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Section A :
Physique théorique.

A variational principle for the equilibrium of hard sphere systems

by

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ABSTRACT. — We show that the equilibrium state of an infinite system of interacting hard spheres can be obtained in the grand canonical formalism by means of a variational principle. We give also a simple application deriving the Salsburg-Zwanzig-Kirkwood expressions for correlation functions of the equilibrium state of one dimensional systems of hard spheres.

§ 1 INTRODUCTION AND NOTATIONS

The aim of this paper is to prove the validity, for a system of classical hard spheres, of a variational analogue to that established in ref [*1*] in the case of lattice systems.

Let us consider a system of classical identical particles in R^ν interacting through a symmetric translationally invariant many body potential $\tilde{\Phi}(X)$: i. e. let the energy of a configuration $X = \{ x_1, \ldots, x_n \} \subset R^\nu$ be given by

$$U_{\tilde{\Phi}}(X) = \sum_{S \subset X} \tilde{\Phi}(S) \qquad (1)$$

(*) The results of this paper will be included in the thesis (« doctorat d'État ès Sciences Physiques ») of one of us (S. M. S.) to be submitted at the Aix-Marseille university (June 1968, C. N. R. S. reg. AO 2290).

We shall consider only interactions having a hard core of fixed radius a; this means that we suppose

$$\tilde{\Phi}(X) = \Phi_a(X) + \Phi(X)$$

where $\Phi_a(x_1, x_2) \equiv 0$ if $|x_1 - x_2| \geq a$ and $\Phi_a(x_1, x_2) = +\infty$ if $|x_1 - x_2| < a$ and $\Phi_a(x_1, \ldots, x_k) \equiv 0$ if $k \geqslant 2$ and the potential $\Phi(X)$ is defined to have arbitrary but finite values if the configuration X contains two points, at least, at a distance smaller than a.

We call E_a the space of « physical » configurations i. e. the space of finite (void or not) configurations X such that $|x_i - x_j| \geq a$ if $i \neq j$ and $x_i, x_j \in X$; we introduce a metric topology on E_a by defining

$$d(X, Y) = \max_i \min_j |x_i - y_j| + \max_j \min_i |x_i - y_j| \tag{2}$$

if $X = \{x_1, \ldots, x_n\}$ and $Y = \{y_1, \ldots, y_m\}$. If $X \in E_a$:

$$U_{\tilde{\Phi}}(X) = \sum_{S \subset X} \Phi(S) = U_{\Phi}(X)$$

We call $E_a^\Lambda \subset E_a$ the space of physical configurations contained in $\Lambda \subset R^\nu$. Note that the presence of hard cores implies that (if ρ_{cp} denotes the close paking density, N(X) the number of points in X and V(Λ) the volume of the region Λ) we have

$$\frac{N(X)}{V(\Lambda)} \leq \rho_{cp} + \varepsilon(\Lambda) \tag{3}$$

and $\varepsilon(\Lambda)$ can be chosen to be a decreasing function approaching 0 as $V(\Lambda) \to \infty$ if we restrict us to consider only cubic Λ's. On E_a we introduce a measure dX as

$$\int_{E_a} \cdot dX = \sum_{n \geq 0} \int_{E_a} \cdot \frac{dx_1 \ldots dx_n}{n!} \tag{4}$$

this means that if $f \in C(E_a)$ and has a compact support (i. e. $f(x) \equiv 0$ if $N(X) \geq n_0$ and $f(X) \equiv 0$ if $X \not\subset \Lambda_0$ where Λ_0 is a bounded set) and if we regard $f(X)$ as a symmetric function on $(R^\nu)^n$ then:

$$\int_{E_a} f(X) dX = \sum_{n \geq 0} \int_{E_a} f(x_1, \ldots, x_n) \frac{dx_1 \ldots dx_n}{n!} \tag{5}$$

The potentials $\Phi(X)$ restricted to $X \in E_a$ can be regarded as functions on E_a (putting $\Phi(\phi) = 0$) which we continue to call Φ. Let $\mathcal{B}_0$ be the set of continuous finite range potentials which are then described by a continuous function on E_a with compact support.

If $\Phi \in \mathcal{B}_0$ we have, if 0 denotes the origin of R^ν:

$$0 \leq \sup_{0 \in X \in E_a} \sum_{0 \in S \subset X} \frac{|\Phi(S)|}{N(S)} = \|\Phi\| < +\infty \tag{6}$$

It is easy to see that $\mathcal{B}_0$ is a separable normed space in the norm defined by (6). Let $\mathcal{B}$ be the Banach space obtained by completing $\mathcal{B}_0$ in the norm (6).

§ 2 THE THERMODYNAMIC LIMIT AND THE CORRELATION FUNCTIONALS

Let $\Phi \in \mathcal{B}$, then from (6) it follows that $U_\Phi(X)$ is defined $\forall X \in E_a$ and is continuous on E_a. Hence we can define the partition function $Z_\Lambda(\Phi)$ associated to a bounded region Λ as

$$Z_\Lambda(\Phi) = \int_{E_a^\Lambda} e^{-U_\Phi(X)} dX \tag{7}$$

and the pressure as

$$P_\Lambda(\Phi) = V(\Lambda)^{-1} \lg Z_\Lambda(\Phi) \tag{8}$$

where the inverse temperature β and the chemical potential μ are absorbed in the interaction.

Then we can state the following theorem.

THEOREM 1: If $\Phi \in \mathcal{B}$

i) the limit

$$\lim_{\Lambda \to \infty} P_\Lambda(\Phi) = P(\Phi) \tag{9}$$

exists on the net of increasing cubes Λ [1]

ii) the functional $\Phi \to P(\Phi)$ is convex and continuous on $\mathcal{B}$ and

$$|P(\Phi) - P(\Psi)| \leq \rho_{cp} \|\Phi - \Psi\| \qquad \forall \Psi \in \mathcal{B} \tag{10}$$

where ρ_{cp} is the close paking density.

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[1] Because of the hard core one could obtain here and in what follows the same results considering $\Lambda \to \infty$ in more general ways [*12*].

To prove this theorem we observe that

$$P_\Lambda(\Phi) - P_\Lambda(\Psi) = \frac{d}{d\lambda} P_\Lambda(\Phi + \lambda(\Psi - \Phi))\Big|_{\lambda=\eta} \qquad 0 \leq \eta \leq 1 \tag{11}$$

but using (6):

$$\begin{aligned} &\left| \frac{d}{d\lambda} P_\Lambda(\Phi + \lambda(\Psi - \Phi)) \right| \\ &\quad \leq \frac{1}{V(\Lambda)} Z_\Lambda(\Phi + \lambda(\Psi - \Phi))^{-1} \int_{E_a^\Lambda} e^{-U_{\Phi+\lambda(\Psi-\Phi)}(X)} \,|\, U_\Phi(X) - U_\Psi(X) \,|\, dX \\ &\quad \leq \left(\max_{E \in X_a^\Lambda} \frac{N(X)}{V(\Lambda)} \right) \| \Phi - \Psi \| \leq (\rho_{cp} + \varepsilon(\Lambda)) \| \Phi - \Psi \| \end{aligned} \tag{12}$$

hence:

$$| P_\Lambda(\Phi) - P_\Lambda(\Psi) | \leq (\rho_{cp} + \varepsilon(\Lambda)) \| \Phi - \Psi \|$$

now the proof runs exactly on the same way as the proof of Theorem 1 ref [*2*] if one notes that for finite range hard core many body potentials statement *i*) is well known [*3*] [*4*].

Now we study the relation between the correlation functionals and the tangent plane to the graph of P_Λ and P: the functional $\alpha_{\Lambda\Phi} \in \mathcal{B}^*$ defined by:

$$\alpha_{\Lambda\Phi}(\Psi) = - \left. \frac{dP_\Lambda(\Phi + \lambda\Psi)}{d\lambda} \right|_{\lambda=0} = V(\Lambda)^{-1} Z_\Lambda(\Phi)^{-1} \int_{E_a^\Lambda} dX e^{-U_\Phi(X)} U_\Psi(X) \tag{13}$$

defines the unique tangent plane to the graph of P_Λ and we can interprete it as the averaged correlation functional [*2*] [*5*].

It follows from (12) that

$$| \alpha_{\Lambda\Phi}(\Psi) | \leq (\rho_{cp} + \varepsilon(\Lambda)) \| \Psi \| \text{ hence } \| \alpha_{\Lambda\Phi} \| \leq (\rho_{cp} + \varepsilon(\Lambda)) \tag{14}$$

Let now $T \subset \mathcal{B}$ denote the set of potentials such that the graph of P has a unique tangent plane at $\Phi \in T$: i. e. the set of $\Phi \in \mathcal{B}$ such that there exists an unique functional $\alpha_\Phi \in \mathcal{B}^*$ such that

$$P(\Phi + \Psi) \geq P(\Phi) - \alpha_\Phi(\Psi) \tag{15}$$

we have then.

THEOREM 2: Let $\Phi \in \mathcal{B}$

i) If $\Phi \in T$ the limit

$$\lim_{\Lambda \to \infty} \alpha_{\Lambda\Phi}(\Psi) = \alpha_\Phi(\Psi)$$

exists $\forall \Psi \in \mathcal{B}$ and defines the tangent plane to the graph of P(.) at Φ.

ii) If, for a given Ψ, $-\frac{d}{d\lambda}P(\Phi+\lambda\Psi)\Big|_{\lambda=0}=\alpha_\Phi(\Psi)$ exists, then for such a Ψ

$$\lim_{\Lambda\to\infty}\alpha_{\Lambda\Phi}(\Psi)=\alpha_\Phi(\Psi) \tag{16}$$

and a necessary and sufficient condition in order that $\Phi\in T$ is that $\frac{d}{d\lambda}P(\Phi+\lambda\Psi)\Big|_{\lambda=0}$ exists $\forall\Psi\in\mathcal{B}$.

iii) The set T contains a countable intersection of open dense subsets of $\mathcal{B}$.

iv) If we separate the chemical potential $\Phi^{(1)}$ form the many body potential Φ' (defined as $\Phi'^{(1)}=0$, $\Phi'^{(k)}=\Phi^{(k)}$ if $k\neq 1$) and consider the potential $\beta\Phi\equiv(\beta\Phi^{(1)},\beta\Phi')$ then there is a dense set $T'\subset\mathcal{B}'$ (where $\mathcal{B}'$ denotes the space of potential Φ' such that $\Phi'^{(1)}=0$) such that, if $\Phi'\in T'$, the potential $(\beta\Phi^{(1)},\beta\Phi')\in T$ almost everywhere in β and $\Phi^{(1)}$ with respect to the Lebesgue measure on the plane $(\beta,\Phi^{(1)})$.

The proof of this theorem follows the same path of that of theorems 2, 3 of ref [*2*] and will be omitted.

Remark: All the results obtained until now can be derived, without any change, substituting the norm (6) on $\mathcal{B}_0$ by $\sup_{X\subset E_a}\left|\frac{U_\Phi(X)}{N(X)}\right|$ and considering instead of $\mathcal{B}$ the completion of $\mathcal{B}_0$ with respect to this new norm.

§ 3 VARIATIONAL PRINCIPLE FOR EQUILIBRIUM

In recent works [*6*] [*7*] it has been shown that the states of a classical system can be regarded as states over a certain C*-algebra $\mathfrak{A}$ subjected to certain conditions whose physical meaning is that the probability of configurations having an infinite number of particles in finite regions is zero.

In the case at hand the algebra $\mathfrak{A}$ can be defined as follows: let Λ be an open set, let $C_0(E_a^\Lambda)$ be the espace of continuous complex functions on E_a having compact support contained in E_a^Λ. If $f\in C_0(E_a^\Lambda)$ we define $Sf\in C(E_a)$ as

$$Sf(X)=\sum_{T\subset X}f(T)\qquad\forall X\in E_a \tag{17}$$

As a consequence of the hard core $\sup_X |Sf(X)| < +\infty$: if M_f is the maximum of f then

$$|Sf(X)| \leq \sum_{T \subset X} |f(S)| = \sum_{T \subset X \cap \Lambda} |f(S)| \leq M_f 2^k$$

where k is the maximum number of hard spheres which can be contained in Λ.

The algebra $\mathfrak{A}$ is defined as the closed (in the sup-norm) subalgebra of $C(E_a)$ generated by the functions of the form Sf, $f \in C_0(E_a^\Lambda) \forall \Lambda \subset R^\nu$, Λ bounded and open.

Now suppose that for each $\Lambda \subset R^\nu$, bounded and open, we are given a measure $\mu_\Lambda \geq 0$ on E_a^Λ such that:

i)
$$\mu_\Lambda(E_a^\Lambda) = 1 \tag{18}$$

ii) If $\Lambda' \supset \Lambda$ and $f \in C_0(E_a^\Lambda)$ then:

$$\int_{E_a^\Lambda} \mu_\Lambda(dX) f(X) = \int_{E_a^{\Lambda'}} \mu_{\Lambda'}(dX') f(X' \cap \Lambda) \tag{19}$$

then if $f \in C_0(E_a^\Lambda)$ the formula

$$\rho(Sf) = \int \mu_\Lambda(dX)(Sf)(X) \tag{20}$$

which as is easily seen is independent on the arbitiarity of Λ, can be used to define, by linearity and continuity, a state over $\mathfrak{A}$ since the set of elements of the form Sf is dense in $\mathfrak{A}$ as a consequence of the relation

$$(Sf_1)(X) \cdot (Sf_2)(X) = (S(f_1 \times f_2))(X)$$

where

$$(f_1 \times f_2)(X) = \sum_{T \subset X} f_1(T) f_2(X/T)$$

Let $\mathcal{F}_0$ be the subset of the set E of states over $\mathfrak{A}$ obtained in this way. The following theorem holds:

THEOREM 3: $\mathcal{F}_0 \equiv E$.

The proof has been given by Ruelle [*6*] under more general conditions but a slightly different formalism. The technical part is considerably simplified taking into account that we are interested only in the hard core case. The spirit of the proof of this theorem is to observe first that in our case the set $\mathcal{F} \subset E$ introduced in the mentioned reference coincides with E and secondly use theorem 5.1 of the same reference (taking the group G to contain only the identity) and prove that $\mathcal{F} \equiv \mathcal{F}_0$. We leave to the interested reader the translation in the formalism of this paper of the referred points of ref [6].

On the algebra $\mathfrak{A}$ one can define the space translations as automorphisms of $\mathfrak{A}$ into itself through:

$$(\tau_x(Sf))(X) = (Sf)(X - x) \qquad \forall x \in R^\nu \tag{21}$$

this operator can be interpreted as the translation by x.

Let $E \cap \mathfrak{L}^\perp$ be the set of states on $\mathfrak{A}$ invariant under all τ_x, $\forall x \in R^\nu$. Then the following theorem due to Robinson-Ruelle [7] holds:

THEOREM 4: It is possible to define a functional $\rho \to S(\rho)$ on $E \cap \mathfrak{L}^\perp$ such that

i) $S(\rho) = -\infty$ for all $\rho \in E \cap \mathfrak{L}^\perp$ such that $\mu_\Lambda(dX)$ is not dX-continuous of every Λ open and bounded.

ii) if $\rho \in E \cap \mathfrak{L}^\perp$ and $\frac{\mu_\Lambda(dX)}{dX} = f_\Lambda(X)$ then

$$S(\rho) = \lim_{\Lambda \to \infty} - \int f_\Lambda(X) \lg f_\Lambda(X) \frac{dX}{V(\Lambda)} \tag{22}$$

iii) $\rho \to S(\rho)$ is affine on $E \cap \mathfrak{L}^\perp$ and upper semi-continuous in the $\mathfrak{A}$-topology over $E \cap \mathfrak{L}^\perp$.

We observe only that the proof of this theorem can be simplified with respect to the more general proof given in the paper [7] taking into account the hard cores and theorem 3. Again the formalism of the reference in question is slightly different than ours, in particular if we call $S_0(\rho)$ the functional defined in ref [7] it differs from the $S(\rho)$ introduced in theorem 4 by an additive constant $S(\rho) = S_0(\rho) + 1$.

Now the variational principle we are going to prove will be that the equilibrium state ρ is such that $S(\rho) - U(\rho) = \max$, where $U(\rho)$ is the mean energy. Hence in order to formulate it we need of the definition of $U(\rho)$ which is given through the following theorem:

THEOREM 5: Let $\Phi \in \mathfrak{B}$, the limit

$$\lim_{\Lambda \to \infty} V(\Lambda)^{-1} \int \mu_\Lambda(dX) U_\Phi(X) \tag{23}$$

exists $\forall \rho \in E \cap \mathfrak{L}^\perp$ and defines an affine functional $U_\Phi(\rho)$ on $E \cap \mathfrak{L}^\perp$, which is also continuous in the $\mathfrak{A}$-topology over $E \cap \mathfrak{L}^\perp$.

Since $U_{\Phi\Lambda}(\rho) = V(\Lambda)^{-1} \int \mu_\Lambda(dX) U_\Phi(X)$ is such that

$$U_{\Phi\Lambda}(\rho) \leq (\rho_{cp} + \varepsilon(\Lambda)) \| \Phi \|$$

it will be sufficient to prove the theorem in the case $\Phi \in \mathcal{B}_0$. Let $b < \frac{a}{4}$ and let $\theta_0(X)$ be a function which is zero if $X \cap S_b = \phi$ where S_b is the sphere with radius b and center at the origin and $\theta_0(X) = \varepsilon(x_i)$ if $x_i \in X \cap S_b$ where $\varepsilon(\xi) \geq 0$ is a continuous function with support in S_b and such that $\int_{S_b} \varepsilon(\xi) d\xi = 1$. θ_0 is a continuous function on E_a. Let us define $A_\Phi^{\theta_0} \in \mathfrak{A}$ as:

$$A_\Phi^{\theta_0}(X) = \sum_{S \subset X} \frac{\theta_0(S)\Phi(S)}{N(S)} = S\left(\frac{\theta_0 \Phi}{N}\right)(X) \tag{24}$$

where $\frac{\theta_0\Phi}{N}$ is defined as $\left(\frac{\theta_0\Phi}{N}\right)(X) = \theta_0(X)\frac{\Phi(X)}{N(X)}$ if $X \neq \phi$ and zero if $X = \phi$ and $\frac{\theta_0\Phi}{N} \in C_0(E_a^{\Lambda_0})$ if Λ_0 is a sufficiently great cube centered at the origin. Now it is easily seen that if $\Lambda \supset X \in S_b$ then:

$$\int_\Lambda d\xi (\tau_\xi A_\Phi^{\theta_0})(X) = \int_\Lambda d\xi A_\Phi^{\theta_0}(X - \xi) = U_\Phi(X) \tag{25}$$

Let $\rho \in E \cap \mathfrak{L}^\perp$, then if Λ is a cube centered at the origin and $\Lambda \supset \Lambda_0$

$$\rho(A_\Phi^{\theta_0}) = \int \mu_\Lambda(dX) A_\Phi^{\theta_0}(X)$$

but if $\tilde{\Lambda}$ is the largest cube centered at the origin such that $\tilde{\Lambda} + \Lambda_0 \subset \Lambda$ we can write $\left(\text{since } \operatorname{supp}_{X \in \tilde{\Lambda}} \tau_x \left(\frac{\theta_0\Phi}{N}\right) \subset \Lambda\right)$:

$$\rho(A_\Phi^{\theta_0}) = \frac{1}{V(\tilde{\Lambda})} \int_{\tilde{\Lambda}} d\xi \int_\Lambda \mu_\Lambda(dX) (\tau_\xi A_\Phi^{\theta_0})(X) \tag{26}$$

if now $\tilde{\tilde{\Lambda}}$ is the smallest cube centered at the origin such that $\Lambda + S_b \subset \tilde{\tilde{\Lambda}}$, we have that (26) can be written as

$$\rho(A_\Phi^{\theta_0}) = \int_{E_a^\Lambda} \mu_\Lambda(dX) \left(\int_{\tilde{\tilde{\Lambda}}} d\xi \tau_\xi A_\Phi^{\theta_0}(X) - \int_{\tilde{\tilde{\Lambda}}/\tilde{\Lambda}} d\xi \tau_\xi A_\Phi^{\theta_0}(X) \right) =$$

$$= \frac{1}{V(\tilde{\Lambda})} \int_{E_a^\Lambda} \mu_\Lambda(dX) U_\Phi(X) - \frac{1}{V(\tilde{\Lambda})} \int_{E_a^\Lambda} \mu_\Lambda(dX) \int_{\tilde{\tilde{\Lambda}}/\tilde{\Lambda}} d\xi \tau_\xi A_\Phi^{\theta_0}(X)$$

but the second term in the last equality can be majorized by:

$$\frac{V(\tilde{\tilde{\Lambda}}/\tilde{\Lambda})}{V(\tilde{\Lambda})} \| A_\Phi^{\theta_0} \| \xrightarrow[\Lambda \to \infty]{} 0$$

hence letting $\Lambda \to \infty$ we get

$$\rho(A_\Phi^{\theta_0}) = \lim_{\Lambda \to \infty} \int_{E_a^\Lambda} \mu_\Lambda(dX) \frac{U_\Phi(X)}{V(\Lambda)} = U_\Phi(\rho) \qquad (27)$$

this formula shows the existence of the limit and also that the functional $\rho \to U_\Phi(\rho)$ is $\mathfrak{A}$-continuous on $E \cap \mathfrak{L}^\perp$.

We can now discuss the variational principle:

THEOREM 5: Let $\Phi \in \mathcal{B}$ then

$$P(\Phi) = \sup_{\rho \in E \cap \mathfrak{L}^\perp} (S(\rho) - U_\Phi(\rho))$$

the proof of this theorem is exactly the same as that given in the case of a lattice system [*1*] [*11*].

This allows us to prove the following form of the Gibbs phase rule:

THEOREM 6: If $\Phi \in T$, where T is the set introduced in theorem 2;

i) the function $\rho \to S(\rho) - U_\Phi(\rho)$ on $E \cap \mathfrak{L}^\perp$ reaches its maximum P_Φ at exactly one point $\rho_\Phi \in E \cap \mathfrak{L}^\perp$,

ii) if $\Phi \in T$ and α_Φ is the functional defined by theorem 2, then

$$\alpha_\Phi(\Psi) = U_\Psi(\rho_\Phi) \qquad \forall \Psi \in \mathcal{B} \qquad (29)$$

iii) if $\Phi \in T$ the « equilibrium state » corresponding to the interaction Φ is an extremal point of $E \cap \mathfrak{L}^\perp$.

The proof of this theorem is again the same as that given by Ruelle in the case of a lattice system if we remark that the set of translates of the elements $A_\Phi^{\theta_0} \forall \theta_0$, $\forall \Phi \in \mathcal{B}_0$ is dense in the subset of $\mathfrak{A}$ determined by the functions f which are zero on the empty set.

§ 4 APPLICATIONS

In this section we study a particularly simple application of the variational principle: we shall find the pressure and the correlation functions of a one dimensional system with nearest neighbour interactions.

Let a be the radius of the hard core of a system of hard spheres on a line. Let $\Phi(x)$ be a two-body potential defined for $x \geqslant a$, continuous and zero for $x \geqslant 2a$.

Let C be the class of states of the system which have the property that the probability of finding a particle at x, knowing that there is a particle at $x_0 < x$ and that there are no particles between them, depends only on $x - x_0$ and not on the possible positions of other particles located at points $y < x_0$.

Hence a state $\rho_\sigma \in \mathrm{C}$ can be described uniquely by giving a function $\sigma(x) \geq 0$ which represents the probability for a particle to be at $x > 0$ knowing that there is a particle in 0 and that there are no particles between 0 and x. The function $\sigma(x)$ cannot be assigned arbitrarily (for instance one should have $\int \sigma(x)dx \leqslant 1$ and $\int x\sigma(x)dx < +\infty$: the first constraint expresses the fact that $\sigma(x)$ is a probability density and the second one that the specific volume in the state ρ_σ is finite).

At the thermodynamic equilibrium we expect that, as a consequence of the nearest neighbour caracter of the interaction, the equilibrium state ρ belongs to C; hence we can find it by maximizing $\mathrm{S}(\rho_\sigma) - \mathrm{U}_{[-\mu,\Phi]}(\rho_\sigma)$ over C.

To avoid convergence problems we consider only the variational problem on a smaller set $\mathrm{C}_0 \subset \mathrm{C}$ of states: i. e. for the set C_0 of states ρ_σ such that σ verifies the following inequalities

$$\begin{array}{ll} \int \sigma(x)dx \leq 1 & \int \sigma(x)\,|\lg x\,|\,dx < +\infty \\ \int x\sigma(x)dx < +\infty & \int x\sigma(x)\,|\lg x\,|\,dx < +\infty \end{array} \tag{30}$$

If [0, L] is a finite interval then the functions $f_{\mathrm{L}}(\mathrm{X})$ introduced in (22) which define the measure $\mu_{\mathrm{L}}(d\mathrm{X})$ are given, as a consequence of the physical meaning of σ, by

$$f_{\mathrm{L}}^{(n)}(\{x_1 \ldots x_n\}) = g_0(x_1)\,\sigma(x_2 - x_1)\ldots\sigma(x_n - x_{n-1})\int_{\mathrm{L}-x_n}^{\infty}\sigma(\xi)d\xi,$$
$$n \geq 1 \quad x_1 \leqslant x_2 \leqslant \ldots x_n$$
$$f_{\mathrm{L}}^{(o)}(\phi) = \int_{\mathrm{L}}^{+\infty} g_0(\xi)d\xi \tag{31}$$

where the function $g_0(x)$ is an unknown function whose meaning is to be the probability density of finding a particle at x knowing that there are no particles between 0 and x.

If we impose the normalization and compatibility conditions (18), (19), we find

$$\int_0^{+\infty} \sigma(x)dx = 1 \tag{32}$$

$$g_0(x) = \delta_\sigma \int_x^{+\infty} \sigma(\xi)d\xi \qquad \text{where} \qquad \delta_\sigma^{-1} = \int_0^{+\infty} \xi\sigma(\xi)d\xi \tag{33}$$

Then applying the definitions (22) and (23) we find

$$S(\rho_\sigma) = -\delta_\sigma \int \sigma(x) \lg \sigma(x)dx$$

$$U_{[-\mu,\Phi]}(\rho_\sigma) = \delta_\sigma \int_0^{+\infty} \sigma(x)(\Phi(x) - \mu)dx$$

where μ is the chemical potential and $\delta_\sigma = \left(\int_0^{+\infty} \xi\sigma(\xi)d\xi\right)$ is the density. The variational equations for σ give for the function σ_0 maximizing $S(\rho_\sigma) - U_{[-\mu,\Phi]}(\rho_\sigma)$ the expression:

$$\sigma_0(x) = e^{\mu-\Phi(x)}e^{-px} \tag{34}$$

where p is the value of $S(\rho_\sigma) - U_{[\mu,\Phi]}(\rho_\sigma)$ at ρ_{σ_0}.

Equation (32) then gives the equation of state

$$\int_a^{\infty} e^{\mu-\Phi(x)}e^{-px}dx = 1 \tag{35}$$

or also

$$\delta_{\sigma_0}^{-1} = \frac{\int_a^{\infty} xe^{-\Phi(x)-px}dx}{\int_a^{\infty} e^{-\Phi(x)-px}dx} \tag{36}$$

We verify easily also that $\frac{\partial p}{\partial \mu} = \delta_{\sigma_0}$. The physical interpretation of σ_0 shows that the two point correlation function is given by:

$$\rho_\sigma^{(2)}(x_2 - x_1) = \delta_{\sigma_0}[\sigma(x_2 - x_1) + (\sigma . \sigma)(x_2 - x_1) + \dots] = \delta_{\sigma_0} \sum_{k=1}^{\infty} \sigma^{(k)}(x_2 - x_1) \tag{37}$$

where $\sigma^{(k)}$ is the k^{th} power of σ in the convolution product; we observe that, as a consequence of the fact that $\sigma_0(x) = 0$, $x \leq a$, the sum appearing in (37) is a finite sum for each x.

More generally if we put

$$\tilde{\sigma}_0(x) = \sum_{k=1}^{\infty} \sigma_0^{(k)}(x) \tag{38}$$

we have

$$\rho^{(n)}(x_1 \dots x_n) = \delta_{\sigma_0}\tilde{\sigma}_0(x_2 - x_1) \dots \tilde{\sigma}_0(x_n - x_{n-1}) \tag{39}$$

From the integral representation

$$\tilde{\sigma}_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i\omega x} \frac{\sigma_0(\omega)}{\left[\frac{1-\sigma_0(\omega)}{\omega}\right]} \frac{d\omega}{\omega + i\varepsilon} \tag{40}$$

which follows from (38), if $\sigma_0(\omega) = \int_{-\infty}^{+\infty} e^{i\omega x}\sigma_0(x)dx$ we find

$$\lim_{x\to\infty} \tilde{\sigma}_0(x) = \delta_{\sigma_0} \tag{41}$$

which proves that the $\rho^{(n)}$ are clustering.

If we confront all these results with the known state equations and correlation functions [*8*], [*9*], [*10*] we find a complete agreement which is an *a posteriori* confirmation of the correctness of the procedure.

This procedure can be generalized to states with a « memory » longer than one but the results are not so simple as in the presented case (« memory » one) and the variational equations are much more complicated, but anyway these techniques could be used to obtain lower bounds for the pressure and approximate correlation functions in given models.

§ 5 REMARK ON ROTATIONAL INVARIANCE

Generally in the continuous case one requires not only translational invariance but also rotational invariance. The results obtained until now do not allow us to deduce immediately any interesting result about rotationally invariant potentials. To obtain again the results obtained in this paper for translationally invariant potentials one has to introduce the rotationally invariant potentials at the beginning by defining $\mathcal{B}$ as the set of many body potentials satisfying (6) and invariant under the euclidean group.

At this point all the results of § 2 can be obtained in the same way, one only has to note that the functional $\alpha_{\Lambda\Phi}$ introduced in formula (13) will correspond to correlation functions averaged on the euclidean group and not only on the translation group. The results of § 3 will be obtained by taking the set $E \cap \mathfrak{L}^{\perp}$ to be set of states invariant under the euclidean group.

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