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S. Aubry

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Complete devil's staircase in the one-dimensional lattice gas

Comment on « one-dimensional lattice gas and the universality of the devil's staircase » by S. E. Burkov

S. Aubry

Laboratoire Léon Brillouin, CEN Saclay, 91191 Gif sur Yvette Cedex, France

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Résumé. — Nous calculons explicitement la forme exacte de l'escalier du diable complet du modèle de gaz sur réseau. Nous montrons ainsi que le comportement de la transition de phase commensurable-incommensurable dépend essentiellement des interactions à longue distance. Nous mettons en question les propriétés d'universalité suggérées par Burkov.

Abstract. — We calculate explicitly the exact form of the complete devil's staircase for the lattice gas model. Thus, we show that the behaviour at the commensurate-incommensurate phase transition essentially depends on the long distance interactions. We question the assertion of Burkov about the universality properties of the devil's staircase.

The devil's staircase, calculated by Burkov in his interesting paper [1], can also be explicitly calculated by the same method that we used in the first exact calculation of a complete devil's staircase in 1978 [2]. In addition, our method has the advantage of having a rigorous mathematical foundation [3]. Our initial model was a variation on the discrete Frenkel-Kontorova model where the sine periodic potential was replaced by a piece-wise parabolic periodic potential. It was transformed into an integer model which had a similar form to the lattice gas model considered by Burkov. The details of these calculations in reference [2] were given in appendix A3 of reference [4b]. We also noted that the model studied by Bak and Bruinsma [5] could also be transformed into such a lattice gas model [6]. In addition by using a result given in reference [3c], which was essentially devoted to obtaining rigorous results applicable to quite a more general class of models, it was pointed out that our proofs and exact results could be extended unchanged to models with any kind of long range interactions given some necessary convexity conditions. The purpose of this comment is not to reproduce the substance of papers already published or about to appear but,

- 1) to show how our method, which is simpler, can be applied to the model studied by Burkov. Thus, we find again the equation of the devil's staircase given by Burkov,
- 2) to question the universality properties of the devil's staircase suggested by Burkov.

The one-dimensional lattice gas model [1] with Hamiltonian

$$H_N = \sum_{n=1}^N \left\{ \sum_{m=1}^{\infty} U_m(x_{n+m} - x_n) - \mu \right\}, \quad (1)$$

is included in the class of models (34) of reference [6] where for each $U_m(x)$ there exists a positive constant C_m such that for all x , $U_m''(x) > C_m > 0$. (Many rigorous results were given for this class of models in reference [3].) (Note that if this condition is not satisfied, the devil's staircase of (1) may not exist.) When the atomic mean distance, l , which is the inverse of the atomic concentration, c , i.e.

$$l = \lim_{N \rightarrow \infty} \frac{x_N - x_0}{N} = \frac{1}{c}, \quad (2)$$

is fixed, the ground-state of model (1) is given by (see ref. [6] or [3a, 3b, 3c])

$$x_n = \text{Int}(nl + \alpha) \quad (3)$$

where α is an arbitrary phase. The energy per atom with condition (2) is

$$\psi(l) - \mu = \lim_{N \rightarrow \infty} H_N/N, \quad (4)$$

and can be written

$$\psi(l) = \sum_{m=1}^{\infty} \psi_m(l), \quad (5)$$

with

$$\psi_m(l) = \langle U_m(x_{n+m} - x_n) \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N U_m(x_{n+m} - x_n). \quad (6)$$

The method for calculating $\psi_m(l)$ is the same as that for calculating (A3-11) in reference [4b] or (13-b) in reference [6]. By inspection of the results in reference [4b] or [6], we readily find

$$\psi_m(l) = (ml - \text{Int } ml) [U_m(1 + \text{Int}(ml)) - U_m(\text{Int}(ml))] + U_m(\text{Int } ml). \quad (7)$$

For the real model (with l not fixed) the concentration $c = 1/l$ is determined by minimizing the « grand potential » (1). Thus unlike our models in references [2, 4 or 6], the quantity which has to be minimized is not the energy per atom but the grand potential per unit length (since the total number of particles is not conserved). Instead of having a devil's staircase $l(\mu)$ where l is the atomic mean distance and μ is a tensile force (that is the opposite of a pressure) the devil's staircase of model (1) describes the concentration $c = 1/l$ of particles as a function of the chemical potential μ . The minimization of the grand potential (1) per unit length, which is from equation (4)

$$\bar{\psi}(c) = \frac{\psi(l) - \mu}{l} = c\psi\left(\frac{1}{c}\right) - \mu \cdot c, \quad (8)$$

yields

$$\mu = \psi\left(\frac{1}{c}\right) - \frac{1}{c} \psi'\left(\frac{1}{c}\right). \quad (9)$$

This is the implicit equation of the devil's staircase $c(\mu)$ of model (1) for which we are looking. Using (7) this equation becomes

$$\mu = \sum_{m=1}^{\infty} \left[\left(1 + \text{Int} \left(\frac{m}{c} \right) \right) U_m \left(\frac{m}{c} \right) - \text{Int} \left(\frac{m}{c} \right) U_m \left(1 + \text{Int} \left(\frac{m}{c} \right) \right) \right] \quad (10)$$

which is identical to equation (5) as given by Burkov in reference [1]. It is clear that the behaviour of $c(\mu)$ at the commensurate-incommensurate transitions reflects the properties of the interaction $U_m(x)$ for large x and m . Since for sake of brevity we cannot give the details of the calculations here, we suggest that the interested reader should convince himself by checking for example the cases in which for all m :

$$U_m(x) = \exp(-\gamma x), \quad (11a)$$

and

$$U_m(x) = \frac{1}{x^\alpha} \quad (\alpha > 1), \quad (11b)$$

in the vicinity of the registered commensurability $c = 1$. In the first case, (11a), the well known logarithmic behaviour

$$1 - c(\mu) \simeq \frac{-\gamma}{\ln(\mu_c - \mu)}, \quad (12a)$$

is found, while in the second case

$$1 - c(\mu) \simeq \left(\frac{\mu_c - \mu}{(\alpha + 1) K_\alpha} \right)^{1/\alpha} \quad \text{where} \quad K_\alpha = \sum_{n=1}^{\infty} \frac{1}{n^\alpha}. \quad (12b)$$

Apparently this behaviour is not universal and only depends on the properties of $U_m(x)$ for large x and large m . The universality properties claimed by Burkov are not clearly connected to any physical observation and appear only as a generic property of a mathematical nature for the irrational numbers.

In our opinion, the hierarchical construction of the devil's staircase proposed by Burkov is an artefact of his method of calculation. Indeed, we have shown above that there exists a straight forward calculation of the devil's staircase of (1) which does not involve any details of continued fraction expansions as in reference [1]. Moreover, the generation of the steps of the devil's staircase as proposed by Burkov does not appear reasonable since, for example, there exist steps generated at order two which are infinitely small while at order 3 some of them can be large. It is necessary to consider the metric (that is the width of the steps) of the devil's staircase for a good description of the generation of the steps, while these purely topological consideration although not wrong mathematically are physically misleading. We proposed in reference [7] another hierarchy which corresponds to the generation of steps which approximately are in decreasing order of width. This corresponds to the well known construction of the set of rational numbers. We start from the two rational $\frac{0}{1}$ and $\frac{1}{1}$. At first order we generate the sequence $\frac{0}{1}, \frac{1}{2}$ and $\frac{1}{1}$. At second order we generate $\frac{0}{1}, \frac{1}{3}, \frac{2}{3}, \frac{1}{2}, \frac{1}{1}$, at third order $\frac{0}{1}, \frac{1}{4}, \frac{1}{3}, \frac{2}{5}, \frac{1}{2}, \frac{3}{5}, \frac{3}{4}, \frac{1}{1}$ and so on. The next sequence is obtained from the previous one by inserting between two consecutive rationals of the sequence $r_n/s_n, r_{n+1}/s_{n+1}$ the new rational $r_n + r_{n+1}/s_n + s_{n+1}$.

Let us also note that Burkov considers it obvious that the Cantor set called M_1 in his paper is self-similar. This is a metric property from which he concludes that M_1 has measure zero which means, in our terminology, that the devil's staircase is complete [2]. In fact, the devil's staircase

could be incomplete [2] and then this set M_1 has finite measure. Of course in this case the Cantor set M_1 cannot be self-similar. It is not self-similar even when M_1 has zero measure, at least in the case when the long range interactions decrease fast enough. In a forthcoming paper we will present the proof for the existence of an incomplete devil's staircase in the Frenkel-Kontorova model for a small periodic potential [8] which confirms our early predictions [2]. Thus a rigorous proof for the completeness of the devil's staircase in the case of the lattice gas model is needed. This proof, which is in fact very simple, can be found in reference [6].

Finally, although we do not believe the physical interpretation of the hierarchical construction in the form proposed by Burkov by using the continued fraction expansion of irrational numbers, this method of expansion turns out to be very useful for understanding the « transition by breaking of analyticity » [2] which is closely related to the stochasticity threshold [9] but such a transition does not exist in model (1). The physical meaning of this expansion becomes very transparent by considering the renormalization group approaches used to investigate this kind of transition [10].

(I apologize to Prof. Burkov and to the reader that my early works on the devil's staircase are not easily available in the literature because they are incompletely published in journal which have only a limited readership. This was due largely to serious difficulties with their publication.)

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