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On the Yang–Lee distribution in the β plane

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Abstract. An earlier result obtained by Elvey giving the Yang–Lee distribution in the β plane for one-dimensional continuum systems of particles with hard cores and nearest-neighbour 'rational step potentials' is here extended to general nearest-neighbour potentials.

1. Introduction

Let $\Omega^{(z)}$, $\Omega^{(\beta)}$, denote the Yang–Lee (1952) distribution in the z plane and β plane, respectively, each distribution arising from the family $\{G(\beta, z, L)\}$ of grand partition functions at inverse temperature β, fugacity z, and length L. Using the inversion integral for Laplace transforms, it was shown in Penrose and Elvey (1968) that $\Omega^{(z)}$ may be determined uniquely as a system of analytic arcs for one-dimensional continuum systems with potential given by:

$$u(r) \equiv \begin{cases} +\infty, & 0 < r < b \\ \phi(r), & b \leqslant r \leqslant 2b \\ 0, & 2b < r \end{cases} \tag{1}$$

where ϕ is real and of bounded variation. This result did *not* extend to $\Omega^{(\beta)}$, though it was implied by the arguments of Penrose and Elvey (1968) that $\Omega^{(\beta)}$ was contained in a system of arcs.

In a subsequent note (Elvey 1973) it was shown that $\Omega^{(\beta)}$ *coincides* with this system of arcs provided that ϕ is a finite sum of rational step functions. In the present work the result for $\Omega^{(\beta)}$ is extended to general nearest-neighbour potentials, using a method† (cf Elvey 1974) introduced to obtain similar results for lattice gases.

2. Statement of results

Consider a classical system of particles with potential given by (1), moving on a line of length L and having grand partition function $G(\beta, z, L)$. Since β is the variable of interest here, dependence of G on z will not usually be shown from now on. As in Penrose and Elvey (1968), the equation of state (at positive values of β and z) may be used to obtain a complete analytic function (eg Saks and Zygmund 1965), say P, with branches $p_1(\beta), \ldots, p_k(\beta) \ldots$ at any point $\beta \in \mathbb{C}, z$ having a fixed (possibly complex) value, z_0.

† The basic idea (use of a corollary of Vitali's convergence theorem in an indirect proof that $\Omega = S$) was suggested to me (Elvey 1974) by an (anonymous) referee—to whom I am grateful.

Moreover, P is determined from the relation (cf Penrose and Elvey 1968, lemma 1 with β and z interchanged; also Elvey 1973):

$$z_0\psi(\beta, p) = 1,$$

where

$$\psi(\beta, p) = \int_0^\infty \exp[-\beta u(r) - pr].$$

In the sequel it will be shown that Ω coincides with a set, say S, defined as follows (cf Elvey 1974, § 4): $S = S_1 \cup S_2$, where

$S_1 \equiv \{\beta \in \mathbb{C}: P$ has a branch point of largest real part at $\beta\}$;

$S_2 \equiv \{\beta \in \mathbb{C}: P$ has no branchpoint of largest real part but at least two branches of largest real part at $\beta\}$.

In these terms, the proof will be accomplished through two propositions, namely:

Proposition A
(1) $S_1 \subset \bar{S}_2$
(2) S is closed
(3) $\Omega \subset S$

Proposition B
(1) S contains no domain
(2) $S \supset \Omega$.

In view of the close correspondence of this scheme of proof (and some of the details) with the work of Elvey (1974) and parts of Penrose and Elvey (1968) and Elvey (1973), only brief indications and references to corresponding proofs in the earlier papers will be given (except in the proof of proposition B(2)).

3. Outline of the proof

For any $\beta \in \mathbb{C}$, P has only a finite number (depending on β) of branches of equal real part; and hence, only a finite number (say $\nu(\beta)$) of branches of largest real part (cf Penrose and Elvey 1968, § 3). Consequently:

If $\beta_0 \in S_1$ and $\nu(\beta_0) \equiv \nu_0$ then there is a deleted neighbourhood of β_0 on which each p_r has an expansion of form:

$$p_r(\beta) = w_0 + \sum_{s=1}^{\infty} b_{rs}[(\beta - \beta_0)^{1/\nu_0}]^s$$

where $(\beta - \beta_0)^{1/\nu_0}$ takes the same value for all s and, for $1 \leqslant r \leqslant \nu_0$, $p_r(\beta_0) \equiv w_0$ has largest real part†. It follows that $\exp(p_r)$ has a similar expansion:

$$\exp(p_r(\beta)) = \exp(w_0) + \sum_{s=1}^{\infty} B_{rs}[(\beta - \beta_0)^{1/\nu_0}]^s$$

† Compared with all other branches of P.

and that the functions $\exp(p_r)$ have *co-maximal moduli* on a deleted neighbourhood of β_0. By applying the maximum modulus theorem to the functions $F_{mn} \equiv g_m/g_n$, for $1 \leqslant m < n \leqslant \nu_0$, where

$$g_k(\zeta) \equiv \exp(w_0) + \sum_{l=1}^{\infty} B_{kl}\zeta^l$$

on the closure of a suitable neighbourhood of the origin, one concludes (cf Elvey 1974, p 105) that every neighbourhood of $\beta_0 \in S_1$ contains a point of S_2; which proves A(1).

To prove A(2), it suffices to use the defining properties of S to show that $\mathbb{C}\setminus S$ is *open*; and this is an immediate consequence of the basic property that all branches of P are everywhere continuous. The deduction of A(3) is now most simply effected by showing that $\beta \in \mathbb{C}\setminus S \Rightarrow \beta \in \mathbb{C}\setminus\Omega$, as in Penrose and Elvey (1968, § 4) with the roles of β and z interchanged. To prove B(1), one may use the method of Penrose and Elvey (1968, § 3) (again with β and z interchanged) to show that a necessary condition for S_2 to contain a domain is that $\psi(p) = \psi(p-\mathrm{i}\omega)$ for some real constant ω and all p. The definition of ψ shows, however, that this condition is violated. Since S_1 comprises branch points (of largest real part) it consists of isolated points; and in view of proposition A(1), that is: $S_1 \subset \bar{S}_2$, it follows that S contains no domain and, moreover, that S has no isolated points.

Note that the proofs that S consists of analytic arcs, and that $\mathbb{C}\setminus S$ is simply-connected follow at once from the arguments of Penrose and Elvey (1968, theorem 2), with β and z interchanged. Hence we may assume in the rest of the present proof that S_2 consists of arcs.

Since it is mainly in proving B(2) that the methods of Penrose and Elvey (1968) and Elvey (1973) break down (because, even when L is finite, $G(\beta, L)$ has in general infinitely many zeros in the β plane) for general nearest-neighbour potentials, we give this proof in more detail, though it closely parallels that of Elvey (1974, proposition 3).

Since S is closed (by A(2)) and Ω is closed (by the definition of 'limit points of zeros') it is enough, in view of A(1), to show that $\Omega \supset S_2$. To this end, suppose *not*; and let $\beta_0 \in S_2\setminus\Omega$. Then it follows that there is a neighbourhood, say $\mathcal{N}(\beta_0)$, on which $G(\beta, L)$ does not vanish for all sufficiently large L; so that a definite, regular branch of $[G(\beta, L)]^{1/L}$ may be defined on $\mathcal{N}(\beta_0)$. Since ϕ is of bounded variation, it must also be bounded below:

$$\mathrm{Inf}\{\phi(r) : b \leqslant r \leqslant 2b\} \equiv \delta$$

where δ is a finite real number. Consequently, outside the hard cores, the total potential energy per particle is uniformly bounded below:

$$\sum_{1 \leqslant j < k \leqslant m} \phi(x_k - x_j) \geqslant -(m-1)|\delta|.$$

It follows that

$$U(x)_m \equiv \sum_{1 \leqslant j < k \leqslant m} u(x_k - x_j) \geqslant -m|\delta|$$

for all possible (ordered) configurations of the m particles on $[0, L]$. (This is, of course, just a simple example of the general 'stability condition'; see, eg Ruelle 1969). Thus we have at once (with $z = z_0$):

$$|G(\beta, L)|^{1/L} \equiv \left| 1 + \sum_{m=1}^{\infty} \frac{z_0^m}{m!} \int_{[0,L]^m} \exp[-\beta U(x)_m] \, d(x)_m \right|$$
$$\leqslant \exp\{|z_0| \exp\{|\delta| \max[\mathrm{Re}\, \beta : \beta \in \mathscr{D}]\}\}$$

which gives a uniform bound for $|G(\beta, L)|^{1/L}$ over any compact subset, $\mathscr{D}$, of $\mathscr{N}(\beta_0)$.

From the uniformly bounded family of analytic functions

$$\{[G(\beta, L)]^{1/L} : L > A, \ \beta \in \mathscr{D}\}$$

where A is any sufficiently large number, one can, by a corollary (eg Titchmarsh 1939, p 169) of the Vitali convergence theorem, extract a uniformly convergent subsequence, say $\{[G(\beta, L_k)]^{1/L_k}\}$, whose limit function, say g, is therefore regular on $\mathscr{D}$. Since S contains no domain (by B(1)), one may, without loss of generality, suppose that $[G(\beta', L_k)]^{1/L_k}$ tends to $\exp[p_1(\beta')]$ when $k \to \infty$ and $\beta' \in \mathscr{D} \setminus S$. This being so for all such β', we conclude that g coincides with $\exp(p_1)$ on $\mathscr{D}$. On the other hand, by hypothesis, $\mathscr{D}$ contains points of S_2; and if β'' is such a point then at β'', p_1 is not the unique branch of largest real part, making it impossible for $[G(\beta'', L_k)]^{1/L_k}$ to tend to $\exp[p_1(\beta'')]$. This contradiction proves proposition B(2).

Finally, since $\Omega \subset S$ and $S \subset \Omega$, we deduce that Ω coincides with S, as originally asserted.

4. Remarks

It appears that the scheme of proof outlined here could be used for very general (stable) potentials—even in two or three dimensions—provided only that adequate information about the poles of the complete analytic function generated by the equation of state was obtainable. This seems to me to be the most promising approach to the problem of determining the Yang–Lee distribution for general systems.

One loss in the present method of proof (as compared with that of Penrose and Elvey 1968 and Elvey 1973) is that no formula can be derived for the density of limit points of zeros (at least, not as a direct consequence of the proof given here); but this loss is balanced by the greater generality of the indirect proof.

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