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On the Statistical Mechanics of One-Dimensional Coulomb Systems

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Abstract. The method of functional integration is applied to classical one-dimensional Coulomb systems. The eigenvalues of the interaction matrix are given explicitly. One (and only one) negative eigenvalue is found as required by a theorem established by Kac. This feature is expressed in a modified Kac–Siegert inversion formula and in an appropriate representation of the Grand Partition Function of a multi-component system in a box. The one-component system (the jellium) is studied next. A new generating function is obtained for this model and a brief comparative analysis is made between its transfer matrix, diffusion equations and euclidean field theory formulations. This is effected with a view to investigating the occurrence of uni-axial periodic density oscillations in the two- and three-dimensional versions of the jellium model. Correlation functions and thermodynamic limits are not dealt with in this paper.

1. Introduction

We consider classical Coulomb systems with one, two or more components. The one-component system is a limiting case of the two-components model in that it consists of an assembly of particles, of charge q, enclosed in a box Λ and immersed in a uniform background of opposite charge. This well-known model is also called jellium, electron gas or one-component plasma.

A physical property of central interest in the one-dimensional version of these models is the (non)-crystalline nature of the (two-)one-component(s) system [2, 5]. With a view to investigating the occurrence of uni-axial periodic density oscillations in the two- and three-dimensional versions of the jellium model, we have re-formulated the one-dimensional case with free boundary conditions (the box) and, for finite Λ, we have examined certain connections between different formulations used in describing its equilibrium properties. The thermodynamic limit is not dealt with in this paper.

The exact statistical mechanics of one-dimensional Coulomb systems has been investigated in the early sixties [1] and further developed in recent years [5, 8]. The present work is based in particular on Edwards' and Lenard's 1962 paper [2] on the method of functional integration and its application to the two-components system, on Baxter's 1964 paper [3] where the one-component system is obtained as a limit of the two-components model and on Baxter's 1963 and Kunz's 1974 papers [4, 5] on the one-component model respectively treated by means of a generating function method and by means of a transfer matrix method.

In the first section we consider an ordered assembly of charged particles in a box and study the eigenvalues of the corresponding Coulomb matrix. In agreement with a theorem established by Kac [6] we find one, and only one, negative eigenvalue. We establish next a modified Kac–Siegert inversion formula used to represent the canonical Boltzmann factor of the assembly as a certain Gaussian average. We proceed in constructing a representation of the Grand Canonical Partition Function Ξ for a multicomponents system as a weighted average of a given generating function. At this point, we compare our results with those of E. and L. established under different boundary conditions: the generating functions are the same, i.e. the elementary solution of a diffusion equation with, in general, complex absorption coefficient, while the representations for Ξ differ.

In the second section we consider the one-component system and examine three formulations. The first one (F_1) is new. It is based on an application of the modified Kac–Siegert inversion formula to the inter-particle Coulomb energy while the one-body particle-background interactions are combined with the (one-body) field variables. The Grand Partition Function is obtained as a weighted average of a generating function which satisfies a diffusion equation with a complex and inhomogeneous absorption coefficient. The second formulation (F_2) is based on an appropriate limit of the two-components systems. It turns out that the absorption coefficient obtained differs from that given by Baxter (Ref. 3, section VI) except in the low fugacity limit. The third formulation (F_3) is based on the fact that the potential energy of an ordered electron gas can be written as a sum of harmonic oscillator potentials with equidistant minima equal to the inverse background density. On this basis, Baxter [4] developed a generating function method to investigate the thermodynamic limit of the model. His generating function is a solution of a first-order differential equation with displaced argument. On the same basis Kunz [5] developed a transfer matrix method to investigate the thermodynamic limit of the model as well as its n-points correlation functions. The fundamental eigenvector of the transfer matrix is also a solution of a first-order differential equation with displaced argument. Since both equations go into one another under minor change of argument we shall designate them as Baxter–Kunz (B.K.) equations. As a preliminary to further investigations, we briefly examine the connections between these three formulations. Explicit transformations leading from F_1 to F_2 and from F_1 to F_3 are given. However, since the thermodynamic limit is not treated in the present paper, we do not make contact with the boundary conditions of the Baxter generating function or the Kunz eigenvector, only with the differential equations that they satisfy.

From this comparative analysis, as well as from other examples such as lattice antiferromagnetism, follows that the occurrence of spatially inhomogeneous states in dense systems seems to be intimately connected with complex absorption coefficients. However, our lack of knowledge concerning the mathematical properties of e.g. the diffusion equation with complex absorption coefficient is the reason why there is no claim of rigor in this section. Nevertheless, it is expected that the links established between the transfer matrix, the diffusion equation and the field theory formulation will prove useful in future work.

In the third section we propose to investigate the possible occurrence, at moderate density, of periodic density oscillations in the two- and three-dimensional versions of the one-component plasma [7] by means of a euclidean field theory based on a given free-energy density with complex interaction term.

2. The Multi-Components System

The system considered consists of a one-dimensional assembly of n particles of arbitrary charges q_j $(j=1,\ldots,n)$ and of position co-ordinates x_j in the box $\Lambda=[a,b]$ with $a \leqslant x_1 \leqslant \ldots \leqslant x_n \leqslant b$. These particles interact via the one-dimensional Coulomb potential $C_{jk}=-|x_j-x_k|$. The potential energy $V(q=\{q_j\}, x=\{x_j\})$ of the system is accordingly

$$V(q,x)=\tfrac{1}{2}\sum_{j,k} C_{jk}q_jq_k \quad j,k=1,\ldots,n.$$

Considering V as a bilinear form in the q_i and C_{jk} as the elements of a matrix C, we are interested in the elements B_{jk} of the inverse matrix $B=C^{-1}$. This matrix occurs quite naturally if we perform a Legendre transformation aimed at eliminating the charges q_j in terms of the potentials v_j acting on the jth particle and produced by all the others, i.e. if we construct

$$W(v,x)=\sum_j q_jv_j - V(q,x)$$

clearly

$$v_j=\sum_k C_{jk}q_k$$

$$q_j=\sum_k B_{jk}v_k$$

$$W(v,x)=\tfrac{1}{2}\sum_{j,k} B_{jk}v_jv_k.$$

Explicit calculation of the B_{jk} elements confirms the structure of the matrix B expected from the theory of Gaussian Markoff processes except, perhaps, for the value of its B_{11} and B_{nn} elements. More precisely, we find

$$B_{kk}=\frac{1}{2(x_{k+1}-x_k)}+\frac{1}{2(x_k-x_{k-1})} \quad k\neq 1,n$$

$$B_{kk+1}=B_{k-1k}=\frac{-1}{2(x_{k+1}-x_k)} \quad k\neq 1,n$$

$$B_{k-1k}=B_{kk-1}=\frac{-1}{2(x_k-x_{k-1})} \quad k\neq 1,n$$

$$B_{1n}=B_{n1}=\frac{-1}{2(x_n-x_1)}$$

$$B_{11}=\frac{-1}{2(x_n-x_1)}+\frac{1}{2(x_2-x_1)}$$

$$B_{nn}=\frac{-1}{2(x_n-x_1)}+\frac{1}{2(x_n-x_{n-1})}$$

all other B_{jk} being zero. The electrostatic energy of the system then becomes

$$W(v,x) = -\frac{(v_n+v_1)^2}{4(x_n-x_1)} + \frac{(v_n-v_{n-1})^2}{4(x_n-x_{n-1})} + \cdots + \frac{(v_2-v_1)^2}{4(x_2-x_1)}$$

or, if we introduce the eigenvalues

$$\mu_n = -(x_n - x_1) \quad \mu_k = (x_{k+1} - x_k) \quad k \neq n$$

and the eigenvectors

$$a_n = \frac{1}{\sqrt{2}}(v_n + v_1) \quad a_k = \frac{1}{\sqrt{2}}(v_{k+1} - v_k) \quad k \neq n$$

W becomes

$$W = \frac{1}{2}\sum_{k=1}^{n} \frac{a_k^2}{\mu_k}.$$

Clearly we have one negative eigenvalue $\mu_n = -(x_n - x_1)$ and this is in agreement with a theorem established by Kac [6] which tells us, without actually giving it explicitly, that the matrix C_{jk} possesses one and only one negative eigenvalue. It follows that the form W is indefinite, a fact which prevents a direct application of the Kac–Siegert inversion formula to the Boltzmann factor $\exp[-\beta W]$, $\beta = (k_B T)^{-1}$ being the natural temperature. An appropriate modification of this formula is proposed below.

In what follows it will be convenient to express the physical variables in dimensionless form. For this purpose let $q_j = \sigma_j |q|$ where $|q|$ is the charge unit, let $\varphi_j = \beta|q|v_j$, $\alpha_k = \beta|q|a_k$, let $y_j = \bar{\rho}x_j$ where $\bar{\rho}$ is a reference density not further specified, let $y_a = \bar{\rho}a$, $y_b = \bar{\rho}b$, $r = y_b - y_a = \bar{\rho}L$ if $L = b - a$ and let $\lambda = \beta q^2/\bar{\rho}$ be the coupling constant; then

$$\beta V(q,x) = \lambda V(\sigma, y)$$

and

$$\beta W(v,x) = \frac{1}{\lambda} W(\varphi, y).$$

We now wish to reproduce the Boltzmann factor $\exp[-\lambda V]$ by an appropriate transformation of $\exp[-(1/\lambda)W]$. If all eigenvalues μ_k were positive, this would easily be achieved (Kac–Siegert formula) in making the Gaussian average of

$$\exp\left[i\sum_k \sigma_k \varphi_k\right],$$

i.e. in taking the n-dimensional Fourier transform of

$$\frac{(\det B(y))^{1/2}}{(2\pi\lambda)^{n/2}} \exp\left[-\frac{1}{\lambda}W(\varphi, y)\right].$$

However, since μ_n is negative, we have first to convert α_n into an imaginary field variable.[1]) Transcribed in terms of the φ_j this means to set, for instance

$$\sqrt{2}\alpha_n = \varphi_n + \varphi_1 = 2iu$$

$$\varphi_n - \varphi_1 = v$$

and to shift all other v_k by an imaginary component

$$\varphi_k = iu + \phi_k$$

then

$$\sum_j \sigma_j \varphi_j = iu\left(\sum_j \sigma_j\right) + (\sigma_n - \sigma_1)\tfrac{1}{2}v + \sum_{j=2}^{n-1} \sigma_j \phi_j$$

and we notice that the coefficient of iu is exactly the total charge of the system.

Defining next

$$V_k = \exp[i\sigma_k(\phi_k + iu)]$$

$$P_0(k+1,k) = P_0(\phi_{k+1}, y_{k+1}|\phi_k, y_k)$$

$$= (4\pi\lambda(y_{k+1} - y_k))^{-1/2} \exp\left[-\frac{(\phi_{k+1} - \phi_k)^2}{4\lambda(y_{k+1} - y_k)}\right]$$

$$F_0(n,1,u) = (\pi\lambda(y_n - y_1))^{-1/2} \exp\left[-\frac{u^2}{\lambda(y_n - y_1)}\right]$$

we indeed find that $\exp[-\lambda V(\sigma, y)]$ can be written as a certain Gaussian average

$$\exp[-\lambda V(\sigma,y)] \equiv \left\langle \prod_{k=1}^{n} V_k \right\rangle = \int du\, dv\, d\phi_n \cdot \delta(\phi_n - \tfrac{1}{2}v)\, F_0(n,1,u)\, V_n$$

$$\times \prod_{k=1}^{n-1} d\phi_k\, P_0(k+1,k)\, V_k\, \delta(\phi_1 + \tfrac{1}{2}v) \tag{2.1}$$

the convention being made that all the integrations over field variables are taken over $R = [-\infty, \infty]$ unless otherwise specified. This is the modified Kac–Siegert inversion formula required by the problem. We notice that, given $\sum_j \sigma_j$, the integration over u can be performed and we get

$$\int du(\pi\lambda(y_n - y_1)^{-1/2} \exp\left[-\frac{u^2}{\lambda(y_n - y_1)} - \left(\sum_j \sigma_j\right)u\right]$$

$$= \exp[\tfrac{1}{4}\lambda(y_n - y_1)(\textstyle\sum \sigma_j)^2] = \exp\left[\tfrac{1}{4}\beta(x_n - x_1)\left(\sum_j q_j\right)^2\right].$$

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[1]) Clearly if all μ_k were negative, as in totally ferromagnetic systems, all α_k, i.e. all φ_j, would be made purely imaginary field variables and one would have the Gaussian average of $\exp[-\sum_j \sigma_j \varphi_j]$.

It can also be remarked that the Coulomb potential can still be considered as the covariance function of two variables, namely $\langle\varphi_j\varphi_k\rangle$ provided it is understood that $\langle\varphi_j\varphi_k\rangle = \langle(\phi_j + iu)(\phi_k + iu)\rangle$. Lastly, we obtain the Canonical Partition Function as

$$\mathcal{Q}_n(r,\lambda,\bar{\rho}) = (\bar{\rho})^{-n}\int_{y_a}^{y_b} dy_n \ldots \int_{y_a}^{y_2} dy_1\langle V_n \ldots V_1\rangle.$$

In order to construct the Grand Partition Function it will be convenient to fix two particles at the boundary of the domain, namely $y_1 = y_a$, $y_n = y_b$, $\sigma_1 = \sigma_2$, $\sigma_n = \sigma_b$ and to generate the Grand Canonical Ensemble beginning with $n = 2$. Since

$$\exp[\lambda\sigma_a\sigma_b(y_b - y_a)]$$
$$= \int du\,dv\,F_0(b,a,u)\exp[-(\sigma_a+\sigma_b)u + i(\sigma_b-\sigma_a)\tfrac{1}{2}v]\,P_0(\tfrac{1}{2}v,y_b|-\tfrac{1}{2}v,y_a)$$

it is useful to define

$$F(b,a,u,v) \equiv \exp[-\lambda\sigma_a\sigma_b(y_b-y_a) - (\sigma_b+\sigma_a)u + i(\sigma_b-\sigma_a)\tfrac{1}{2}v]\,F_0(b,a,u) \qquad (2.2)$$

which will permit us to put $\sigma_b = \sigma_a = 0$ if eventually convenient and to start accordingly with the normalized distribution FP_0, namely

$$1 = \int du\,dv\,F(b,a,u,v)\,P_0(\tfrac{1}{2}v,y_b|-\tfrac{1}{2}v,y_a).$$

As a matter of comparison, E. and L. ([2], eq. 20) start from

$$1 = \int dv\,P_0(v,r|0,0).$$

If the system consists of several components with charges σ_α, $\alpha = (1,\ldots,s)$, to which we assign dimensionless fugacities $z_\alpha = \varkappa_\alpha/\bar{\rho}$ where $\varkappa_\alpha = \lambda_0^{-1}\exp[\beta\mu_\alpha]$, λ_0 being the de Broglie thermal wavelength and μ_α the chemical potentials, the next term of Ξ reads

$$\sum_{\alpha=1}^{s} z_\alpha \int_{y_a}^{y_b} dy \int du\,dv\,d\phi F(b,a,u,v)\cdot P_0(\tfrac{1}{2}v,y_b|\phi,y)\exp[i\sigma_\alpha\phi - \sigma_\alpha u]\,P_0(\phi,y|-\tfrac{1}{2}v,y_a).$$

Proceeding term by term in the usual way we arrive at the following representation of the Grand Canonical Partition Function

$$\Xi = \int du\,dv\,F(b,a,u,v)\,P(\tfrac{1}{2}v,y_b|-\tfrac{1}{2}v,y_a) \qquad (2.3)$$

where the generating function $P(\phi,y|\phi',y')$ is given in integral form by

$$P(\phi,y|\phi',y') = P_0(\phi,y|\phi',y') + \sum_{\alpha=1}^{s} z_\alpha \int_{y'}^{\check{} } dy'' \int d\phi''\,P_0(\phi,y|\phi'',y'')$$
$$\times\exp[i\sigma_\alpha\phi'' - \sigma_\alpha u]\,P(\phi'',y''|\phi',y').$$

It is the elementary solution (i.e. with $P(\phi,y|\phi',y)=\delta(\phi-\phi')$) of the diffusion equation

$$\frac{\partial P}{\partial y}=\lambda\frac{\partial^2 P}{\partial\phi^2}+\left(\sum_{\alpha=1}^{s} z_\alpha e^{i\sigma_\alpha\phi-\sigma_\alpha u}\right)P. \tag{2.4}$$

Inspection of the eigenvalues of the above equation indicates that the latter are independent of u. This means that we can perform a canonical transformation to eliminate u from the diffusion equation. Indeed, with

$$Q(\phi,y|\phi',y')=\exp\left[-iu\left(\frac{\partial}{\partial\phi}+\frac{\partial}{\partial\phi'}\right)\right]P(\phi,y|\phi',y';u)\exp\left[iu\left(\frac{\partial}{\partial\phi}+\frac{\partial}{\partial\phi'}\right)\right]$$

we obtain Q as the elementary solution of

$$\frac{\partial Q}{\partial y}=\lambda\frac{\partial^2 Q}{\partial\phi^2}+\left(\sum_{\alpha} z_\alpha e^{i\sigma_\alpha\phi}\right)Q \tag{2.5}$$

which is E. and L. ([2], eq. 33) with some obvious changes of notation. Lastly, it is often convenient to extract from P and Q the term giving rise to the perfect gas pressure, i.e. to write

$$Q=\exp\left[\sum_{\alpha=1}^{s} z_\alpha(y-y')\right]R.$$

Then R is the elementary solution of the diffusion equation

$$\frac{\partial R}{\partial y}=\lambda\frac{\partial^2 R}{\partial\phi^2}-U(\phi)\,R \tag{2.6}$$

where

$$U(\phi)=\sum_{\alpha=1}^{s} z_\alpha(1-e^{i\sigma_\alpha\phi}) \tag{2.7}$$

plays the role of a generally complex absorption coefficient. For the two-components plasma of opposite charge ($\sigma_+=-\sigma_-=1$) and of equal concentration ($z_+=z_-=z$), $U(\phi)$ becomes real and positive, a situation investigated in detail by Edwards and Lenard [2].

Assuming that the generating function $R(\phi,y|\phi',y')$ has been found we construct

$$P(\phi,y|\phi',y';u)=\exp\left[\sum_{\alpha=1}^{s} z_\alpha(y-y')\right]R(\phi+iu,y|\phi'+iu,y')$$

through continuation of R in the complex φ plane and obtain finally, for the system considered, the Partition Function in the form

$$\Xi=\exp\left[\sum_{\alpha=1}^{s} z_\alpha r\right]\int du\,dv\,F(b,a,u,v)\,R(\tfrac{1}{2}v+iu,y_b|-\tfrac{1}{2}v+iu,y_a) \tag{2.8}$$

instead of

$$\Omega = \exp\left[\sum_{\alpha=1}^{s} z_\alpha r\right] \int dv\, R(v, r|0, 0)$$

as Edwards and Lenard obtained for the case where the system of particles is in contact with an infinite reservoir ($y \leqslant y_a$) exchanging particles with the system, the reservoir plus the system being electrically neutral as a whole. We have questioned their statement (p. 780) that it would be incorrect to consider the system with free boundary conditions (the box). We can indeed consider $\Lambda = [a, b]$ to be a portion of the frontier of a two-dimensional domain playing the role of reservoir. While it is quite obvious that the thermodynamics of the system will not be affected by the different boundary conditions, it is not said that the latter should not influence the correlation functions.

3. The One-Component System

This model consists of an assembly of particles of charge $q_j = q_+$, $\forall_j$, enclosed in a box $\Lambda = [a, b]$ and immersed in a uniform background of opposite charge. Recent work by Kunz [5, 9] and the author [7, 9], and by Brascamp and Lieb [8] in the case of spinless Fermions, has revived interest in the equilibrium properties of this model, first investigated by Baxter [3, 4] by means of two different methods. In this section three formulations are examined together with some of their inter-connections.

The first formulation (F_1) is new. We start from the potential energy for a system of n particles and apply the modified Kac–Siegert inversion formula to the Coulomb interaction between the particle only while the one-body particle background interaction is combined with the one-body field variable. With $-|q|\bar{\rho}$ designating the background charge density we have

$$V = V_{pp} + V_{pb} + V_{bb}$$

or

$$\beta V = \tfrac{1}{2} \sum_{j,k} (-)\lambda |y_j - y_k| + \sum_j \lambda \psi(y_j) - \tfrac{1}{2}\lambda \int_{y_a}^{y_b} dy\, \psi(y) \tag{3.1}$$

where

$$\psi(y) = \int_{y_a}^{y_b} dy' |y - y'| = (y - \tfrac{1}{2}(y_a + y_b))^2 + \tfrac{1}{4}(y_b - y_a)^2.$$

Combining the one-particle factor $\exp[-\lambda\psi(y_k)]$ with V_K to form

$$U_k = \exp[i\phi_k - u - \lambda\psi(y_k, r)]$$

we obtain the Canonical Partition Function as

$$\mathcal{Q}_1 = \exp[\tfrac{1}{6}\lambda r^3](\bar{\rho})^{-n} \int_{y_a}^{y_b} dy_n \ldots \int_{y_2}^{y_2} dy_1 \langle U_n \ldots U_1 \rangle$$

the Gaussian average being defined exactly as in (2.1). Proceeding here as in the first section, but with the factors V_k being replaced by the factors U_k, we obtain the following representation of the Grand Partition Function

$$Z = A \int du\, dv\, F(b, a, u, v)\, G(\tfrac{1}{2}v + iu, y_b | -\tfrac{1}{2}v + iu, y_a; \psi) \tag{3.2}$$

with

$$A = \exp[\tfrac{1}{6}\lambda r^3 + z_+ r - \lambda(\sigma_a \psi_a + \sigma_b \psi_b)] \tag{3.3}$$

the generating function $G(\phi, y|\phi', y'; \psi)$ being the elementary solution of the diffusion equation

$$\frac{\partial G}{\partial y} = \lambda \frac{\partial^2 G}{\partial \phi^2} - z_+(1 - e^{i\phi - \lambda\psi(y)})\, G. \tag{3.4}$$

The second formulation (F_2) is based on an appropriate limit of the generating function R of (2.6) for a two-component plasma ($s = 2$, $z_\alpha = z_+, z_-$, $\sigma_\alpha = \sigma_+, \sigma_-$). The idea is that the homogeneous background can be obtained as a limit of a system of particles whose charges tend to zero while their density tends to infinity in such a way that their charge density remains finite. Contact with Baxter's version [3] of the problem is made, revealing a discrepancy in the respective prescriptions given to obtain the limit. We argue as follows: let $\sigma_+ = +1$, $\sigma_- = -\varepsilon$ and let

$$\bar{\rho} U(\phi) = \varkappa_+(1 - e^{i\phi}) + \varkappa_-(1 - e^{-i\varepsilon\phi})$$

then it is true that for any fixed temperature, volume and ε

$$\rho_+ = \varkappa_+ + \not{f}_+(\varkappa_+, \varepsilon\varkappa_-, \varepsilon^2 \varkappa_-, \ldots)$$

$$\rho_- = \varkappa_- + \not{f}_-(\varkappa_+, \varepsilon\varkappa_-, \varepsilon^2 \varkappa_-, \ldots)$$

where $\not{f}_+$, $\not{f}_-$ are bounded functions. Let $\varepsilon \to 0$, $\varkappa_- \to \infty$ with $\varepsilon\varkappa_- = \rho$. Then $\not{f}_{+,-} = \not{f}_{+,-}(z_+, \rho, 0, \ldots)$ and since $\varepsilon \not{f}_- \to 0$ we have from the second equation

$$\lim_{\substack{\varepsilon \to 0 \\ \varkappa_- \to \infty}} \varepsilon\varkappa_- = \lim_{\substack{\varepsilon \to 0 \\ \varkappa_- \to \infty}} (\varepsilon\varkappa_- + \varepsilon \not{f}_-(\varkappa_+, \varepsilon\varkappa_-, \ldots)) = \rho$$

On the other hand, if we require charge neutrality, in the mean, we must have

1. $\rho_+ = \varkappa_+ + \not{f}_+(\varkappa_+, \rho, 0, \ldots) = \rho.$

Consequently our prescription is

$$\lim_{\substack{\varepsilon \to 0 \\ \varkappa_- \to \infty}} \varepsilon\varkappa_- = \varkappa_+ + \not{f}_+(\varkappa_+, \rho, 0, \ldots) = \rho \tag{3.5}$$

which implies $\varkappa_+ = \varkappa_+(\rho)$ or $\rho = \rho(\varkappa_+)$ whereas Baxter's prescription is

$$\lim_{\substack{\varepsilon \to 0 \\ \varkappa_- \to \infty}} \varepsilon\varkappa_- = \varkappa_+ = \rho.$$

From (3.5) it follows that the limiting absorption coefficient U_1 of U for the jellium model becomes

$$\bar{\rho} U_1 = \varkappa_+(1 - e^{i\phi}) + i\rho(\varkappa_+)\,\phi \tag{3.6}$$

instead of $i\varkappa_+\phi$ in the last term ([3], section VI). It also follows that we consistently recover $\rho(\varkappa_+) = \varkappa_+ \langle\!\langle \exp[i\phi] \rangle\!\rangle$ where $\langle\!\langle \ldots \rangle\!\rangle$ represents the normalized field and space average of the particle density operator as required by the charge neutrality condition. At this stage it is convenient to choose the reference density $\bar{\rho}$, so far unspecified, to be $= \rho(\varkappa_+)$. The limiting absorption coefficient then becomes, with $z_+ = \varkappa_+/\rho(\varkappa_+)$

$$U_1 = z_+(1 - e^{i\phi}) + i\phi.$$

Lastly, it is clear that in letting $\varkappa_- \to \infty$, $\varepsilon \to 0$, the background contributes an infinite perfect gas pressure to the total pressure of the system. Since by definition of the jellium model its background is passive in this respect, the contribution has to be subtracted from the total pressure. A final point concerns the choice of σ_a and σ_b. We can choose any combination $\sigma_{a,b} = +1, -\varepsilon$, the boundary particles being of the background type or not. Keeping σ_a, σ_b for generality, the proposed Partition Function of the one-component system in a box Λ reads accordingly

$$Z = \exp[z_+ r] \int du\, dv\, F(b, a, u, v)\, K(\tfrac{1}{2}v + iu, y_b | -\tfrac{1}{2}v + iu, y_a) \tag{3.7}$$

where the generating function $K(\phi, y|\phi', y')$ is the elementary solution of the diffusion equation

$$\frac{\partial K}{\partial y} = \lambda \frac{\partial^2 K}{\partial \phi^2} - (z_+(1 - e^{i\phi}) + i\phi)\, K. \tag{3.8}$$

In order to test the content of this equation and to establish a point of contact with (3.4) we examine the zeroth order contribution in z_+ to K at fixed λ, thus disregarding charge neutrality. We should recover the pre-integral factor A of (3.2), i.e. the Boltzmann factor of the background, together with the potential energy of the boundary particles minus their interaction. In zeroth order, we have

$$\frac{\partial K_0}{\partial y} = \lambda \frac{\partial^2 K_0}{\partial \phi^2} - i\phi K_0.$$

The elementary solution of this particular equation is known. It reads

$$K_0 = \left(-\frac{\beta}{2\pi} \frac{\partial^2 F}{\partial \phi\, \partial \phi'} \right)^{1/2} \exp[-\beta F(\phi, y|\phi', y')]$$

with

$$\beta F = \frac{(\phi - \phi')^2}{4\lambda(y - y')} + i(y - y')\frac{\phi + \phi'}{2} + \frac{\lambda}{12}(y - y')^3.$$

Constructing $K_0(\frac{1}{2}v + iu, y_b | -\frac{1}{2}v + iu, y_a)$ and using (2.2) for $F(b,a,u,v)$ we then get

$$Z_0 = \int du\, dv (4\pi\lambda r)^{-1} \exp\left[-\frac{u^2}{\lambda r} - \frac{v^2}{4\lambda r} + u(r - \sigma_a - \sigma_b) + \tfrac{1}{2} iv(\sigma_b - \sigma_a) \right]$$

$$\cdot \exp\left[-\lambda \sigma_a \sigma_b r - \frac{\lambda}{12} r^3 \right]$$

$$= \exp\left[\frac{\lambda r}{4} (r - \sigma_a - \sigma_b)^2 - \frac{\lambda r}{4} (\sigma_b - \sigma_a)^2 - \lambda \sigma_a \sigma_b r - \frac{\lambda}{12} r^3 \right]$$

$$= \exp\left[\tfrac{1}{6} \lambda r^3 - (\sigma_a + \sigma_b) \frac{\lambda r^2}{2} \right]$$

which is exactly $A(z_+ = 0)$ of (3.3) since $\psi_a = \psi_b = \frac{1}{2} r^2$.

In the third formulation of the electron gas model [4, 5] one starts again from the potential energy (3.1) for a system of n particles in the box $\Lambda = [a,b]$ and exploits the property that for an ordered configuration βV can be written as

$$\beta V = \beta V_0(n,r) + \lambda \sum_j (y_j - y_j^0)^2 \quad y_j \leqslant y_{j-1} \; \forall_j$$

i.e. a sum of harmonic oscillation potentials having their minima at $y_j^0 = j - (r+1)/2$ and a constant

$$\beta V_0 = -\tfrac{1}{6} \lambda (r-n)^3 + \frac{\lambda}{12} n - \frac{\lambda}{4} n (r-n)^2.$$

As mentioned in the Introduction, Baxter [4], on this basis, developed a generating function method to investigate the thermodynamic limit of the model. His generating function $g(x)$ is a solution of the differential equation

$$\frac{dg(x)}{dx} = \varkappa e^{-\lambda x^2} g(x+1).$$

On the same basis, Kunz [5] developed a transfer matrix method to investigate the thermodynamic limit and the n-points correlation functions of the model. The fundamental eigenvector of the transfer matrix is a solution of the equation

$$\frac{\zeta d\Psi(u)}{du} = -e^{-\lambda(u-1)^2} \Psi(u-1).$$

It is our purpose to establish some relationship between the three formulations which relate the generating functions G of (3.4) to K of (3.8) and G to B.K. equations. Let us begin with the connection between G and K. We first perform a change of variables $(\phi, y) \to (\Phi, s)$ with

$$\Phi = \phi + i\lambda\psi(y)$$

$$s = y - \tfrac{1}{2}(y_a + y_b)$$

then $G(\phi, y)$ becomes $G(\Phi, s)$ and we have

$$\left(\frac{\partial G}{\partial y}\right)_{\Phi} = \left(\frac{\partial G}{\partial s}\right)_{\Phi} + \left(\frac{\partial \Phi}{\partial y}\right)_{\Phi}\left(\frac{\partial G}{\partial \Phi}\right)_{s}$$

$$\left(\frac{\partial^2 G}{\partial \phi^2}\right)_{y} = \left(\frac{\partial^2 G}{\partial \Phi^2}\right)_{s}.$$

With

$$\left(\frac{\partial \Phi}{\partial y}\right)_{\phi} = 2i\lambda s$$

the new equation for $G(\Phi, s)$ becomes

$$\frac{\partial G}{\partial s} = \lambda \frac{\partial^2 G}{\partial \Phi^2} - 2i\lambda s \frac{\partial G}{\partial \Phi} - z_+(1 - e^{i\Phi})\, G.$$

Next, in making the Ansatz

$$G(\Phi, s|\Phi', s') = \exp\left[is\Phi - is'\,\Phi' + \frac{\lambda}{3}(s^3 - s'^3)\right] \tilde{K}(\Phi, s|\Phi', s')$$

we find, with a little bit of algebra, that $\tilde{K}$ satisfies the equation

$$\frac{\partial \tilde{K}}{\partial s} = \lambda \frac{\partial^2 \tilde{K}}{\partial \Phi^2} - (z_+(1 - e^{i\Phi}) + i\Phi)\, \tilde{K}$$

which is formally the same as (3.8) for K. The initial conditions being the same, $\tilde{K} = K$ if they exist.

In order to make contact with B.K. equations, we take advantage of the fact that the absorption coefficient of equation (3.4) for G is periodic in ϕ with period 2π. This means that we can construct a generating function $\bar{G}(\phi, y|\phi', y')$ solution of the same differential equation (3.4) but with initial condition

$$\delta_{2\pi}(\phi - \phi') = \sum_{\nu=-\infty}^{+\infty} \delta(\phi - \phi' + 2\pi\nu).$$

The new generating function is periodic in ϕ and ϕ'. Assuming that it can be decomposed into the form

$$\bar{G}(\phi, s|\phi', s') = \sum_{n=-\infty}^{+\infty} e^{in(\phi - \phi')} f_n(s) f_{-n}(-s')$$

we find

$$\frac{df_n(s)}{ds} = -\lambda n^2 f_n(s) - z_+ f_n(s) + z_+ e^{-\lambda\psi(s)} f_{n-1}(s)$$

and, making the Ansatz

$$f_n(s) = \exp[-\lambda n^2 s - z_+ s - \tfrac{1}{3}\lambda n^3 + \lambda n(\tfrac{1}{12} + \tfrac{1}{4}r^2)]\,\varphi_n(s) \tag{3.9}$$

we obtain

$$\frac{d\varphi_n(s)}{ds} = z_+ e^{-\lambda(s-n+1/2)^2}\varphi_{n-1}(s),$$

an equation which reveals a key property of $\varphi_n(s)$, namely that $\varphi_n(s) = \varphi(s-n)$. It follows that in setting $s-n = x-\frac{1}{2}$, $\varphi(x-\frac{1}{2}) = g(x)$ and $z_+ = z$ we obtain Baxter differential equation ([4], eq. 26)

$$\frac{dg(x)}{dx} = z\,e^{-\lambda x^2} g(x+1),$$

whereas in setting $s-n = u+\frac{1}{2}$, $\varphi(u+\frac{1}{2}) = \Psi(-u)$ and $z_+ = \zeta^{-1}$ we obtain Kunz equation ([5], eq. 16)

$$\zeta\frac{d\Psi(u)}{du} = -e^{-\lambda(u-1)^2}\psi(u-1).$$

4. Long-Range Ordering in One-Component Coulomb Systems

In this section we briefly comment on the question of long-range ordering in one-component Coulomb systems [7].

In using a method of transfer matrix Kunz [5] proved, for almost all values of the coupling constant λ, the suspected crystalline nature of the one-dimensional electron gas with free boundary conditions. He also showed that for periodic boundary conditions, the constant density is obtained as an average over a unit cell of the former inhomogeneous density. It is in fact this sensitivity to boundary conditions which, in part, motivated the work reported in the first section. The transfer matrix method has thus proved extremely useful to investigate the nature of the states of the system. However, it is very difficult to imagine how this method could be generalized to higher dimension owing to the long-range nature of the Coulomb interactions.

On the other hand, the diffusion equation method is equivalent to a one-dimensional euclidean field theory based on a free energy density given by

$$\mathcal{L}_2^{(1)} = \frac{1}{4}\left(\frac{dv}{dx}\right)^2 - 2K_B T z\cos\beta q v$$

for the two-components system, by

$$\mathcal{L}_1^{(1)} = \tfrac{1}{2}\rho q\psi(x) + \frac{1}{4}\left(\frac{dv}{dx}\right)^2 - K_B T z\, e^{i\beta q v - \beta q\psi(x)}$$

and

$$\mathcal{L}_1^{(1)} = \frac{1}{4}\left(\frac{dv}{dx}\right)^2 + iq\rho(z)\,v - K_B T z\, e^{i\beta q v}$$

for the one-component system in the version (F_1) and (F_2). Advantages of this formulation are i) elimination of the particle ordering, ii) short-range nature of the inverse Coulomb potential and local character of the interaction term, iii) it can be generalized to dimension $\nu > 1$. We have, indeed, at least formally

$$\mathscr{H}_1^{(\nu)} = \frac{1}{z(\nu-1)\,\pi}(\nabla v)^2 + \tfrac{1}{2}\rho q\psi(x) - K_B T{:}\,e^{i\beta q v - \beta q\psi(x)}\,{:}$$

and

$$\mathscr{H}_1^{(\nu)} = \frac{1}{z(\nu-1)\,\pi}(\nabla v)^2 + iq\rho v - K_B T{:}\,e^{i\beta q v}\,{:} \tag{3.10}$$

where the dots represent the usual Wick ordering. It follows that in understanding how periodic density oscillations come about at $\nu = 1$ in the field versions, perhaps in using the version F_1, we might be able to investigate the conjecture and heuristic mean-field theory advanced [7] that uni-axial long-range ordering (periodic density oscillations) may occur in $\nu > 1$ one-component systems at

$$\lambda^{(\nu)} = \beta q^2 \rho^{(\nu-2)/\nu} = \lambda_c^{(\nu)}\,(\text{M.F.T.}) = \frac{2\pi}{\nu - 1}.$$

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