Properties of a One-Dimensional Coulomb Gas

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The BBKGY equations for N identical, impenetrable, charged particles which move in one dimension and lie in a charge neutralizing background, are shown to separate into N uncoupled equations for the sequence of N reduced distributions. The potential relevant to any subgroup of s adjoining particles is that of an s-dimensional harmonic oscillator whose frequency is the plasma frequency of the aggregate. The s-particle spatial equilibrium distribution reveals that particle vibrations remain centered about fixed, uniformly distributed sites as ϱ/T goes from zero to infinity, where ϱ is particle density and T is temperature. Thus it is concluded that the system suffers no change in phase for all ϱ and T.

1. Introduction

In this paper we consider a one-dimensional aggregate of N identical charged particles which move in a charge neutral background which extends over the spatial interval $(-L/2, L/2)$. The particles are further constrained so that they are impenetrable. Whereas the equilibrium properties of closely related systems have been studied in detail [1, 2], kinetic analyses have for the most part been restricted to numerical studies [3, 4]. Furthermore, in these previous investigations, particles were not constrained to be impenetrable.

In the present work, a general simplifying property of the BBKGY sequence, relevant to this configuration, is derived. Namely, it is found that the hierarchy separates into N uncoupled equations for the sequence of N reduced distributions. The potential relevant to any such subgroup of s labeled, adjoining particles, is that of an s-dimensional harmonic oscillator whose frequencies are equal to the plasma frequency of the aggregate.

The general solution for each such reduced distribution is obtained and explicit forms are written down for the normalized equilibrium distributions at a given temperature. The one-particle distribution, for the first labeled particle, in configuration space, is found to be one half a gaussian with local maximum at $x = -L/2$ and local minimum at $x = +L/2$. This asymmetry is a consequence of the constraint of impenetrability and distinguishability of particles in one dimension.

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The s-particle equilibrium distribution is found to contain the Debye distance as a parameter. Apart from fixed constants, the square of this length is equal to T/ϱ, where T is temperature and ϱ is particle number density. It is found that as T/ϱ diminishes from ∞ to 0, the s-particle spatial distribution passes from a flat distribution to one which is peaked at uniform intervals. The exact form of the many-particle distribution function reveals that at all points of this variation, particle migrations remain centered about sites fixed at uniform intervals. These findings are in accord with those of Kunz [5], who studied the same configuration as described herein, through a partition-function approach. Although results are left in quadrature form, Kunz concludes that, "the system is in a crystalline state, at all temperatures and densities". Van Hove [6] reaches the same conclusion for a collection of finite-sized rigid particles in one dimension, through calculation of the free energy of the configuration.

Partition-function analyses of Lenard [1], and Baxter [2] for the analogous system of penetrable charged particles were interpreted to imply a form of particle binding which reduced the effective number of particles by one half. A molecular-field-type phase transition for a one-dimensional Coulomb system on a circle was reported by Schotte and Truong [7].

2. BBKGY Equations

We consider N particles of charge-σ which lie in a one-dimensional space of length L. The space is uniformly charged with total neutralizing charge

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$N\sigma$. The Coulomb potential for this system [1, 2] is given by

$$U = -2\pi\sigma^2 \left(\sum_{i<j}^{N} \sum^{N} |x_i - x_j| - \varrho \sum_i x_i^2 \right), \quad (1)$$

where $\varrho = N/L$ is number density and x_i is the coordinate of the i^{th} particle. The second term in (1) represents the interaction between the N particles and the uniform background.

The Hamiltonian for this system appears as

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + U(x_1, \ldots, x_N). \quad (2)$$

With this form at hand, we may construct the Liouville equation for the N-particle distribution $f_N(x^N, p^N)$, where x^N denotes the N-dimensional vector, $x_1, \ldots, x_N$, and similarly for p^N. There results

$$\frac{\partial f_N}{\partial t} + \sum_i^N \frac{p_i}{m} \frac{\partial f_N}{\partial x_i} - \sum_i^N \frac{\partial U}{\partial x_i} \frac{\partial f_N}{\partial p_i} = 0. \quad (3)$$

Writing di for $\mathrm{d}x_i \mathrm{d}p_i$, standard reduction [8] of the second term in (3) gives

$$\int \mathrm{d}(s+1) \ldots \mathrm{d}N \sum_{i=1}^{N} \frac{p_i}{m} \frac{\partial f_N}{\partial x_i} = \sum_{i=1}^{s} \frac{p_i}{m} \frac{\partial}{\partial x_i} f_s. \quad (4)$$

The remainder summation vanishes due to the boundary conditions,

$$f_N(x^N, p^N, t) = 0 \quad \text{at} \quad x^N = \left(-\frac{L}{2}\right)^N \quad \text{and} \quad \left(\frac{L}{2}\right)^N. \quad (5)$$

To reduce the third term in (3) first we note

$$\frac{1}{2\pi\sigma^2} \frac{\partial U}{\partial x_1} \frac{\partial f_N}{\partial p_1} = \left[-\sum_{i<j}\sum \frac{\partial u_{ij}}{\partial x_1} + \varrho \sum_i \frac{\partial u_i}{\partial x_1} \right] \frac{\partial f_N}{\partial p_1}$$
$$= \left[-\left(\frac{\partial u_{12}}{\partial x_1} + \cdots + \frac{\partial u_{1N}}{\partial x_1} \right) + \varrho \frac{\partial u_1}{\partial x_1} \right] \frac{\partial f_N}{\partial p_1}. \quad (6)$$

Here we have written

$$u_{ij} \equiv |x_i - x_j|, \quad u_i = x_i^2. \quad (7)$$

Furthermore we are assuming impenetrability of particles so that

$$x_1 < x_2 < x_3 < \cdots < x_N. \quad (8)$$

Equation (16) then reduces to

$$\frac{1}{2\pi\sigma^2} \frac{\partial U}{\partial x_1} \frac{\partial f_N}{\partial p_1} = [(N-1) + \varrho\, 2 x_1] \frac{\partial f_N}{\partial p_1}.$$

Similarly,

$$\frac{1}{2\varrho\sigma^2} \frac{\partial U}{\partial x_2} \frac{\partial f_N}{\partial p_2}$$
$$= \left[-\left(\frac{\partial u_{21}}{\partial x_2} + \frac{\partial u_{23}}{\partial x_2} + \cdots + \frac{\partial u_{2N}}{\partial x_2} \right) + \varrho \frac{\partial u_2}{\partial x_2} \right] \frac{\partial f_N}{\partial p_2},$$
$$\frac{1}{2\pi\sigma^2} \frac{\partial U}{\partial x_2} \frac{\partial f_N}{\partial p_2} = [(N-3) + 2\varrho x_2] \frac{\partial f_N}{\partial p_2}.$$

In like manner, for the i^{th} term we find

$$\frac{1}{2\pi\sigma^2} \frac{\partial U}{\partial x_i} \frac{\partial f_N}{\partial p_i} = [(N - 2i + 1) + 2\varrho x_i] \frac{\partial f_N}{\partial p_i}.$$

Collecting these terms gives,

$$\sum_{i=1}^{N} \frac{\partial U}{\partial x_i} \frac{\partial f_N}{\partial p_i} = 4\pi\sigma^2 \sum_{i=1}^{N} \left[\frac{(N - 2i + 1)}{2} + \varrho x_i \right] \frac{\partial f_N}{\partial p_i}. \quad (9)$$

With the additional boundary condition

$$f_N(x^N, p^N, t) = 0 \quad \text{at} \quad p^N = \infty^N \quad (10)$$

it follows that

$$\int \mathrm{d}(s+1) \ldots \mathrm{d}N \frac{\partial U}{\partial x_i} \frac{\partial f_N}{\partial p_i} = 0,$$
$$i = s+1, \ldots, N. \quad (11)$$

Thus, the integral of (9) becomes,

$$4\pi\sigma^2 \int \mathrm{d}(s+1) \ldots \mathrm{d}N \sum_{i=1}^{s} \left[\frac{(N-2i+1)}{2} + \varrho x_i \right] \frac{\partial f_N}{\partial p_i}$$
$$= 4\pi\sigma^2 \sum_{i=1}^{s} \left[\frac{(N-2i+1)}{2} + \varrho x_i \right] \frac{\partial f_s}{\partial p_i}. \quad (12)$$

Combining (4) and this last result (12), we obtain

$$\frac{\partial f_s}{\partial t} + \sum_{i=1}^{s} \frac{p_i}{m} \frac{\partial}{\partial x_i} f_s$$
$$- 4\pi\sigma^2 \sum_{i=1}^{s} \left[\frac{(N-2i+1)}{2} + \varrho x_i \right] \frac{\partial}{\partial p_i} f_s = 0. \quad (13)$$

Thus we find that for a one-dimensional Coulomb gas of impenetrable particles, the BBKGY equations degenerate into N uncoupled equations for the sequence $\{f_s\}$, $s = 1, \ldots, N$.

3. Effective Hamiltonian and Solutions

The effective potential which enters (13) is given by

$$U_s(1, \ldots, s) = \sum_{i=1}^{s} \bar{U}_i(x_i),$$
$$\bar{U}_i = \tfrac{1}{2} m \omega_p^2 [(x_i + \lambda_i)^2 - \lambda_i^2],$$
$$\lambda_i = \frac{N - 2i + 1}{2\varrho}, \quad \omega_p^2 = \frac{4\pi\varrho\sigma^2}{m}. \quad (14)$$

Thus the potential "seen" by the sub group of particles 1 through s is that of an s-dimensional harmonic oscillator with constant effective spring constant $m\omega_p^2$, varying displacement of origin, λ_i, and varying depression of energy, $\frac{1}{2}m\omega_p^2\lambda_i^2$.

The Hamiltonian for this same group of particles is given by

$$H_s(1,\ldots,s)=\sum_{i=1}^{s}\left[\frac{p_i^2}{2m}+\tilde{U}_i(x_i)\right]\equiv\sum_{i=1}^{s}E_i(x_i,p_i). \tag{15}$$

Since the energy of this sub group is separable, the orbits are independent [9]. Thus, N constants of the motion for our s-particle group are the energies $\{E_i\}$. (Here we are suppressing the origin-of-time constant so that a single particle in one dimension has only one constant of motion [8].) It follows that the general solution to (13) is given by

$$f_s(1,\ldots,s)=g(E_1,\ldots,E_s), \tag{16}$$

where g is an arbitrary function.

In equilibrium at the temperature T one obtains

$$f_{s,\,\mathrm{eq}}(1,\ldots,s)=A_s\exp\{-\beta H_s(1,\ldots,s)\},\quad \beta\equiv 1/k_\mathrm{B}T. \tag{17}$$

Equivalently,

$$f_{s,\,\mathrm{eq}}=\prod_{i=1}^{s}f_{1,\,\mathrm{eq}}(i),\quad f_{1,\,\mathrm{eq}}(i)=A_1\exp[-\beta H_1(i)]. \tag{18}$$

4. Asymmetry of Distributions

With f_s representing probability density,

$$\int f_s(1,\ldots,s)\,\mathrm{d}l\ldots\mathrm{d}s=1$$

we obtain [together with the constraint, (8)],

$$f_s=\frac{1}{(\sqrt{2\pi m k_\mathrm{B}T})^s}\frac{1}{\left(\sqrt{\frac{\pi}{2}}\lambda_\mathrm{D}\right)^s}\cdot\prod_{i=1}^{s}\frac{\exp[-(p_i^2/2mk_\mathrm{B}T)-(x_i+\lambda_i)^2/2\lambda_\mathrm{D}^2]}{\mathrm{erf}\left(\frac{\frac{L}{2}+\lambda_i}{\sqrt{2}\lambda_\mathrm{D}}\right)+\mathrm{erf}\left(\frac{\frac{L}{2}-\lambda_i}{\sqrt{2}\lambda_\mathrm{D}}\right)}. \tag{19}$$

Here we have written λ_D for the Debye distance,

$$\lambda_\mathrm{D}^2=\frac{k_\mathrm{B}T}{m\omega_p^2}=\frac{k_\mathrm{B}T}{4\pi\varrho\sigma^2},$$

and $\mathrm{erf}\,x$ represents the error integral [10]

$$\mathrm{erf}\,x=\frac{2}{\sqrt{\pi}}\int_0^x e^{-z^2}\mathrm{d}z\sim\frac{2x}{\sqrt{\pi}},\quad x\ll 1\qquad\sim 1,\quad x\gg 1. \tag{20}$$

The s-particle configuration density, ϱ_s, is related to f_s as

$$\varrho_s(x_1,\ldots,x_s)=\int f_s\,\mathrm{d}p_1\ldots\mathrm{d}p_s.$$

There follows,

$$\varrho_s=\frac{1}{\left(\sqrt{\frac{\pi}{2}}\lambda_\mathrm{D}\right)^s}\prod_{i=1}^{s}\frac{\exp[-(x_i+\lambda_i)^2/2\lambda_\mathrm{D}^2]}{\mathrm{erf}\left(\frac{\frac{L}{2}+\lambda_i}{\sqrt{2}\lambda_\mathrm{D}}\right)+\mathrm{erf}\left(\frac{\frac{L}{2}-\lambda_i}{\sqrt{2}\lambda_\mathrm{D}}\right)}. \tag{21}$$

This density enjoys the pseudo-normalization (i.e., with condition (8) relaxed over integration),

$$\int\varrho_s\,\mathrm{d}x_1\ldots\mathrm{d}x_s=1.$$

Note particularly that

$$\varrho_1(x_1)=\frac{1}{\sqrt{\frac{\pi}{2}}\lambda_\mathrm{D}}\frac{\exp[-(x_1+\lambda_1)^2/2\lambda_\mathrm{D}^2]}{\mathrm{erf}\left(\frac{\frac{L}{2}+\lambda_1}{\sqrt{2}\lambda_\mathrm{D}}\right)+\mathrm{erf}\left(\frac{\frac{L}{2}-\lambda_1}{\sqrt{2}\lambda_\mathrm{D}}\right)},\quad \lambda_1=\frac{N-1}{2\varrho}\cong\frac{L}{2}. \tag{22}$$

It follows that in the accessible configuration space $\left(-\frac{L}{2}\leqq x_1\leqq+\frac{L}{2}\right)$, the probability of locating particle No. 1 is maximum at $-L/2$ and minimum at $L/2$. This asymmetric property is a consequence of the impenetrability constraint (8).

5. Phase Properties

Returning to the s-particle configuration distribution function (21), we see that in the limits:

a) $\lambda_\mathrm{D}\to\infty,\quad \varrho_s\to L^{-s}$,

b) $\lambda_\mathrm{D}\to 0,\quad \varrho_s\to\prod_{i=1}^{s}\delta(x_i+\lambda_i)$.

Note that the constraint (8) reappears in limit (b). To understand the significance of the limiting forms (a) and (b), we refer to the expression for λ_D given above. Thus, $\lambda_\mathrm{D}\to\infty$ corresponds either to $T\to\infty$

or $\varrho \to 0$, both of which extremes diminish the Coulomb interaction between particles and background. The interparticle force in one dimension is constant. The opposite limit, $\lambda_D \to 0$, corresponds either to $T \to 0$ or $\varrho \to \infty$, in which cases the interaction between particles and background is most pronounced resulting in a rigid spatial ordering of the N particles. This change from a uniform, flat distribution at $(\varrho/T) = 0$ to a distribution of uniformly spaced particles at the limiting value $(\varrho/T) = \infty$, resembles a continuous transition from the gaseous phase to the solid phase. However, the form (21) indicates that particles "remember" their centers of displacement $(x_i = -\lambda_i)$ throughout the change in ϱ/T. In this sense the system maintains its crystalline property for all ϱ and T [5].

6. Conclusions

The BBKGY sequence for N equally charged, impenetrable, identical particles which move in a charge neutral one-dimensional space were shown to separate into N uncoupled equations for the respective N reduced distributions. The Hamiltonian for any sub group of connected particles includes a summational potential of harmonic oscillator terms with constant frequency but varying displacement of origin and varying depression of energy. Explicit forms were obtained for the coordinate and momentum parts of the equilibrium s-particle reduced distribution.

The spatial component of this distribution was found to contain the Debye distance as a parameter, or equivalently ϱ/T. In varying this parameter from ∞ to 0 it was found that the s-particle coordinate distribution passed from a constant (flat) function of s coordinates to a product of s delta functions centered at uniform intervals over the length of the aggregate. However, at all points of this change, particle-coordinate variations remain centered about what might be termed "lattice sites". Thus one may conclude that there is no change in phase of the system at any ϱ or T.

The key constraint of this analysis is that of impenetrability of particles. In two and three dimensions [11], this constraint has little consequence. However in one dimension we see that impenetrability of particles implies distinguishability of particles.

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[1] A. Lenard, J. Math. Phys. **2**, 682 (1961).
[2] R. Baxter, Proc. Cambridge Phil. Soc. **59**, 779 (1963).
[3] J. Dawson, Phys. Fluids **5**, 445 (1962).
[4] E. Lieb and D. C. Mattis, Mathematical Physics in One Dimension, Academic Press, New York 1966.
[5] H. Kunz, Ann. Physics **85**, 303 (1974).
[6] L. Van Hove, Physica **XVI**, 137 (1950).
[7] K. D. Schotte and T. T. Truong, Phys. Rev. A **22**, 2183 (1980).
[8] R. L. Liboff, Introduction to the Theory of Kinetic Equations. Krieger Publishing, Huntington, New York 1979.
[9] H. Goldstein, Classical Mechanics, Addison Wesley, Cambridge (Mass.) 1951.
[10] M. Abramowitz and I. Stegun, Handbook of Mathematical Functions (Section 7), Dover, New York 1965.
[11] R. L. Liboff, J. Math. Phys. **7**, 999 (1966).