Charge Correlations in a Harmonic Trap

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A system of N classical Coulomb charges trapped in a harmonic potential displays shell structure and orientational ordering. The local density profile is well understood from theory, simulation, and experiment. Here, pair correlations are considered for this highly inhomogeneous system for both the fluid and ordered states. In the former, it is noted that there is a close relationship to pair correlations in the uniform OCP. For the ordered state, it is shown that the disordered "tiling" is closely related to the ground state Thomson sites for a single sphere.

1 Introduction

Harmonically trapped Coulomb charges form a shell structure in their local density profile at sufficiently strong coupling. An ordering of the particles within the shells occurs at still stronger coupling. This behavior is now well understood at strong coupling from both experiment and simulation [1–6] and from theory (shell models) [6–8]. Recently, Monte Carlo simulation and density functional theory have been applied across the entire fluid phase [9, 10]. The theoretical approaches make clear the essential role of pair correlations in the formation of shells. Somewhat surprisingly, it was found that good shell structure could be obtained using the pair correlations for a uniform one component plasma (OCP) as an approximation to the true correlations of the highly non-uniform trap. The objective here is to report some initial studies of pair correlations among charges in a trap under conditions of strong shell structure in both the fluid and ordered states. The primary observations are:

- The distribution of pairs in the trap in their fluid state is well represented by that for the three dimensional OCP for particle number $N \gtrsim 50$, even at strong coupling where shell structure is prominent.
- Angular correlations for particles within a given shell in the fluid phase are similar to those obtained from the uniform three dimensional OCP if the pair distance of the latter is reinterpreted as the chord length for two points in the shell.
- Angular correlations for charges confined to a single sphere in the fluid phase are almost identical to those for the two dimensional OCP with the pair distance interpreted as the chord length.
- Angular correlations in the ordered phase can be represented by the solutions to the Thomson problem [11] broadened by thermal disorder.

2 Pair correlations - fluid phase

Consider a one component system of Coulomb charges q. The two cases of interest here are a system of charges in a harmonic trap, and the same system of charges in a uniform neutralizing background (OCP). Only equilibrium

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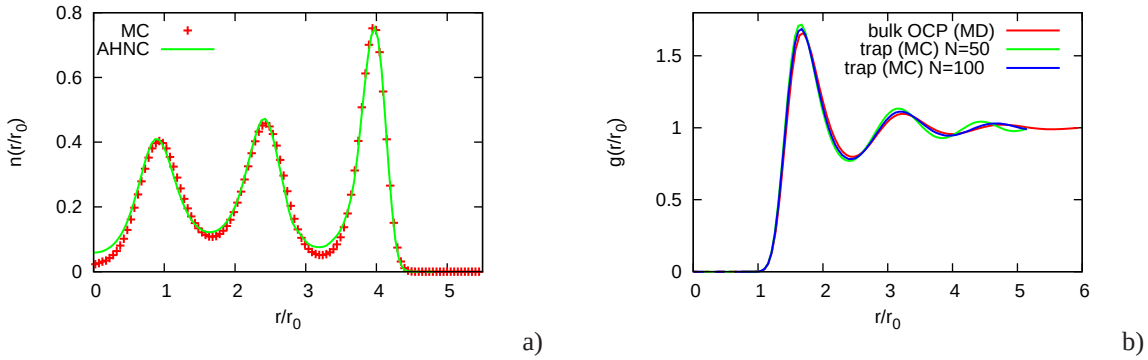

a) b)

Fig. 1: Density profile for $N = 100$ charges in trap showing shell structure ($\Gamma = 50$) (**a**). Comparison of distribution of pairs for particles in trap with that for particles in bulk OCP ($\Gamma = 50$) (**b**).

correlations are considered so the statistical properties are determined from the potential energies

$$U_T\left(\{r_i\}\right) = \sum_{i=1}^{N} \frac{1}{2} m\omega^2 r_i^2 + \frac{1}{2}\sum_{i\neq j}^{N} \frac{q^2}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{1}$$

$$U_{OCP}\left(\{r_i\}\right) = \frac{1}{2}\sum_{i\neq j}^{N} \frac{q^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i=1}^{N} n \int d\mathbf{r}' \frac{q^2}{|\mathbf{r}_i - \mathbf{r}'|} + n^2 \frac{1}{2} \int d\mathbf{r}' d\mathbf{r}'' \frac{q^2}{|\mathbf{r}' - \mathbf{r}''|}. \tag{2}$$

Here $n = N/V$, where the volume is taken to be spherical with radius R.

Usually, the OCP is considered in the thermodynamic limit ($N, V \to \infty, n = N/V$ =constant) where it is spatially uniform. This will be referred to as the bulk OCP. However, the charges in the trap and those of the OCP constitute the same system for finite N [12], which is shown by performing the integrals in (2) to give

$$U_{OCP} = \frac{1}{2}\sum_{i\neq j}^{N} \frac{q^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{2\pi q^2}{3} n \sum_{i=1}^{N} r_i^2 + \frac{8\pi q^2}{5} nNR^2. \tag{3}$$

Thus U_{OCP} is equivalent to U_T, up to a constant which does not contribute to the equilibrium ensemble. Both systems are self-bound at a maximum radius R_0 (when $R > R_0$). Force equilibrium on a particle for the trap $m\omega^2 R_0 = q^2 N/R_0^2$ and similarly for the OCP $4\pi q^2 n R_0/3 = q^2 N/R_0^2$ determine R_0. Thus for the same N in the trap and OCP, their volume and average density are the same. In particular $n_{OCP} = n_T = 3m\omega^2/4\pi q^2$ and $R_0^3 = q^2 N/m\omega^2$. This also implies $\omega_p^2 = 3\omega^2$, where $\omega_p^2 = 4\pi n_{OCP} q^2/m$ defines the plasma frequency. In this context, the bulk OCP corresponds to a harmonic trap with infinite filling, and the shell structure for particles in a trap can be understood as finite volume effects for the OCP. The terminology here will be OCP for finite N and bulk OCP for the thermodynamic limit. Simulations using periodic boundary conditions describe the bulk OCP.

In reference [9] a theory for the density profile in the trap was developed in terms of the pair correlations within the trap. For practical purposes it was found that the corresponding bulk OCP pair correlations could be used, giving an accurate approximation for the shell structure. This is illustrated in Fig. 1a for $N = 100$, and coupling strength $\Gamma \equiv \beta q^2/r_0 = 50$ (where r_0 is the mean distance for a pair defined by $4\pi n r_0^3/3 = 1$ and $n = N/V$ is the density). Results from the adjusted hypernetted chain theory (AHNC) and Monte Carlo are given, showing their good agreement. In spite of the above equivalence of the OCP and trap for finite N, it is surprising that the correlations for the uniform bulk OCP could be the same as those for the trap with strong shell structure. Nevertheless, this is the case as shown in Fig. 1b. The agreement is quite reasonable for $N = 50$ and improves with increasing N. This plot gives the distribution of pairs within the trap from Monte Carlo simulation, without reference to where the center of mass of the pair is located. Thus it is not the pair correlation function defined relative to the center of the trap, which would indeed reflect its spatial inhomogeneity. In Fig. 1b the contributions to a given r come from all pairs at that distance anywhere within the trap. The bulk three dimensional OCP pair correlation function is determined from molecular dynamics simulation.

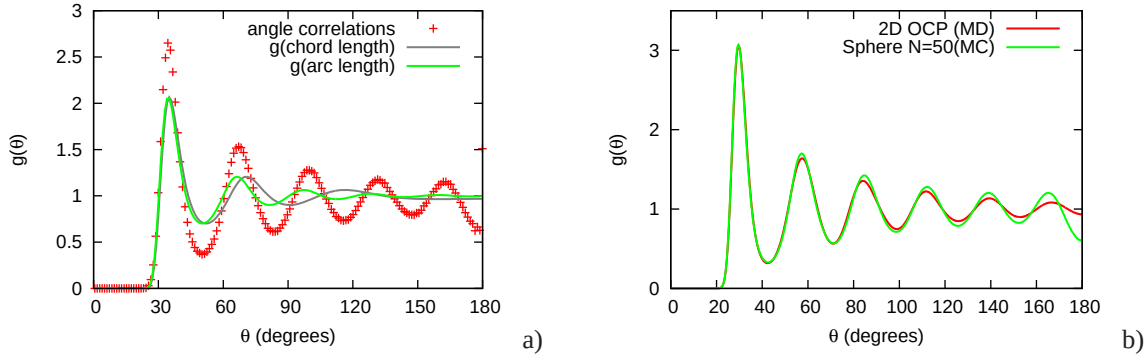

Fig. 2: Angular correlations for particles in the outer shell compared to those for a 3d bulk OCP ($N = 44$, $\Gamma = 100$) (**a**). Pair correlation function for particles confined to a single sphere ($N = 50$) compared to that for a 2d bulk OCP with distance interpreted as arc length ($\Gamma = 126$) (**b**).

This agreement is possible because the property being calculated depends only on the relative separation of pairs, a translationally invariant property. The trap Hamiltonian can be expressed in terms of its center of mass and relative coordinates by a canonical transformation. For averages of properties depending only on pair separation the center of mass coordinate can be integrated out leaving a translationally invariant potential. For sufficiently large N (e.g., $N = 50$) most pairs are away from the trap surface and the pair distribution behaves like that for the bulk OCP. A detailed demonstration of this will be given elsewhere.

3 Angular correlations - fluid phase

Next consider the particles within a chosen shell, defined by the domain between the minima on either side of a peak in the radial density profile (see Fig. 1a). An initial particle is chosen and the number of particles at an angle θ relative to the first is calculated. In the fluid phase there is rotational symmetry about the line from the origin to the first particle, so only one angle is required for this correlation function. In practice the results obtained by Monte Carlo simulation are an average over the radial annulus of the shell for both members of a pair.

Fig. 2a shows the angular correlation function from molecular dynamics simulation of $N = 44, \Gamma = 100$, for which there are two shells with 8 and 36 particles. The correlation function is for the larger outer shell. Also shown are two results from the same molecular dynamics simulation of the three dimensional OCP at the same value of Γ, but with two interpretations for the pair separation. In one case, the usual Euclidean distance between particles is chosen, i.e. the chord length. In the second case the argument of the bulk OCP pair correlation function is interpreted as the larger arc length. The figure shows a definite improvement in relative agreement with the trap correlations in the second case. Absolute agreement is not expected since the trap data is averaged over the annulus whereas the OCP data is calculated for points at the maximum of the outer shell only. In this context the location of the peaks is the relevant test for qualitative comparison.

The complication of a finite shell width can be mitigated by increasing the coupling constant Γ, leading to a sharpening of the shells into smaller annulae. This is limited since ordering within the shells occurs at some maximum value of Γ for the fluid state. The correlations are then very different (see below) and not related to those of the bulk OCP. To explore the interesting relationship of Fig. 2a under more controlled conditions, consider the idealized case of charges confined to a single spherical shell of zero width. The correlations are now constrained to a two dimensional surface and the appropriate comparison is with correlations in the two dimensional OCP. This is demonstrated in Fig. 2b where the angular correlations for particles constrained to the sphere at $\Gamma = 126$ are compared to those for the two dimensional (Coulomb potential) OCP pair correlation function *with the distance reinterpreted as the arc length*. The remarkable agreement suggests a mathematical relationship between the two quite different systems. Why should the two systems find agreement when their geometry (metric) is adjusted? This will be discussed elsewhere.

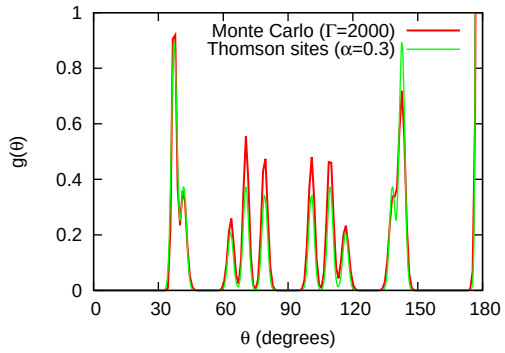

Fig. 3 Comparison of the angular correlations among particles in the outer shell with those for the thermally broadened Thomson sites ($N = 38$).

4 Angular correlations - ordered phase

At sufficiently large Γ rotational symmetry is broken and the particles within each shell become ordered. The ground state configuration for $\Gamma \to \infty$ is well studied by simulation and theory. In particular, a shell model using the correlation energy for the Thomson sites (minimum energy configuration for charges on a sphere) gives an excellent description of the trap ground state energy [8]. In fact, the ground state positions for a given shell from quenched molecular simulation are very close to the Thomson sites on a sphere of the same size and particle number. Due to the spherical geometry, the ordering is not regular in general and depends on the particle number. It is tempting to consider the Thomson sites as the analogue of a fundamental lattice for these spherical crystals.

To test this picture the angular correlations for particles of one shell of a trap with those for the corresponding Thomson sites are compared. At finite Γ, the Thomson site charges have kinetic energy and are represented by

$$f(\theta) = \sqrt{\frac{\alpha}{\pi}} e^{-\alpha(\theta-\theta_0)^2},$$

where θ_0 are the Thomson sites and α is a function of Γ. Configuration data for the Thomson sites can be found at [13]. Fig. 3 shows this comparison for a trap with 38 particles (32 in the outer shell) at $\Gamma = 2000$. The corresponding Thomson correlations are shown for $\alpha = 0.3$. The very good agreement provides initial support for this picture of Thomson sites as a fundamental spherical "lattice". A detailed test requires further analysis to study how structure appears as Γ is increased, other values of N for which very different order occurs, and a comparison with configurations for nearby metastable states. This will be reported elsewhere.

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