = 0$

$$\begin{aligned} &k_B T \frac{\partial}{\partial \mathbf{q}_1} F_{12}(\mathbf{q}_1 \mathbf{q}_2) + F_{12} \frac{\partial}{\partial \mathbf{q}_1}(U_{12} + U_1 + U_2) \\ &+ n \int d\mathbf{q}_3 \, \frac{\partial}{\partial \mathbf{q}_1} U_{13}(\mathbf{q}_1 \mathbf{q}_3)(F_1 F_2 F_3 + F_1 g_{23} + F_2 g_{31} + F_3 g_{12}) = 0 \,. \end{aligned} \tag{53}$$

In the integral term, only the contribution from $F_1 g_{23}$ is finite, the other terms vanish, with the result

$$\begin{aligned} k_B T \frac{\partial}{\partial \mathbf{q}_1}\{F_1 F_2 \ + \ g_{12}(\mathbf{q}_1 \mathbf{q}_2)\} + (F_1 F_2 + g_{12}) \frac{\partial}{\partial \mathbf{q}_1}(U_{12} + U_1 + U_2) \\ + n F_1 \frac{\partial}{\partial \mathbf{q}_1} \int d\mathbf{q}_3 \, U_{13}(\mathbf{q}_1 \mathbf{q}_3) g_{23}(\mathbf{q}_2 \mathbf{q}_3) = 0 \,. \end{aligned} \tag{54}$$

In order to derive an analytical solution including screening effects, we neglect the correlation function g_{12} in the second parenthesis on the left. This corresponds to the neglect of ladder type diagrams [13]. We introduce relative and center of mass coordinates,

$$\mathbf{q}_1 - \mathbf{q}_2 = \mathbf{q} \quad \mathbf{q}_1 + \mathbf{q}_2 = 2\mathbf{R} \,,$$

and assume weak inhomogeneity, such that $F(q_1) \approx F(R)$, $U(q_1) \approx U(R)$, therefore $\frac{\partial}{\partial \mathbf{q}}(F_1 F_2) \approx 0$, and $\frac{\partial}{\partial \mathbf{q}}(U_1 + U_2) \approx 0$. Further we use that U_{12} depends only on the relative coordinate and assume that $\frac{\partial}{\partial \mathbf{R}} g_{12}(\mathbf{q}; \mathbf{R}) \ll \frac{\partial}{\partial \mathbf{q}} g_{12}(\mathbf{q}; \mathbf{R})$, Then we write, explicitly indicating species

$$\begin{aligned} &\frac{\partial}{\partial \mathbf{q}} g_{ab}(\mathbf{q}; \mathbf{R}) \ + \ \frac{1}{k_B T} F_a(R) F_b(R) \frac{\partial}{\partial \mathbf{q}} U_{ab}(\mathbf{q}) \\ &\qquad + \sum_c \frac{n_c}{k_B T} F_a(R) \frac{\partial}{\partial \mathbf{q}_1} \int d\mathbf{q}_3 \, U_{ac}(\mathbf{q}_1 - \mathbf{q}_3) g_{bc}[\mathbf{q}_2 - \mathbf{q}_3; (\mathbf{q}_2 + \mathbf{q}_3)/2] = 0 \,. \end{aligned} \tag{55}$$

Now let us assume U_{ab} to be the Coulomb potential. We apply $\frac{\partial}{\partial \mathbf{q}_1}$ to Eq. (55) and recall the Green function of the Poisson equation

$$\Delta_q U = -4\pi e_a e_b \delta(|\mathbf{q}_1 - \mathbf{q}_2|) \,,$$

allowing us to transform Eq. (55) to

$$\Delta_q g_{ab}(\mathbf{q}; \mathbf{R}) = \frac{4\pi e_a e_b}{k_B T} F_a F_b \delta(r) + F_a(R) \sum_c \frac{4\pi n_c e_a e_c}{k_B T} g_{bc}(\mathbf{q}; \mathbf{R}) \,, \tag{56}$$

where $r \equiv |\mathbf{q}_1 - \mathbf{q}_2|$). We introduce the ansatz

$$g_{ab}(\mathbf{q}; \mathbf{R}) = \frac{1}{k_B T} e_a e_b g(r) F_a(\mathbf{R}) F_b(\mathbf{R})$$

in Eq. (56) and obtain

$$\Delta g(r) = 4\pi\delta(r) + \sum_c \frac{4\pi n_c e_c^2}{k_B T} F_c(\mathbf{R}) g(r) \,. \tag{57}$$

For $r \neq 0$, we get

$$\Delta g(r) = \kappa^2 g(r) \tag{58}$$

with

$$\kappa^2(\mathbf{R}) = \sum_c \frac{4\pi n_c e_c^2}{k_B T} F_c(\mathbf{R}) \,. \tag{59}$$

The solution is

$$g(r) = -A \frac{e^{-\kappa r}}{r} \,,$$

where the constant A is determined from the condition

$$\sum_b n_b e_b F_b(\mathbf{R}) \int dr \, g_{ab}(r) = e_a$$

with the result $A = 1$. Thus, in this approximation, the full pair correlation function is given by

$$g_{ab}(r;\mathbf{R}) = -F_a(\mathbf{R}) F_b(\mathbf{R}) \frac{e_a e_b}{k_B T} \frac{e^{-\kappa(\mathbf{R}) r}}{r} \,, \tag{60}$$

i.e. we have obtained the Debye pair correlation function in local approximation which contains a space-dependent screening constant κ.

4.2. Screening and short range forces

We assume that the single particle distributions occur only as pre-factors and in κ like in (59). We follow the papers [34], [35] and write for the pair distribution function which now includes ladder type contributions and, in addition short range contributions and screening corrections.

$$F_{ab}(r;\mathbf{R}) = F_a(R) F_b(R) \exp\{-\beta V_{ab} - \beta V'_{ab}\} \left[1 + \sum_c n_c \int \cdots \right] . \tag{61}$$

Here, V_{ab} is the Coulomb potential, and V'_{ab} is an *additional* short range potential, e.g., the hard sphere potential or the Kelbg-potential, but *not* the Debye or the Yukawa potential. However, (61) leads to divergent results for large distances between the particles a and b. Therefore, according to Schmitz [35], the Coulomb potential is iteratively replaced by a screened potential. This is performed as follows. We use the alternative definition for the distribution function and get from (55) after integration over $\mathbf{q}_1$ with U_{ab} now being the Coulomb potential V_{ab}

$$g_{ab}(\mathbf{q}_1\mathbf{q}_2) \frac{1}{k_B T} V_{ab} + \sum_c \frac{n_c}{k_B T} F_c \int V_{ac}(\mathbf{q}_1\mathbf{q}_3) g_{bc}(\mathbf{q}_2\mathbf{q}_3) d\mathbf{q}_3 = 0 \,. \tag{62}$$

The equation (62) is the famous screening equation having a solution of the type (60). The idea of Schmitz was to eliminate the Coulomb potential from (61) using Eq. (62). The result is (now the relative variables are r and $\mathbf{r}_3$)

$$\begin{aligned} F_{ab}(r;\mathbf{R}) \;&= F_a(R) F_b(R) \exp\{g_{ab} - \beta V'_{ab}\} \Big\{ 1 + \sum_c n_c \int d\mathbf{r}_3 \\ &\qquad \times [\Phi_{ac} g_{bc} + \Phi_{bc} g_{ac} + \Phi_{ab} g_{bc}] + \cdots \Big\} \,, \end{aligned} \tag{63}$$

where $\Phi_{ab}(r) = \exp(g_{ab} - \beta V'_{ab}) - 1 - g_{ab}$, see also Ref. [36].

4.3. Thermodynamics from the Pair Distribution Function

The excess free energy is given in terms of F_{ab} via the charging procedure

$$F - F^{id} = \frac{1}{2}\sum_{ab}\int_0^1 \frac{d\lambda}{\lambda}\left\{V_{ab}(r) + V'_{ab}\right\} F_{ab}(r, R; \lambda) d\mathbf{r} d\mathbf{R}. \tag{64}$$

We omit the details of the calculations and arrive at

$$\begin{aligned} F - F^{id} \;&=\; -k_B T \sum_{ab}\int d\mathbf{R} F_a(R) F_b(R)\Bigg\{\frac{1}{4}\frac{\kappa^3}{12\pi} + \frac{\pi}{3} n_a n_b \left(\frac{e_a e_b}{k_B T}\right)^3 \ln(\kappa R_{ab}) \\ &\quad + 2\pi n_a n_b R_{ab}^3 K_0(\xi_{ab}) + \mathcal{O}(n^{3/2}\ln n)\Bigg\}. \end{aligned} \tag{65}$$

Here we used $\xi_{ab} = -e_a e_b/(D_0 k_B T R_{ab})$, where R_{ab} is the hard-sphere contact distance. In Eq. (65), there is an implicit R-dependence via κ, and we introduced the virial function, $K_0(\xi)$, which is given by

$$\begin{aligned} K_0(\xi) \;&= \frac{1}{6}\xi^3\left[Ei(\xi) - \ln|3\xi| - 2C + \frac{11}{6}\right] - \frac{1}{6}e^{\xi}(2 + \xi + \xi^2) \\ &= -\frac{1}{3} - \frac{1}{2}\xi - \frac{1}{2}\xi^2 - \frac{1}{6}\xi^3(C + \ln 3) + \sum_{m=4}^{\infty}\frac{\xi^m}{m!(m-3)}, \end{aligned} \tag{66}$$

with Ei denoting the exponential-integral-function, and $C = 0.5772$ is Euler's constant. This result is applicable for large e^2, but for small densities.

As an example, we give two values: $K_0(10) = .3756 * 10^4$, $K_0(-10) = .4537 * 10^3$. The function with the positive argument corresponds to an attractive interaction leading to association (i.e. to bound states). It is one order of magnitude larger than the function with the negative argument, which is related to the repulsive case. For very large (positive) $\xi_{ab} = \xi$, we have:

$$F - F^{id} = -k_B T \int d\mathbf{R} F_1 F_2 \left\{\frac{\kappa^3}{12\pi} + 4\pi n^2 R_0^3 \frac{1}{\xi} e^{\xi} + \cdots\right\}. \tag{67}$$

Here, for all species, the same hard sphere radius $R_{ab} = R_0$ was used, for simplicity. From the free energy (65) or (67), respectively, any thermodynamic function may be determined.

A detailed discussion of thermodynamic functions and especially of the transition from mesoscopic clusters to macroscopic systems is given in Ref. [37], in this volume.

5. Conclusion

In summary, the aim of this paper was to briefly review certain theoretical techniques which can be used to describe many particle systems spatially confined in a trap. The main assumption in all derivations was a separation of length scales: we assumed that there are two well separated length scales, namely the extension R_{trap} of the trap and the correlation length r_{corr} of the interacting particles. We assumed that $R_{trap} \gg r_{corr}$. This is frequently the case, in particular, for a large trap, for high density or short range interactions. This allowed us to use the local approximation for the many-particle distribution functions, where R enters the homogeneous equations as a parameter. Of course, in general, this distinction is not possible, and one can go beyond the local approximation by performing gradient expansions.

A particular case where it might be necessary to go beyond the local approximation are finite systems containing only several (up to a few thousand) particles. Also, the transition from a mesoscopic to a macroscopic system [37] has to be considered more carefully. Nevertheless, the theoretical schemes given in this paper should be useful for future work on trapped charged particles in general and dusty plasmas in particular.

Acknowledgment

This work is supported by the Deutsche Forschungsgemeinschaft via SFB–TR 24. One of us (WDK) wants to thank Ronald Redmer (Institute of Physics, Rostock University) for hospitality.

References

[1] Major F, Gheorge V and Werth G 2005 *Charged Particle Traps. Physics and Techniques of Charged Particle Field Confinement* (Heidelberg: Springer)

[2] Filinov A , Bonitz M, and Lozovik Yu E 2001, *Phys. Rev. Lett.* **86** 3851

[3] Totsuji H, Totsuji C, Ogawa T and Tsuruta K 2005 *Phys Rev E* **71** 045401(R)

[4] Ludwig P, Kosse S and Bonitz M 2005 *Phys Rev E* **71** 046403

[5] Bonitz M, Block D, Arp O, Golubnichiy V, Baumgartner H, Ludwig P, Piel A, and Filinov A 2006, *Phys. Rev. Lett.* **96** 075001

[6] Dubin D H E and O'Neil T M 1999 *Rev Mod Phys* **71** 87

[7] Bonitz M, Filinov V S, Fortov V E, Levashov P R, and Fehske H 2005 *Phys. Rev. Lett.* **95** 235006

[8] Ichimaru S 1982 *Rev Mod Phys* **54** 1017

[9] Totsuji H, Kishemoto T, Totsuji C and Tsuruta K 2002 *Phys Rev Lett* **88** 125002

[10] Totsuji C, Liman M S, Tsuruta K and Totsuji H 2003 *Phys Rev E* **68** 017401

[11] Totsuji H, Liman M S, Totsuji C and Tsuruta K 2004 *Phys Rev E* **70** 016405

[12] Rosenfeld Y 1994 *Phys Rev E* **49** 4425

[13] Bonitz M 1998 *Quantum Kinetic Theory* (Stuttgart/Leipzig: Teubner)

[14] Kadanoff L P and Baym G 1962 *Quantum Statistical Mechanics* (Redwood City, California: Addison-Wesley)

[15] Ebeling W, Kraeft W D and Kremp D 1976 [1979] *Theory of Bound States and Ionization Equilibrium in Plasmas and Solids* (Berlin [Moscow]: Akademie-Verlag [Mir])

[16] Kremp D, Schlanges M and Kraeft W D 2005 *Quantum Statistics of Nonideal Plasmas* (Berlin/Heidelberg: Springer)

[17] Greiner W, Neise L and Stöcker H 1987 *Theoretische Physik, Band 9: Thermodynamik und Statistische Mechanik* (Harri Deutsch: Thun)

[18] Nolting W 1992 *Theoretische Physik Vol 5 Quantenmechanik* (Zimmermann-Neufang: Ulmen)

[19] Bonitz M and Dufty J W 2004, *Cond. Matt. Phys.* **7** 483

[20] Kraeft W D, Kremp D, Ebeling W and Röpke G 1986 *Quantum Statistics of Charged Particle Systems* (Berlin[New York]: Akademie–Verlag[Plenum])

[21] Tsytovich V, Gusein–Zade N, and Morfill G 2004 *IEEE Trans Plasma Sci* **32** 637

[22] Tsytovich V 2005 *Contr Plasma Phys* **45** 533,544

[23] Morita T 1959 *Progr Theor Phys (Japan)* **22** 757

[24] Kraeft W D, Schlanges M and Vorberger J 2002 *Phys Rev E* **66** 046405

[25] Kraeft W D 2005 *J Phys: Conf Series* **11** 131-138

[26] Kelbg G 1963 *Ann. Physik (Leipzig)* **12** 219

[27] Ebeling W, Hoffmann H J and Kelbg G 1967 *Beitr Plasmaphys* **7** 233

[28] Klimontovich Yu L and Kraeft W D 1974 *High Temp Physics (USSR)* **12** 212-19

[29] Klimontovich Yu L and Kraeft W D 1974 *Teor Mat Fiz* **19** 364-70

[30] Filinov A, Bonitz M and Ebeling W 2003 *J Phys A Math Gen* **36** 5957

[31] Filinov A, Golubnychiy V, Bonitz M, Ebeling W and Dufty J W 2004 *Phys Rev E* **70** 046411

[32] Ebeling W, Filinov A, Bonitz M, Filinov V and Pohl T 2005 *J Phys A Math Gen* (accepted)

[33] Golubnychiy V 2004 *PhD thesis* (University of Kiel)

[34] Falkenhagen H and Ebeling W 1971 *Ionic Interactions Vol 1* (Academic Press Inc: New York & London)

[35] Schmitz G 1968 *Ann Physik (Leipzig)* **21** 31

[36] Meeron E 1957 *J Chem Phys* **26** 804

[37] Kraeft W D and Bonitz M 2006 *J Phys*, this volume