Archives

Ref. TH. 797

ANALYTICITY PROPERTIES OF A LATTICE GAS

G. Gallavotti and S. Miracle-Sole
Institut des Hautes Etudes Scientifiques
91 - Bures sur Yvette, France

and

Derek W. Robinson
CERN - Geneva

A B S T R A C T

Analyticity properties of the pressure, and the correlation functions, in the chemical potential, temperature, and the interaction potentials are given for a system of classical particles on a lattice interacting through many-body potentials.

67/858/5 - TH. 797
22 June 1967

The purpose of this note is to give certain analyticity properties of a system of classical particles on a lattice interacting through many-body potentials. We prove analyticity of the pressure, and the correlation functions, in the chemical potential, temperature, and the interaction potentials. Our methods are those first developed by Dobrushin et al.[1] for two-body potentials. Results are obtained by combination of two features. Firstly we use the structure of an integral equation for the correlation functions and secondly we utilise a symmetry property of the pressure as a functional of the interaction potentials. Physically these properties are of interest because it is known that for the values of the thermodynamic parameters in the domain of analyticity the lattice gas is in a single phase state. Thus such results delimit the regions where phase transitions are possible.

Let Z^ν be a ν dimensional lattice and assume that at each lattice point there can be either 0 or 1 particles and hence a finite configuration X of the system is specified by a finite subset $X \subset Z^\nu$. We suppose that the particles interact through symmetric translationally invariant many-body potentials $\Phi^{(k)}(x_1,\dots,x_k)$ and we regard these potentials as a function Φ on the finite subsets X, of Z^ν, defined by $\Phi(X) = \Phi^{(k)}(x_1,\dots,x_k)$ if $X = \{x_1,\dots,x_k\}$. In what follows we consider only those interactions Φ which involve a finite number of particles and which are such that

$$\|\Phi\| = \sum_{0 \in S \subset Z^\nu} |\Phi(S)| < +\infty$$

We denote this set of interactions by $\mathcal{B}_0$ and we use the notation $\Phi = (\Phi^{(1)}, \Phi')$ where Φ' is the interaction obtained from Φ by setting the one particle potential $\Phi^{(1)}$ equal to zero. The one-particle potential can be interpreted as $-\mu$, where μ is the chemical potential. The energy $U_\Phi(X)$ of a finite configuration of particles on the subset $X \subset Z^\nu$ with interaction Φ is

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

If $x_1 \in X$ we denote by $X^{(1)}$ the set $X/\{x_1\}$ obtained from X by subtracting the point x_1 and we introduce the definition

$$U_{\Phi}^{1}(X) = \sum_{x_1 \in S \subset X} \Phi(S)$$

To complete our notation let $\mathcal{E}$ be the Banach space of bounded functions on the finite non-empty sets of Z^{ν} equipped with the sup-norm topology and, denoting by $N(X)$ the number of points of the configuration X, define $\alpha \in \mathcal{E}$ by $\alpha(X) = 1$ if $N(X) = 1$ and $\alpha(X) = 0$ if $N(X) > 1$.

Integral Equations

The correlation functions $\rho_{\beta,\Phi}$ (β is the inverse temperature) of the classical lattice system can be regarded as elements of the space $\mathcal{E}$ satisfying the following equations (for details, cf. Ref. [2]).

$$\rho_{\beta,\Phi} = \frac{e^{-\beta\Phi^{(1)}}}{1+e^{-\beta\Phi^{(1)}}}\,\alpha + \mathcal{H}_{\beta,\Phi}\,\rho_{\beta,\Phi}$$

where the operator $\mathcal{H}_{\beta,\Phi}$ on $\mathcal{E}$ is defined by

$$(\mathcal{H}_{\beta,\Phi}\varphi)(X) = \frac{e^{-U^{1}_{\beta\Phi}(X)}}{1+e^{-U^{1}_{\beta\Phi}(X)}}\left[\varphi(X^{(1)}) + \sum_{\substack{T\neq\emptyset\\ T\cap X=\emptyset}} K_{\beta\Phi'}(X,T)\big(\varphi(X^{(1)}\cup T)-\varphi(X\cup T)\big)\right]$$

for all $\varphi \in \mathcal{E}$, and the kernel $K_{\beta\Phi'}(X,T)$ has the property that for fixed X

$$\sum_{\substack{T\cap X=\emptyset\\ T\neq\emptyset}} |K_{\beta\Phi'}(X,T)| \leq \left[\exp\left(e^{\beta\|\Phi'\|}-1\right)-1\right]$$

[$\varphi(X^{(1)})$ has to be interpreted as zero if $N(X) = 1$]. It follows that the norm on $\mathcal{E}$ of the operator $\mathcal{H}_{\beta,\Phi}$ is majorized by

$$\|\mathcal{H}_{\beta,\Phi}\| \leq \frac{e^{-\beta\Phi^{(1)}}e^{\beta\|\Phi'\|}}{1+e^{-\beta\Phi^{(1)}}e^{\beta\|\Phi'\|}}\left[2\exp\left(e^{\beta\|\Phi'\|}-1\right)-1\right]$$

Thus we see that there exists a function $f(\xi)$ defined on the positive axis, $f(\xi) = -\log 2e^{\xi}\left[\exp(e^{\xi}-1)-1\right]$, such that

$$-\beta\Phi^{(1)} < f(\beta\|\Phi'\|)$$

implies that $\|\mathcal{H}_{\beta,\Phi}\| < 1$. Note that $f(\xi)$ satisfies

$$\lim_{\xi\to 0} f(\xi) = +\infty \tag{1}$$

Now with the same methods as Refs. [2),3)] it is possible to prove that if $\|\mathcal{H}_{\beta_0,\Phi_0}\| < 1$ then the correlation functions $\rho_{\beta,\Phi} \in \mathcal{E}$ are an analytic vector for β, Φ around β_0, Φ_0. Explicitly we have that for n arbitrary vectors $\Psi_1, \Psi_2, \ldots, \Psi_n \in \mathcal{B}_0$ the vector

$$\rho_{\beta,\, \Phi + \sum_{i=1}^{n} \lambda_i \Psi_i}$$

is an analytic vector in $(\beta, \lambda_1, \ldots, \lambda_n)$ around $(\beta_0, 0, \ldots, 0)$. The same analyticity property can be proven for the pressure $P(\beta, \Phi)$.

Symmetry Property

We next prove a symmetry property for the pressure $P(\beta, \Phi)$. Let the operator $\mathcal{L} : \mathcal{B}_0 \to \mathcal{B}_0$ be defined by

$$(\mathcal{L}\Phi)(X) = (-1)^{N(X)} \sum_{S\supset X} \Phi(S) \tag{2}$$

(Note that $\mathcal{L}^2 = 1$) and then by direct calculation we can verify that

$$U_\Phi(X) - U_{\mathcal{L}\Phi}(\Lambda/X) = N(\Lambda)A_\Phi - N(\Lambda/X)(A_\Phi + A_{\mathcal{L}\Phi}) + \sum\nolimits_\Lambda(X) \quad \text{if } X\subset\Lambda \tag{3}$$

where Λ is a finite subset of Z^ν, A_Φ is defined by

$$A_\Phi = \sum_{0\in S\subset Z^\nu} \frac{\Phi(S)}{N(S)} \tag{4}$$

and $\sum_\Lambda(X)$ is a surface term, i.e., $\sum_\Lambda(X)$ is such that

$$\lim_{\Lambda\to\infty} \frac{1}{V(\Lambda)} \sup_{X\subset\Lambda} \left|\sum\nolimits_\Lambda(X)\right| = 0$$

From definitions (2) and (4) it readily follows that $A_\Phi + A_{\mathcal{L}\Phi} = 0$ and thus from (3) we deduce that the pressure $P(\beta, \Phi)$, defined by

$$P(\beta,\Phi) = \lim_{\Lambda\to\infty} \frac{1}{V(\Lambda)} \log \sum_{X\subset\Lambda} e^{-\beta U_\Phi(X)}$$

has the symmetry property

$$P(\beta,\Phi) + \frac{1}{2} A_{\beta\Phi} = P(\beta,\mathcal{L}\Phi) + \frac{1}{2} A_{\beta\mathcal{L}\Phi} \tag{5}$$

This is the many-body generalization of a well-known formula (cf. Ref.[4]).

Now if $\|\mathcal{H}_{\beta_0,\mathcal{L}\Phi_0}\| < 1$ we have deduced that both $P(\beta,\mathcal{L}\Phi)$ and $\rho_{\beta,\mathcal{L}\Phi}$ are analytic in β and $\Phi \in \mathcal{B}_0$ around β_0, Φ_0. Therefore (5) implies that under the same condition $P(\beta,\Phi)$ and $\rho_{\beta,\Phi}$ are also analytic in β, $\Phi \in \mathcal{B}_0$ around β_0, Φ_0. Hence we have deduced that $P(\beta,\Phi)$ and $\rho_{\beta,\Phi}$ are analytic around β, Φ if one of the two following inequalities is satisfied

$$\left.\begin{aligned} -\beta\Phi^{(1)} &< f(\beta\|\Phi'\|) \\ -\beta(\mathcal{L}\Phi)^{(1)} &< f(\beta\|(\mathcal{L}\Phi)'\|) \end{aligned}\right\} \tag{6}$$

However, from (2) we find that

$$(\mathcal{L}\Phi)^{(1)} = -\Phi^{(1)} - \sum_{0\in S} \Phi'(S) \tag{7}$$

and hence we see that if

$$-f(\beta_0\|\Phi_0'\|) - f(\beta_0\|(\mathcal{L}\Phi_0)'\|) < -\beta_0 \sum_{0\in S} \Phi_0'(S) \tag{8}$$

we have analyticity of the pressure and the correlation functions in β around β_0, in Φ' around Φ_0', and for all values of $\Phi^{(1)}$. But, due to (1) this last inequality (7) must surely be satisfied if β_0 is sufficiently small.

A simple explicit example which illustrates the nature of the analyticity domain obtained above is given by choosing $\Phi^{(2)} \geqslant 0$ and $\Phi^{(k)} = 0$ for $k > 2$. In this case we find from (6) and (7) that we have analyticity if either of the inequalities

$$0 \leqslant z < \tfrac{1}{2} e^{-\beta C} \left[\exp(e^{\beta C} - 1) - 1 \right]^{-1}$$

$$z > 2\, e^{2\beta C} \left[\exp(e^{\beta C} - 1) - 1 \right]$$

is satisfied, where $z = \exp(-\beta \Phi^{(1)})$ is the activity and

$$C = \| \Phi^{(2)} \| = \sum_{0 \in S} \Phi^{(2)}(S)$$

Let us conclude by observing that a property similar to (5) follows for the correlation functions. To deduce this property introduce for any X an interaction $\chi_X \in \mathcal{B}_0$ by the definition

$$\chi_X(S) = 0 \quad \text{if } \nexists\, a \in Z^\nu \text{ such that } X + a = S$$

$$\chi_X(S) = 1 \quad \text{if } \exists\, a \in Z^\nu \text{ such that } X + a = S$$

and then we have

$$\rho_{\beta,\Phi}(X) = - \left. \frac{d P(\beta, \Phi + \lambda \chi_X)}{\beta\, d\lambda} \right|_{\lambda = 0}$$

From this equation and

$$\mathcal{L} \chi_X = \sum_{\substack{S \subset X \\ S \neq \emptyset}} (-1)^{N(S)} \chi_S$$

we deduce the property

$$\rho_{\beta,\Phi}(X) = \sum_{S \subset X} (-1)^{N(S)} \rho_{\beta, \mathcal{L}\Phi}(S)$$

where we take $\quad , \; (\emptyset) \equiv 1$.

Acknowledgements

Two of us (G.G. and S.M-S.) are indebted firstly to D. Ruelle and J.L. Lebowitz for helpful discussions and to the latter for an account of the work of Dobrushin et al., secondly to Professor L. Motchane for his kind hospitality at the I.H.E.S., and finally, to Professor J. Prentki for his hospitality at CERN.

References

1) - R.L. Dobrushin et al. (to be published).

2) - G. Gallavotti and S. Miracle-Sole - "Correlation Functions of a Lattice System" I.H.E.S. Preprint (1967).

3) - D. Ruelle - Ann.Phys. 25, 109 (1963).

4) - C.N. Yang and T.D. Lee - Phys.Rev. 87, 410 (1952).