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Must Thermodynamic Functions Be Piecewise Analytic?

David Ruelle[1]

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There seems to be no general theoretical argument to support the idea that thermodynamic functions are piecewise analytic. We suggest that nonanalyticity may be associated with Gibbs states which are quasiperiodic under space translations, or have a more general nonperiodic ("turbulent") behavior.

KEY WORDS: Thermodynamic functions; nonanalyticity; quasiperiodicity; turbulence.

It is a natural idea that thermodynamic functions should be piecewise analytic. For instance, in the case of a classical system of particles, the pressure should depend piecewise analytically on the temperature, the chemical potential, and more generally on parameters describing the interaction between particles. This should be true at least in the case of short-range forces (for long-range forces there are negative results due to Israel,[(5)] Section V.2).

In favor of the idea of piecewise analyticity are the analyticity results which have been obtained for dilute systems. For instance if the truncated correlation functions[2] at activity z are denoted by $z^n\varphi^z(x_1, \ldots, x_n)$ we have the relations

$$\varphi^{z_0+z_1}(x_1, \ldots, x_m) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int dy_1 \cdots dy_n \, \varphi^{z_0}(x_1, \ldots, x_m, y_1, \ldots, y_n) \tag{1}$$

[1] Institut des Hautes Etudes Scientifiques, 35, Route de Chartres, 91440 Bures-sur-Yvette, France.

[2] Also called "cluster functions" of the correlation functions.

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which are formally true in general, but are known to hold exactly, with absolutely convergent series and integrals, for sufficiently small z_0, z_1, and suitable short-range interactions (see Ruelle,[7] Exercise 4.F). The relations (1) do not contain explicitly the interactions [these occur in the Ursell functions $\varphi^0(x_1, \ldots, x_m)$]; they are one reason of a general nature to suggest analyticity of the pressure as a function of z [using the analyticity of the density $z\varphi^z(x_1)$].

If one tries to pursue this idea, one meets a problem in the region where the substance is in a crystal state (if such a state exists). In order for the $\varphi^z(x_1, \ldots, x_n)$ to have some kind of decrease at infinity as functions of the difference variables $x_2 - x_1, \ldots, x_n - x_1$, one is led to taking them periodic rather than invariant under translations $x_i \mapsto x_i + a$ [and rotations $x_i \mapsto Rx_i$)[3]]. One might hope that (1) holds with these new functions. Unfortunately, if (1) makes any sense the φ^z must have a periodicity independent of z, contrary to physical expectation (crystals are compressible). One conclusion is that the φ^z do not have strong enough decrease at infinity to make the right hand side of (1) convergent. [In fact, Gruber and Martin[3] have recently shown that, in a crystal, neither $\varphi^z(x_1,x_2)$ nor $\varphi^z(x_1,x_2,x_3)$ could decrease fast when $x_2 - x_1 \to \infty$.] For our argument, however, the main point is that we have lost any method of a general nature to show that the pressure is an analytic function of z.[4]

Looking at things differently, we may try to construct systems with nonanalytic thermodynamic functions. A possible model for nonanalytic behavior is provided by maps of the circle, for instance,

$$\theta \mapsto \theta + \alpha + \beta \cos\theta \pmod{2\pi}$$

For fixed β, there are infinitely many intervals of values of the parameter α for which the above map has attracting periodic orbits. In the complement of the intervals the behavior is different. For one-parameter families of maps f_α of the circle (with suitable differentiability conditions), Herman[4] has shown that there is in general a set with positive Lebesgue measure of values of the parameter α for which f_α does not have an attracting periodic orbit. The sets corresponding to periodic and nonperiodic behavior have both positive measure, and are very mixed, so that a function describing the system is likely to be nonanalytic. It is not hard to construct many-particle systems which at *zero temperature*, exhibit the type of nonanalytic behavior just discussed (intervals of periodicity in a quasiperiodic background). Such

[3] These periodic functions φ^z correspond to periodic correlation functions which by average over translations (and rotations) reproduce the original correlation functions.

[4] It may be noted that there are general relations between differentiability of thermodynamic functions and decrease at infinity of truncated correlation functions (see, for instance, Duneau, Souillard, and Iagolnitzer[2]).

systems have been discussed by Aubry,[1] and there is experimental evidence that they exist in nature. The question is whether the nonanalyticity encountered in these systems persists at temperatures different from zero. An example would be a crystal with alternating layers of atoms A and B where the stochiometric ratio of A to B would go through intervals of rational values in a background of irrational values as the activity of A is varied.

The above example suggests that nonanalyticity of thermodynamic functions might be missed because it leads to messy experiments.

Our discussion has linked the analyticity of thermodynamic functions with the behavior of the underlying physical system under translations. Mathematically, this corresponds to the behavior of Gibbs states under translations. We have encountered translation invariance, periodicity, and quasiperiodicity. It would be interesting to find also examples of "turbulent" behavior as one sees in other types of dynamical systems (see Ruelle[8]).

We have discussed only continuous systems, and the arguments presented above do not apply to lattice systems with discrete spin. For such systems, Pirogov and Sinai[6] have in fact obtained relatively general results of piecewise analyticity.

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