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Stable Potentials I

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Abstract. We discuss a conjecture of Ruelle concerning *stable* potentials on a group. For the groups $\boldsymbol{Z}_2, \boldsymbol{Z}_3, \boldsymbol{Z}_4$, and $\boldsymbol{Z}_6$ any stable potential can be written as the sum of a non-negative function and a function of non-negative type. This is not true for the groups $\boldsymbol{Z}_k$ (k odd, $\geqq 5$). For the Euclidean group $\boldsymbol{R}^\nu$ the question is open.

§ 1

The following theorem is due to David Ruelle [1]. Let φ be a real valued, even, upper semicontinuous function on a Euclidean space $\boldsymbol{E}$. Let

$$\begin{cases} U_1 = 0 \\ U_n = \sum_{1 \leqq i < j \leqq n} \varphi(x_i - x_j) \end{cases} \qquad (n = 2, 3, \ldots) \tag{1}$$

The following conditions are equivalent:

$$\text{(a)} \quad \sum_{i=1}^{n} \sum_{j=1}^{n} \varphi(x_i - x_j) \geqq 0 \tag{2}$$

for all $n \geqq 1$ and all $(x_1, \ldots, x_n)$ in $\boldsymbol{E}^n$.

(b) There is a constant B such that

$$U_n(x_1, \ldots, x_n) \geqq -nB \tag{3}$$

for all $n \geqq 1$ and all $(x_1, \ldots, x_n)$ in $\boldsymbol{E}^n$.

(c) For all bounded Lebesgue measurable sets $\Lambda \subset \boldsymbol{E}$ and all positive numbers z and β the series

$$\Xi = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \int_\Lambda dx_1 \ldots \int_\Lambda dx_n e^{-\beta U_n} \tag{4}$$

converges.

The importance of this theorem is that the quantity Ξ has a fundamental significance in the statistical mechanics of classical systems in thermal equilibrium (it is the Grand Partition Function of Gibbs). φ is called the two-particle potential function, or simply the potential,

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and the equivalent conditions (a) and (b) are referred to as *stability*. We shall denote the class of stable potentials by $\mathcal{S}$. It is easy to see that the following condition is also equivalent to stability:

(a′) For all n, all $x_1, x_2, \ldots, x_n$ in $\boldsymbol{E}$ and all $\lambda_1, \lambda_2, \ldots, \lambda_n \geqq 0$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \varphi(x_i - x_j)\, \lambda_i \lambda_j \geqq 0 . \tag{5}$$

In this form the condition is reminiscent of the property of being of non-negative type. φ is of non-negative type if for all n, all $(x_1, x_2, \ldots, x_n)$ in $\boldsymbol{E}^n$, and all complex $\lambda_1, \lambda_2, \ldots, \lambda_n$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \varphi(x_i - x_j)\, \bar{\lambda}_i \lambda_j \geqq 0 . \tag{6}$$

Evidently a function of non-negative type belongs to $\mathcal{S}$. Furthermore, every function of the form

$$\varphi(x) = \psi(x) + \chi(x) , \tag{7}$$

with ψ of non-negative type and $\chi(x) \geqq 0$ for all x in $\boldsymbol{E}$, belongs to $\mathcal{S}$. We write this

$$\mathcal{B} + \mathcal{P} \subseteqq \mathcal{S} \tag{8}$$

where $\mathcal{P}$ denotes the class of non-negative valued functions and $\mathcal{B}$ those of non-negative type. Ruelle has speculated [2] that perhaps equality holds in (8) so that every stable potential (subject perhaps to general smoothness assumptions) is of the form (7). If this be true, then the possibility of the decomposition (7) offers a further characterization of the functions possessing properties (a), (b), and (c) of Ruelle's theorem. The purpose of this paper is to examine the status of this conjecture.

§ 2

We take the point of view that the natural mathematical setting of this problem is as follows. Let $\boldsymbol{G}$ be an Abelian group and let $\mathcal{L}$ be the real linear space of real-valued, even, functions φ on $\boldsymbol{G}$,

$$\varphi(x) = \varphi(-x) \quad \text{for all} \quad x \in \boldsymbol{G} . \tag{9}$$

Let

$$\mathcal{P} = \{\varphi \in \mathcal{L} : \varphi(x) \geqq 0 \quad \text{for all} \quad x \in \boldsymbol{G}\} \tag{10}$$

and

$$\mathcal{B} = \left\{ \varphi \in \mathcal{L} : \sum_{i=1}^{n} \sum_{j=1}^{n} \varphi(x_i - x_j)\, \bar{z}_i z_j \geqq 0 \right. \\ \left. \text{for all} \quad x_1, \ldots, x_n \in \boldsymbol{G} \quad \text{and all complex} \quad z_1, \ldots, z_n \right\} . \tag{11}$$

Furthermore, let

$$\mathcal{S} = \left\{ \varphi \in \mathcal{L} : \sum_{i=1}^{n} \sum_{j=1}^{n} \varphi(x_i - x_j)\, \lambda_i \lambda_j \geqq 0 \right. \\ \left. \text{for all} \quad x_1, \ldots, x_n \in \boldsymbol{G} \quad \text{and all} \quad \lambda_1, \ldots, \lambda_n \geqq 0 \right\}. \tag{12}$$

The inclusion (8) holds, and we are concerned with the question whether in general equality is the case or not.

We examine this question for the simplest special case, namely for the group $\boldsymbol{G} = \boldsymbol{Z}_n$ ($n \geqq 2$), the group of integers under addition modulo n. We let the elements of $\boldsymbol{Z}_n$ be denoted by k, l, m, etc. and write φ_m for the value of a function φ on $\boldsymbol{Z}_n$ at the point m. We use $+$ for the group operation in $\boldsymbol{Z}_n$, but this ambiguous notation will not cause misunderstanding.

The sets $\mathcal{P}, \mathcal{B}, \mathcal{S} \subset \mathcal{L}$ form *convex cones*. That is, if φ and ψ are two functions belonging to them, so does $\alpha\varphi + \beta\psi$ for any $\alpha, \beta \geqq 0$. Furthermore, if we view $\mathcal{L}$ as a real finite dimensional Euclidean space with its usual topology, these cones are topologically closed. A closed convex cone $\mathcal{T}^+$ may be associated with any subset $\mathcal{T} \subseteqq \mathcal{L}$ as follows

$$\mathcal{T}^+ = \left\{ f \in \mathcal{L} : \sum_{m \in \boldsymbol{Z}_n} f_m \varphi_m \geqq 0 \quad \text{for all} \quad \varphi \in \mathcal{T} \right\}. \tag{13}$$

$\mathcal{T}^+$ is called the *polar cone* of $\mathcal{T}$. The operation of taking the polar cone reverses set-inclusion relations. Furthermore $\mathcal{T}^{++}$ is the closed convex hull of $\mathcal{T}$, i.e. the smallest closed convex cone containing $\mathcal{T}$. In particular, if $\mathcal{T}$ is already a closed convex cone then $\mathcal{T} = \mathcal{T}^{++}$. For proof of these and other simple propositions concerning convex cones see [3].

The cones $\mathcal{P}$ and $\mathcal{B}$ are self-dual

$$\mathcal{P} = \mathcal{P}^+ \tag{14}$$

and

$$\mathcal{B} = \mathcal{B}^+ . \tag{15}$$

The first of these relations is obvious from the definition. The second is shown as follows. For every $\varphi \in \mathcal{L}$ we introduce its Fourier transform $\hat{\varphi} \in \mathcal{L}$ by

$$\hat{\varphi}_m = \frac{1}{n} \sum_{k \in \boldsymbol{Z}_n} \varphi_k e^{-\frac{2\pi i}{n} km} = \frac{1}{n} \sum_{k \in \boldsymbol{Z}_n} \varphi_k \cos\left(\frac{2\pi}{n} km\right), \tag{16}$$

so that conversely

$$\varphi_m = \sum_{k \in \boldsymbol{Z}n} \hat{\varphi}_k \cos\left(\frac{2\pi}{n} km\right). \tag{17}$$

By a famous theorem of Bochner the set $\mathcal{B}$ may be characterized as

$$\mathcal{B} = \{\varphi \in \mathcal{L} : \hat{\varphi} \in \mathcal{P}\} . \tag{18}$$

On the other hand the Fourier transformation (16) preserves the inner product

$$\sum_{m \in \mathbf{Z}_n} \varphi_m \psi_m = \sum_{m \in \mathbf{Z}_n} \hat{\varphi}_m \hat{\psi}_m \tag{19}$$

for any $\varphi, \psi \in \mathscr{L}$. From this remark, and from (18) and (14) we conclude (15).

The dual cone $\mathscr{S}^+$ may be obtained as follows. According to the definition $\varphi \in \mathscr{S}$ if and only if

$$\sum_{m \in \mathbf{Z}_n} \varphi_m \sum_{k \in \mathbf{Z}_n} \lambda_{m+k} \lambda_k \geqq 0 \tag{20}$$

for all λ with $\lambda_k \geqq 0$ $(k \in \mathbf{Z}_n)$. Let then

$$\mathscr{R} = \left\{ \mu \in \mathscr{L} : \mu_m = \sum_{k \in \mathbf{Z}_n} \lambda_{m+k} \lambda_k, \ \lambda_k \geqq 0 \quad \text{for all} \quad k \in \mathbf{Z}_n \right\}; \tag{21}$$

then we have

$$\mathscr{S} = \mathscr{R}^+ . \tag{22}$$

Taking the dual

$$\mathscr{S}^+ = \mathscr{R}^{++}, \tag{23}$$

i.e., $\mathscr{S}^+$ is the closed convex hull of the set $\mathscr{R}$.

The inclusion (8) is equivalent to its dual which, in view of (14) and (15) reads

$$\mathscr{S}^+ \subseteqq \mathscr{P} \cap \mathscr{B} . \tag{24}$$

Moreover, equality holds if and only if equality holds in (8). Thus we have reduced our problem to the following question: Is there a common element of $\mathscr{P}$ and $\mathscr{B}$ not in $\mathscr{S}^+$?

§ 3

The simplest case is $n = 2$. The group $\mathbf{Z}_2$ has two elements 0, 1. We have then

$$\mathscr{P} = \{\varphi : \varphi_0 \geqq 0, \varphi_1 \geqq 0\} \tag{25}$$

and

$$\mathscr{B} = \{\varphi : \hat{\varphi}_0 = \tfrac{1}{2}(\varphi_0 + \varphi_1) \geqq 0, \hat{\varphi}_1 = \tfrac{1}{2}(\varphi_0 - \varphi_1) \geqq 0\} . \tag{26}$$

Therefore any element of $\mathscr{P} \cap \mathscr{B}$ satisfies

$$0 \leqq \varphi_1 \leqq \varphi_0 . \tag{27}$$

We also have in this case

$$\mathscr{R} = \{\varphi : \varphi_0 = \lambda_0^2 + \lambda_1^2, \varphi_1 = 2\lambda_0 \lambda_1 \quad \text{for some} \quad \lambda_0, \lambda_1 \geqq 0\} . \tag{28}$$

This shows that

$$\mathscr{P} \cap \mathscr{B} \subseteqq \mathscr{R} ; \tag{29}$$

because for a φ satisfying (27) it suffices to take

$$\begin{cases} \lambda_0 = \frac{1}{2}(\sqrt{\varphi_0+\varphi_1} + \sqrt{\varphi_0-\varphi_1}) \\ \lambda_1 = \frac{1}{2}(\sqrt{\varphi_0+\varphi_1} - \sqrt{\varphi_0-\varphi_1}) \end{cases} \tag{30}$$

which shows $\varphi \in \mathcal{R}$. But (29) implies

$$\mathcal{P} \cap \mathcal{B} \subseteqq \mathcal{R}^{++} = \mathcal{S}^{+}, \tag{31}$$

so that from (24) we get

$$\mathcal{P} \cap \mathcal{B} = \mathcal{S}^{+} \tag{32}$$

and its dual

$$\mathcal{P} + \mathcal{B} = \mathcal{S}. \tag{33}$$

Thus for $\boldsymbol{Z}_2$ every stable function is the sum of a non-negative function and a function of non-negative type.

We have looked at $\boldsymbol{Z}_3$ and $\boldsymbol{Z}_4$ in a similar way and found that the same conclusion holds[1].

Let us now consider $\boldsymbol{Z}_5$. A real even function φ is given here by the three real numbers φ_0, $\varphi_1 = \varphi_4$ and $\varphi_2 = \varphi_3$. $\varphi \in \mathcal{P}$ if and only if $\varphi_0, \varphi_1, \varphi_2 \geqq 0$. Using the notation

$$c_j = \cos\left(\frac{2\pi}{5} j\right) \tag{34}$$

we have the following necessary and sufficient conditions for $\varphi \in \mathcal{B}$

$$\begin{cases} \varphi_0 + 2\varphi_1 + 2\varphi_2 \geqq 0, \\ \varphi_0 + 2c_1\varphi_1 + 2c_2\varphi_2 \geqq 0, \\ \varphi_0 + 2c_2\varphi_1 + 2c_1\varphi_2 \geqq 0. \end{cases} \tag{35}$$

Elements $\mu \in \mathcal{R}$ have the form

$$\begin{cases} \mu_0 = \lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2, \\ \mu_1 = \lambda_0\lambda_1 + \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_4 + \lambda_4\lambda_0, \\ \mu_2 = \lambda_0\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_4 + \lambda_3\lambda_0 + \lambda_4\lambda_1, \end{cases} \tag{36}$$

where $\lambda_0, \lambda_1, \ldots, \lambda_4 \geqq 0$. Suppose now that an element $\varphi \in \mathcal{R}^{++} = \mathcal{S}^{+}$ has the property that $\varphi_2 = 0$. Since φ is a linear combination, with positive coefficients, of elements $\mu \in \mathcal{R}$ we conclude that for these μ it must also be true that $\mu_2 = 0$. An inspection of (36) reveals that, for such μ, $\lambda_k = 0$ for at least three values of k successive in the cyclical order. The form of such μ is then

$$\begin{cases} \mu_0 = \lambda_k^2 + \lambda_{k+1}^2, \\ \mu_1 = \lambda_k\lambda_{k+1}, \\ \mu_2 = 0, \end{cases} \tag{37}$$

[1] Explicit calculation in the Appendix.

and so

$$\mu_0 \geqq 2\mu_1 . \tag{38}$$

But this inequality is preserved by linear combination with positive coefficients. This shows that for $\varphi \in \mathscr{S}^+$ such that $\varphi_2 = 0$ the inequality

$$\varphi_0 \geqq 2\varphi_1 \tag{39}$$

holds. It is now easy to see that $\varphi \in \mathscr{P} \cap \mathscr{B}$ exists such that $\varphi \notin \mathscr{S}^+$. Indeed if $\varphi_0, \varphi_1 \geqq 0$ but $\varphi_2 = 0$, and

$$-2c_2\varphi_1 \leqq \varphi_0 < 2\varphi_1 \tag{40}$$

then (39) does not hold but (35) does. This shows that for $\boldsymbol{Z}_5$ the strict inclusion

$$\mathscr{P} \cap \mathscr{B} \supset \mathscr{S}^+, \tag{41}$$

and therefore

$$\mathscr{P} + \mathscr{B} \subset \mathscr{S} \tag{42}$$

holds.

This argument generalizes in the natural manner to $\boldsymbol{Z}_n$ for odd $n \geqq 5$. Thus we have found that on $\boldsymbol{Z}_n$ (odd $n \geqq 5$) *there exist stable functions which are not decomposable into the sum of a non-negative function and one of non-negative type.*

For $\boldsymbol{Z}_6$, on the other hand, it can be shown that such a decomposition is always possible. The question for the group of physical interest, the ν-dimensional Euclidean group $\boldsymbol{R}^\nu$, is open.

Appendix

We show here that for $\boldsymbol{Z}_3$ and $\boldsymbol{Z}_4$ Ruelle's conjecture holds, i.e., that

$$\mathscr{P} \cap \mathscr{B} \subseteqq \mathscr{S}^+ .$$

In the case of $\boldsymbol{Z}_3$

$$\mathscr{P} = \{\varphi : \varphi_0, \varphi_1 \geqq 0\}$$

$$\mathscr{B} = \{\varphi : \hat{\varphi}_0 = \tfrac{1}{3}(\varphi_0 + 2\varphi_1) \geqq 0, \hat{\varphi}_1 = \tfrac{1}{3}(\varphi_0 - \sqrt{3}\varphi_1) \geqq 0\}$$

so that

$$\mathscr{P} \cap \mathscr{B} = \{\varphi : 0 \leqq \sqrt{3}\varphi_1 \leqq \varphi_0\} .$$

Furthermore,

$$\mathscr{R} = \{\varphi : \varphi_0 = \lambda_0^2 + \lambda_1^2 + \lambda_2^2,\ \varphi_1 = \lambda_0\lambda_1 + \lambda_1\lambda_2 + \lambda_2\lambda_0, \text{ with } \lambda_0, \lambda_1, \lambda_2 \geqq 0\} .$$

Given $\varphi \in \mathscr{P} \cap \mathscr{B}$, we take then

$$\lambda_0 = \tfrac{1}{3}(\sqrt{\varphi_0 + 2\varphi_1} + 2\sqrt{\varphi_0 - \varphi_1}),$$

$$\lambda_1 = \lambda_2 = \tfrac{1}{3}(\sqrt{\varphi_0 + 2\varphi_1} - \sqrt{\varphi_0 - \varphi_1}) .$$

Then $\lambda_0, \lambda_1, \lambda_2 \geqq 0$ and so

$$\varphi \in \mathscr{R} \subseteqq \mathscr{R}^{++} = \mathscr{S}^{+}.$$

The analogous conditions for $\boldsymbol{Z}_4$ are

$$\mathscr{P} = \{\varphi : \varphi_0, \varphi_1, \varphi_2 \geqq 0\},$$

$$\mathscr{B} = \{\varphi : \hat{\varphi}_0 = \tfrac{1}{4}(\varphi_0 + 2\varphi_1 + \varphi_2) \geqq 0, \hat{\varphi}_1 = \tfrac{1}{4}(\varphi_0 - \varphi_2) \geqq 0, \\ \hat{\varphi}_2 = \tfrac{1}{4}(\varphi_0 - 2\varphi_1 + \varphi_2) \geqq 0\},$$

$$\mathscr{P} \cap \mathscr{B} = \{\varphi : \varphi_0 \geqq \varphi_2 \geqq 0, \varphi_0 + \varphi_2 \geqq 2\varphi_1 \geqq 0\},$$

$$\mathscr{R} = \{\varphi : \varphi_0 = \lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2, \varphi_1 = \varphi_3 = \lambda_0\lambda_1 + \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_0, \\ \varphi_2 = 2\lambda_0\lambda_2 + 2\lambda_1\lambda_3, \quad \text{with} \quad \lambda_0, \lambda_1, \lambda_2, \lambda_3 \geqq 0\}.$$

For any $\varphi \in \mathscr{P} \cap \mathscr{B}$ we take

$$\lambda_0 = \tfrac{1}{4}(\sqrt{\varphi_0 + 2\varphi_1 + \varphi_2} + \sqrt{\varphi_0 - 2\varphi_1 + \varphi_2} + 2\sqrt{\varphi_0 - \varphi_2}),$$

$$\lambda_1 = \lambda_3 = \tfrac{1}{4}(\sqrt{\varphi_0 + 2\varphi_1 + \varphi_2} - \sqrt{\varphi_0 - 2\varphi_1 + \varphi_2}),$$

$$\lambda_2 = \tfrac{1}{4}(\sqrt{\varphi_0 + 2\varphi_1 + \varphi_2} + \sqrt{\varphi_0 - 2\varphi_1 + \varphi_2} - 2\sqrt{\varphi_0 - \varphi_2})$$

showing that $\varphi \in \mathscr{R} \subseteqq \mathscr{S}^{+}$ too.

References

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