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Equilibrium Equations and Symmetries of Classical Coulomb Systems

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In this paper we establish the validity of the BBGKY equilibrium equations for Coulomb states which have been obtained as thermodynamic limit of finite volume states. We also give a new derivation of the l-sum rules for phases constructed by the cluster expansion. These sum rules are interpreted as Ward identities associated to a symmetry of the screening phase.

KEY WORDS: Coulomb systems; BBGKY equations; sum rules; symmetries.

1. INTRODUCTION

The starting point of many theoretical investigations on the physics of charged fluids and plasmas at equilibrium is the so-called BBGKY (*Born–Bogoliubov–Green–Kirkwood–Yvon*) *hierarchy* of equations.[1,2] This hierarchy is a set of relations between the N and $N+1$ point functions which have the form

$$\nabla_1 \rho(q_1 \ldots q_N) = e_{\alpha(1)} E(x_1) \rho(q_1 \ldots q_N) + \int dq\, F(q_1, q)(\rho(q_1 \ldots q_N q) - \rho(q)\rho(q_1 \ldots q_N)) \quad (1.1)$$

We used the notation $q = (\alpha, x)$ with α the species of the particle located at x, e_α its charge, and $\int dq = \int_{\mathbb{R}^\nu} dx \sum_\alpha$. $F(q_1, q_2) = -e_{\alpha(1)} e_{\alpha(2)} \nabla_1 \phi(x_1 - x_2)$ is the force, $\rho(q_1), \rho(q_1 q_2), \ldots$ are the singlet, doublet, ... distributions defined in the usual way, and $E(x)$ is the electric field due to all the charges (system's charges plus external and boundary charges). These equilibrium

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equations are easily derived in a finite volume Gibbs ensemble and they are usually *assumed* to still hold after the thermodynamic limit for the correlation functions of the infinitely extended state.

In a series of papers,[3–5] assuming the validity of (1.1) in the thermodynamic limit, it has been shown that under certain clustering conditions, the long range of the Coulomb force imposes additional constraints on the correlations, which are typical for charged systems. The first one is the *local neutrality* which reads in a homogeneous state

$$\sum_\alpha e_\alpha \rho_\alpha = 0 \qquad [\rho_\alpha = \rho(\alpha, x)] \tag{1.2}$$

The others are *the multipolar sum rules*

$$\int dq\, e_\alpha Y_l(x) \rho(q \mid q_1 \ldots q_N) = 0 \tag{1.3}$$

$$l = 0, 1, \ldots, \qquad N = 1, 2, \ldots$$

where

$$\rho(q \mid q_1 \ldots q_N) = \frac{\rho(q q_1 \ldots q_N)}{\rho(q_1 \ldots q_N)} + \sum_{i=1}^{N} \delta_{q, q_i} - \rho(q) \tag{1.4}$$

$$[\delta q_1, q_2 = \delta_{\alpha(1),\alpha(2)} \delta(x_1 - x_2)]$$

is the *excess particle density* at q in the presence of any N particles $\alpha(1) \ldots \alpha(N)$ fixed at $x_1 \ldots x_N$, and Y_l is an harmonic polynomial of order l. The sum rules (1.3) express that the multipole moments of order l of the charge density induced by specifying the positions of any N particles vanish.

On the other hand, several recent works have been devoted to the construction of the thermodynamic limit (in two and three dimensions) by means of correlation inequalities[6] and cluster expansions.[7,8] The purpose of this note is to supplement these results by showing explicitly that the states so obtained obey the equilibrium equation (1.1) and the sum rules (1.2), (1.3). We find in fact that these states, which are translation invariant, are always locally neutral and verify (1.1) with $E(x) = 0$. One should recall here that in one dimension there exist solutions of the hierarchy (1.1) with nonvanishing electric field (θ states or dielectric states).[9]

In Section 2, we briefly recall the functional integration formalism and the results of[6–8] that we need in the sequel. We show in Section 3 that the correlations satisfy a regularized version of the BBGKY hierarchy in all the cases where the thermodynamic limit has been constructed. Moreover, the correlations obey the ordinary hierarchy (1.1) whenever they cluster faster than $|x|^{-1}$ ($\nu = 3$). We establish in Section 3 that the local neutrality is generally true and that the l-sum rules hold when there are sufficiently strong clustering properties. In particular, the states of Refs. 7, 8 (several components and jellium), which are known to be exponentially clustering, satisfy (1.1) [with $E(x)=0$], (1.2), and (1.3) for all l, N. This provides a new derivation of the l-sum rules which does not use the BBGKY. [Actually we have to use the local neutrality to prove the BBGKY equations (1.1)].

Our result (BBGKY and the l-sum rules) rely on two simple identities in the Sine-Gordon representation: the integration by parts formula and the translation of a Gaussian measure. These identities imply that Eqs. (1.1), (1.2), (1.3) are true at finite volume up to terms depending on the boundaries. We then use the estimates of Refs. 6–8 to show that these additional contributions vanish in the thermodynamic limit.

It is interesting to remark that the l-sum rules can be considered as the "Ward identities" corresponding to the formal local phase transformations $z_\alpha \to z_\alpha \exp[ie_\alpha Y(x)]$ in the activity phase, where $Y(x)$ is an harmonic function. This is discussed in more detail in the last section.

2. DEFINITION AND PROPERTIES OF THE MODEL

2.1. The Model

We consider a system of s species of particles, species α having the charge e_α. The e_α are multiples of a unit charge e_0. The particles interact via a two-body potential $\phi(q_1, q_2) = e_{\alpha(1)} e_{\alpha(2)} V(x_1 - x_2)$. We carry out the details for dimensions $\nu = 3$; for $\nu = 1$ or 2, see the comments at the end of Sections 3 and 4. $V(x_1 - x_2)$ will be chosen of positive type: it contains the Coulomb potential plus a short-range potential in order to insure stability. Typically we shall take

$$V(x_1 - x_2) = \frac{1 - \exp(-d|x_1 - x_2|)}{4\pi|x_1 - x_2|}, \qquad d > 0 \tag{2.1}$$

We could also consider the regularized Coulomb potential

$$V(x_1 - x_2) = \int dz \int dz' \, \frac{\chi(x_1 - z)\chi(x_2 - z')}{4\pi|z - z'|} \tag{2.2}$$

where

$$\chi(x) \in \mathscr{S}(\mathbb{R}^3), \quad \chi(x) = \chi(|x|), \quad \chi(x) = 0, \quad |x| \geqslant R, \quad \int dx\, \chi(x) = 1$$

The *potential of N particles* is

$$U((q)_N) = \sum_{1 \leqslant i < j \leqslant N} e_{\alpha(i)} e_{\alpha(j)} V(x_i - x_j) \tag{2.3}$$

with the notation

$$(q)_N = (q_1 \ldots q_N), \qquad q_j = (\alpha(j), x_j),$$

The *grand canonical partition function* in a finite volume Λ is defined by

$$\Xi_\Lambda(\beta, z) = \sum_N \frac{z^n}{N!} \int_{\Lambda^N} d(x)_N \exp[-\beta U((q)_N)] \tag{2.4}$$

The multi-index $N = (N_1 \ldots N_s)$ specifies the number of particles of each species present and

$$\frac{z^N}{N!} = \prod_{\alpha=1}^{s} \frac{z_\alpha^{N_\alpha}}{N_\alpha!}$$

The *finite volume correlation functions* are

$$\rho_\Lambda((q)_N) = \Xi^{-1} z^N \sum_M \frac{z^M}{M!} \int_{\Lambda^M} d(x')_M \exp[-\beta U((q)_N (q')_M)] \tag{2.5}$$

2.2. Existence of the Thermodynamic Limit

The existence of the infinite volume limit of the thermodynamic functions has been established in great generality by Lieb and Lebowitz.[10] Existence of the limit of the correlation functions has only been established under more restrictive conditions that we now recall.

2.2.1. Charge Symmetric Systems[6]

Condition CS. (i) for any α, there exists a species α' such that $e_\alpha = -e_{\alpha'}$; (ii) if α and α' are such that $e_\alpha = -e_{\alpha'}$, then $z_\alpha = z_{\alpha'}$.

Theorem 1. If condition CS holds, then for all β, z the thermodynamic limit of the finite volume correlation functions exists and is translation invariant.

2.2.2. Plasma Phase[7,8]

Condition P

i. $\beta e^2 / l_D$ is small with $l_D = (\beta \sum_{\alpha=1}^{s} z_\alpha e_\alpha^2)^{-1/2}$

ii. $\sum_{\alpha=1}^{s} e_\alpha z_\alpha = 0$

iii. $z_\alpha / \max_\alpha(z_\alpha) \geqslant C > 0$

iv. In the definition of $\Xi_\Lambda, \rho_\Lambda((q)_N)$, $V(x_1 - x_2)$ introduced in (2.1) is replaced by

$$V_\Lambda(x_1, x_2) = (-\Delta_\Lambda)^{-1}(x_1, x_2) - (-\Delta_\Lambda + d^2)^{-1}(x_1, x_2) \tag{2.6}$$

where Δ_Λ is the Laplacian with Dirichlet boundary conditions on Λ.

Theorem 2. If condition P holds, the thermodynamic limit of the finite volume correlation functions exists, is translation invariant, and has the exponential clustering property.

This theorem has recently been improved; Imbrie has been able to handle the jellium system. This formally corresponds to the case $z_s \to \infty$ with $z_s e_s$ fixed, or in other words, to relax condition P(iii).[8] Federbush has considered particular Coulomb systems where conditions P(ii) and P(iv) have been relaxed.[11]

2.3. The Sine-Gordon Representation

To prove the above theorems, it was useful to represent a Coulomb system as a (Euclidean) field theory.[12]

Let $d\mu_V(\phi)$ be a Gaussian measure on $\mathscr{S}'(\mathbb{R}^\nu)$ of covariance $V(x_1 - x_2)$; $d\mu_V(\phi)$ exists when V is of positive type, and with the choice (2.1), the support of $d\mu_V(\phi)$ is the set of continuous functions on $\mathbb{R}^\nu$—see Ref. 7.

The basic identity relating statistical mechanics to Gaussian integrals is

$$\exp\left[-\beta U((q)_N)\right] = \int d\mu_V(\phi) \prod_{j=1}^{N} \left\{ :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} \tag{2.7}$$

with

$$:\exp\left[i\phi(f)\right]: = \exp\left[\frac{1}{2}\int dx\, dy\, f(x) V(x-y) f(y)\right] \exp\left[i\phi(f)\right]$$

The partition function can then be written as

$$\Xi_\Lambda(\beta, z) = \int d\mu_V(\phi) \exp\left\{ \sum_{\alpha=1}^{s} z_\alpha \int_\Lambda dx\, :\exp\left[i\sqrt{\beta}\, e_\alpha \phi(x) \right]: \right\} \tag{2.8}$$

Introducing the perturbed Gaussian measure

$$d\mu_\Lambda^{\beta,z}(\phi) = \Xi_\Lambda^{-1}(\beta, z) \exp\left\{ \sum_{\alpha=1}^{s} z_\alpha \int_\Lambda dx\, :\exp\left[i\sqrt{\beta}\, e_\alpha \phi(x) \right]: \right\} d\mu_V(\phi) \tag{2.9}$$

and the notation

$$\langle - \rangle_\Lambda = \int - \, d\mu_\Lambda^{\beta,z}(\phi)$$

the finite volume correlation functions are given by

$$\rho_\Lambda((q)_N) = \left\langle \prod_{j=1}^{N} \left\{ z_{\alpha(j)} :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} \right\rangle_\Lambda \tag{2.10}$$

We now gather some bounds on correlations that we shall need in the sequel.

Lemma. (i) Systems satisfying condition (CS) or (P) obey the bounds uniformly in Λ ($\nu = 3$):

$$\left\langle \prod_{j=1}^{N} \left\{ :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} \phi^{p}(x) \right\rangle_{\Lambda} \leqslant C \qquad N = 0, 1, \ldots, \qquad p = 0, 1$$

(ii) If (P) holds the truncated correlations

$$\left\langle \prod_{j=1}^{N} \left\{ :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} ; \phi(x) \right\rangle$$

have an exponential clustering as $|x| \to \infty$, ($\langle - \rangle = \lim_{\Lambda \to \mathbb{R}^{\nu}} \langle - \rangle_{\Lambda}$; $\langle A; B \rangle = \langle AB \rangle - \langle A \rangle \langle B \rangle$).

The proof of the lemma follows from the methods developed by Imbrie.[8] In the charge symmetric situation, the part (i) can be deduced from an infrared bound.[6]

3. THE BBGKY EQUILIBRIUM EQUATION

As stated in the Introduction, we introduce a regularized form of the BBGKY equations. Define for any $m > 0$

$$D^{m}(x_1 - x_2) = \left[V(1 + m^2 V)^{-1} \right](x_1, x_2) \tag{3.1}$$

as the kernel of the operator $V(1 + m^2 V)^{-1}$ where V is the integral operator (2.1), and set $F^{m}(x) = -\nabla D^{m}(x)$, $F^{m}(q_1, q_2) = e_{\alpha(1)} e_{\alpha(2)} F^{m}(x_1 - x_2)$. Notice that $D^{m}(x)$ is differentiable for $x \neq 0$, has finite directional derivatives at $x = 0$, and decays exponentially fast as $|x| \to \infty$ for $m > 0$ [if V is the Coulomb potential without short-range regularization, $D^{m}(x)$ reduces to $(1/4\pi|x|)\exp(-m|x|)$, the Yukawa potential; see (B.7) in Appendix B].

Definition. A state satisfies the regularized BBGKY equation if

$$\begin{aligned} -\int dx_1 (\nabla f)(x_1) \rho(q_1 \ldots q_N) &= \beta \lim_{m \to 0} \int dx_1\, f(x_1) \sum_{j=2}^{N} F^{m}(q_1, q_j) \rho(q_1 \ldots q_N) \\ &\quad + \beta \lim_{m \to 0} \int dx_1\, f(x_1) \\ &\quad \times \int dq\, F^{m}(q_1, q)(\rho(q_1 \ldots q_N q) - \rho(q)\rho(q_1 \ldots q_N)) \end{aligned} \tag{3.2}$$

for all $f \in \mathscr{S}$.

Theorem 3. If a Coulomb system obeys either condition (CS) or (P), then its infinite volume state satisfies the regularized BBGKY hierarchy.

Corollary. If a Coulomb system obeys either conditions (P) or condition (CS) with the clustering property

$$|\rho((q)_N q) - \rho((q)_N)\rho(q)| \leqslant \frac{C}{\left[d((x)_N, x)\right]^{1+\epsilon}}, \qquad \epsilon > 0 \tag{3.3}$$

$[d((x)_N, x) =$ Euclidean distance], then its infinite volume state satisfies the ordinary BBGKY hierarchy.

The tool to prove Theorem 3 is the integration by parts formula for Gaussian measure[13] and the bounds of the lemma. We also introduce a regularized form of this formula, which will be useful to handle the thermodynamic limit.

If $d\mu(\phi)$ is a Gaussian measure with smooth covariance $V(x, y) = \int d\mu(\phi)\,\phi(x)\phi(y)$ and $F(\phi)$ is a smooth functional on $C^0(\mathbb{R}^\nu)$ we have

$$\int d\mu(\phi)\,\phi(x)F(\phi) = \int dy\, V(x, y) \int d\mu(\phi)\, \frac{\delta F(\phi)}{\delta\phi(y)} \tag{3.4}$$

For any real λ, define the function $G(x) = \int d\mu(\phi)\,F(\phi){:}\exp[i\lambda\phi(x)]{:}$. We then obtain from (3.4) the following formula {replacing there $F(\phi)$ by ${:}\exp[i\lambda\phi(x)]{:}\,F(\phi)$, see Appendix A}

$$(\nabla G)(x) = i\lambda \int dy \left[\nabla_x V(x, y)\right] \int d\mu(\phi)\ {:}\exp\left[i\lambda\phi(x)\right]{:}\ \frac{\delta F(\phi)}{\delta\phi(y)} \tag{3.5}$$

It is easy to check that an application of (3.5) to the representation (2.10) of the correlations yields the finite volume BBGKY equations. From this point of view, these are similar to the ordinary Schwinger–Dyson equations of field theory, which are also derived by integration by parts.

The regularized integration by parts formula reads[14]

$$\int d\mu(\phi)\,\phi(x)F(\phi) = \int dy\, D^m(x, y) \int d\mu(\phi)\, \frac{\delta F(\phi)}{\delta\phi(y)} + m^2 \int dy\, D^m(x, y) \int d\mu(\phi)\,\phi(y)F(\phi) \tag{3.6}$$

where $D^m(x, y)$ is related to V by the formula (3.1). As before, we deduce from (3.6) the identity

$$\begin{aligned}(\nabla G)(x) = {} & i\lambda \int dy \left[\nabla_x D^m(x, y)\right] \int d\mu(\phi)\ {:}\exp\left[i\lambda\phi(x)\right]{:}\ \frac{\delta F(\phi)}{\delta\phi(y)} \\ & + i\lambda m^2 \int dy \left[\nabla_x D^m(x, y)\right] \int d\mu(\phi)\ {:}\exp\left[i\lambda\phi(x)\right]{:}\phi(y)F(\phi) \\ & + \lambda^2 \nabla_x\left[V(x,x) - D^m(x,x)\right] G(x)\end{aligned} \tag{3.7}$$

Notice that if the covariance $V(x, y)$ is translation invariant, $V(x,x)$ and $D^m(x,x)$ are constant and the last term of (3.7) vanishes.

Proof of Theorem 3. We calculate the gradient of the finite volume correlation function (2.10) with the help of the regularized integration by parts formula (3.7). The result differs from the regularized BBGKY equations by terms depending both on m and Λ. We then use the lemma to show that these terms vanish in the limit $\Lambda \to \mathbb{R}^3$ and $m \to 0$. We perform the proof for systems obeying condition (CS) [with the translation invariant interaction (2.1)]. The plasma case, which involves boundary conditions on the Laplacian in (2.6), can be treated in the same way (see Appendix B).

Applying (3.7) to (2.9), (2.10) with

$$F(\phi) = \Xi^{-1}\exp\left\{ \sum_{\alpha=1}^{s} z_\alpha \int_\Lambda dx \, :\exp\left[i\sqrt{\beta}\, e_\alpha \phi(x) \right]: \right\} \times \prod_{j=2}^{N} \left\{ z_{\alpha(j)} :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\}$$

yields

$$\begin{aligned}\nabla_{x_1} \rho_\Lambda(q_1 \cdots q_N) = {} & \beta e_{\alpha(1)} \sum_{j=2}^{N} e_{\alpha(j)} F^m(x_1 - x_j) \rho_\Lambda(q_1 \cdots q_N) \\ & + \beta e_{\alpha(1)} \sum_{\alpha=1}^{s} e_\alpha \int_\Lambda dx\, F^m(x_1 - x) \rho_\Lambda(q_1 \cdots q_N q) \\ & + R_\Lambda^m(x_1) \end{aligned} \tag{3.8}$$

with

$$R_\Lambda^m(x_1) = m^2 \sqrt{\beta}\, e_{\alpha(1)} \int dy \times F^m(x_1 - y) \left\langle \prod_{j=1}^{N} \left\{ z_{\alpha(j)} :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} \phi(y) \right\rangle_\Lambda \tag{3.9}$$

Using the estimate (i) of the lemma (with $p = 1$) and the fact that $F^m(x)$ is integrable for any $m > 0$ (see Appendix B) with

$$\int dx\, |F^m(x)| \leqslant C_1 m^{-1} \tag{3.10}$$

we get

$$|R_\Lambda^m(x_1)| \leqslant C\sqrt{\beta}\, |e_{\alpha(1)}| m^2 \int dx\, |F^m(x)| \leqslant C_2 m \tag{3.11}$$

where C_2 is independent of Λ.

We multiply Eq. (3.8) by a function $f(x_1) \in \mathscr{S}(\mathbb{R}^3)$ and integrate on x_1.

By (3.10) and the lemma (i), all the integrands are majorized uniformly in Λ by integrable functions. Using (3.11) and taking the limit $\Lambda \to \mathbb{R}^3$ we then get by dominated convergence

$$\left| -\int dx_1\,(\nabla f)(x_1)\rho(q_1 \ldots q_N) - \beta \sum_{j=2}^{N} \int dx_1\, f(x_1) F^m(q_1, q_j)\rho(q_1 \ldots q_N) \right.$$

$$\left. -\beta \int dx_1\, f(x_1) \int dq\, F^m(q_1, q)\rho(q_1 \ldots q_N q) \right| \leqslant mC_2 \int dx\,|f(x)| \qquad (3.12)$$

Under the hypothesis of Theorem 3, we shall prove in the next section the local neutrality $\sum_{\alpha=1}^{s} e_\alpha \rho(q) = 0$. Using this and taking the limit $m \to 0$ in (3.12) yields the regularized BBGKY equation (3.2).

Proof of the Corollary. We have

$$\lim_{m \to 0} F^m(x) = F(x) = -(\nabla V)(x)$$

and $|F^m(x)| \leqslant C|x|^{-2}$ uniformly in m. If condition (P) holds or if one has the clustering property (3.3), one can take the limit $m \to 0$ in (3.2) by dominated convergence to get the BBGKY equations in the weak sense

$$-\int dx_1\,(\nabla f)(x_1)\rho(q_1 \ldots q_N)$$

$$= \beta \int dx_1\, f(x_1) \sum_{j=2}^{N} F(q_1, q_j)\rho(q_1 \ldots q_N) + \beta \int dx_1\, f(x_1) \int dq\, F(q_1 q)$$

$$\times \left[\rho(q_1 \ldots q_N q) - \rho(q_1 \ldots q_N)\rho(q)\right] \qquad (3.13)$$

To conclude the proof we use general theorems on distributions. It follows from (3.13) that the derivatives of order 1 of $\rho(\alpha_1 x_1, q_2 \ldots q_N)$ (considered as distributions of x_1) are functions, and therefore $\rho(\alpha_1, x_1, q_2 \ldots q_N)$ are continuous functions of x_1 (Ref. 15, p. 189). The fact that these derivatives are continuous functions implies in turn that $\rho(\alpha_1 x_1, q_2 \ldots q_N)$ are continuously differentiable in x_1 (Ref. 15, p. 61). From this we conclude that the BBGKY equations hold in the ordinary sense. ■

Remarks.

(1) In dimension $\nu = 2$ and for system obeying the same conditions P [with (i) repaced by β small], Theorem 2 and the Lemma still hold. We then get the validity of the ordinary BBGKY equation by the same method.

(2) By the work of Imbrie,[8] jellium systems in dimensions 2 and 3 also satisfy Theorem 2 and the Lemma in the range of convergence of the cluster expansion. We then get for them the ordinary BBGKY equation as in Theorem 3.

(3) In the charge symmetric case and $\nu = 2$, we first construct the thermodynamic limit of finite volume systems defined by (2.4), (2.5) with V replaced by $V(1 + m^2 V)^{-1}$ (Yukawa system) and call $\rho^m((q)_N)$ the corre-

sponding correlation functions. We then define the Coulomb state for $\nu = 2$ by $\rho((q)_N) = \lim_{m\to 0}\rho^m((q)_N)$ (the limit exists by correlation inequalities[6]). If the $\rho((q)_N)$ cluster as in (3.3), one can check that the ordinary BBGKY equation holds.

(4) For charge symmetric systems in one dimension, the same remark applies. General one-dimensional charged systems (including the jellium) have been shown to satisfy the equilibrium equations in Refs. 16 and 9.

(5) A slightly different regularized hierarchy was introduced in Ref. 16 (using a spatial cutoff instead of the Yukawa cutoff), and this hierarchy was shown to be equivalent to the classical KMS condition.

4. THE *l*-SUM RULES

In this section, we present a new derivation of the l-sum rules (1.2), (1.3) based on the Sine-Gordon representation. We first prove the local neutrality (1.2) which is seen to be generally true in homogeneous phases, irrespective of the value of the parameters β, z and of the cluster properties (Theorem 4). In fact, to establish its validity, one uses only a bound uniform with respect to Λ which is expected to hold in great generality. We then derive the l-sum rules for systems obeying the condition (P), where the cluster properties play an important role (Theorem 5).

Theorem 4. If the thermodynamic limit of the finite volume correlation functions (2.5) exists [with the potential as in (2.1) or (2.6)], is translation invariant, and if

$$\left.\begin{array}{r}|\rho_\Lambda(q)| \leqslant C\\ |\langle\phi(x)\rangle_\Lambda| \leqslant C\end{array}\right\} \quad \text{uniformly with respect to } \Lambda \tag{4.1}$$

then the local neutrality $\sum_{\alpha=1}^{s} e_\alpha \rho(q) = 0$ holds.

Corollary. Coulomb systems satisfying condition (CS) or (P) are locally neutral.

Theorem 5. Coulomb systems satisfying the condition (P) obey the l-sum rules (1.3) for all l, N.

The basic identity which will generate the local neutrality and the sum rules is the formula of translation of a Gaussian measure, which we now recall. Let $d\mu(\phi)$ be a Gaussian measure with smooth covariance $V(x, y)$ and $g(x) \in \mathscr{S}(\mathbb{R}^\nu)$. The formula for the change of variable $\phi(x) \to \phi(x) + g(x)$ in the integral $\int d\mu(\phi)\, F(\phi)$ is[13]

$$\int d\mu(\phi)\, F(\phi) = \int d\mu(\phi)\, F(\phi + g)\exp\left[-\frac{1}{2}(g, V^{-1}g) - (\phi, V^{-1}g)\right] \tag{4.2}$$

We see *formally* on (4.2) that the measure $d\mu(\phi)$ is invariant under translations g which belong to the kernel of V^{-1} (i.e., $V^{-1}g = 0$). For a Coulomb kernel, as $V^{-1} = d^{-2}(-\Delta + d^2)(-\Delta)$, $d\mu(\phi)$ will be invariant under translations by harmonic functions Y with $(\Delta Y)(x) = 0$ for all $x \in \mathbb{R}^\nu$. The local neutrality and the l-sum rules are the differential expression of this invariance. Technically, we have first to approximate $Y(x)$ by a function with compact support. The resulting boundary terms are then shown not to contribute in the thermodynamic limit as a consequence of the Lemma.

Proof of Theorem 4. Consider $P_\Lambda(\beta, z) = |\Lambda|^{-1}\ln \Xi_\Lambda(\beta, z)$, $\Xi_\Lambda(\beta, z)$ represented by the functional integral (2.8), and perform the translation $\phi(x) \to \phi(x) + tk(x)$, $k(x) \in C_0^\infty(\mathbb{R}^3)$ and $t \in \mathbb{R}$. We get from (4.2)

$$P_\Lambda(\beta, z) = |\Lambda|^{-1}\ln \int d\mu_V(\phi) \exp\left[-\frac{t^2}{2}(k, V^{-1}k) - t(\phi, V^{-1}k)\right]$$
$$\times \exp\left\{ \sum_{\alpha=1}^{s} z_\alpha \int_\Lambda dx \exp\left[i\sqrt{\beta}\, e_\alpha tk(x)\right] :\exp\left[i\sqrt{\beta}\, e_\alpha \phi(x)\right]: \right\} \qquad (4.3)$$

Since $P_\Lambda(\beta, z)$ is independent of t, we have

$$|\Lambda| \frac{d}{dt} P_\Lambda(\beta, z) = i\sqrt{\beta} \int_\Lambda dx\, k(x) \sum_{\alpha=1}^{s} e_\alpha \rho(\alpha x) - \int_\Lambda dx\, (V^{-1}k)(x)\langle\phi(x)\rangle_\Lambda = 0 \qquad (4.4)$$

The first term on the right-hand side of (4.4) tends as $\Lambda \to \mathbb{R}^3$ to $(\sum_{\alpha=1}^{s} e_\alpha \rho_\alpha)$ $\int dx\, k(x)$ by dominated convergence [with $\rho_\alpha = \lim_{\Lambda\to\mathbb{R}^3} \rho_\Lambda(\alpha x)$]. Using the bound (4.1) we thus get from (4.4)

$$\left| \sum_{\alpha=1}^{s} e_\alpha \rho_\alpha \right| \leqslant \frac{C}{\sqrt{\beta}} \frac{\int dx\, |(V^{-1}k)(x)|}{|\int dx\, k(x)|} \qquad (4.5)$$

We now choose $k(x)$ as follows for any positive R:

$$k(x) = \begin{cases} 1, & |x| \leqslant R \\ 0, & |x| \geqslant R+1 \end{cases} \qquad |k(x)| \leqslant 1 \qquad (4.6)$$

and $|(\Delta^p k)(x)| \leqslant C$ uniformly with respect to R, $p = 1, 2$. Since $(V^{-1}k)(x)$ $= d^{-2}(-\Delta + d^2)(-\Delta)k(x)$ is only nonzero for $R < |x| < R + 1$, $\int dx\, |(V^{-1}k)(x)|$ is of the order of R^2, and therefore (4.5) implies

$$\left| \sum_{\alpha=1}^{s} e_\alpha \rho_\alpha \right| \leqslant C_1 R^{-1}$$

Since R is arbitrary, Theorem 4 is proven. ■

The corollary is obvious since for (CS) systems $\langle\phi(x)\rangle_\Lambda = 0$ and for (P) systems, (4.1) is a particular case of the Lemma (i).

Remark. We expect that homogeneous charged systems are always locally neutral, and that the bound (4.1) is generally true, even in non-screened phases. (4.1) holds in the high-temperature two-dimensional phase, as well as in the high-temperature phases of jellium systems for $\nu = 2, 3$. The local neutrality can also be verified explicitly in one dimension.[6]

Proof of Theorem 5. We do the translation $\phi(x) \to \phi(x) + tg(x)$, $g(x) \in C_0^\infty(\mathbb{R}^3)$, $t \in \mathbb{R}$, in a general correlation function (2.10). This gives

$$\rho_\Lambda(q_1 \ldots q_N) = \Xi^1(\beta, z) \int d\mu_V(\phi) \exp\left[-\frac{t^2}{2}(g, V^{-1}g) - t(\phi, V^{-1}g) \right]$$
$$\times \exp\left\{ \sum_{\alpha=1}^{s} z_\alpha \int_\Lambda dx \exp\left[i\sqrt{\beta}\, e_\alpha t g(x) \right] :\exp\left[i\sqrt{\beta}\, e_\alpha \phi(x) \right]: \right\}$$
$$\times \prod_{j=1}^{N} \left\{ z_{\alpha(j)} \exp\left[i\sqrt{\beta}\, e_{\alpha(j)} t g(x_j) \right] :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} \tag{4.7}$$

Taking the derivative at $t = 0$ and using the identity (4.4) we find

$$i\sqrt{\beta} \sum_{j=1}^{N} g(x_j) e_{\alpha(j)} \rho_\Lambda(q_1 \ldots q_N)$$
$$+ i\sqrt{\beta} \int_\Lambda dx\, g(x) \sum_{\alpha=1}^{s} e_\alpha \left[\rho_\Lambda(q_1 \ldots q_N q) - \rho_\Lambda(q_1 \ldots q_N) \rho_\Lambda(q) \right]$$
$$= \int_\Lambda dx\, (V^{-1}g)(x) \left\langle \prod_{j=1}^{N} \left\{ z_{\alpha(j)} :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} ; \phi(x) \right\rangle_\Lambda \tag{4.8}$$

We can take the limit $\Lambda \to \mathbb{R}^3$ in (4.8) using a dominated convergence theorem together with the bound of the Lemma (i)

$$i\sqrt{\beta} \sum_{j=1}^{N} g(x_j) e_{\alpha(j)} \rho(q_1 \ldots q_N)$$
$$+ e\sqrt{\beta} \int dq\, g(x) e_\alpha \left[\rho(q_1 \ldots q_n q) - \rho(q_1 \ldots q_N) \beta(q) \right]$$
$$= \int dx\, (V^{-1}g)(x) \left\langle \prod_{j=1}^{N} \left\{ z_{\alpha(j)} :\exp\left[i\sqrt{\beta}\, e_{\alpha(j)} \phi(x_j) \right]: \right\} ; \phi(x) \right\rangle \tag{4.9}$$

Choosing $g(x)$ of the form $g(x) = Y_l(x)k(x)$, where $Y_l(x)$ is an harmonic polynomial of order l and $k(x)$ is as in (4.6), we see that $(V^{-1}g)(x)$ has its support in the shell $R < |x| < R + 1$ where it is of the order R^l. With the exponential clustering of the Lemma (ii), we therefore find that the right-hand side of (4.9) is bounded by $CR^{l+2}\exp(-\kappa R)$, $\kappa > 0$. The result of the theorem now follows when we let $R \to \infty$ in (4.9).

Remark. It is clear from the proof of the theorem that the l-sum rule will hold whenever the correlations occurring in the right-hand side of (4.9) decay faster than any inverse power. This is known to be the case in the high-temperature phase for $\nu = 2, 3$, including jellium systems.

5. CONCLUDING REMARKS

In this section, we discuss at an heuristic level symmetry properties that should possess Coulomb states which obey the l-sum rules.

Formula (4.7) shows that, up to boundary terms, the translation of the random field $\phi(x)$ yields an identity which can be viewed as invariance of the state under the transformation $z_\alpha \to z_\alpha \exp[ie_\alpha Y(x)]$ in the space of activities. The sum rules are then the Ward identities associated with this symmetry.

Alternatively the symmetry can be formulated as the invariance of the state under translations in the space of chemical potential or external fields. Denote by $\rho_\Lambda((q)_N, \mu)$ and $\rho((q)_N, \mu) = \lim_{\Lambda \to \mathbb{R}^3} \rho_\Lambda((q)_N, \mu)$ the correlations as functions of the chemical potentials $\mu = (\mu_1 \ldots \mu_s)$, with $\mu_\alpha = \beta^{-1} \ln z_\alpha$. We derive easily, setting $e = (e_1 \ldots e_s)$,

$$\begin{aligned} &\frac{\partial}{\partial \lambda} \rho_\Lambda((q)_N, \mu + \lambda e)\Big|_{\lambda=0} \\ &\quad = \sum_{\alpha=1}^{s} e_\alpha \frac{\partial}{\partial \mu_\alpha} \rho_\Lambda((q)_N, \mu) \\ &\quad = \sum_{\alpha=1}^{s} e_\alpha \rho_\Lambda((q)_N, \mu) \\ &\qquad + \int_\Lambda dx \sum_{\alpha=1}^{s} e_\alpha [\rho_\Lambda((q)_N q, \mu) - \rho_\Lambda((q)_N, \mu) \rho_\Lambda(q, \mu)] \end{aligned} \tag{5.1}$$

Taking the formal infinite volume limit of (5.1) yields

$$\sum_{\alpha=1}^{s} e_\alpha \frac{\partial}{\partial \mu_\alpha} \rho((q)_N, \mu) = \int dq\, e_\alpha \rho(q \,|\, (q)_N) = 0 \tag{5.2}$$

as a result of the $l = 0$ sum rule (1.3) Equation (5.2) is the differential form of the invariance of the state under translations in the e direction in μ space, i.e.,

$$\rho((q)_N, \mu) = \rho((q)_N, \mu + \lambda e) \tag{5.3}$$

In other words the state depends only on that part of the vector μ which is perpendicular to e. This invariance property was found to be true by Lieb and Lebowitz for the pressure $p(\beta, \mu)$, as an expression of local neutrality of the state.[10] We see that the same invariance for the whole state would be equivalent to the full set of electroneutrality sum rules. The equations (5.2), (5.3) can be checked in one dimension by explicit calculations, but we did not prove them for $\nu > 1$. In the plasma phase, this would require showing some screening in a situation where $\sum_{\alpha=1}^{s} e_\alpha z_\alpha \neq 0$ [i.e., relaxing condition P(ii)], which would involve controlling surface charge effects. Some recent progress in this direction has been made in Ref. 11. Notice that if (5.3) holds in some domain of μ space, the state depends there only on $(s-1)$ activity parameters, and hence the condition P(ii) does not imply any restriction, but is simply a choice of a particular parametrization in this domain.

The general l-sum rules can be interpreted as follows. Consider now the state as a functional of space-dependent chemical potential (i.e., external fields) $\mu(x) = (\mu_1(x) \ldots \mu_s(x))$ and denote it by $\rho_\Lambda(q_n), \mu(\cdot))$ and $\rho(q)_N, \mu(\cdot))$. The infinitesimal action of a translation in the direction $eY(x)$ is

$$\frac{\partial}{\partial\lambda} \rho_\Lambda((q)_N, \mu(\cdot) + \lambda e Y(\cdot))\Big|_{\lambda=0}$$

$$= \sum_{j=1}^{N} e_{\alpha(j)} Y(x_j) \rho_\Lambda((q)_N, \mu(\cdot)) + \int_\Lambda dx \sum_{\alpha=1}^{s} e_\alpha Y(x)$$

$$\times \left[\rho_\Lambda((q)_N q, \mu(\cdot)) - \rho_\Lambda((q)_N, \mu(\cdot)) \rho_\Lambda(q, \mu(\cdot))\right] \quad (5.4)$$

Choosing $Y(x)$ harmonic on $\mathbb{R}^3$ and taking again the formal infinite volume limit gives

$$\frac{\partial}{\partial\lambda} \rho((q)_N, \mu + \lambda e Y(\cdot))\Big|_{\lambda=0} = \int dq\, e_\alpha Y(x) \rho(q \mid (q)_N) = 0 \quad (5.5)$$

by the general l-sum rules (1.3). This would correspond formally to the global symmetry

$$\rho((\rho)_N, \mu) = \rho((q)_N, \mu + \lambda e Y(\cdot)) \quad (5.6)$$

with $Y(x)$ harmonic. Physically (5.6) says that in the plasma phase, the state does not change in an external harmonic potential. More precisely, if one constructs a state starting at finite volume with an arbitrary charge distribution at the boundary (generating an harmonic field in the bulk), its thermodynamic limit should not depend on these boundary charges when the parameters correspond to the plasma phase (high temperature, low density). This invariance was proven by Fröhlich and Pfister[17] in the special case of a planar uniform charge distribution (i.e., a plane condensor generating a constant field) by means of correlation inequalities. These symmetries should play an important role in understanding the structure of Coulomb states and their equilibrium equations.

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APPENDIX A

We prove the formulas (3.5) and (3.7) under the condition that $\nabla_x V(x, y)$ and $\nabla_x V(x,x)$ exist for all x and y.

Proof of (3.5).

$$\begin{aligned}(\nabla G)(x) &= \nabla_x\left\{\exp\left[\frac{1}{2}\lambda^2 V(x,x)\right]\int d\mu(\phi)\exp[i\lambda\phi(x)]F(\phi)\right\}\\ &= \frac{\lambda^2}{2}\left[\nabla_x V(x,x)\right]G(x)\\ &\quad+\exp\left[\frac{1}{2}\lambda^2 V(x,x)\right]\nabla_x\int d\mu(\phi)\exp[i\lambda\phi(x)]F(\phi) \qquad (A.1)\end{aligned}$$

To calculate $\nabla_x \int d\mu(\phi)\exp[i\lambda\phi(x)]F(\phi)$, we consider

$$\begin{aligned}&\frac{1}{h}\int d\mu(\phi)\left\{\exp[i\lambda\phi(x+h)]-\exp[i\lambda\phi(x)]\right\}F(\phi)\\ &= \frac{1}{h}\int d\mu(\phi)\int_0^1 d\epsilon\,\frac{d}{d\epsilon}\exp\{i\lambda\epsilon[\phi(x+h)-\phi(x)]\}\exp[i\lambda\phi(x)]F(\phi)\\ &= \frac{i\lambda}{h}\int d\mu(\phi)\int_0^1 d\epsilon\,[\phi(x+h)-\phi(x)]\\ &\quad\times\exp[i\lambda\epsilon\phi(x+h)+i\lambda(1-\epsilon)\phi(x)]F(\phi)\end{aligned}$$

Using the integration by parts formula (3.4), this can be expressed as

$$\begin{aligned}&\frac{-\lambda^2}{h}\int_0^1 d\epsilon\,\{\epsilon[V(x+h,x+h)-V(x,x+h)]\\ &\qquad+(1-\epsilon)[V(x+h,x)-V(x,x)]\}\\ &\quad\times\int d\mu(\phi)\exp[i\lambda\epsilon\phi(x+h)+i\lambda(1-\epsilon)\phi(x)]F(\phi)\\ &\quad+\frac{i\lambda}{h}\int_0^1 d\epsilon\int dy\,[V(x+h,y)-V(x,y)]\\ &\quad\times\int d\mu(\phi)\exp[i\lambda\epsilon\phi(x+h)+i\lambda(1-\epsilon)\phi(x)]\frac{\delta F(\phi)}{d\phi(y)}\end{aligned}$$

(A.2)

Because of the regularity of the covariance, $\phi(x)$ can be taken as continuous function of x, see Ref. 7. In the limit $h \to 0$ we finally get

$$-\lambda^2 \int_0^1 d\epsilon \left[(1-2\epsilon) \nabla_x V(x,y)|_{y=x} + \epsilon \nabla_x V(x,x) \right]$$
$$\times \int d\mu(\phi) \exp\left[(i\lambda\phi(x)) F(\phi) \right]$$
$$+ i\lambda \int dy\, \nabla_x V(x,y) \int d\mu(\phi) \exp\left[i\lambda\phi(x) \right] \frac{\delta F(\phi)}{\delta\phi(y)}$$

This combined with (A.1) proves (3.5). The formula (3.7) is proven in the same way.

APPENDIX B

To treat the plasma case, we have to replace $F^m(x-y)$ everywhere in the proof of Theorem 3 by $F_\Lambda^m(x,y) = -\nabla_x D_\Lambda^m(x,y) D_\Lambda^m(x,y)$ defined as in (3.1) with V replaced by V_Λ (2.6).

Following Ref. 7 [let us remark that our d^2 is their $(dl_D)^{-2}$] we have

$$\begin{aligned} D_\Lambda^m &= V_\Lambda\left(1 + m^2 V_\Lambda\right)^{-1} \\ &= \left\{ \left[(-\Delta_\Lambda)^{-1} - (-\Delta_\Lambda + d^2)^{-1} \right]^{-1} + m^2 \right\}^{-1} \\ &= \left[d^{-2}\Delta_\Lambda^2 - \Delta_\Lambda + m^2 \right]^{-1} \\ &= \frac{d^2}{r_+^2 - r_-^2} \left[(-\Delta_\Lambda + r_-^2)^{-1} - (-\Delta_\Lambda + r_+^2)^{-1} \right] \end{aligned} \tag{B.1}$$

where $r_\pm^2 = 2d^2[1 \pm (1 - 4m^2 d^{-2})^{1/2}]$. For d fixed and m small, we have

$$d^2 > r_+^2 > r_-^2 > m^2 \tag{B.2}$$

Using the methods of the images[13] and (B.1), it is easy to obtain the following:

(i) For every x and y, the following derivatives exist and

$$|\nabla_x D_\Lambda^m(x,y)| \leqslant C \tag{B.3}$$

$$|\nabla_x D_\Lambda^m(x,x)| \leqslant C \tag{B.4}$$

with C uniform in Λ and m.

(ii) For $|x-y|$ large enough

$$|D_\Lambda^m(x,y)| \leqslant C_1 \exp(-r_- |x-y|) \tag{B.5}$$

$$|\nabla x D_\Lambda^m(x,y)| \leqslant C_1 \exp(-r_- |x-y|) \tag{B.6}$$

where C_1 is uniform in Λ.

(B.3)–(B.6) provide the uniform bounds needed in the proof of Theorem 3.

Moreover, we find from (B.1)

$$\lim_{\Lambda\to\mathbb{R}^3} D^m_\Lambda(x, y) = D^m(x-y)$$
$$= \frac{d^2}{r_+^2 - r_-^2}\left[\frac{\exp(-r_-|x-y|) - \exp(-r_+|x-y|)}{4\pi|x-y|}\right] \qquad (B.7)$$

and (B.2) together with

$$\int dx \left|\nabla_x\left[\frac{\exp(-r|x|)}{4\pi|x|}\right]\right| = C_0 r^{-1}$$

leads to (3.10).

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