



HAL
open science

Two-dimensional commensurate soliton structures

G.V. Uimin, V.L. Pokrovsky

► **To cite this version:**

G.V. Uimin, V.L. Pokrovsky. Two-dimensional commensurate soliton structures. Journal de Physique Lettres, 1983, 44 (21), pp.865-870. 10.1051/jphyslet:019830044021086500 . jpa-00232275

HAL Id: jpa-00232275

<https://hal.science/jpa-00232275>

Submitted on 4 Feb 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

LE JOURNAL DE PHYSIQUE - LETTRES

J. Physique — *LETTRES* 44 (1983)L-865-L-870

1^{er} NOVEMBRE 1983, PAGE L- 865

Classification

Physics Abstracts

05.50 — 64.60C — 75.10H

Two-dimensional commensurate soliton structures

G. V. Uimin and V. L. Pokrovsky

L. D. Landau Institute for Theoretical Physics,
ul. Kosygina, 2, Moscow 117940, U.S.S.R.

(Reçu le 11 avril 1983, révisé le 1^{er} septembre, accepté le 9 septembre 1983)

Résumé. — Nous avons trouvé un diagramme de phase correspondant à des structures de soliton ancré à deux dimensions dans le cas d'une interaction répulsive $\mathcal{U}(x)$ entre solitons avec $\mathcal{U}''(x) > 0$. Nous montrons que la fugacité critique de la structure de soliton commensurable est proportionnelle à $\mathcal{U}''(l)$, où l est la période de cette structure.

Abstract. — A phase diagram of pinned soliton structures in two dimensions has been found for a repulsive interaction $\mathcal{U}(x)$ between solitons with $\mathcal{U}''(x) > 0$. The critical fugacity of the commensurate soliton structure is shown to be proportional to $\mathcal{U}''(l)$, where l is the period of this structure.

The commensurate-incommensurate phase transition is associated with spontaneous creation of linear defects — solitons or domain lines. In the one-dimensional case at zero temperature the soliton pinning by a lattice leads to a complicated sequence of commensurate soliton phases [1]. The same sequence arises in an anisotropic 2D system at $T = 0$, where solitons are linear defects and not point defects as in the 1D case. A commensurate soliton structure in two dimensions melts at some finite temperature. This possibility has been previously proposed by Villain [2]. The purpose of this work is to represent the phase diagram of a 2D system in the region of existence of commensurate soliton phases.

There are two main physical realizations of our problem. The first one can be presented by a system of soliton lines, or a system of particles placed into a weak substrate potential, i.e., by a 2D discrete Sine-Gordon model. The second possibility corresponds to a highly anisotropic lattice gas of particles with a strong attracting interaction along the Y -axis and a repulsive interaction along the X -axis. Similar structures have been experimentally observed on the surfaces [211] of W and Mo [3].

According to [4], commensurate soliton structures at $T = 0$ exist in the range of the chemical potential μ between μ_{c_1} and μ_{c_2} , where μ_{c_1} is defined by the vanishing of the soliton energy, and μ_{c_2} is the point of a soliton depinning. When $\mu > \mu_{c_2}$ the repulsion of solitons prevails, resulting in a continuous degree of freedom, i.e. the acoustic mode, of the soliton superstructure, whereas at $\mu_{c_1} < \mu < \mu_{c_2}$ the pinning energy prevails and a soliton system can be considered as a 1D lattice gas with the Hamiltonian

$$\mathcal{H} = -\mu \sum_m n_m + \sum_{m,p>0} \mathcal{U}_p n_m n_{m+p} \quad (1)$$

where m is an integer labelling valleys of the pinning potential, \mathcal{U}_p is the interaction energy of solitons and $n_m = 0, 1$ are the occupation numbers. The function \mathcal{U}_p is assumed to be positive, convex and monotonically decreasing to zero at $p \rightarrow \infty$.

The total set of phases at $T = 0$ can be described as a branching sequence (so-called « complete devil's staircase »). In the leading nearest-neighbour interaction one gets the principal sequence of phase transitions *versus* μ :

$$\dots - \langle p - 1 \rangle - \langle p \rangle - \langle p + 1 \rangle - \dots$$

The basic structural element $\langle p \rangle$ consists of solitons with separation p . At $\mu = \mu_{p,p-1}$ the energies of phases $\langle p \rangle$ and $\langle p - 1 \rangle$ coincide. The next-nearest soliton interaction lifts this degeneracy and one finds the new dimerized phase $\langle p - 1, p \rangle$ in between two « pure » phases $\langle p - 1 \rangle$ and $\langle p \rangle$. Hence, a more complicated sequence of phase transitions :

$$\dots - \langle p - 1 \rangle - \langle p - 1, p \rangle - \langle p \rangle - \langle p, p + 1 \rangle - \langle p + 1 \rangle - \dots$$

If more and more long-distance interactions are added, more bifurcations would take place and a new phase $\langle A B \rangle$ would be created between any two *neighbouring* phases $\langle A \rangle$ and $\langle B \rangle$. We call *neighbouring* phases $\langle p - 1 \rangle$ and $\langle p \rangle$, $\langle p - 1, p \rangle$ and $\langle p \rangle$, but not $\langle p - 1, p \rangle$ and $\langle p, p + 1 \rangle$. We denote by $\langle A \rangle$ the periodic structure with the elementary cell A. The symbol $\langle A B \rangle$ denotes the periodic structure formed as the dimerized sequence of A and B. For any rational concentration $c = p/q$ the corresponding periodic structure can be constructed by expanding c into the continuous fraction [5].

The $\Delta\mu(c)$ regions of the existence of the complicated soliton structures decrease with the growing of their periods $q(c)$ according to the law $\Delta\mu \sim q^{\alpha} \mathcal{U}''(q)$ (the exact formulas for $\Delta\mu(c)$ were derived in [6, 7]).

At $T \neq 0$ the fluctuation of soliton lines has to be taken into account. Let $Z = \exp(-E_0/T)$ be the fugacity of a kink on a soliton line and E_0 be the energy of a kink. In the spirit of the transfer-matrix method we shall consider the evolution of our system along the Y -direction, playing the rôle of time. If $Z \ll p^{-1}$, one can consider the evolution of a 1D system of particles (traces of soliton lines) interacting with one another *via* the one-dimensional potential $\mathcal{U}(x_n - x_m)$. Kinks change the arrangement of particles.

For any pair of neighbours $\langle A \rangle$ and $\langle B \rangle$ in the « complete devil's staircase » there exists a range of μ in the vicinity of $\mu_{A,B}$ and a range of Z between $\min(Z_A^c, Z_B^c)$ and $\max(Z_{A^2B}^c, Z_{AB^2}^c)$, where Z_A^c is the critical fugacity of the phase $\langle A \rangle$. In this range the elementary cells A and B can be considered as new indivisible competing particles. Only kinks permutating the neighbours A B into B A and *vice versa* will be taken into account. We neglect the probability of a kink between A and A or between B and B, since the energies of the resulting excitations are too large (see Fig. 1).

We introduce a fictitious lattice with the sites occupied with either a particle A or a particle B. Moreover, because $n_A + n_B = 1$ a spin-like description may be applied. We consider particles A and B on the fictitious lattice as spin-down and spin-up states $\sigma_z = \pm 1/2$. It is convenient to take for the vacuum state the lattice occupied at each site by a particle A. Then the transfer-matrix acts on the orthonormal set of vectors, describing a displacement of A- and B-particles along the row :

$$| \sigma_{m_1}^+ \sigma_{m_2}^+ \dots \sigma_{m_k}^+ \rangle$$

The transfer-matrix is defined by its diagonal matrix elements and those off-diagonal elements which correspond to the existence of one kink only. The appearance of a kink can be described as the action of the operator $\sigma_{m_j \pm 1}^+ \sigma_{m_j}^-$. For instance, acting with $\sum_m \sigma_m^+ \sigma_{m+1}^-$ on the sequence ... A A A B B B ... we get ... A A B A B B ... This implies the shifting of a spin-up excitation (B)

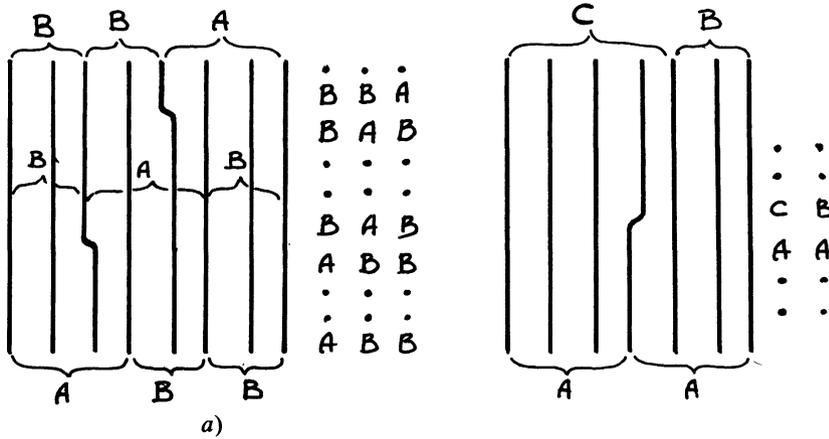


Fig. 1. — Particles A, B and C correspond to the structures $\langle p^2, p - 1 \rangle$, $\langle p, p - 1 \rangle$ and $\langle p^3, p - 1 \rangle$, only A and B being competing ones among these. The kinks, depicted in the l.h.s. of this figure are allowed ones, the other one (r.h.s.) transforming the sequence A A into C B is not allowed, because the self-energy of C-particle is too large. Structures of fictitious lattices are also presented.

by one site to the left on a fictitious lattice. Our approach is a slightly modified version of that used in the Pokrovsky-Talapov model near the C-I transition [2], in the 2D ANNNI model [8], and in the asymmetric clock model [9]. Villain and Bak [8] also introduced the fictitious lattice, but their « particles » or « fermions » were domain walls $+++|---$..., rather than « particles » we have introduced above.

Dislocations in our treatment are described by the following row-to-row configuration :

$$\begin{array}{ccccccc} A & A & |B| & |B| & \dots & |B| & A & A \\ A & A & A & A & ..A & A & A & A \end{array}$$

If the length l of particles in a real lattice exceeds 2 dislocations are irrelevant. Here we assume l to be a large quantity.

The Hamiltonian corresponding to the transfer-matrix has the following form :

$$\mathcal{H} = - Z \sum_m (\sigma_m^+ \sigma_{m+1}^- + \sigma_m^- \sigma_{m+1}^+) + h \sum_m \sigma_m^z + \lambda \sum_m \sigma_m^z \sigma_{m+1}^z \tag{2}$$

where

$$h = 2(\mu - \mu_{AB})/T(l_A + l_B); \quad \lambda = (\mathcal{U}_{l_{AB}-1} - 2\mathcal{U}_{l_{AB}} + \mathcal{U}_{l_{AB}+1})/T. \tag{3}$$

Here l_A and l_B are the periods of the $\langle A \rangle$ and $\langle B \rangle$ phases. Obviously, $l_{AB} = l_A + l_B$.

The first term in the r.h.s. of equation 2 corresponds to the migration of soliton lines, the second term describes a small difference of the energy of the particles A and B at zero temperature, the third term represents the interaction between the neighbouring particles in the fictitious lattice.

Hamiltonian (2) is exactly the Hamiltonian of the XXZ-model in an external magnetic field. Using the well-known properties of the XXZ-model [10, 11] we obtain the critical fugacity of the phase $\langle A B \rangle$:

$$Z_{AB}^c = \lambda/2 \quad (h = 0) \tag{4}$$

and the equation of the phase boundary near the critical point $Z = Z_{AB}^c, h_c = 0$:

$$h_{AB}(Z) = \pm 8 \pi Z_{AB}^c \exp \left\{ - \pi^2/2 \sqrt{2} \sqrt{(Z_{AB}^c - Z)/Z_{AB}^c} \right\}. \tag{5}$$

The phase boundary of the commensurate phase $\langle A \rangle$ ($\langle B \rangle$) is defined by the equation :

$$\mu_{A(B)}(T) = \mu_{AB} \mp T(l_A + l_B) Z. \quad (6)$$

Between all these boundaries an incommensurate phase I_{AB} consisting of particles A and B is stable. Its origin and properties are the same as those for any 2D incommensurate phase. Particularly, the shift of a Bragg peak corresponding to the soliton superstructure is proportional to $|\mu - \mu_{A(B)}(T)|^{1/2}$ or $|h - h_{A(B)}(Z)|^{1/2}$ [12]. All the incommensurate phases transform continuously one into another. The schematic picture of the phase diagram between phases $\langle A \rangle$ and $\langle B \rangle$ is shown in figure 2.

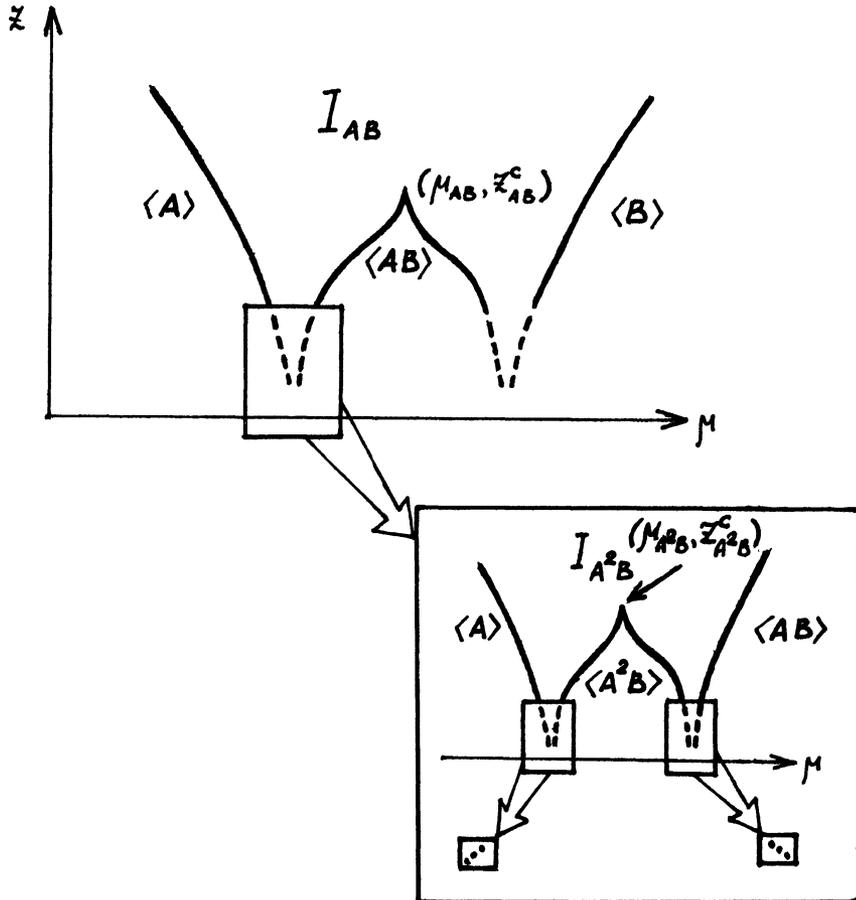


Fig. 2. — Typical fragment of the « complete devil's staircase » is shown. This looks like the phase diagram presented in [13].

For the structure of the type $\langle A^k B \rangle$ or $\langle A B^k \rangle$ with large k and with solitons interacting with one another *via* a power-like potential the consideration has to be modified slightly, since the critical fugacities of the sets consisting of different phases $\langle A^k B \rangle$, $\langle A^{k\pm 1} B \rangle$, etc., are close. In the vicinity of the critical point of the phase $\langle A^k B \rangle$ only the « particles » $A^k B$, $A^{k+1} B$ and $A^{k-1} B$ have to be considered. The problem can be reduced to the investigation of the Hamiltonian of planar magnet with the spin $S = 1$ in the external magnetic field,

$$\mathcal{H} = -Z \sum (S_m^+ S_{m+1}^- + S_m^- S_{m+1}^+) - h \sum S_m^z + \lambda \sum_m (S_m^z)^2. \quad (7)$$

The same consideration can be applied to the sequence of the main commensurate phases $\langle p \rangle$ even in the case of an exponential decay of the particle interaction. This problem (at a zero magnetic field) has been considered in [14, 15]. The 1D quantum spin-1 model with Hamiltonian (7) has been shown to be equivalent to the 2D classical XY model. Including the external magnetic field one obtains the region of commensurate and incommensurate phases similar to figure 2. The critical behaviour remains almost the same as before.

The general phase diagram is schematically depicted in figure 3. For definiteness, we put the period p_0 of the initial commensurate (solitonless) phase equal to 2. The phase diagram consists of an infinite number of peaks, corresponding to different commensurate soliton structures. The width $\Delta\mu$ of a peak decreases as $q^{\mathcal{U}''(q)}$ and the critical fugacity Z^c decreases as $\mathcal{U}''(q)$ with an increase of the period q . The critical temperature $T_c(q)$ behaves as $[\ln \mathcal{U}''(q)]^{-1}$.

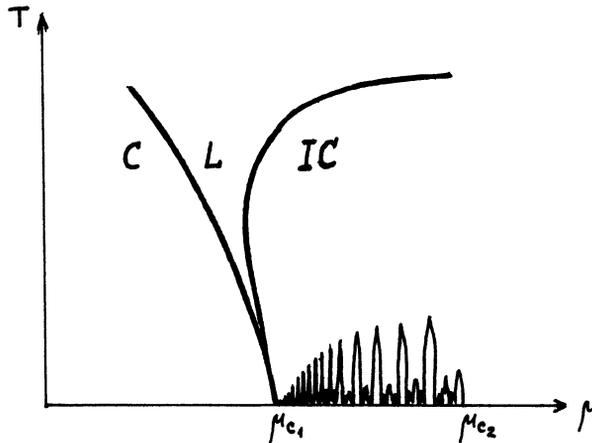


Fig. 3. — Phase diagram for an overlayer with the period $p_0 = 2$ along the X-axis. The commensurate, liquid and incommensurate phases are denoted as C, L and IC, respectively. The location of a region of liquid phase can be explained by the approach presented in [8, 16].

Any bifurcation of the commensurate phases can be represented as a scaling transformation of the phase diagram, as is shown in figure 2. The scaling picture is complete, since the critical behaviour is the same near any critical curve. In such a system phase transitions at zero temperature have been shown to be continuous and to take place at points of a Cantor set along the μ -axis. This Cantor set of points turns into a set of ranges associated with the incommensurate phase at any finite temperature.

We have also calculated the structure factor $S(k)$ of the incommensurate phase I_{AB}

$$S(\mathbf{k}) = \sum_{\mathbf{r}_i, \mathbf{r}_j} \langle \exp(i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)) \rangle$$

for an interpretation of the X-ray and neutron scattering patterns. It is given by

$$S(k) \sim (\delta k)^{-2+\eta}, \quad \eta = \frac{k_0^2(l_B - l_A)^2}{2\pi^2 y} \tag{8}$$

where k is assumed to be close to some Bragg vector k_0 and $\delta k = k - k_0$ is assumed to be directed along X-axis for the sake of simplicity, y is the critical exponent of the energy operator for the 8-vertex model given by the expression [17] :

$$y = 2 - \frac{2}{\pi} \arccos(\lambda/2Z).$$

The dependence of the exponent η on y is substantial only in a close vicinity of the critical point ($Z \approx Z_{AB}^c$, $h \approx 0$). Far from this point the exponent $y = 1$ in agreement with the results obtained by Schulz, den Nijs and others.

The Bragg vector set k_0 for the incommensurate structures is defined by the following equations

$$k_0 = 2\pi \times (\text{integer}) / (\frac{1}{2}(l_A + l_B) + \langle \sigma_z \rangle (l_A - l_B)).$$

The detailed version will be published elsewhere.

References

- [1] BURKOV, S. E., POKROVSKY, V. L., UIMIN, G., *J. Phys. A* **15** (1982) L-645.
 - [2] VILLAIN, J., in *Ordering in Strongly Fluctuating Condensed Matter Systems*, ed. by T. Riste (Plenum, New York) 1980.
 - [3] LYUKSYUTOV, I. F., MEDVEDEV, V. K., YAKOVKIN, I. N., *ZhETF* **80** (1981) 2452.
 - [4] AUBRY, S., *Ferroelectrics* **24** (1980) 52;
POKROVSKY, V. L., *J. Physique* **42** (1981) 762.
 - [5] POKROVSKY, V. L., UIMIN, G. V., *J. Phys. C* **11** (1978) 3535;
HUBBARD, J., *Phys. Rev. B* **17** (1978) 494.
 - [6] BAK, P., BRUINSMA, R., *Phys. Rev. Lett.* **49** (1982) 249.
 - [7] BURKOV, S. E., SINAI, Ya. G. (to be published).
 - [8] VILLAIN, J., BAK, P., *J. Physique* **42** (1981) 657.
 - [9] OSTLUND, S., *Phys. Rev. B* **24** (1981) 398.
 - [10] LIEB, E. H., WU, F. Y., in *Phase transitions and Critical Phenomena* (Academic, London) 1972 v. I.
 - [11] YANG, C. N., YANG, C. P., *Phys. Rev.* **50** (1966) 327.
 - [12] POKROVSKY, V. L., TALAPOV, A. L., *Phys. Rev. Lett.* **42** (1979) 65;
LUTHER, A. and POKROVSKY, V. L., unpublished.
 - [13] SCHULZ, H. J., *Phys. Rev. Lett.* **46** (1981) 1685.
 - [14] LUTHER, A., SCALAPINO, D. J., *Phys. Rev. B* **16** (1977) 1153.
 - [15] DEN NIJS, M. P. M., *Physica IIIA* (1982) 273.
 - [16] COPPERSMITH, S. N., FISHER, D. S., HALPERIN, B. I., LEE, P. A., BRINKMAN, W. F., *Phys. Rev. Lett.* **46** (1981) 549.
 - [17] BAXTER, R. J., *Phys. Rev. Lett.* **26** (1971) 834.
-