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# Phase diagram of the modified *XY* model

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**Abstract.** A modified two-dimensional *XY* model, in which the energy of the nearest-neighbour interaction is a function with two minima, has been considered. The extrema of Hamiltonian have been classified and transformations to a dual model and Coulomb gas have been performed. It has been shown that a large depth of an additional minimum of the interaction function can lead to the splitting of the phase transition into two. One of them (of the Ising type) is connected with appearance of solitons of an infinite length, and the second one with dissociation of pairs of vortices with half of the circulation quantum. A corresponding phase diagram is constructed. It is proposed that recursion relations of the Migdal–Kadanoff moving bonds approximation can be modified. This new version shows the presence of a line of true fixed points in the *XY* model, and can be applied for studying the modification of the *XY* model introduced in this paper. The modified *XY* model can be applied for describing the behaviour of superfluid $^3$He thin films.

## 1. Introduction

The $U(1)$-symmetric Hamiltonian of a traditional *XY* model can be given in the form:

$$H = \sum_{(jj')} V(\varphi_j - \varphi_{j'}) \tag{1}$$

where the variables $\varphi_j$ assuming the values on the circumference $-\pi \leqslant \varphi_j \leqslant \pi$, are defined at the sites of a two-dimensional (2D) lattice; summation is performed over the nearest-neighbour pairs, and the interaction has the form:

$$V(\Delta\varphi) = -V_0 \cos(\Delta\varphi). \tag{2}$$

Variables $\varphi_j$ can be thought of as, say, rotation angles of some planar magnetic moments with respect to a certain fixed direction.

Though rigorous long-range order is impossible in 2D continuously degenerated systems (Peierls 1936, Landau 1937, Mermin and Wagner 1966, Hohenberg 1967), in the case of the Abelian symmetry group $U(1)$ a transition between the phases with the algebraic and exponential decay of the correlation function can occur due to dissociation of vortex pairs. (Berezinskii 1970, 1971a, b, Kosterlitz and Thouless 1973). The type of singularities of thermodynamical functions at the transition point was found by Kosterlitz (1974) by means of the renormgroup transformation for the Coulomb gas of the vortices. The free energy and all its derivatives are continuous at the transition point. The transition of such kind will hereafter be referred to as the BKT transition.

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Small deviations of the interaction function from (2) are irrelevant for the character of the phase transition. Berezinskii (1971b) and Villain (1975) proposed to study the model (1) with the interaction function $V(\Delta\varphi)$, given by:

$$W_{\mathrm{BV}}(\Delta\varphi) \equiv \exp\left(-\frac{1}{T}V(\Delta\varphi)\right) = \sum_{p=-\infty}^{\infty} \exp\left(-\frac{(\Delta\varphi - 2\pi p)^2}{2J}\right) \qquad (3)$$

where $J$ is some constant. In contrast to (2) this interaction function allows for rigorous transformation of the partition function of model (1) to that of 2D Coulomb gas (Villain 1975, José *et al* 1977).

In recent years some authors (Swendsen 1982, Domany *et al* 1984, van Himbergen 1984), using numerical simulations have shown that a drastic change in the type of interaction in a 2D $XY$ model can affect the character of a phase transition. It can become a first-order transition (Domany *et al* 1984, van Himbergen 1984) or even split into two successive ones (Swendsen 1982).

The principal purpose of this paper is to prove by analytical methods that the BKT transition can split into two. We perform this for model (1) with the interaction which is noticeably different from (2) or (3) (but which corresponds to the same form of the ground state).

A physical system where the splitting of the BKT transition can occur is a thin film of superfluid $^3$He-A (Korshunov 1985a). Stein and Cross (1979) have pointed out that since the order parameter degeneracy space for $^3$He-A thin films is $U(1) \times Z_2$, two independent phase transitions can occur in such a system: an ordinary BKT transition and that of the Ising type associated with the breaking of the discrete symmetry. We consider the case when an Ising-type transition takes place at a temperature higher than that of the BKT transition (the inverse sequence is impossible, see Halsey 1985). For the values of the spin-orbital coupling $g_{\mathrm{D}}$ lower than some critical value $g_{\mathrm{D}}^{\mathrm{c}}$ the BKT transition will be split into two independent transitions (Korshunov 1985a). One of them can be associated with the dissociation of half-vortex pairs and the other is of the Ising type. The temperature of this second Ising-type transition tends to zero for $g_{\mathrm{D}} \to 0$. The total number of transitions is three.

In the case of real films the inequality $g_{\mathrm{D}} > g_{\mathrm{D}}^{\mathrm{c}}$ is likely to hold, although the value of the spin-orbital coupling $g_{\mathrm{D}}$ is small in absolute value. Fortunately, the effective value of $g_{\mathrm{D}}$ can be diminished by means of a magnetic field perpendicular to the film (Tešanović 1984), making thus possible the experimental observation of the splitting of the BKT transition. With an increase in the magnetic field the splitting of the transition should be precursed by a deviation of the superfluid density jump at the transition point from its universal value for $^3$He films, as given by Stein and Cross (1979) and Brusov and Popov (1981). At the triple point the increase in the superfluid density jump will be fourfold and, therefore, experimentally observable.

If submonolayer films of $^3$He on $^4$He do exhibit p-pairing superfluidity, as has been proposed by Edwards *et al* (1977), the splitting of the BKT transition would be possible not only in the 2D analogue of the A phase, but also in the planar phase (Korshunov 1985a).

Since the modified $XY$ model considered here and $^3$He-A films at temperatures lower than that of the discrete symmetry breaking are characterised by exactly the same set of relevant topological excitations (consisting of ordinary vortices, closed soliton loops and solitons terminating at half-vortices, see § 2), we can expect them to exhibit isomorphic phase diagrams. The existence of solitons in $^3$He-A films is due to non-triviality of the

corresponding relative homotopy group (cf Mineev and Volovik 1978). Variation of two relevant parameters of the modified $XY$ model can be related to variation of temperature and magnetic field in the case of $^3$He-A film.

In contrast to the $^3$He-A film, which allows for only a qualitative analysis similar to that of § 2 of this paper (which may seem not too convincing) the modified $XY$ model can be investigated with quite a number of methods.

In § 3 we make use of the duality transformation relating the $XY$ models to so-called SOS models with discrete variables. In § 4 a new version of the Migdal–Kadanoff recursion relation is introduced. This version demonstrates the existence of lines of true fixed points and can be applied for the investigation of the model considered. In § 5 the partition function of the modified $XY$ model is rigorously transformed into that of a system of strings and charges on a lattice. The representation containing explicit Ising-type variables is also derived. These different approaches not only reaffirm a possibility of the BKT transition splitting in a much more rigorous manner, but also show some other features of the phase diagram of the modified $XY$ model.

A short account of the principal results of this paper have been published previously (Korshunov 1985b). Later the same model has been independently introduced and investigated by Lee and Grinstein (1985). Their reasoning is close to that of §§ 2 and 5 of this paper and leads (not unexpectedly) to the same conclusions. These authors point out that the model considered can be applied for the description of some kinds of two-dimensional liquid crystals.

## 2. Definition of the model. Low-temperature analysis

We shall consider modification of the $XY$ model, in which $V(\Delta\varphi)$ is an even periodic function of $\Delta\varphi$, having at $\Delta\varphi = \pi$ an extra minimum of almost the same depth as that of the main minimum at $\Delta\varphi = 0$ (figure 1). The specific form of the function $V(\Delta\varphi)$ convenient for the analysis will be chosen in § 3. We assume so far that the difference in the depth of the main and additional minima is $V_1$, and the value of the second derivative of $V$ with respect to $\Delta\varphi$ at the points of the both minima is the same and equals $V_2 \gg V_1$.

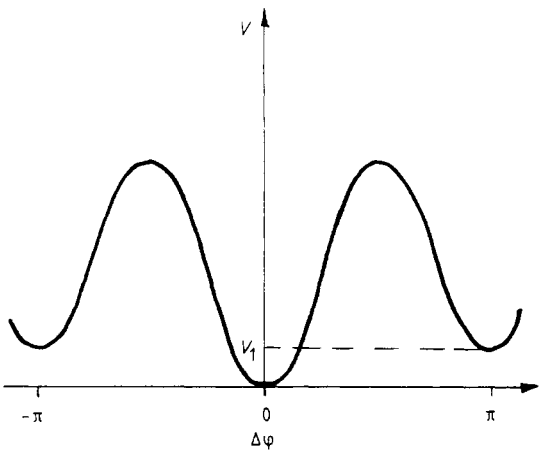


**Figure 1.** Energy of the nearest-neighbour interactions as a function of $\Delta\varphi$.

In a low-temperature analysis of the partition function of the model with continuously degenerate symmetry it is necessary to consider not only the ground state (corresponding to the absolute minimum of energy) but also the states corresponding to the local minima of the Hamiltonian and small fluctuations in the vicinities of all these minima (spin waves). This ensures an algebraic decay of the correlation function $\langle \exp i(\varphi_j - \varphi_l)\rangle$ at large distances:

$$\langle \exp i(\varphi_j - \varphi_l)\rangle \sim |\boldsymbol{r}_j - \boldsymbol{r}_l|^{-2\Delta}. \tag{4}$$

In the harmonic approximation $\Delta = T/(4\pi V_2)$.

Among the states corresponding to the Hamiltonian local minima we shall first deal with vortices. Figure 2(*a*) presents an example of a vortex with minimal circulation. In a continuous approximation vortices are topologically stable point singularities. The vortex circulation is quantised and can only acquire the values multiple to $2\pi$.

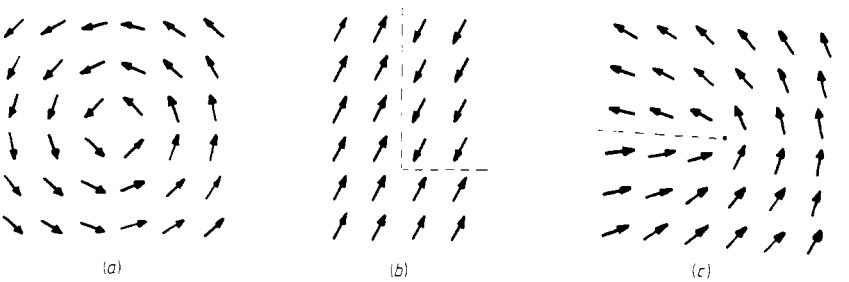


**Figure 2.** Configurations of $\varphi_j$, which are the Hamiltonian local minima: (*a*), vortex; (*b*), soliton; (*c*), soliton terminating at half-vortex.

At large distances the interaction of vortices is logarithmic (and proportional to $2\pi V_2$). For $T \ll V_2$ only small bound vortex pairs are present, situated far one from another. Their existence leads to a slight renormalisation of the exponent $\Delta$ entering equation (4).

For the interaction function of the chosen type the Hamiltonian (1) possesses also such local minima as solitons, i.e. linear singularities upon which $\varphi$ is changed by $\pi$ (figure 2(*b*)). Solitons may be closed or may terminate on vortices with the half-integer number of circulation quanta. In the simplest case the vortices with circulation of $\pm\pi$, which we shall call half-vortices, serve as end points of solitons (figure 2(*c*)). The direct interaction of half-vortices is logarithmic, just as in the case of ordinary vortices, but the interaction constant is less by a factor of four. However, half-vortices can exist only as end points of solitons having finite energy per unit length.

At $T \ll V_1$ the concentration of closed soliton loops and half-vortex pairs, connected by solitons, is low. Their influence only slightly modifies the behaviour of the correlation function $\langle \exp i(\varphi_j - \varphi_l)\rangle$. The free energy of solitons decreases with increasing temperature, and at $T \sim V_1$ is likely to vanish.

A soliton, as a topological singularity, is unstable, since the states it separates can be transformed one into another by continuous deformation. A gap in a closed soliton can be obtained if a pair of half-vortices is created. Running around the soliton these half-vortices are capable of destroying it completely. Nevertheless, this cannot prevent solitons from being the Hamiltonian extrema, so they should be taken into account (with the corresponding weight) while evaluating the partition function.

For $T \ll V_2$ the solitons behave (from the viewpoint of statistical mechanics) as domain walls in the Ising model. Due to strong logarithmic interaction of soliton end-points, the solitons cannot have free ends but should form closed loops with, possibly, small gaps which are not significant for the correlation functions and can only slightly shift the temperature of the phase transition at $T = T_{c1} \sim V_1$.

For $T > T_{c1}$ the solitons of infinite length are present in the system. Since any two distant points happen to be separated by a large number of infinite solitons, on each of which $\varphi$ is changed by $\pi$, the correlation function $\langle \exp i(\varphi_j - \varphi_l) \rangle$ decays exponentially at large distances.

The solitons do not affect the behaviour of the correlation function $\langle \exp 2i(\varphi_j - \varphi_l) \rangle$. At a temperature exceeding $T_{c1}$, as well as at a similar temperature it decays algebraically, since for $T \ll V_2$ the helicity modulus remains finite. For $T > T_{c1}$ the term linear in distance in the interaction of half-vortices related to the soliton free energy is absent. The interaction becomes purely logarithmic and with a further increase in temperature half-vortices behave as vortices in an ordinary $XY$ model. At $T = T_{c2} \sim (\pi/8)V_2$ another phase transition takes place: the dissociation of half-vortex pairs, so that the correlation function $\langle \exp 2i(\varphi_j - \varphi_l) \rangle$ also decays exponentially at higher temperatures.

If in 2D continuously degenerate systems the spontaneous symmetry breaking is defined as an algebraic decay of the corresponding correlation functions, the model under consideration for $T_{c1} < T < T_{c2}$ is in an intermediate phase, in which the spontaneously broken symmetry with respect to a group of 2D rotations $U(1)$ turns out to be partially restored (for rotations by the angles which differ by $\pi$). In other words, only factorisation of the group $U(1)$ by $Z_2$ is spontaneously violated in this case. Therefore we can relate the phase transition taking place at $T = T_{c1}$ to the group $Z_2$ (the subgroup of $U(1)$), though due to the absence of rigorous long-range order in $\varphi$ the Ising-type variable defining the ordering cannot be introduced.

## 3. Transformation to solid-on-solid model

José *et al* (1977) and Knops (1977) showed that the partition function of the model (1) with an accuracy of the non-singular factor is equal to that of the so-called solid-on-solid (SOS) model with the Hamiltonian:

$$\tilde{H} = \sum_{(jj')} \tilde{V}(n_j - n_j') \tag{5}$$

in which the integer variables $n_j$ are defined at the sites of the dual lattice, and summation is performed over the pairs of nearest-neighbours. The interaction $\tilde{V}(\Delta n)$ is related to $V(\Delta\varphi)$ by the Fourier transformation for the corresponding weight functions:

$$\exp[-\tilde{V}(\Delta n)] = \int_{-\pi}^{\pi} \frac{d(\Delta\varphi)}{2\pi} \exp\left(-\frac{1}{T}V(\Delta\varphi) + i(\Delta\varphi)(\Delta n)\right)$$

(the temperature is included into the definition of $\tilde{H}$). SOS models are widely used for studying the crystal surfaces (see, e.g., Weeks 1980).

In case $V(\Delta\varphi)$ is of the form shown in figure 1, the even function $\tilde{V}(\Delta n)$ can be presented as a sum of two terms, one of them increasing monotonically with $|\Delta n|$, and the other depending on the parity of $\Delta n$ only. It is convenient to choose the interaction $\tilde{V}(\Delta n)$ in the form:

$$\tilde{V}(\Delta n) = \tfrac{1}{2}J(\Delta n)^2 - K\exp(i\pi\Delta n) \tag{6}$$

which is a generalisation of a purely quadratic interaction of the discrete gaussian model (Berezinskii 1971b, Chui and Weeks 1976). For $\tilde{V}(\Delta n)$ defined by equation (6) the interaction function $V(\Delta\varphi)$ of the $XY$ model dual to (5) can be expressed through the $J$-dependent Berezinskii–Villain function (3):

$$\exp\left(-\frac{1}{T}V(\Delta\varphi)\right) = W_{\mathrm{BV}}(\Delta\varphi) + \tanh K W_{\mathrm{BV}}(\Delta\varphi - \pi). \tag{7}$$

$j \ll 1 \ll K$ corresponds to the case of $V_1 \ll T \ll V_2$ with $V_1 \approx Te^{-2K}$, $V_2 \approx T/J$.

For $K = \infty$ all the variables $n_j$ are simultaneously either even or odd. If $J \ll 1$, the system is in a roughened state, i.e., the square surface width diverges and the free energy of the step (of double height) per unit length is zero. For $1 \ll K < \infty$ there can exist domain walls between these roughened 'vacua'. These domain walls possess high energy of 2 K per unit length, and consequently, the finite free energy (the entropy can be estimated from the above by the magnitude of the order of unity). Only small 'islands' of one 'vacuum' are present in the other, and the ordering with respect to the Ising variables $\sigma_j = \exp(i\pi n_j)$ is retained. The symmetry of the Hamiltonian (5) with respect to a simultaneous shift of all the variables $n_j$ is broken only partially, i.e., for the shift by an odd number of units. For the dual $XY$ model this corresponds to the phase with partially broken continuous symmetry.

Van der Eerden and Knops (1978) and Swendsen (1978) established a relationship between the correlation function of the $XY$ model and the step free energy of the dual SOS model. The finiteness of the free energy of a unit height step as in the case of $J \ll 1 \ll K$ corresponds to an exponential decay of the correlation function $\langle \exp i(\varphi_j - \varphi_l)\rangle$. Analogously, the zero free energy of the double height step corresponds to an algebraic decay of the correlation function $\langle \exp 2i(\varphi_j - \varphi_l)\rangle$. So, for $J \ll 1 \ll K$ the $XY$ model, dual to (5), is in the intermediate phase, described in the previous section.

With decreasing $K$ the free energy of the domain wall for the variable $\sigma_j$ (coinciding with the free energy of the unit height step) decreases and vanishes at some critical value of $K$. In terms of the $XY$ model this phase transition of the SOS model corresponds to the transition to the phase with an algebraic decay of the correlation function $\langle \exp i(\varphi_j - \varphi_l)\rangle$, i.e., to a completely ordered phase (we use the word 'ordered', while speaking about the $XY$ model, in the sense of algebraic decay of the corresponding correlation functions). It should be noted that in a dual representation it has become possible to introduce the Ising-type variable $\sigma_j = \exp(i\pi n_j)$, with the ordering of which one of the phase transitions of the system is related. The variable $\sigma_j$ is dual to the Ising variable, which we would like to but cannot introduce in the $XY$ model. A completely ordered (atomically-smooth) phase of the SOS model with a fixed $\langle n_j\rangle$ corresponds to a completely disordered phase of the $XY$ model. The model is sure to be in this phase for $J, K \gg 1$. So, the investigation of the dual model confirms the existence of three different phases in the $XY$ model with the interaction given by equation (7).

## 4. New version of the Migdal–Kadanoff recursion relations

### *4.1. Characteristic features of the method*

The recursion relations of the Migdal–Kadanoff 'moving bonds' approximation (Migdal 1975, Kadanoff 1976) are approximate renormalisation transformation, giving the lower bound for the free energy. They are obtained if some bonds are moved from one pair of

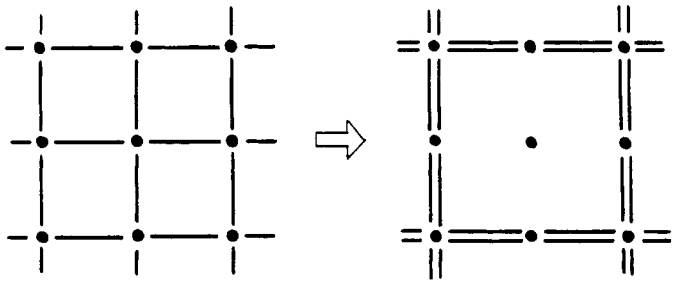

**Figure 3.** Bonds moving scheme for the considered version of the Migdal–Kadanoff relations.

sites to the others (for instance, in a way, as is shown in figure 3). This bond moving allows one to perform some summations in the partition function and obtain the Hamiltonian with renormalised interaction defined on a lattice with doubled intersite spacing.

For the case of the SOS model (5) with the nearest-neighbour interaction application of the bond moving scheme of figure 3, and subsequent summation leads to the following transformation for the weight function $W(n) \equiv \exp[-\tilde{V}E(n)]$

$$W_R(n) = \sum_{n'=-\infty}^{\infty} W^2(n-n')W^2(n'). \tag{8}$$

Transformation (8) is a successive squaring of the weight function $W(n)$ and of its Fourier transform, which is a weight function of the dual model. Application of the bond moving procedure directly to the $XY$ model leads to a transformation differing from equation (8) by a sequence of the squaring of the weight function $W(n)$ and of its Fourier transform. In repeated application of the recursion relations the difference between these two methods vanishes. We find it more convenient to use relation (8) for the weight function of the SOS model.

In the case of a discrete gaussian model the substitution of the weight function

$$W^{(0)}(n) = \exp(-\tfrac{1}{2}Jn^2) \tag{9}$$

into equation (8) yields

$$W^{(1)}(n) = \exp(-\tfrac{1}{2}Jn^2)f^{(1)}(n) \tag{10}$$

where

$$f^{(1)}(n) = \begin{cases} Y_2^0 & \text{for even } n \\ Y_2^1 & \text{for odd } n \end{cases}$$

and

$$Y_q^p = \sum_{s=p(\mathrm{mod}\,q)} \exp(-\tfrac{1}{2}Js^2) \tag{11}$$

for example

$$Y_2^1 = \sum_{s=\pm 1,\pm 3,\ldots} \exp(-\tfrac{1}{2}Js^2).$$

It seems worth mentioning that a weight function of the form (10) corresponds to an interaction of the form (6) with a non-zero $K$.

Now applying (8) to (10) we obtain

$$W^{(2)}(n) = \exp(-\tfrac{1}{2}Jn^2) f^{(2)}_{(n)} \tag{12}$$

where $f^{(2)}_{(n)}$ is an even periodic function of $n$ with a period equal to 4. Further use of this procedure shows that for the $i$th iteration $W^{(i)}(n)$ differs from $W^{(0)}(n)$ by the factor $f^{(i)}(n)$, which is an even periodic function of the period equal to $2^i$.

When $W(n)$ is expressed in such terms, the value of $J$ is not renormalised. However, the effective temperature of the model can be renormalised, since it depends on both $J$ and $f(n)$. In particular, the renormalisation of the effective temperature to zero corresponds to renormalisation of the charges $f_n \equiv f(n)/f(0)$ to zero for all $n \neq 0$. The roughened phase corresponds to a fixed point with all non-zero $f_n$, whose position smoothly varies with $J$.

It has been shown both numerically and analytically (Migdal 1975, José *et al* 1977, Ito 1985) that in the case of 2D $XY$ models (or, equivalently, SOS models) Migdal–Kadanoff recursion relations have only one true fixed point, a trivial one. For high enough initial temperatures (in the SOS representation) we arrive only at quasi-stationary points of the recursion relations, with an exponentially small rate of effective temperature renormalisation (José *et al* 1977, Ito 1985), though the high-temperature phase should correspond to a line of true stationary points (Kosterlitz 1974).

In this paper we propose a modification of the iteration procedure in the spirit of the traditional renormalisation group approach. Its application (i) does not require any numerical computation, (ii) results in appearance of a line of true stationary points and (iii) last but not least, provides a possibility to study a SOS model with the interaction of the form (6).

In our formulation each iteration leads to doubling the period of the function $f(n)$ and the number of independent charges $f_n$. We would like to close this procedure by approximating the function $f(n)$, obtained at some (say, $i$th) step, by a function of the structure which function $f(n)$ had at the previous $((i-1)$th) step.

The simplest way is to average the values of $f(n)$ which were equal one to another at the $(i-1)$th step and have become different at the $i$th step.

### 4.2. *One-charge approximation*

Consider the simplest case with one independent charge:

$$f(n) = \begin{cases} 1 & n = 0 \pmod 2 \\ f_1 & n = 1 \pmod 2. \end{cases}$$

Applying equation (8) to $W(n) = W^{(0)}(n)f(n)$ we get

$$f^{\mathrm{R}}(n) = \begin{cases} Y^0_4 + Y^2_4 f^4_1 & n = 0 \pmod 4 \\ (Y^1_4 + Y^3_4) f^2_1 & n = 1, 3 \pmod 4 \\ Y^0_4 f^4_1 + Y^2_4 & n = 2 \pmod 4. \end{cases}$$

The $J$-dependent functions $Y^p_q$ are defined by equation (11). Averaging $f^{\mathrm{R}}(0)$ and $f^{\mathrm{R}}(2)$ and normalising we get:

$$f^{\mathrm{R}}_1 = \frac{2\gamma f^2_1}{1 + f^4_1} \tag{13}$$

where $\gamma = Y^1_2/Y^0_2$. With increasing $J$ from zero to infinity, $\gamma$ decreases from unity to zero.

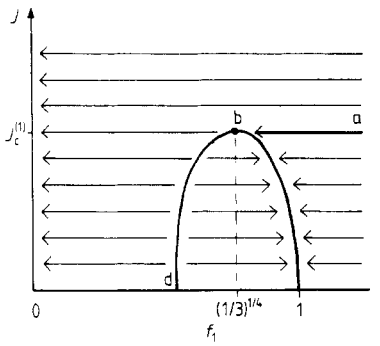


**Figure 4.** Renormalisation group trajectories of the one-charge approximation for the recursion relations.

At $\gamma < \gamma_c = (16/27)^{1/4}$ transformation (13) has only one fixed point—the trivial low-temperature stationary point $f_1 = 0$. For $\gamma > \gamma_c$ it has also two non-trivial fixed points, one of which is stable. With decreasing $\gamma$ these points move closer one to another and at $\gamma = \gamma_c$ merge into one point. It will be convenient to present the renormalisation group trajectories corresponding to continuous version of equation (13):

$$\frac{\partial f_1}{\partial \xi} = \left(\frac{2\gamma f_1}{1+f_1^4} - 1\right) f_1 \tag{14}$$

in coordinates $(f_1, J)$ (figure 4). Here $\xi$ is the logarithm of the lattice constant. The line of non-trivial stable fixed points terminates at $J = J_c^{(1)} \approx 1.44$. For comparison we would like to mention that a self-consistent approximation for the sine–Gordon model, approximating the discrete gaussian model, gives $J_c = (\pi/2) \approx 1.57$ (Saito 1978), but the numerical simulation for a discrete gaussian model shows that $J_c \approx 1.37$ (Shugard *et al* 1978). The areas of the phase diagram corresponding to the roughened and low-temperature phases are separated by the separatrix ab and the line of unstable fixed points bd.

It seems worth mentioning that the family of renormalisation group trajectories (figure 4) coincides with (to an accuracy of the smooth transformation leading to the straightening of the trajectories) those of a Coulomb gas corresponding to a discrete gaussian model depicted in figure 5 in accordance with the Kosterlitz (1974) results. One can use equation (14) to obtain the law of the critical behaviour of the correlation radius

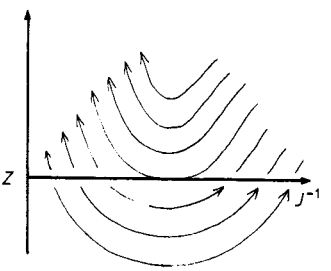


**Figure 5.** Renormalisation group trajectories of a two-dimensional Coulomb gas, $J$ is inversely proportional to the prelogarithmic factor in the interaction of the charges, $Z$ is their fugacity.

for the correlation function $\langle \exp i(\varphi_j - \varphi_l)\rangle$. It proves to be the same as that found by Kosterlitz (1974).

So, our procedure even in the simplest approximation provides an adequate description of the roughening transition in a discrete gaussian model (corresponding to the initial value of $f_1$ equal to unity). The one-charge approximation considered above cannot certainly provide any detailed information on the properties of low-temperature phase for different initial values of $f_1$ and $J$.

### *4.3. Two-charge approximation*

If $f(n)$ has the form:

$$f(n) = \begin{cases} 1 & n = 0 \pmod 4 \\ f_1 & n = 1; 3 \pmod 4 \\ f_2 & n = 2 \pmod 4 \end{cases} \tag{15}$$

application of equation (8) and subsequent summation and normalisation yields

$$f_1^{\mathrm{R}} = \frac{\gamma(1+\gamma_4)(1+f_2^2)f_1^2}{1+2\gamma_4 f_1^4 + f_2^4}$$

$$f_2^{\mathrm{R}} = 2\frac{f_1^4 + \gamma_4 f_2^2}{1+2\gamma_4 f_1^4 + f_2^4} \tag{16}$$

with $\gamma_4 = Y_4^2/Y_4^0 \equiv \gamma(4J)$

For small $J$ transformations, equations (16) possess seven fixed points in the region of non-negative values of parameters $f_1$ and $f_2$. Their position on the plane $f_1, f_2$ is plotted in figure 6 together with the trajectories corresponding to the continuous version of equations (16). Points $A_0$, $A_1$ and $A_2$ are stable and represent low temperature (smooth),

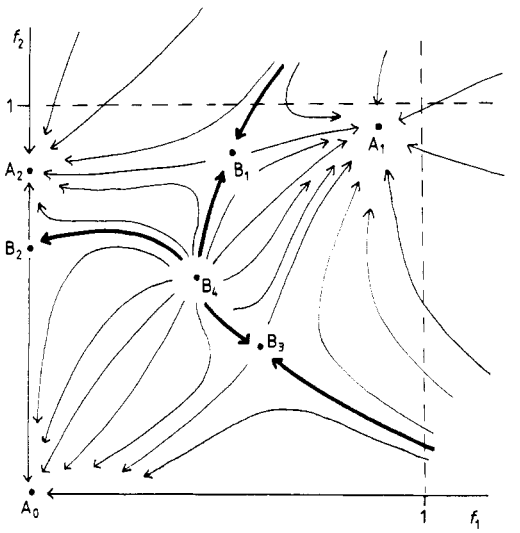


**Figure 6.** Renormalisation trajectories of the two-charge approximation for recursion relations.

roughened and intermediate phases, respectively. Points $B_1$, $B_2$ and $B_3$ are saddle-points, and point $B_4$ is an unstable knot. Phase borders coincide with the separatrices shown by bold lines in figure 6. The intermediate phase is smooth with respect to the odd height steps and is roughened with respect to the even height steps.

With varying $J$ the position of stationary points changes. At $J = (1/4)J_c^{(1)} \approx (0.36)$ points $A_2$ and $B_2$ merge into one point, which vanishes for higher $J$. With further increase in $J$, points $B_3$ and $B_4$ merge and vanish, and at least (at $J \approx J_c^{(1)}$) points $A_1$ and $B_1$ also merge and vanish.

Interaction (6) corresponds to the initial values of parameters $f_1$ and $f_2$ equal to $e^{-2K}$ and 1, respectively. The phase diagram for the Hamiltonian with such an interaction obtained on the basis of equations (16) is depicted in figure 7(*a*) in coordinates $(K^{-1}, J)$. The same phase diagram can be interpreted as a phase diagram of the $XY$ model with interaction (7). The ordered (superfluid) phase of the $XY$ model is denoted by S, the disordered phase by N and the intermediate one by I.

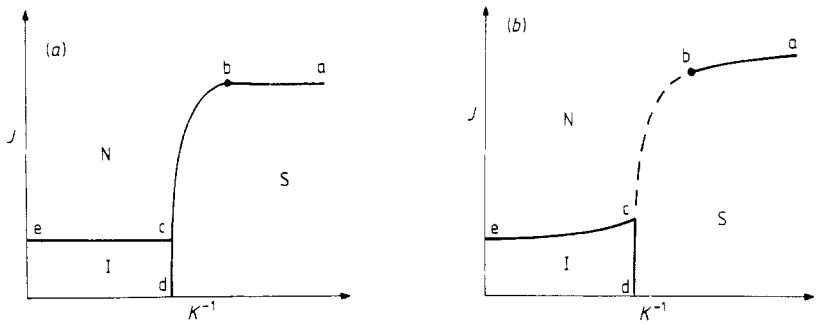


**Figure 7.** Phase diagram of a modified $XY$ model with interaction (7): (*a*), obtained by means of the recursion relations (§ 4); (*b*), obtained by the perturbation theory (§ 5) S, ordered phase I, intermediate phase; N, disordered phase.

The one-charge approximation considered earlier corresponds to $f_2 \equiv 1$. In this case there are only two non-trivial singular points corresponding to $A_1$ and $B_1$. They merge and vanish at $J = J_c^{(1)}$. Therefore, the allowance made for renormalisation of $f_2$ leads to a shift of the line of stable fixed points and to a change in the value of $J$, at which it terminates. The character of the behaviour of renorm group trajectories in the vicinity of the end-point of the A-type fixed points line remains the same as in the one-charge approximation. The account taken of the renormalisation of $f_2$ makes it possible also to separate two different low-temperature phases of the SOS model, the true low-temperature (smooth) phase and the intermediate one introduced in § 3. They correspond to disordered and intermediate phases of the $XY$ model.

## 5. Coulomb gas representation

Since $\exp i\pi(n_j - n_j')$ acquires only the values equal to $\pm 1$, the partition function of model (5) with interaction (6) with an accuracy of a non-singular factor can be written as:

$$z = \sum_{n_j=-\infty}^{\infty} \sum_{y_{jj'}=0,1} \exp\left( \sum_{(jj')} [\tfrac{1}{2}J(n_j - n_{j'}')^2 + 2K^* y_{jj'})^2 + i\pi(n_j - n_{j'})y_{jj'}] \right) \tag{17}$$

where variables $y_{jj'} = 0.1$ are defined at lattice bonds, and $K^*$ is related to $K$ by the Kramers–Wannier duality relation (Kramers and Wannier 1941):

$$\sinh 2K \times \sinh 2K^* = 1.$$

Chui and Weeks (1976) showed that the partition function of the discrete gaussian model can be transformed to that of a 2D lattice Coulomb gas. The partition function given by equation (17) can be transformed analogously. One can substitute summation over $n_j$ by integration, introducing $\delta$-functional factors in the form

$$\frac{1}{2\pi}\sum_{m_j} \exp(2\pi \mathrm{i} m_j n_j)$$

and then perform gaussian integration in $n_j$, obtaining (with an accuracy of a non-singular factor)

$$Z = \sum_{m_j=-\infty}^{\infty} \sum_{y_{jj'}=0.1} \exp\left( -\tfrac{1}{2}\sum_{j,l} [m_j - \tfrac{1}{2}(\operatorname{div} \mathbf{y})_j] G_{jl} \times [m_l - \tfrac{1}{2}(\operatorname{div} \mathbf{y})_l] - 2K^* \sum_{(jj')} y_{jj'} \right) \tag{18}$$

where

$$G_{jl} = \frac{(2\pi)^2}{J} \int\int_{-\pi}^{\pi} \frac{\mathrm{d}k_x}{2\pi} \frac{\mathrm{d}k_y}{2\pi} \frac{\exp \mathrm{i}\boldsymbol{k}(\boldsymbol{r}_j - \boldsymbol{r}_l)}{4\sin^2(k_x/2) + 4\sin^2(k_y/2)}$$

and

$$(\operatorname{div} \mathbf{y})_j = y_{j,j+e_x} + y_{j,j+e_y} - y_{j-e_x,j} - y_{j-e_y,j}.$$

The partition function (18) is that of a system of strings defined on lattice bonds and of charges located at lattice sites. Strings (corresponding to $y = 1$) possess the energy $2K^*$ per unit length. The charges $M_j/2 = m_j - \frac{1}{2}(\operatorname{div} \mathbf{y})_j$ can acquire half-integer values at the sites, where an odd number of strings converge, and integer values at the other sites. All the strings are either closed or terminate at half-integer charges. The interaction of charges $G_{jl}$ is logarithmic at large distances.

The properties of charges and strings coincide with those of vortices and solitons (cf § 2). The existence of representation (18) (in which continuous degrees of freedom have been integrated out) justifies the analysis of § 2, carried out without spin waves being taken into account.

In equation (18) $m_j - \frac{1}{2}(\operatorname{div} \mathbf{y})_j$ can be substituted by $M_j/2$ if the constraints $M_j = (\operatorname{div} \mathbf{y})_j \pmod 2$ are imposed. In case these conditions are written as factors in the form

$$\tfrac{1}{2}\sum_{\sigma_j=\pm 1} \exp\{\tfrac{1}{2}\mathrm{i}\pi\sigma_j [M_j - (\operatorname{div} \mathbf{y})_j]\} \tag{19}$$

the summation over $y_{jj'}$ can be easily performed, leading to:

$$Z \sim \sum_{M_j=-\infty}^{\infty} \sum_{\sigma_j=\pm 1} (-1)^{\sum_j \frac{1}{2}M_j\sigma_j} \exp\left( -K\sum_{(jj')} \sigma_j\sigma_{j'} - \tfrac{1}{2}\sum_{j,l} \tfrac{1}{2}M_j G_{jl} \tfrac{1}{2}M_l \right) \tag{20}$$

where the condition of total neutrality ($\Sigma_j M_j = 0$) has been taken into account.

The partition function (20) differs from the product of the Ising model and 2D Coulomb gas partition functions only by a 'phase factor' $\pm 1$ included into each term. This peculiar interaction of the variables $\sigma_j$ and $M_j$ can be taken into account in the framework of the perturbation theory (of the low-temperature expansion type). For $J^{-1} = K = \infty$ only the terms with all $M_j = 0$ and all $\sigma_j$ equal to each other are non-zero in the partition function (20). In terms of the initial $XY$ model this corresponds to an intermediate phase, serving as 'the background' for the perturbation theory of this section. For $J^{-1}$, $K \gg 1$ only the terms with small-size bound pairs of charges $M_j/2$ and small separate regions of turned over $\sigma_j$ are important in the partition function (20), i.e., we remain for certain in the intermediate phase. Let us consider now the influence of the interaction of variables $\sigma_j$ and $M_j$.

For $J = 0$ we have a pure Ising model, in which the phase transition occurs at $K = K_c = \frac{1}{2}\ln(1 + \sqrt{2})$ (Kramers and Wannier 1941). For $0 < J \ll 1$ one can perform summation over $M_j$, assuming these charges to be bound into neutral small-size pairs, their mutual interaction leading only to a slight renormalisation of $J$. Such summation results in an additional ferromagnetic interaction of variables $\sigma_j$, decreasing at large distances as $r^{-\pi/2J_R}$ ($J_R$ is the renormalised value of $J$). For the phase with half-vortices bound in pairs, $\pi/2J_R \geqslant 4$, and this additional interaction cannot lead to a change in the character of the Ising transition and in the values of critical exponents (cf Fisher *et al* 1972). It only results in a decrease in the critical value of $K$, exponentially small in $J$.

For $K = \infty$ we have a Coulomb gas of the charges $M_j/2$, in which the phase transition associated with dissociation of pairs of the smallest charges $M_j/2 = \pm 1/2$ (corresponding to half-vortices) occurs with increasing $J$. For $K < \infty$ we can consider the influence of Ising variables on the interaction of charges $M_j/2$. Performing in (20) summation over $\sigma_j$, for the configuration with only two non-zero charges $M_j/2$ we get that the interaction of ordinary vortices (even $M_j$) does not change and the term $-\ln\langle\sigma_j\sigma_l\rangle$ is added to the interaction of half-vortices. For large $K$, when $\langle\sigma_j\rangle \neq 0$, an addition of this term is equivalent to a decrease in the fugacity of half-vortices, and leads only to an exponentially small increase in the critical value of $J$. An algebraic decay of the correlation function $\langle\sigma_j\sigma_l\rangle$, corresponding to the critical point of the Ising transition, results in an increase of prelogarithmic factor in the half-vortex interaction by $1/4$. For $K < K_c$ we have

$$-\ln\langle\sigma_j\sigma_l\rangle \simeq \frac{1}{r_c}|\boldsymbol{r}_j - \boldsymbol{r}_l|$$

so in the interaction of half-vortices there appears a linear-in-distance term related to the soliton free energy. Therefore, in this case an increase in $J$ up to the value corresponding to the effective screening of the logarithmic interaction does not cause dissociation of vortex pairs. The line of the phase transition, where dissociation of half-vortices occurs through the Kosterlitz mechanism, terminates at the line corresponding to the vanishing of the soliton free energy.

For $K = 0$ the $XY$ model under consideration turns into the Villain–Berezinskii model. For small $K$ no second minimum is present in the interaction function $V(\Delta\varphi)$ and the phase transition proceeds through dissociation of pairs of ordinary vortices but at smaller values of $J$.

The results of the perturbation theory analysis of this section are summarised in figure 7(*b*) as a phase diagram in the coordinates $(K^{-1}, J)$. The phases are denoted as in figure 7(*a*). On line ab, dissociation of pairs of ordinary vortices takes place, and on line ce, dissociation of pairs of half-vortices. On line cd the soliton free energy vanishes. The

phase transition on lines ab, ce and cd (or at least on their parts lying not too close to the triple point c) should occur continuously. In the area lying to the left from the segment bc the logarithmic interaction of half-vortices is too weak for them to be bound in pairs. Therefore, the phase transition on the segment bc should proceed directly into a disordered phase, but in a different way than on the segment ab (either with other critical exponents, or rather by the first-order transition). In the vicinity of line bc in contrast to the case of small $J$, solitons cannot be treated as continuous linear objects, since in this case the logarithmic interaction of soliton end-points is not strong enough for them to be bound in pairs. The phase transition on line bc should be related not to vanishing of the soliton free energy, but rather to the transition of the half-vortex gas to a plasma phase, caused by the screening of the total interaction (which includes logarithmic and linear terms). In case it is a first-order phase transition (and it seems such is the case) it is not clear whether it is reasonable to put forward the question about its primary cause. Such a first-order transition can also be treated as the one caused by anharmonicity of the interaction function (Pokrovsky and Uimin 1973). The value of the helicity modulus (superfluid density) jump at the transition line bc should vary continuously from its universal value for vortex pairs dissociation (point b) to a four-times higher universal value for half-vortex pairs dissociation (point c).

It should be noted that the phase diagram produced by our new version of the Migdal–Kadanoff recursion relations (figure 7(*a*)) is rather similar to that obtained in this section (figure 7(*b*)). In it the line of direct phase transitions from an ordered phase to a disordered one is also divided into two segments by point b, where the analyticity of this line is broken.

In terms of the initial $XY$ model $J$ corresponds to dimensionless temperature and $2JK^*$ to dimensionless soliton energy (depending on the magnetic field for the case of $^3$He-films). Some of the thermodynamic paths (i.e., lines $JK^* = \text{constant}$) are sketched in figure 7 by broken lines. They can cross either one (ab or bc) or two (cd and ce) lines of phase transitions.

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## References

Berezinskii V L 1970 *Zh. Eksp. Teor. Fiz.* **59** 907 *(Sov. Phys.-JETP* **32** 493)
—— 1971a *Zh. Eksp. Teor. Fiz.* **61** 1144 *(Sov. Phys.-JETP* **34** 610)
—— 1971b *Thesis* L D Landau Institute for Theoretical Physics, Moscow (unpublished)
Brusov P N and Popov V N 1981 *Zh. Eksp. Teor. Fiz.* **80** 1564
Chui S T and Weeks J D 1976 *Phys. Rev.* B **14** 4978
Domany E, Schick M and Swendsen R 1984 *Phys. Rev. Lett.* **52** 1535
Edwards D O, Feder J D and Nayak V S 1977 in *Quantum Fluids and Solids* ed. S B Trickey, E D Adams and J W Duffy, (New York, London: Plenum) p 375
van der Eerden J P and Knops H J K 1978 *Phys. Lett.* **66A** 334
Fisher M E, Ma S-k and Nickel B G 1972 *Phys. Rev. Lett.* **29** 917
Halsey T C 1985 *J. Phys. C: Solid State Phys.* **18** 2437
van Himbergen J P 1984 *Phys. Rev. Lett.* **53** 5
Hohenberg P C 1967 *Phys. Rev.* **158** 383
Ito K R 1985 *Phys. Rev. Lett.* **54** 2383

José J V, Kadanoff L P, Kirkpatrick S and Nelson D R 1977 *Phys. Rev.* B **16** 1217
Kadanoff L P 1976 *Ann. Phys.* **100** 359
Knops H J F 1977 *Phys. Rev. Lett.* **39** 766
Korshunov S E 1985a *Zh. Eksp. Teor. Fiz.* **89** 531
—— 1985b *Pis'ma Zh. Eksp. Teor. Fiz.* **41** 216
Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
Kramers H A and Wannier G H 1941 *Phys. Rev.* **60** 252
Landau L D 1937 *Zh. Eksp. Teor. Fiz.* **7** 627
Lee D H and Grinstein G 1985 *Phys. Rev. Lett.* **55** 541
Mermin N and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
Migdal A A 1975 *Zh. Eksp. Teor. Fiz.* **69** 1457
Mineev V P and Volovik G E 1978 *Phys. Rev.* B **18** 3197
Peierls R 1936 *Helv. Phys. Acta VII Suppl.* **2** 81
Pokrovsky V L and Uimin G V 1973 *Phys. Lett.* **45A** 467 (*Zh. Eksp. Teor. Fiz.* **65** 1691)
Saito Y 1978 *Z. Phys.* B **32** 75
Shugard W J, Weeks J D and Gilmer G H 1978 *Phys. Rev. Lett.* **31** 549
Stein D L and Cross M C 1979 *Phys. Rev. Lett.* **42** 504
Swendsen R H 1978 *Phys. Rev.* B **17** 1370
—— 1982 *Phys. Rev. Lett.* **49** 1302
Tešanović Z 1984 *Phys. Lett.* **100A** 158
Villain J 1975 *J. Physique* **36** 581
Weeks J D 1980 *Order in Strongly Fluctuating Condensed Matter Systems* ed. T Riste (New York, London: Plenum) p 293