Generalization of the
Berezinskii-Kosterlitz-Thouless theory to higher
vortex densities

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Abstract

The Berezinskii-Kosterlitz-Thouless theory for superfluid films is gen-
eralized in a straightforward way that (a) corrects for overlapping vortex-
antivortex pairs at high pair density and (b) utilizes a dielectric approx-
imation for the polarization of the vortex system and a local field cor-
rection. Generalized Kosterlitz equations are derived, containing higher
order terms, which are compared with earlier predictions. These terms
cause the total pair density to remain finite for temperatures above the
transition so that it is not necessary to introduce an ad hoc cut-off, as
opposed to the original Berezinskii-Kosterlitz-Thouless theory. The low-
temperature bound pair phase is destabilized for small vortex core energy.
The behaviour of the stiffness constant and of the correlation length close
to the transition is not affected by the higher order terms. A first-order
transition as suggested by other authors is not found for any values of the
parameters. The pair density is calculated for temperatures below and
above the transition. Possible experiments and the applicability of the
extended approach are discussed. The approach is found to be applicable
even in a significant temperature range above the transition.

1 Introduction

Two-dimensional and quasi-two-dimensional systems with a two-component or-
der parameter and short-range interactions typically fall into the universality
class of the two-dimensional $XY$ model. The behaviour of such systems, e.g.,
superconducting films, superfluid films and thin planar magnets, close to their
phase transition is usually well described by the Berezinskii-Kosterlitz-Thouless
(BKT) theory [1, 2]. The discovery of the high-temperature superconductors,
which consist of weakly coupled superconducting layers, has led to renewed interest in this theory [3]. In BKT theory the phase transition is supposed to take place through the unbinding of spontaneously created vortex-antivortex pairs. For temperatures up to the transition temperature $T_c$ the predictions of BKT theory typically agree quite well with experimental results. There are several essentially equivalent mathematical formulations of the BKT theory [2, 4, 5, 6, 7]. Here, we follow Halperin’s presentation [8], which is founded upon the heuristic approach of Kosterlitz and Thouless [8].

The BKT theory treats the interaction between different vortex-antivortex pairs through a suitable renormalization of the intra-pair interaction. This approximation is best justified if pairs are small and far apart. The so-called Kosterlitz equations, which are derived in BKT theory, relate the density of vortex-antivortex pairs of given size and the screening of the vortex-antivortex interaction at given separation to one another. Nelson and Kosterlitz [9] and Halperin [8] predict the general form of higher order terms of these equations, but do not derive the coefficients. Amit et al. [10] utilize field-theoretical methods to derive a universal relation between the coefficients of two higher order terms. One would like to know the higher order terms, including the coefficients, to see if the typical BKT behaviour, which is found in experiment, survives in their presence.

Without these terms the BKT theory suffers from the following weakness: If taken literally it predicts a diverging vortex density for $T > T_c$. This result cannot be correct. The creation of one vortex-antivortex pair costs at least twice the core energy. The density of pairs should thus be governed by a Boltzmann factor containing this energy. In the BKT theory, a cut-off length $\xi_+$ is introduced ad hoc to obtain finite results. The length $\xi_+$ is meant to represent the average separation between free vortices. In a system of zero overall vorticity, all vortices and antivortices can be grouped into pairs. Thus $\xi_+$ is not very well-defined. The concept of “free vortices” does not naturally fit into the theory. It is unsatisfactory that such a cut-off is necessary at all. It seems that an important contribution to the density has been neglected.

Different objections are put forward by Gabay and Kapitulnik [11]. These authors argue that one should use the Clausius-Mossotti formula [12] for the dielectric constant to take local field effects into account. Several authors [13, 14, 15] predict the breakdown of the BKT theory for small vortex core energy and the appearance of a first-order transition. These papers are inspired by Monte Carlo simulations [14, 17], which indicate the presence of such a transition for low vortex core energies. Minnhagen and Wallin [13] employ a linear screening theory to obtain generalized Kosterlitz equations. It seems that local field effects are not included in their approach (see below) and that the restriction that vortices may only be created in neutral pairs is not taken into account. Furthermore, the authors use different sets of self-consistency equations below and above the critical temperature, whereas one would welcome an approach which predicts a phase transition without having to assume its presence be-
forehand. In Refs. [14] and [15] phase diagrams are derived that do not match the BKT result for high core energies, $E_c > q^2$, where the BKT theory should be applicable. Here, $q^2$ is the coupling constant appearing in the unscreened vortex-antivortex interaction $V(r) = q^2 \ln(r/r_0)$. Experimental evidence for a first-order transition does not seem to exist as of yet.

In the following sections, a generalized BKT theory is proposed, which is based on straightforward physical ideas and takes the points mentioned above into consideration. A geometric correction, which avoids the diverging density, is employed. For the derivation of the screening of the intra-pair interaction, we start from an exact expression of linear response theory and then take the polarization of the vortex system and local field effects into account. We end up with higher order terms in both Kosterlitz equations. These terms are compared with the predictions mentioned above and the generalized equations are discussed. It is shown that these equations describe the vortex system even in a significant temperature range above the transition.

2 Geometric correction at high pair density

Let $\nu(r) \, dr$ be the areal density of vortex-antivortex pairs of sizes between $r$ and $r + dr$. Then the total density of pairs is

$$ n = \int_{r_0}^{\infty} \, dr \, \nu(r), $$

where $r_0$ is the minimum pair size, which is of the order of the Ginzburg-Landau coherence length.

The BKT ansatz for the pair density is

$$ \nu(r) \, dr = \frac{N_0^2}{r^2} \, 2\pi r \, dr \, \exp(-2\beta E_c) \exp[-\beta V_{\text{eff}}(r)], $$

where $N_0$ is the number of possibilities to place a vortex in an area $r^2$, $\beta = 1/T$ is the inverse temperature (we set $k_B = 1$ throughout the paper), $E_c$ is the core energy of a vortex and $V_{\text{eff}}$ is the effective intra-pair interaction. The expression for the pair density contains a geometric factor $2\pi r \, dr$, which represents the area of the circular ring in which the separation vector resides, and a Boltzmann factor $\exp(-\beta[2E_c + V_{\text{eff}}(r)])$, which contains the energy of the pair.

We now understand why the total density diverges for $T > T_c$. In this temperature regime we expect the effective interaction to be screened, i.e. $\lim_{r \to \infty} V_{\text{eff}}(r) = \text{const}$. Thus $\nu(r) \, dr \propto r \, dr$ for large $r$. Equation (1) then implies that the total density $n$ diverges with the system size squared. As noted above, this result cannot be correct since the energy of a pair is at least $2E_c > 0$. Hence, an important effect must have been neglected in Eq. (2). As explained in the following, the error lies in the enumeration of pairs.
The idea of BKT theory is to group the vortices and antivortices into neutral pairs and to describe the interaction between different pairs through the renormalization of the intra-pair interaction. However, we must not group the vortices and antivortices arbitrarily. For the approximation to be best justified, we must form pairs as small as possible. We now imagine that we fill the system with pairs, starting from the smallest ones (of size $r_0$). The probability that we add a pair of size $r$ contains the geometric term and the Boltzmann factor present in Eq. (2). Furthermore, we must make sure that the enumeration remains consistent. If we placed the vortex of the new pair closer than a distance $r'$ to the antivortex of another pair, where $r'$ is the size of the latter pair, the new vortex and the old antivortex should be considered a pair. In that case, we would have miscounted the pairs. Our ansatz is to introduce an additional factor in the density, which denotes the probability that the pairs are placed properly. This probability is determined by the distribution of the smaller pairs already present.

A new pair of size $r$ be tentatively placed anywhere in the system. The probability that the new vortex is not placed closer than $r'$ to the antivortex of any pair of size $r'$ is $1 - \nu(r') / \pi r'^2$, since $\nu(r') / \pi r'^2$ is the density of such pairs. The probability that the new vortex is not placed closer than $r'$ to the antivortex of any pair of size $r' < r$ is then given by

$$\prod_{r' < r} \left[1 - \nu(r') / \pi r'^2\right] = \prod_{r' < r} \exp \left[-\nu(r') / \pi r'^2\right]$$

$$= \exp \left[-\pi \int_{r_0}^{r} dr' r'^2 \nu(r')\right].$$

(3)

The probability that the placement of the new pair does not violate the enumeration rule is just the square of the last expression since a corresponding condition must be satisfied for the antivortex. Thus we obtain

$$\nu(r) dr = \frac{N_0^2}{r_0} 2\pi r dr \ exp(-2\beta E_c) \ exp[-\beta V_{\text{eff}}(r)]$$

$$\times \exp \left[-2\pi \int_{r_0}^{r} dr' r'^2 \nu(r')\right]$$

(4)

instead of Eq. (2).

This integral equation for $\nu(r)$ can be solved by transformation into a differential equation for $Y(r) = \int_{r_0}^{r} dr' r'^2 \nu(r')$. The solution is

$$\nu(r) = \frac{2\pi r n^* \ exp[-\beta V_{\text{eff}}(r)]}{1 + 4\pi^2 n^* \int_{r_0}^{r} dr' r'^3 \ exp[-\beta V_{\text{eff}}(r)]},$$

(5)

where $n^* = N_0^2 / r_0^4 \ exp(-2\beta E_c)$.
However, Eq. (4) is more suitable for the derivation of the corresponding generalized Kosterlitz equation. Employing the fugacity

\[ y(r) = \sqrt{\frac{r^3 \nu(r)}{2\pi}} \]  

(6)

and the logarithmic length scale \( l = \ln(r/r_0) \) as defined in the BKT theory, we obtain, by taking the logarithm of Eq. (4) and differentiating with respect to \( l \),

\[ \frac{dy}{dl} = \left( 2 - \beta \frac{dV_{\text{eff}}}{dl} \right) y - 2\pi y^3. \]  

(7)

Defining the dielectric constant as the ratio of bare and effective forces,

\[ \epsilon = \frac{dV/dr}{dV_{\text{eff}}/dr} = \frac{dV/dl}{dV_{\text{eff}}/dl}, \]  

(8)

assuming a logarithmic form of the potential, \( V = q^2 \ln(r/r_0) = q^2 l \), and defining the stiffness constant of BKT theory by

\[ K(l) = \frac{\beta q^2}{2\pi \epsilon(l)} \]  

(9)

we eventually find

\[ y' = (2 - \pi K)y - 2\pi y^3. \]  

(10)

This equation contains the additional term \(-2\pi y^3\) as compared with the original Kosterlitz equation. The corresponding initial condition,

\[ y_0 = y(l = 0) = N_0 \exp(-\beta E_c), \]  

(11)

is the same as in BKT theory since the geometric correction results in a factor of unity in Eq. (4) for the smallest pairs.

The additional term in Eq. (10) is proportional to \( y^3 \) as predicted by Halperin [8]. It is also of the same form and has the same sign as the term found by Amit et al. [10]. Note that the notation of Ref. [10] differs from the usual one of BKT theory [8]. The implications of this term are discussed in Sec. 4. Here, we only note that since \( y \geq 0 \) by definition and \( y' < 0 \) for sufficiently large \( y \), the fugacity \( y \) is bounded for any \( K \), whereas \( y \) diverges for \( T > T_c \) in the original BKT theory. Equation (10) then implies that the density \( \nu \) falls off at least as fast as \( r^{-3} \) for large \( r \) so that the total density \( n \) also remains finite.

3 Polarization and local field correction

The question arises of whether higher order terms have also to be included in the second Kosterlitz equation in order to consistently describe higher vortex
densities. To address this question we first rederive the equation for the stiffness coefficient $K$ starting from linear response theory and then discuss the necessary changes due to finite vortex densities. In the present section we use the language of the Coulomb gas model, i.e., we view the vortices as charged hard-core particles interacting via the two-dimensional Coulomb potential $V = q^2 \ln(r/r_0)$.

In linear response theory the dielectric function $\varepsilon(k) = V(k)/V_{\text{eff}}(k)$ is derived,

$$\frac{1}{\varepsilon(k)} = 1 - \frac{2\pi\beta}{k^2} g(k), \quad (12)$$

where $g(k)$ is the Fourier transform of the charge (vorticity) density correlation function,

$$g(r) = \langle \rho(0) \rho(r) \rangle. \quad (13)$$

The macroscopic dielectric constant is defined as

$$\frac{1}{\varepsilon_{\infty}} \equiv \lim_{k \to 0} \frac{1}{\varepsilon(k)}. \quad (14)$$

Assuming that $1/\varepsilon_{\infty}$ is finite, we see from Eq. (12) that $\lim_{k \to 0} g(k)$ and $\lim_{k \to 0} \frac{dg(k)}{dk}$ have to vanish so that $\varepsilon_{\infty}$ is finite.

$$\frac{1}{\varepsilon_{\infty}} = 1 - 2\pi \beta \frac{1}{2} \left. \frac{d^2 g}{dk^2} \right|_{k \to 0}$$

$$= 1 - \pi \beta \int d^2 r \ g(r) \left. \frac{d^2}{dk^2} e^{-ik \cdot r} \right|_{k \to 0}$$

$$= 1 + \pi \beta \int r^2 \ g(r) \ r^2 \cos^2 \phi$$

$$= 1 + \pi \beta \int r^3 g(r). \quad (15)$$

Here, we always have $1/\varepsilon_{\infty} < 1$.

One now defines a scale-dependent dielectric constant $\varepsilon(r)$,

$$\frac{1}{\varepsilon(r)} = 1 + \pi \beta \int_{r_0}^r dr' \ r'^3 g(r'), \quad (16)$$

which includes the contribution of pairs of sizes $r' \leq r$ only. Since we employ a hard-disk model we have introduced a lower cut-off $r_0$ in the integral. Note that $\varepsilon(r)$ is not the Fourier transform of $\varepsilon(k)$ as given by Eq. (12).

Since the correlation function $g$ is not known exactly we need an approximation for this quantity. As discussed above, we can always decompose the vortex system into neutral pairs. We expect the correlation function to consist of three terms: (a) A $\delta$-function term denoting the autocorrelation. This term is irrelevant because of the lower cut-off $r_0$. (b) A term from the partner of
the test vortex, which should be proportional to the pair size distribution \( \nu(r) \).

c) A term from the polarization of the other pairs. Here, we make the usual assumption that only smaller pairs are polarized in the field of a large one \[6\].

Neglecting the autocorrelation term, we write

\[
g(r) = g_{\text{pair}}(r) + g_{\text{pol}}(r).
\]

The relation between \( g_{\text{pair}} \) and the pair density \( \nu \) is given by

\[
g_{\text{pair}}(r) = -\frac{q^2 \nu(r)}{\pi r},
\]

(18)

taking into account that \( \nu \) has already been integrated over the angle. To determine \( g_{\text{pol}} \) we employ a dielectric approximation. We assume that the smaller pairs form a dielectric gas characterized by the dielectric constant \( \epsilon(r) \), which is to be obtained self-consistently. The appearance of \( \epsilon(r) \) instead of \( \epsilon_{\infty} \) is a result of the approximation that only pairs smaller than \( r \) contribute to the screening.

If two test charges, \( q \) at 0 and \( -q \) at \( r' \), are brought into a neutral medium with dielectric constant \( \epsilon(r') \), the total charge density, including the polarization charges, is given by

\[
\rho_t(r) = \frac{q}{\epsilon(r')} \delta(r) - \frac{q}{\epsilon(r')} \delta(r - r').
\]

(19)

In the present approach the effect of screening is to reduce the charges of a pair of size \( r \) to the effective values \( \pm q/\epsilon(r) \). Thus, the effect of screening on the correlation function can be expressed as

\[
g(r) = g_{\text{pair}}(r) + g_{\text{pol}}(r) = -\frac{q^2 \nu(r)}{\pi r \epsilon^2(r)}.
\]

(20)

From Eq. (16) we get

\[
\frac{1}{\epsilon(r)} = 1 - \pi \beta q^2 \int_{r_0}^{r} dr' \frac{\nu(r')}{\epsilon^2(r')},
\]

(21)

Employing the definitions (6) and (9), we obtain

\[
\frac{2\pi K}{\beta q^2} = 1 - \frac{8\pi^4}{\beta q^2} \int_0^l dl' g^2(l') K^2(l')
\]

(22)

and, after differentiating with respect to \( l \),

\[
K' = -4\pi^3 g^2 K^2.
\]

(23)

This equation is identical to the one obtained in BKT theory.

In the above considerations the smaller vortex-antivortex pairs are treated as a continuous polarizable medium. In particular, local field effects are neglected
in the correlation function given by Eq. (20). Consequently, the dielectric constant of Eq. (21) does not include these effects, either. Here, we employ a Clausius-Mossotti type formula to obtain a better approximation for $\epsilon$. In two dimensions the relation between the dielectric constant neglecting local field effects, $\epsilon_a$, and the full dielectric constant $\epsilon$ is given by

$$\epsilon = 1 + \frac{\epsilon_a}{3 - \epsilon_a}. \quad (24)$$

Taking $\epsilon_a$ from Eq. (16) we thus make the ansatz

$$\frac{1}{\epsilon(r)} = \frac{1 + \frac{3\pi}{2} \beta \int_{r_0}^r dr' r'^3 g(r')}{1 + \frac{\pi}{2} \beta \int_{r_0}^r dr' r'^3 g(r')} = \frac{1 - \frac{3\pi}{2} \beta q^2 \int_{r_0}^r dr' r'^2 \nu(r')/\epsilon^2(r')}{1 - \frac{\pi}{2} \beta q^2 \int_{r_0}^r dr' r'^2 \nu(r')/\epsilon^2(r')} \quad (25)$$

where $g(r)$ is not the (unknown) exact correlation function, but the one without local field corrections, Eq. (20). Inserting the definitions (6) and (9) and expanding for small $y$, we obtain

$$K = \frac{\beta q^2}{2\pi} \left[ 1 + \frac{8\pi^4}{\beta q^2} \int_0^l dl' y^2(l') K^2(l') \right]^2. \quad (26)$$

Differentiation yields

$$K' = -4\pi^3 y^2 K^2 \left[ 1 + \frac{8\pi^4}{\beta q^2} \int_0^l dl' y^2(l') K^2(l') \right]. \quad (27)$$

This expression is similar to the predicted one [8, 9]: The second term on the right hand side is of fourth order in $y$. However, it is not simply proportional to $y^4$. Note that this result is qualitatively different from the one of Amit et al. [10].

These authors effectively perform an expansion for a different small parameter, namely $K - 2/\pi$ instead of $y$, which makes direct comparison difficult.

To second order in $y$, the term in brackets in Eq. (27) is given by $2 - 2\pi K / \beta q^2$, as can be seen from Eq. (20). Thus we find, to fourth order in $y$,

$$K' = -4\pi^3 y^2 K^2 \left( 2 - \frac{2\pi K}{\beta q^2} \right). \quad (28)$$

For pairs of minimum size $r_0$ there is no screening ($\epsilon = 1$) and, therefore, the initial condition reads

$$K_0 \equiv K(l = 0) = \frac{\beta q^2}{2\pi}. \quad (29)$$
Equation (28) can thus be rewritten as
\[ K' = -4\pi^3 y^2 K^2 \left( 2 - \frac{K}{K_0} \right). \] (30)

4 Discussion of the generalized equations

The generalized Kosterlitz equations now have the form
\[ K' = -4\pi^3 y^2 K^2 \left( 2 - \frac{K}{K_0} \right), \] (31)
\[ y' = (2 - \pi K) y - 2\pi^2 y^3, \] (32)

together with the initial conditions given by Eqs. (11) and (29). We proceed to discuss these equations. Note that the equation for \( K' \) contains the initial value \( K_0 = q^2/2\pi T \) as an additional parameter so that the derivatives at a point \((K, y)\) are not exclusively determined by \( K \) and \( y \), as opposed to the original BKT theory.

We are interested in the behaviour of Eqs. (31) and (32) on large length scales, \( l \rightarrow \infty \). The equations have an attractive fixed point at \( K = 0, y = 1/\pi \) and an attractive line of fixed points at \( K \geq 2/\pi, \ y = 0 \). The first fixed point corresponds to a screened interaction at large distances \( (K \rightarrow 0) \); it is the high-temperature fixed point. Contrary to BKT theory, however, where this fixed point is at \( K = 0, \ y = \infty \), the fugacity remains finite. We note here that our approach, which essentially treats all vortices as bound in pairs and thus has no free vortices, predicts the correct, metallic form of screening for the high-temperature phase. Of course one has to check whether the decomposition of the vortex system into pairs is justified for \( T > T_c \). This is done below. The line of fixed points corresponds to a vanishing density of large pairs \( (y \rightarrow 0) \) together with a logarithmic interaction at large distances \( (K \text{ remaining finite}) \). This is the bound-pair phase.

In BKT theory analytical expressions for the trajectories, i.e., for the curves \((K(l), y(l))\), can be found. The same is not true for Eqs. (31) and (32). However, these equations are not difficult to integrate numerically. Since the equations contain the additional parameter \( K_0 \), every initial point now defines its own trajectory. In Fig. 1 trajectories for \( E_c/q^2 = 0.5 \) and several temperatures (thin solid lines) as well as for \( E_c/q^2 = 0.2 \) and several temperatures (dashed lines) are plotted. The dotted lines denote curves of initial values for \( E_c/q^2 = 0.2 \) and \( E_c/q^2 = 0.5 \), respectively, and varying \( T/q^2 \). The trajectories are shown in \( K-y \) space instead of the more usual \( x-y \) space, where \( x = -1 + 2/\pi K \), to emphasize the high-temperature behaviour. The trajectories in \( x-y \) representation are similar to the ones of standard BKT theory.

An important question is which initial values belong to which phase, or put mathematically, which points belong to the basin of attraction of the high-temperature fixed point and of the line of low-temperature fixed points, respectively.
As in the original BKT theory, the two basins of attraction are separated by the initial values which flow to \( K = 2/\pi, \ y = 0 \) in the limit \( l \to \infty \). These points form the so-called separatrix, which can be obtained numerically and is shown in Fig. 1 as the thick solid line. The separatrix is found to lie below the BKT result, i.e., the high-temperature phase is stabilized. This result is not surprising since local field effects tend to increase \( \epsilon \), thereby weakening the renormalized vortex interaction.

Although the trajectories themselves cannot be obtained analytically, limiting forms of the separatrix and the leading temperature dependence of \( K_\infty = K(l \to \infty) \) for \( K_0 \approx 2/\pi \) and \( y \ll 1 \) can be deduced from the recursion relations (31) and (32). First, we consider the renormalized stiffness coefficient \( K_\infty \). For \( T > T_c \), the flow is to the high-temperature fixed point and we have \( K_\infty = 0 \).

At the transition we recover the universal value \( K_\infty = 2/\pi \) of BKT theory. To find the behaviour for \( T < T_c \), we consider Eqs. (31) and (32) to leading order only,

\[
K' = -16\pi y^2, \tag{33}
\]

\[
(y^2)' = -2\pi y^2 \left( K - \frac{2}{\pi} \right). \tag{34}
\]

These equations lead to

\[
K'' = -2\pi K' \left( K - \frac{2}{\pi} \right) \tag{35}
\]

with the initial conditions \( K(0) = \beta q^2 / 2\pi \) and \( K'(0) = -16\pi y_0^2 \). The solution is

\[
K = \frac{2}{\pi} + \sqrt{C/\pi} \coth \left( \sqrt{\pi C l + \arcoth \left( \sqrt{\pi C \left( K_0 - \frac{2}{\pi} \right) / C \right)} \right) \tag{36}
\]

with \( C = \pi(K_0 - 2/\pi)^2 - 16\pi y_0^2 \). In the limit \( l \to \infty \) we thus obtain

\[
K_\infty = \frac{2}{\pi} + \sqrt{\left( K_0 - \frac{2}{\pi} \right)^2 - 16y_0^2}. \tag{37}
\]

We know from the analysis of the fixed points that \( K_\infty = 2/\pi \) at \( T = T_c \). Therefore, to the present order the radicand in Eq. (37) vanishes at the transition. To the same order we thus find

\[
y_0 \cong \frac{1}{4} \left( K_0 - \frac{2}{\pi} \right) \tag{38}
\]

as the limiting form of the separatrix, which is the same result as given by BKT theory.
From the initial conditions (11) and (29) we see that the leading temperature
dependence of the radicand in Eq. (37) is linear so that

\[ K_\infty \approx \frac{2}{\pi} + 4 \sqrt{\frac{B}{q^2}} \left( T_c - T \right) \]

for small \( T_c - T \geq 0 \). Here, \( B \) is some function of the core energy independent
of temperature. Equation (39) also has the same form as in BKT theory. The
typical square-root cusp and the universal jump are thus left unchanged by
the higher order terms.

The same is true for the typical length scale \( \xi_+ \), which is interpreted as the
correlation length of the superconducting order parameter. This length is also
used as the aforementioned cut-off in BKT theory. Here, it does not have such
a significance and we only discuss it for completeness. We define this quantity
as the length scale on which the trajectories start to be drawn towards the high-
temperature fixed point, i.e., we define \( K(r = \xi_+) = 2/\pi \). The length scale \( \xi_+ \)
thus diverges for \( T \to T_c \) from above. For \( T < T_c \) the high-temperature fixed
point never comes into play and we have \( \xi_+ = \infty \). Under the same assumptions
as above and starting again from Eqs. (33) and (34) we find

\[ \ln \frac{\xi_+}{r_0} \approx \frac{1}{\pi \sqrt{16y_0^2 - (K_0 - 2/\pi)^2}}. \]  

Since the radicand is again linear in \( T \) to leading order, we reobtain the BKT
result

\[ \xi_+ \approx r_0 \exp \left( \frac{b q}{\sqrt{T - T_c}} \right) \]

for small \( T - T_c > 0 \) with \( b \) independent of temperature.

The stability of the well-established predictions for \( K_\infty \) and \( \xi_+ \) in the presence
of higher order terms lends additional support to the general concept of
BKT. As far as these quantities are concerned, however, both the original the-
ory and the extension presented here are in agreement with experiment. Thus,
experiments such as measurements of the current-voltage characteristics of superconducting films, which effectively measure \( K \), cannot distinguish between the
two approaches.

Such a distinction may be possible, however, using the total pair density \( n \).
In Sec. 2 we already mentioned that \( y \) is bounded in the present case and that,
therefore, \( n \) must remain finite. We now discuss this point in more detail.

From Eqs. (6) and (3) the total density in natural units is given by

\[ nr_0^2 = 2\pi \int_0^\infty dl \, e^{-2ly^2(l)}. \]

This integral cannot be evaluated analytically since \( y^2(l) \) is unknown. One can,
however, obtain a rigorous statement concerning the continuity of \( n \). Substitution of \( u = e^{-l} \) for \( l \) yields

\[
n r_0^2 = 2\pi \int_0^1 du \, u y^2(u).
\]

In this expression, \( y^2 \) is a continuous function of \( l \), and thus of \( u \). Furthermore, \( y^2 \) is a smooth, i.e. arbitrarily often differentiable, function of the initial values \( K_0 \) and \( y_0 \) for any finite \( l \), see Fig. 1. Thus \( y^2 \) is a smooth function of temperature for finite \( l \) \((u > 0)\). On the other hand, \( y^2 \) is not a smooth, or even continuous, function of \( T \) for \( l = \infty \) \((u = 0)\) since it has a jump at \( T_c \). The integrand in Eq. (43), however, is smooth in \( T \) even for \( u = 0 \). Thus we have an integral over a finite interval over a function that is continuous in the integration variable and smooth in the external parameter \( T \). Under these suppositions the integral \( n r_0^2 \) is a smooth function of temperature even at the transition. This behaviour is connected with the observation that the phase transition is of infinite order [8].

This result is in agreement with BKT theory, where, however, one has to introduce a cut-off \( \xi^+ \) to obtain it. Since the definition of \( \xi^+ \) is somewhat arbitrary, as discussed in Sec. 1, the argument given here appears to be based on firmer grounds.

To obtain numerical results for the total density \( n \), the generalized Kosterlitz equations (31) and (32) are integrated numerically up to \( l = 20 \), corresponding to a system size of \( e^{20} r_0 \), for various values of \( T/q^2 \) and \( E_c/q^2 \). We assume \( N_0 = 1 \). The results for \( y \) are used to approximate the integral in Eq. (42). The results are plotted in Fig. 2. As expected, the density increases with temperature and decreases with increasing core energy. Note that the approach presented here is not limited to \( T/q^2 < 1/4 \), where \( 1/4 \) is the maximum value of \( T_c/q^2 \). The density starts to increase below \( T_c \), but the larger part of the increase takes place above \( T_c \). As expected, there is no feature at \( T_c \) (open circles in Fig. 2). For high temperatures the density saturates. This saturation and in fact the convergence of the density for \( T > T_c \) are due to the geometric correction of Sec. 2. The temperature dependence of the total density is, in principle, experimentally accessible through, e.g., flux noise [20] and NQR [21] measurements on superconducting films.

One may ask whether the theory is still applicable for \( T > T_c \), where the average pair size approaches the typical distance between neighboring pairs. If both quantities are of the same order the decomposition of the vortex system into small pairs becomes meaningless. To address this issue we compare the pair separation \( r_p \) with the average pair size \( \langle r \rangle \). The pair separation is just \( r_p = 1/\sqrt{n} \). The pair size is

\[
\langle r \rangle = \frac{1}{n} \int_{r_0}^{\infty} dr \, r \nu(r) = r_0 \int_{r_0}^{\infty} dl \, \frac{e^{-l} y^2(l)}{\int_{r_0}^{\infty} dl \, e^{-2l} y^2(l)}.
\]

(44)
This quantity can be calculated similarly to the pair density. The result for 
$E_c/q^2 = 0.5$ is depicted in Fig. 3. The important point is that $(r)$ (dashed line) 
remains small compared to $r_p$ (solid line) even in a significant temperature range 
above $T_c$. In this regime large pairs are “broken” in the sense that the interaction 
takes on a screened form for large distances, but nevertheless the pairs do not 
overlap considerably and the decomposition of the vortex system into pairs is 
justified. Therefore, the theory is applicable in the proximity of $T_c$, in addition 
to the low-temperature phase. The inset of Fig. 3 shows the corresponding 
quantities for $E_c/q^2 = 0.05$. One sees that the range of applicability for $T > T_c$ 
is narrower in this case, but it still exists.

We thus have reason to believe that the extended theory is valid in a temperature 
interval around $T_c$ for arbitrary core energy $E_c$, and, therefore, that the 
transition is of infinite order for any $E_c$. This result contradicts Refs. [13, 14, 15], 
which predict a first-order transition for small $E_c/q^2$. However, we cannot ex-
clude the possibility that terms of even higher order in the Kosterlitz equations 
bring about such a transition or that the expansion for small $y$ does not work 
at all for small $E_c/q^2$.

To conclude, straightforward physical models have been presented for higher 
order terms in the Kosterlitz equations. These terms are of a form similar, but 
not identical, to earlier predictions [3, 4]. A geometric correction, which ensures 
the correct enumeration of pairs, leads to the disappearance of the unphysical 
divergence of the total pair density for $T > T_c$. Starting from an exact ex-
pression for the dielectric constant, the polarization of the vortex system and 
local field effects are taken into account, leading to a stabilization of the high-
temperature phase. The behaviour of the stiffness constant and the correlation 
length close to $T_c$ is identical to the predictions of BKT theory so that ex-
periments on these quantities, e.g. measurements of the nonlinear resistance of 
superconducting films, cannot distinguish between the two approaches. The 
employment of the Clausius-Mossotti formula in Sec. 3 does not lead to easily 
testable predictions. However, it is comforting to know that the next higher 
order term in the equation for $K$ does not destroy the BKT behaviour. The 
enumeration rule of Sec. 2, on the other hand, leads to new quantitative predic-
tions for the total pair density even above $T_c$, which can, in principle, be tested 
by flux noise and NQR techniques. In short, it has been shown that the BKT 
approach can be extended in such a way that the temperature regimes below 
and above $T_c$ are treated on equal footing.

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References

[1] V. L. Berezinskii, Zh. Eksp. Teor. Fiz. 61 (1971) 1144 [Sov. Phys. JETP 34 (1972) 610].

[2] J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6 (1973) 1181.

[3] S. Scheidl and G. Hackenbroich, Phys. Rev. B 46 (1992) 14010; K. H. Fischer, Physica C 210 (1993) 179; M. Friesen, Phys. Rev. B 51 (1995) 632; S. W. Pierson, Phys. Rev. B 51 (1995) 6663; C. Timm, Phys. Rev. B 52 (1995) 9751.

[4] J. M. Kosterlitz, J. Phys. C 7 (1974) 1046.

[5] J. V. José, L. P. Kadanoff, S. Kirkpatrick and D. R. Nelson, Phys. Rev. B 16 (1977) 1217.

[6] A. P. Young, J. Phys. C 11 (1978) L453.

[7] P. Minnhagen, Rev. Mod. Phys. 59 (1987) 1001.

[8] B. I. Halperin, in Proceedings of Kyoto Summer Institute 1979—Physics of Low-Dimensional Systems, edited by Y. Nagaoka and S. Hikami (Publication Office, Prog. Theor. Phys., Kyoto) p. 53.

[9] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. 39 (1977) 1201.

[10] D. J. Amit, Y. Y. Goldschmidt and G. Grinstein, J. Phys. A 13 (1980) 585.

[11] M. Gabay and A. Kapitulnik, Phys. Rev. Lett. 71 (1993) 2138.

[12] See, e.g., C. Kittel, Introduction to Solid State Physics (John Wiley & Sons, New York, 1971).

[13] P. Minnhagen and M. Wallin, Phys. Rev. B 40 (1989) 5109.

[14] G.-M. Zhang, H. Chen and X. Wu, Phys. Rev. B 48 (1993) 12304.

[15] G.-H. Ding and B.-W. Xu, Phys. Rev. B 51 (1995) 12653.

[16] J. M. Caillol and D. Levesque, Phys. Rev. B 33 (1986) 499.

[17] J.-R. Lee and S. Teitel, Phys. Rev. Lett. 64 (1990) 1483; ibid. 66 (1991) 2100.

[18] P. Minnhagen, Phys. Rev. B 32 (1985) 3088.

[19] A. Alastuey and F. Cornu, J. Stat. Phys. 66 (1992) 165.

[20] C. T. Rogers, K. E. Myers, J. N. Eckstein and I. Bosovic, Phys. Rev. Lett. 69 (1992) 160.

[21] J. Appel, C. Timm and A. Zabel, J. Low Temp. Phys. 99 (1995) 553.
Figures

Figure 1: Trajectories of the generalized Kosterlitz equations \( \frac{E_c}{q^2} = 0.5 \) and varying \( \frac{T}{q^2} \) (thin solid lines), and for \( \frac{E_c}{q^2} = 0.2 \) and varying \( \frac{T}{q^2} \) (dashed lines). The separatrix is denoted by the thick solid line, the bound-pair phase is below that line. The dotted lines denote initial values \( (l = 0) \) for \( \frac{E_c}{q^2} = 0.2 \) and 0.5, respectively, and varying temperature.

Figure 2: The total pair density \( n \) as a function of \( \frac{T}{q^2} \) for \( \frac{E_c}{q^2} = 0.02, 0.05, 0.1, 0.2, 0.5, 1 \) (from left to right). The open circles denote the respective values of \( T_c/q^2 \) and the corresponding densities.

Figure 3: The average pair size \( \langle r \rangle \) (dashed line) and the average separation between neighboring pairs (solid line) for \( \frac{E_c}{q^2} = 0.5 \). The filled triangle denotes \( T_c \). The inset shows the same quantities for \( \frac{E_c}{q^2} = 0.05 \).
