Il Nuovo Cimento Vol.57-B, Pag. 208-211, 1968 11 Settembre 1968

# On the mechanical equilibrium equations

G. Gallavotti(1)

(1) *Institut des Hautes Etudes Scientifques, Bures s/Yvette*

(ricevuto 19 Giugno 1968; approvato )

The aim of this note is to prove, briefly but rigorously, that at sufficiently small activity (in fact inside the gas region) the infinite volume correlation functions of certain systems of classical identical particles satisfy the *hierarchy* of integro–differential equations which can formally be derived from the Liouville equations for finite systems (see for instance [1]).

The spirit of the proof is simply to consider a finite cubic box with periodic boundary conditions, write down the correlation functions using the grand–canonical formalism and observe that they satisfy the hierarchy of equations; then one takes the limit as the sides of the box tend to infinity and shows that every term of the equations converges to the right thing: the convergence problems arising in this process can be controlled, if the activity is sufficiently small, by using the Kirkwood-Salsburg equations.

**1:** *Conditions on the interaction.*

We shall consider only *finite range* pair potentials $\varphi(\xi)$ belonging to one of the classes $\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$ below:

$\mathcal{C}_1$: $\varphi$ is non negative, once differentiable for $|\xi| > 0$ and $|\mathrm{grad}\varphi|\, e^{-\varphi}$ is continuous on all $\mathbb{R}^d$.

$\mathcal{C}_2$: (i) $\varphi(\xi) = +\infty$ if $|\xi| < a$, $a > 0$,
(ii) $\varphi$ is once differentiable for $|\xi| > a$, bounded below and $|\mathrm{grad}\varphi|\, e^{-\varphi}$ is continuous on all $\mathbb{R}^3$.

$\mathcal{C}_3$: $\varphi$ is the sum of a positive once differentiable potential with continuous gradient and a positive type potential with continuous integrable Fourier transform and continuous gradient.

We observe that if $\varphi \in \mathcal{C}_1 \cup \mathcal{C}_2 \cup \mathcal{C}_3$ then $I(\beta) = \int |e^{-\beta\varphi(\xi)} - 1| d\xi < +\infty$ and that the class $\mathcal{C}_1 \cup \mathcal{C}_2 \cup \mathcal{C}_3$ contains all the physically interesting finite range potentials. We put the mass of the particles equal to one, so the activity will be $z = h^{-3}(2\pi\beta^{-1})^{\frac{3}{2}} e^{\beta\mu}$ where $\mu$ is the chemical potential, $h$ is Planck's constant and $\beta = (k_B T)^{-1}$.

**2.** *Finite volume correlation functions.*

Let $\Lambda$ be a finite cube considered with periodic boundary conditions and with sides of length at least twice the range of the potential. Call $\varphi^\Lambda$ the interaction potential periodized in the box $\Lambda$. Then the energy of a configuration $(p_1,q_1,\ldots,p_n,q_n)$ will be

$$E^\Lambda(p_1,q_1,\ldots,p_n,q_n)=\frac12\sum_i p_i^2+\sum_{i<j}\varphi^\Lambda(q_1,\ldots,q_n)=T(p_1,\ldots,p_n)+U^\Lambda(q_1,\ldots,q_n) \tag{1}$$

The grand canonical partition function and the correlation functions are respectively

$$\begin{aligned}Z_\Lambda=&\sum_{n\ge0}\int_{\Lambda^n}e^{\beta\, n\,\mu}e^{-\beta E^\Lambda(p_1,q_1,\ldots,p_n,q_n)}\frac{dp_1\ldots dq_n}{n!h^{3n}}=\\ =&\sum_{n\ge0}\int_{\Lambda^n}z^n\,e^{-\beta U^\Lambda(q_1,\ldots,q_n)}\frac{dq_1\ldots dq_n}{n!}\end{aligned} \tag{2}$$

$$\rho_\Lambda(p_1,q_1,\ldots,p_n,q_n)=\frac{h^{3n}}{(2\pi\beta^{-1})^{\frac32 n}}e^{-\beta T(p_1,\ldots,p_n)}\widetilde\rho_\Lambda(q_1,\ldots,q_n) \tag{3}$$

$$\widetilde\rho_\Lambda(q_1,\ldots,q_n)=\frac{1}{Z_\Lambda}\sum_{m\ge0}\int_{\Lambda^m}z^{n+m}e^{-\beta U^\Lambda(q_1,\ldots,q_n,q'_1\ldots q'_m)}\frac{dq'_1\ldots dq'_m}{m!} \tag{4}$$

**3.** *Differential equations for* $\rho_\Lambda$.

We observe that if $\varphi\in\mathcal C_1\cup\mathcal C_2\cup\mathcal C_3$ and if $\Lambda$ is a *finite* cube there is no problem in differentiating the *r.h.s.* of (4) with respect to the $q_i$'s.

If we define $W^\Lambda_q(q_1,\ldots,q_n)=\sum_{i=1}^n\varphi^\Lambda(q-q_i)$ we get, differentiating (4) and using the symmetry of $U^\Lambda(q_1,\ldots,q_n,q'_1\ldots q'_m)$ and of $dq'_1\ldots dq'_m$,

$$\begin{aligned}\mathrm{grad}_{q_1}\widetilde\rho_\Lambda(q_1,\ldots,q_n)=&-\beta\,\widetilde\rho_\Lambda(q_1,\ldots,q_n)\,\mathrm{grad}_{q_1}W^\Lambda_{q_1}(q_2,\ldots,q_n)-\\ &-\beta\int_\Lambda\widetilde\rho_\Lambda(q_1,\ldots,q_nq')\mathrm{grad}_{q_1}\varphi^\Lambda(q_1-q')\,dq'\end{aligned} \tag{5}$$

and these equations are one of the forms of the Bogoliubov equations for the equilibrium correlation functions, [1].

**4.** *The infinite volume limit.*

We now want to take the limit as $\Lambda\to\infty$ in both sides of (5): this will be possible if we can prove the existence of the $\lim_{\Lambda\to\infty}\widetilde\rho_\Lambda(q_1,\ldots,q_n,q')$, of an upper bound on

$$\widetilde\rho_\Lambda(q_1,\ldots,q_n)\,\mathrm{grad}_{q_1}W^\Lambda_{q_1}(q_2,\ldots,q_n)$$

which holds uniformly as $q_1,\ldots,q_n$ vary in a bounded region (at fixed $n$) and of an integrable function of $q'$ which majorizes $|\mathrm{grad}_{q_1}\varphi^\Lambda(q_1-q')\widetilde\rho(q_1,\ldots,q_n,q')|$ uniformly in $q_1,\ldots,q_n$ as $q_1,\ldots,q_n$ vary inside a bounded region (at fixed $n$).

The simplest way to see why these convergence and boundedness properties allow us to take the limit on both sides of (5) is to integrate this equation evaluated replacing $q_1$

by $q$ with respect to $q$ from $q_1$ to $q_2$ along a straight path of length $\eta = |q_2 - q_1|$, to use the theorem on the exchange of limits and integrals (which holds as a consequence of the mentioned properties) and to let $\eta \to 0$ after division by $\eta$.

The above properties can be obtained using some known intermediate results about the convergence of the Mayer expansions.

Let $z < e^{-2\beta B-1} I(\beta)^{-1}$ where $B$ is a stability bound, $U^\Lambda(q_1, \ldots, q_n) \geq -n\,B$ and $I(\beta)$ has been defined above ($B$ exists if $\varphi \in \mathcal{C}_1 \cup \mathcal{C}_2 \cup \mathcal{C}_3$), then the following result holds (and is a consequence of the Kirkwood-Salsburg equations with the obvious modifications due to the periodicity of the boundary conditions), [2],[3]:

(1) The limit $\lim_{\Lambda\to\infty} \widetilde{\rho}_\Lambda(q_1, \ldots, q_n) = \widetilde{\rho}(q_1, \ldots, q_n)$ exists and is uniform in the $q_i$'s if the $q_i$'s are contained in a bounded region at fixed $n$).

(2) $\widetilde{\rho}_\Lambda(q_1, \ldots, q_n) \leq \xi^n$ for some $\xi > 0$.

Now, if $z < e^{-2\beta B-1} I(\beta)^{-1}$, the bounds we need for

$$\widetilde{\rho}_\Lambda(q_1, \ldots, q_n)\mathrm{grad}_{q_1} W_{q_1}(q_2, \ldots, q_n), \quad \text{and } |\widetilde{\rho}(q_1, \ldots, q_n, q')\,\mathrm{grad}_{q_1} \varphi^\Lambda(q_1 - q')|$$

are an obvious consequence of property (2) if $\varphi \in \mathcal{C}_3$; if $\varphi \in \mathcal{C}_1 \cup \mathcal{C}_2$ one still obtains these bounds (when $z < e^{-2\beta B-1} I(\beta)^{-1}$) by taking into account, together with (2), the conditions imposed on $(\mathrm{grad}\varphi)\, e^{-\varphi}$ and the following bounds, [3], which hold if $\varphi \in \mathcal{C}_1 \cup \mathcal{C}_2$

$$\widetilde{\rho}_\Lambda(q_1, \ldots, q_n) \leq C^n e^{-\beta\, U^\Lambda(q_1, \ldots, q_n)} \tag{6}$$

where $C > 0$ is a suitable constant.

We are now allowed to take the limit as $\Lambda \to \infty$ in both sides of (5) and deduce, always in the region $z < e^{-2\beta B-1} I(\beta)^{-1}$,

$$\begin{aligned} \mathrm{grad}_{q_1} \widetilde{\rho}(q_1, \ldots, q_n) = &- \beta\, \widetilde{\rho}(q_1, \ldots, q_n)\, \mathrm{grad}_{q_1} W_{q_1}(q_2, \ldots, q_n) - \\ &- \beta \int \widetilde{\rho}(q_1, \ldots, q_n, q')\mathrm{grad}_{q_1} \varphi(q_1 - q')\, dq' \end{aligned} \tag{7}$$

This equation is a form of the infinite volume *hierarchy* of equations, [2], and it is immediately verified that if (7) holds the functions

$$\rho(p_1, \ldots, p_n, q_1, \ldots, q_n) = \frac{h^{3n}}{(2\pi\beta^{-1})^{\frac{3}{2}n}} e^{-\beta T(p_1, \ldots, p_n)} \widetilde{\rho}(q_1, \ldots, q_n)$$

satisfy the Bogoliubov equations in the stationary case:

$$\begin{aligned} &\big\{E(p_1, q_1, \ldots, p_n, q_n); \rho(p_1, q_1, \ldots, p_n, q_n)\big\} + \\ &+ \int \big\{W_\xi(q_1, \ldots, q_n); \rho(q_1, \ldots, q_n, \xi, p_1, \ldots, p_n, \pi)\big\} \frac{d\xi\, d\pi}{h^3} = 0 \end{aligned} \tag{8}$$

where $\{\cdot;\cdot\}$ is the Poisson bracket (the (7) is the form to which (8) reduces if it is evaluated at $p_1 \neq 0$, $p_i = 0$ for $i \neq 1$; and vice versa (7) implies (8) if the momentum distribution of the correlations is Maxwellian at inverse temperature $\beta$).

Since the condition $z < e^{-2\beta B-1} I(\beta)^{-1}$ implies the convergence of the Mayer and the virial series and also strong factorization properties of the correlation functions, [2], one sees that the region $(z, \beta)$ for which (8) has been proved is inside the gaseous phase.

I am indebted to O. Lanford, S. Miracle-Solé and D. Ruelle for comments and reading the manuscript. I am also indebted to L. Motchane for his kind hospitality at the I.H.E.S and to C.N.R.S. for partial financial support.

## References

[1] R.M. Lewis: Journal of Mathematical Physics, **2**, 222, 1961.
[2] D. Ruelle: Annals of Physics, **25**, 109, 1963.
[3] J. Groeneveld: Physics Letters, **3**, 50, 1962.