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Two-Dimensional Commensurate Soliton Structures

G. V. Uimin[1] and V. L. Pokrovsky[1]

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

KEY WORDS: Commensurate–incommensurate phase transition; soliton; kink; transfer-matrix; "complete devil's staricase."

The commensurate–incommensurate phase transition is associated with a 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 two-dimensional (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 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]

[1] L. D. Landau Institute for Theoretical Physics, The Academy of Sciences of the USSR, Moscow.

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According to Ref. 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 soliton energy and μ_{c_2} is the point of soliton depinning. In this variable range a soliton system can be considered as a 1D lattice gas with the Hamiltonian

$$\mathscr{H} = -\mu \sum_m n_m + \sum_{m,p>0} U_p n_m n_{m+p} \tag{1}$$

Here m is an integer labeling valleys of the pinning potential, U_p is the interaction energy of solitons, and $n_m = 0, 1$ are the occupation numbers. The function U_p is assumed to be positive, convex, and monotonically decreasing to zero at $p \to \infty$.

The total set of phases at $T = 0$ can be described as a branching sequence (so-called "complete devil's staircase"). The main soliton sequence, arising from the nearest-neighbor interaction only, consists of simple periodic phases $\langle p \rangle$ with the distance p between nearest solitons. At any bifurcation a new phase $\langle AB \rangle$ arises between any two neighboring phases $\langle A \rangle$ and $\langle B \rangle$. We denote by $\langle A \rangle$ the periodic structure with the elementary cell A. The symbol $\langle AB \rangle$ 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 complicated soliton structures decrease with the growing of their periods $q(c)$ according to the law $\Delta\mu \sim qU''(q)$ (the exact formulas for $\Delta\mu(c)$ were derived in[6,7]).

At $T \neq 0$ the fluctuational energy 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 role of time. If $Z \ll p^{-1}$, one can consider the evolution of a 1D system of particles (traces of soliton lines) interacting one with another via the one-dimensional potential $U(x_n - x_m)$. Kinks change the arrangement of particles.

For any pair of neighbors $\langle A \rangle$ and $\langle B \rangle$ in the "complete devil's staircase" there exists 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 particles. Only kinks permutating the following neighbors AB into BA 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.

We introduce a fictitious lattice with the sites occupied with either a particle A or a particle B, represented by a spin variable σ_Z taking the values $\pm 1/2$, respectively. Then the appearance of the kink can be described as the action of the operator $\sigma_m^+ \sigma_{m+1}^-$ or $\sigma_m^- \sigma_{m+1}^+$. An analogous approach to the 2D systems has been applied in the 2D ANNNI model[8] and in the asymmetric clock model.[9]

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

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

where

$$h = \frac{2}{T(l_A + l_B)} (\mu - \mu_{AB}), \qquad \lambda = \frac{1}{T} (U_{l_A + l_B - 1} - 2U_{l_A + l_B} + U_{l_A + l_B + 1}) \tag{3}$$

Here l_A and l_B are the periods of the A and B phases. Obviously, $l_{AB} = l_A + l_B$. The first term on the right-hand side of Eq. (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; and the third term represents the interaction between the neighboring particles in the fictitious lattice.

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

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

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

$$h_{AB}(Z) = \pm 8\pi Z_{AB}^c \exp\left\{ -\pi^2/2\sqrt{2} \left[(Z_{AB}^c - Z)/Z_{AB}^c \right]^{1/2} \right\} \tag{5}$$

The phase boundary of the commensurate phases $\langle A \rangle$ and $\langle B \rangle$ is defined by the equation

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

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 $|h - h_{AB}(Z)|^{1/2}$ (Ref. 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 Fig. 1.

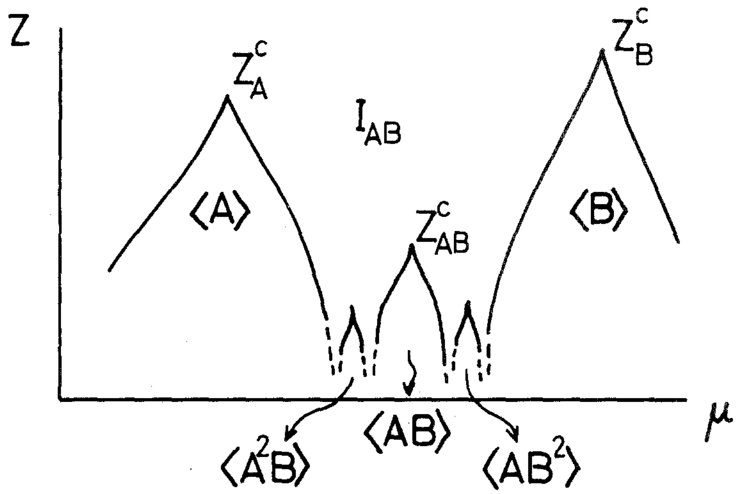

Fig. 1. Typical fragment of the complete devil's staircase is shown. This looks like the phase diagram presented in Ref. 13.

For the structure of the type $\langle A^kB\rangle$ or $\langle AB^k\rangle$ with large k and with solitons interacting one with another via a powerlike potential, the consideration has to be modified slightly, since the critical fugacities of the sets consisting of different phases $\langle A^kB\rangle, \langle A^{k\pm 1}B\rangle$, etc., are close. In the vicinity of the critical point of the phase $\langle A^kB\rangle$ only the "particles" A^kB and $A^{k\pm 1}B$ 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:

$$\mathscr{H} = -Z\sum_m (S_m^+ S_{m+1}^- + S_m^- S_{m+1}^+) - h\sum_m S_m^z + \lambda \sum_m (S_m^z)^2 \tag{7}$$

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 Refs. 14 and 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 Fig. 1. The critical behavior remains almost the same as before.

The general phase diagram is schematically depicted in Fig. 2. 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

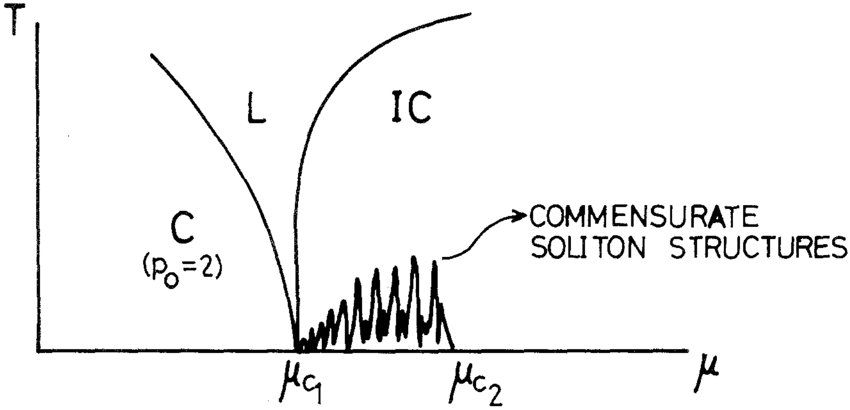

Fig. 2. Phase diagram for an overlayer with the period $p_0 = 2$ along the x axis is shown. The commensurate, liquid, and incommensurate phases are denoted as C, L, and IC, respectively. A location of a region of a liquid phase can be explained by the approach presented in Refs. 16 and 8.

peaks, corresponding to different commensurate soliton structures. The width $\Delta\mu$ of a peak decreases as $qU''(q)$ and the critical fugacity Z^c decreases as $U''(q)$ with an increase of the period q. The critical temperature $T_c(q)$ behaves as $[\ln U''(q)]^{-1}$.

Any bifurcation of the commensurate phases can be represented as a scaling transformation of the phase diagram, as is shown in Fig. 1. The scaling picture is complete, since the critical behavior 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 changes to 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} for the x-ray and neutron scattering. It is given by

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

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 the 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 Bragg vector set k_0 for the incommensurate structures is defined by the following equation:

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

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