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Linear response for confined particles

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Abstract

The dynamics of fluctuations is considered for electrons near a positive ion or for charges in a confining trap. The stationary nonuniform equilibrium densities are discussed and contrasted. The linear response function for small perturbations of this nonuniform state is calculated from a linear Markov kinetic theory whose generator for the dynamics is exact in the short time limit. The kinetic equation is solved in terms of an effective mean field single particle dynamics determined by the local density and dynamical screening by a dielectric function for the nonuniform system. The autocorrelation function for the total force on the charges is discussed.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Consider a system of N charges in a spherical container of radius R. An external potential centered at the origin exerts an attractive central force. The Hamiltonian is

$$H = \sum_{\alpha=1}^{N} \left(\frac{1}{2} m v_\alpha^2 + V_c(r_\alpha) + V_b(r_\alpha) + V_w(r_\alpha) \right) + \frac{1}{2} \sum_{\alpha}^{N} \sum_{\gamma \neq \alpha}^{N} V(r_{\alpha\gamma}) \qquad (1)$$

where $\mathbf{r}_\alpha$ and $\mathbf{v}_\alpha$ are the position and velocity of charge α. The repulsive interaction potential between particles α and γ is denoted by $V(r_{\alpha\gamma})$ where $r_{\alpha\gamma} \equiv |\mathbf{r}_\alpha - \mathbf{r}_\gamma|$. The external 'confinement' potential $V_c(r_\alpha)$ is the same for all particles, and $V_w(r_\alpha)$ is the wall potential that is zero inside the container and infinite otherwise. Charged systems are of direct relevance e.g. to dusty plasmas and ions in traps. For neutral systems $V_b(r_\alpha)$ is the interaction of each particle with a uniform neutralizing background, corresponding to an OCP or jellium with an attractive trap at the origin.

An example that has been studied recently is jellium with a point positive ion of charge number Z at the origin [1, 2]. At equilibrium the electron density is enhanced (partial confinement) near the origin and approaches a uniform limit far from the ion, for sufficiently large R, due to charge neutrality. An opposite extreme is a system of charges in a strong trap such that they are localized in a finite domain away from the wall and their density vanishes outside this domain (complete confinement). There is a continuous mapping between these two limiting cases, controlled by the relative strengths of the repulsion between particles and the strength and form of the confining potential. The discussion of these cases here will be limited to classical statistical mechanics.

2. Equilibrium density

In the absence of a confining potential the equilibrium density may be uniform (charge neutral) or nonuniform (charged). In general the confining potential will induce a nonuniform equilibrium density in any case. Formally it is determined from the exact Yvon–Born–Green equation [3]

$$\frac{\mathrm{d}n(r_1)}{\mathrm{d}r_1} + \beta n(r_1)\frac{\mathrm{d}V_c(r_1)}{\mathrm{d}r_1} = -\beta \int \mathrm{d}\mathbf{r}_2 (n(\mathbf{r}_1,\mathbf{r}_2) - n(\mathbf{r}_1)n_b)\frac{\mathrm{d}V(r_{21})}{\mathrm{d}r_1}, \tag{2}$$

where $n(\mathbf{r}_1, \mathbf{r}_2)$ is the joint density for two charges and n_b is the density of the uniform neutralizing background. A reasonable approximation is the hypernetted chain approximation (HNC) [3, 4],

$$\frac{\mathrm{d}}{\mathrm{d}r_1}\left[\ln n(r_1) + \beta V_c(r_1) - \int \mathrm{d}\mathbf{r}_2 (n(r_2) - n_b)c(r_{21})\right] = 0. \tag{3}$$

The solutions to this equation are quite rich, reflecting the competition between the attraction of V_c and the renormalized repulsion of $c(r_{21})$. They have been described in some detail for the case of the positive ion in jellium [4]. Here we report on some preliminary results for the qualitatively different case of weakly coupled charges in a harmonic trap $V_c(r) = kr^2/2$ with $n_b = 0$. There is then a competition between Coulomb repulsion and trap attraction, with charge density enhanced near the wall or near the center, respectively. These effects are balanced when $\omega_m = \omega_c$, leading to a uniform density at all temperatures. Here $\omega_m = \omega_p/\sqrt{3}$ is the Mie plasma frequency ($\omega_p^2 = 4\pi nq^2/m$) and $\omega_c = \sqrt{k/m}$ is the frequency associated with the harmonic trap. More generally, when $\omega_c > \omega_m$ the charges are increasingly drawn away from the wall at lower temperatures (i.e., kinetic energy relative to trap energy decreases), approaching at $T = 0$ a uniform density for $r < R_0 = (\omega_m/\omega_c)^{2/3}R$ and zero density for $R_0 < r$ [5]. In the opposite case of $\omega_c < \omega_m$ the Coulomb repulsion dominates and the particle density is enhanced at the wall. At lower temperatures the density becomes sharp at the walls—a 'Coulomb explosion' that is restrained by the external walls. This behavior is illustrated in figure 1 for $\omega_c/\omega_m = 2$ and for $\omega_c/\omega_m = 1/2$, at $T = 1, 0.1$ and 0.01.

3. Linear response

Consider a perturbation of the nonuniform equilibrium state by an external potential of the form $U_{\mathrm{ext}}(t) = \sum_{\alpha=1}^{N} V_{\mathrm{ext}}(r_\alpha, t) = \int \mathrm{d}\mathbf{r} V_{\mathrm{ext}}(r, t)\widehat{n}(\mathbf{r})$, where $\widehat{n}(\mathbf{r})$ is the phase function representing the particle density. Then, to linear order in $V_{\mathrm{ext}}(r, t)$ the response of the average particle density to this perturbation is [6]

$$\delta\langle\widehat{n}(\mathbf{r},t)\rangle = \int_0^t \mathrm{d}t' \int \mathrm{d}\mathbf{r}' \chi(\mathbf{r}, \mathbf{r}', t - t')V_{\mathrm{ext}}(r', t'), \tag{4}$$

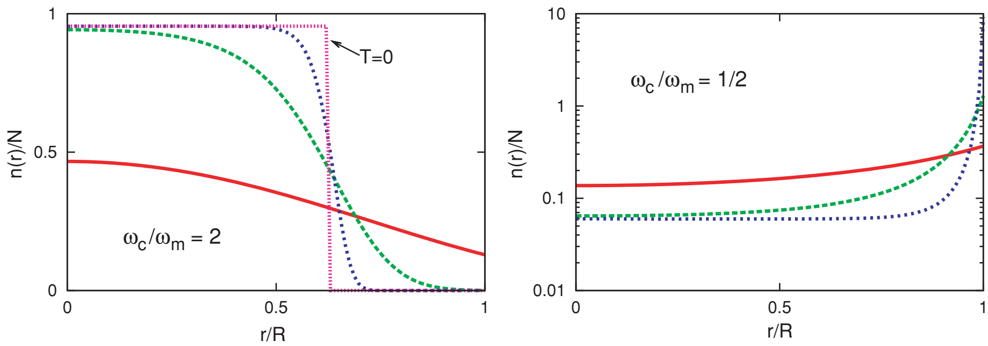

Figure 1. Temperature dependence of densities for trap-dominated (left) and Coulomb-dominated (right) conditions.

with the response function

$$\chi(\mathbf{r}, \mathbf{r}', t) = -\beta\partial_t \langle \widehat{n}(\mathbf{r})\widehat{n}(\mathbf{r}', -t)\rangle_e = \beta\nabla_{\mathbf{r}'} \cdot \langle \widehat{n}(\mathbf{r}, t)\mathbf{j}(\mathbf{r}')\rangle_e. \tag{5}$$

The brackets $\langle\rangle_e$ denote an equilibrium ensemble average. The second equality follows from the conservation law $\partial_t\widehat{n}(\mathbf{r}, t) + \nabla_{\mathbf{r}} \cdot \mathbf{j}(\mathbf{r}, t) = 0$, and the stationarity of the equilibrium ensemble. The response function $\chi(\mathbf{r}, \mathbf{r}', t)$ provides an appropriate object for studying the possible modes of excitation that are supported by the system. An alternative equivalent instrument is the dielectric function $\epsilon(\mathbf{r}, \mathbf{r}'; t)$ defined in analogy with electrodynamics

$$\epsilon^{-1}(\mathbf{r}, \mathbf{r}'; t) \equiv \delta(\mathbf{r} - \mathbf{r}')\,\delta(t) + \int \mathrm{d}\mathbf{r}''\chi(\mathbf{r}, \mathbf{r}''; t)V(|\mathbf{r}'' - \mathbf{r}'|). \tag{6}$$

4. Markov kinetic theory

The evaluation of the response function is a difficult many-body problem. The conditions of interest include both strong confinement and possibly strong charge correlations, so there is no small parameter available for simplifications. Instead, a non-perturbative Markov kinetic theory has been discussed recently in this context [2]. It is based on approximating the formal generator for dynamics in the single particle phase space by its exact form at $t = 0$. This leads to a mean field theory of the linear Vlasov form, but with both the confining potential and the charge–charge potential renormalized by the initial equilibrium correlations. The analysis of [2] can be extended in a straightforward way to the system considered here with the result

$$\chi(\mathbf{r}, \mathbf{r}', t) \rightarrow \int_0^t \mathrm{d}t' \int \mathrm{d}\mathbf{r}_1\overline{\epsilon}^{-1}(\mathbf{r}, \mathbf{r}_1; t - t')\chi_0(\mathbf{r}_1, \mathbf{r}', t'), \tag{7}$$

where $\chi_0(\mathbf{r}'', \mathbf{r}', z)$ is the response function for confined particles without the interparticle interactions $(V(|\mathbf{r} - \mathbf{r}'|) = 0)$

$$\chi_0(\mathbf{r}, \mathbf{r}', t) = -\beta n(\mathbf{r}) \int \mathrm{d}\mathbf{v}\phi(v)\,\mathrm{e}^{-\mathcal{L}_0 t}\mathbf{v} \cdot \nabla_{\mathbf{r}}\delta(\mathbf{r} - \mathbf{r}'), \tag{8}$$

$\phi(v)$ is the Maxwellian, and where the generator $\mathcal{L}_0$ for the effective single particle dynamics is

$$\mathcal{L}_0 = \mathbf{v} \cdot \nabla_{\mathbf{r}} - m^{-1}\nabla_{\mathbf{r}}\mathcal{V}_c(r) \cdot \nabla_{\mathbf{v}}. \tag{9}$$

The renormalized confinement potential is determined from the equilibrium density by $\mathcal{V}_c(r) \equiv -\beta^{-1} \ln n(r)$. Also, $\overline{\epsilon}(\mathbf{r}, \mathbf{r}'; t)$ is

$$\overline{\epsilon}(\mathbf{r}, \mathbf{r}'; t) = \delta(\mathbf{r} - \mathbf{r}')\delta(t) - \int \mathrm{d}\mathbf{r}'' \chi_0(\mathbf{r}, \mathbf{r}'', t)\mathcal{V}(\mathbf{r}'', \mathbf{r}'), \tag{10}$$

where the renormalized charge–charge potential, $\mathcal{V}(\mathbf{r}, \mathbf{r}')$, is defined in terms of the direct correlation function by $\mathcal{V}(\mathbf{r}, \mathbf{r}') = -\beta^{-1} c(\mathbf{r}, \mathbf{r}')$.

Further progress requires evaluation of $\chi_0(\mathbf{r}, \mathbf{r}', t)$ whose dynamics is determined from the effective single particle charge dynamics in the presence of the confinement potential. This can be quite complex over the whole range of weak to strong confinement, and has been discussed in some detail for the case of a central positive ion in jellium [2]. The autocorrelation function for the total force on the charges was studied as a function of the charge number on the central ion. It was found that a simple representation of the single particle trajectories in terms of bound and free states provided an accurate analytical description from weak to strong ion–electron interaction.

Preliminary studies of the harmonic trap suggest the possibility of a simplification in that case as well. As noted above, the low temperature limit leads to a uniform density inside a sphere of radius R_0. Since the effective potential $\mathcal{V}_c(r)$ for the dynamics is determined from this potential, $\chi_0(\mathbf{r}, \mathbf{r}', t)$ becomes the correlation function for free particles inside a sphere. An exact evaluation of the force autocorrelation function in terms of all response frequencies is possible in this case [7].

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