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One-dimensional lattice gas and the universality of the Devil's staircase

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Résumé. — On discute une chaîne discrète d'atomes adsorbés à température nulle. On étudie la structure de la phase incommensurable. Le comportement universel au voisinage de la transition commensurable-incommensurable est tiré de la théorie des nombres.

Abstract. — The discrete chain of adsorbed atoms at zero temperature is studied. The structure of the incommensurate phases is investigated. The universal behaviour near a commensurate-incommensurate phase transition is obtained from number theory.

Recently the effects of discreteness of various incommensurate systems have become the subject of keen interest [1-3]. I shall consider the simplest model exhibiting a Devil's staircase : a one-dimensional lattice gas at zero temperature [4-6]. The system consists of a chain of adsorbed atoms that are in equilibrium with a gas at fixed chemical potential μ . The magnitude of the periodic substrate potential is supposed to be infinite, so atoms are allowed to occupy the minima of the potential relief only. The Hamiltonian is of the form :

$$\mathcal{H} = \sum_{n=1}^N \left\{ \sum_{m=1}^{\infty} U_m (X_{n+m} - X_n) - \mu \right\} \quad (1)$$

where N is the total number of adsorbed atoms, the integers X_n are their coordinates (a lattice constant is put equal to unity) and U_m is the interaction between two atoms separated by $(m-1)$ others (U_1 is a nearest neighbour interaction, U_2 is a next nearest one, etc.). This problem has been solved in references [4, 5] by the linear programming method. The Hamiltonian (1) describes also graphite intercalation compounds, « neutral-ionic » transitions in charge transfer salts [3] and a structure of the incommensurate phase in one-dimensional sine-Gordon chain near commensurate-incommensurate phase transitions. In the latter case solitons are considered as adsorbed atoms and a pinning potential as a substrate [7].

There are some values of the chemical potential corresponding to the commensurate (C)

phase with a rational concentration of atoms $c = p/q < 1$. To obtain the structure of this phase one must present the number c as a continued fraction :

$$\frac{p}{q} = \frac{1}{S_1 + \frac{1}{S_2 + \frac{1}{\ddots + \frac{1}{S_n}}}} \quad (2)$$

The positive integers $S_1, S_2, \dots, S_n$ define the coordinates of all atoms unambiguously [4, 6]. This periodic phase consists of S_n clusters of smaller periods :

$$\langle S_1, S_2, \dots, S_{n-2}, S_{n-1}, S_n \rangle = \langle S_1, \dots, S_{n-2}, S_{n-1} \rangle^{S_n} \langle S_1, \dots, S_{n-2} \rangle, \quad (3)$$

where $\langle S_1, \dots, S_n \rangle$ denotes a phase corresponding to the continued fraction (2). The free energy (1) of this phase is given by the formula :

$$\phi = q^{-1} \left[\sum_{m=1}^{\infty} \{ (p(\tau_m + 1) - mq) U_m(\tau_m) + (mq - p\tau_m) U_m(\tau_m + 1) \} - \mu p \right], \quad (4)$$

where τ_m are the entire part of m/c . The phase $c = p/q$ minimizes the energy (1) in some interval of μ , the critical points $\mu_{\min}(c)$ and $\mu_{\max}(c)$ being obtained from the condition that the formation of a soliton (antisoliton) costs no energy [3] :

$$\mu_{\min}(c) = \bar{\mu}(c), \quad \mu_{\max}(c) = \mu_{\min}(c) + \Delta\mu(c),$$

$$\bar{\mu}(c) = \sum_{m=1}^{\infty} [(\tau_m + 1) U_m(\tau_m) - \tau_m U_m(\tau_m + 1)], \quad (5)$$

$$\Delta\mu(c) = q \sum_{m=1}^{\infty} k [U_{kp}(kq + 1) - 2 U_{kp}(kq) + U_{kp}(kq - 1)]. \quad (6)$$

The functions $U_m(X)$ must be convex $U_m''(X) > 0$ and must tend to zero when m or X tends to infinity.

Now let us consider an incommensurate (I) phase with a given concentration c . The ground state is not periodic and is given by equation (3), where c is presented by an infinite continued fraction $\langle S_1, S_2, \dots \rangle$. It can be shown that at $\mu = \bar{\mu}(c)$ from equation (5) this I-phase minimizes the energy (1). Thus any concentration c is possible, irrational concentration corresponding to the only μ but rational one may have a non-zero stability interval $\Delta\mu$ (6). The structure of the Devil's staircase is different for the cases of finite or of infinite range of interaction. If there exists m^* such that $U_m(X) = 0$ at $m > m^*$ or if $U_m(X) = 0$ for $X > X^*$ then the C-phases with small p and q have a non-zero stability interval $\Delta\mu$ (6). They are separated by the first order phase transitions at the critical points $\mu_{\min}$ and $\mu_{\max}$ (5, 6). The C-phases with large p or q have $\Delta\mu = 0$, so these phases and all I-phases may exist at the critical points only. The staircase has only finite steps. The dependence $c(\mu)$ is ambiguous : if μ is a critical point then there is a finite interval of c corresponding to this μ .

The case of infinite range of interaction is much more complicated. Every C-phase has a non-zero $\Delta\mu$, the dependence $c(\mu)$ is unambiguous, monotonous and continuous. There is no finite step in the staircase. Let us denote M_I the set of points on the μ -axis corresponding to all incommensurate phases. The points of M_I are given by equation (5) where c takes all irrational numbers in $[0, 1]$. Because two different c yield different $\bar{\mu}(c)$ the set M_I is uncountable, it is conti-

num. M_1 consists not only of the critical points but of their limiting points. On the other hand it can be shown that the measure of M_1 is equal to zero. This fact is a consequence of the staircase self-similarity. Namely, the whole staircase can be obtained by the following induction. First we construct only C-phases of the form $c=1/S_1$. They form «first-order steps» of the staircase. Then we construct phases with $c = 1/(S_1 + 1/S_2)$. They form new, second-order staircases analogous to the first-order one between every pair of phases $c = 1/S_1$ and $c = 1/(S_1 + 1)$. So the construction of new order in the staircase excludes some interval of μ -axis allowed for I-phase. Let us denote a_n the interval excluded on n -th step divided by the interval remaining after $(n-1)$ -th step. It is equal to $a_n = \Delta\mu/\delta\mu$ where $\Delta\mu$ is the width of the C-phase $\langle S_1, \dots, S_n \rangle$ (Eq. (6)) and $\delta\mu$ is the distance between two neighbouring phases of the n -th order

$$\delta\mu = q(S_n) [E(S_n + 1) - 2 E(S_n) + E(S_n - 1)] , \quad (7)$$

where $E(S_n) = q\phi + \mu p$ is the energy of the phase $\langle S_1, \dots, S_n \rangle$ (see Fig. 1). The infinite product $(1-a_1).(1-a_2)....(1-a_n)....$ gives the measure of M_1 . Substituting (6) and (7) into it one can see that the product is zero. So M_1 is continuum of zero measure, it is analogous to the Cantor set.

Fig. 1. — The Devil's staircase in the first- and the second-orders. The steps of first-order ($c = 1/S_1$) are shown by thick lines.

Usually, exactly incommensurate phase is destroyed by fluctuations, impurities, etc. But C-phases with very large denominators q are quite observable. Let us consider an I-phase with given concentration c . The continued fraction $\langle S_1, S_2, \dots \rangle$ yields the structure of this phase. It is not periodic. But it can be presented as a limit of the C-phases with large periods q_n . Namely we must cut-off the continued fraction $\langle S_1, \dots, S_n, \dots \rangle$ on the n -th term and consider a C-phase $\langle S_1, \dots, S_n \rangle$ with concentration p_n/q_n close to c . This phase coincides with the initial (incommensurate) one on a large distance q_n . So, I-phase is a limit of the C-phases with increasing periods. They are determined by induction : $q_{n+1} = S_n q_n + q_{n-1}$ [8] giving rise to the exponential increase of q_n at large n :

$$q_n \sim \alpha^n . \quad (8)$$

The exponent α is universal in the following sense : if we consider another irrational concentration $c' \neq c$ and construct the same approximation then $q'_n \sim (\alpha')^n$ with $\alpha' = \alpha$. So α is the same for almost all incommensurate phases. It is equal to [9] :

$$\alpha = \exp\left(\frac{\pi^2}{12 \ln 2}\right). \quad (9)$$

This exponent governs also the accuracy of the approximation :

$$\left|c - \frac{p_n}{q_n}\right| \sim \alpha^{-2n}. \quad (10)$$

Thus the universal mechanism of approaching an I-phase is the increase of the C-phase period by α times. There are some other universalities in this field :

$$(S_1, S_2, \dots, S_n) \sim \beta^n, \quad \beta = \exp\left[\frac{1}{\ln 2} \sum_{m=1}^{\infty} \ln m \cdot \ln\left(1 + \frac{1}{m(m+2)}\right)\right] \approx 2.6. \quad (11)$$

The probability to find $S_n = S$ in the infinite continued fraction equals $\ln[1 + 1/S(S+2)]/\ln 2$ and does not depend on c . The relations (9)-(11) are well known in number theory [8, 9]. More exactly, they must be stated in the metric language : equations (9)-(11) are valid for all irrational concentrations except a set of zero measure (on c -axis). There is an obvious example of such an exception. It is a quadratic irrationality. They all have periodic continued fractions. It is easy to see that equation (8) is still valid but α is not equal to (9) and depends on c . For example the golden mean $c = (\sqrt{5} - 1)/2$ all have $S_n = 1$, $p_n/q_n = F_n/F_{n+1}$ where F_n are the Fibonacci numbers, so $\alpha = (\sqrt{5} + 1)/2$, $\beta = 1$. In conclusion I want to emphasize that the universal relations (9)-(11) are only the consequences of number theory.

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References

- [1] AUBRY, S., *Solid State Surf. Sci.* **8** (1978) 264.
- [2] POKROVSKY, V. L., *J. Physique* **42** (1981) 761.
- [3] BAK, P., BRUINSMA, R., *Phys. Rev. Lett.* **49** (1982) 249.
- [4] HUBBARD, J., *Phys. Rev. B* **17** (1978) 494.
- [5] POKROVSKY, V. L., UIMIN, G., *J. Phys. C* **11** (1978) 3535.
- [6] BURKOV, S. E., SINAI, Ya. G., *Sov. Math. Surveys* (1983).
- [7] BURKOV, S. E., POKROVSKY, V. L., UIMIN, G., *J. Phys. A* **15** (1982) L643.
- [8] KHINTCHIN, A. Ya., *Continued Fractions* (« Nauka », Moscow) 1978 (in Russian).
- [9] KORNFIELD, I. P., FOMIN, S. V., SINAI, Ya. G., *Ergodic Theory* (Springer Verlag) 1982.