Series of effective-field approximations and coherent anomaly in Kosterlitz-Thouless transitions

1994 J. Phys. A: Math. Gen. 27 2313

(http://iopscience.iop.org/0305-4470/27/7/013)

J. Phys. A: Math. Gen. 27 (1994) 2313–2323. Printed in the UK

Series of effective-field approximations and coherent anomaly in Kosterlitz–Thouless transitions

Xiao Hu
Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980, Japan

Received 12 October 1993

Abstract. A series of effective-field approximations are formulated for the Kosterlitz–Thouless transition in the sine–Gordon model by means of the cumulant expansion and the variational method. Effective-field essential singularities $\xi \sim \exp[\bar{\xi}_n(K_c^{[n]} - K)^{-1}]$ are obtained for the correlation length as first derived by Saito in a single approximation. However, a systematic variance of the effective-field critical coefficient $\bar{\xi}_n \sim 2\ln(J/2y_0)/(n+1)\pi$ is found when the order of approximation n increases. The true critical exponent $\bar{\nu}$ of the Kosterlitz–Thouless transition is thus revealed to be less than the effective-field exponent $\bar{\nu}_0$, $\bar{\nu} < \bar{\nu}_0 = 1$, from Suzuki's coherent-anomaly method. The phase transition in the two-dimensional XY model is studied from its relation to the sine–Gordon model. The critical exponent η_c of the spin–spin correlation function at the critical point is found to be $\eta_c = 1/(4 + 1/\pi^2)$.

1. Introduction

Several years ago, Suzuki proposed the coherent-anomaly method (CAM) in the field of critical phenomena [1]. The CAM approach provides non-classical estimates of critical exponents from a series of systematic mean-field (MF) approximations by relating the anomalous behavior of the MF critical coefficient $\bar{\chi}$, defined as

$$\chi \simeq \bar{\chi}(T - T_c)^{-\gamma_0} \qquad (1)$$

when the approximation is improved, to the true critical point and the critical exponent γ:

$$\bar{\chi} \simeq \mathcal{A}(T_c - T_c^*)^{-\gamma+\gamma_0}. \qquad (2)$$

Since then there has been a renewal of interest in effective-field (EF) type theory in critical phenomena with emphasis on the evaluation of the non-classical critical exponent. Efforts have been made on the construction of quickly convergent series of EF approximations and the CAM approach has achieved impressive successes [2, 3]. What seems to be lacking, however, is a study of the applicability of CAM to topological phase transitions.

Since topological orders such as vortices in the two-dimensional XY model [4, 5] cannot be defined in a local region, an MF theory is not straightforward. The ordinary self-consistency formalism by the cluster-decoupling of the relevant Hamiltonian produces a fictitious order parameter, contrary to an analytical theorem [6] and to the results from other approaches [4, 5, 7–13]. Essential singularities of the correlation length and susceptibility in the Kosterlitz–Thouless (KT) type transitions cannot be derived with the naive MF theory, either.

A couple of attempts have been made to grasp the essence of topological phase transitions within an EF scheme [14, 15]. Saito has constructed an EF theory for the roughening phase transition in a crystal-surface system in terms of the sine–Gordon (SG)

0305-4470/94/072313+11$19.50

model by combining the cumulant expansion with the variational method [15, 16]. He was able to obtain an essential singularity denoted by $\tilde{\nu}_0 = 1$ for the correlation length. This EF value $\tilde{\nu}_0 = 1$ differs from the results by other approaches [4, 5, 7–13]. On the other hand, his estimate for the critical exponent $\eta_c = \frac{1}{4}$ of the spin–spin correlation function at the critical point for the *XY* model coincides with the results by RG [7–10].

Our interest is then two-fold. Firstly, we want to clarify the behaviour of Saito's EF theory when higher-order cumulants are taken into account. In this way we may see why the EF value $\tilde{\nu}_0$ differs from the results by other approaches. Secondly, if the EF theory can be extended to a series of approximations, we apply the CAM analysis to derive non-classical estimates of critical exponents. In the present paper we perform cumulant expansion to higher orders and show how a coherent anomaly appears when the terms proportional to the small parameter y_0/J or its square power in higher-order cumulants are taken into account [17].

The series of EF approximations are formulated for the roughening transition in the crystal-surface system in section 2. Section 3 is devoted to study of the *XY* model. Discussions and summary are given in section 4.

2. KT transition in the crystal-surface system

We study the sine–Gordon Hamiltonian for the roughening transition in the crystal-surface system [15, 16],

$$\mathcal{H}_{sG} = J/2\sum_{i,\delta}(h_i - h_{i+\delta})^2 + y_0\sum_i(1-\cos 2\pi h_i) \tag{3}$$

where h_i's are continuous height variables, δ denotes unit vectors and y_0 is positive. The second term, proportional to y_0, preserves the periodicity of the variables in the discrete Gaussian (dG) model which is shown to be equivalent to the Villain model, Coulomb gas model and the *XY* model [10, 18, 19, 15]. The height-variables in the above sine–Gordon Hamiltonian correspond to the magnitudes of vortices in the *XY* model. In the present system, topological effects can be taken into account more easily. Since the positive parameter y_0 is included to restore the symmetry of the dG model, it may be treated as a small parameter compared with the strength of interaction J [15].

We evaluate the free energy of the above system by the cumulant expansion

$$F = F_e - k_B T\sum_{n=1}^{\infty}\frac{(-1/k_BT)^n}{n!}\langle(\mathcal{H}-\mathcal{H}_e)^n\rangle_c \tag{4}$$

around the diagonalized effective Hamiltonian

$$\mathcal{H}_e = k_BT/2\sum_q G^{-1}(q)h_q h_{-q} \tag{5}$$

where $F_e = -k_BT\ln\mathrm{Tr}\exp[-\mathcal{H}_e/k_BT]$ and $\langle Q^n\rangle_c$ is the nth cumulant of Q under $\mathcal{H}_e$. The Green function $G(q)$ in the above effective Hamiltonian is arbitrary, provided that the infinite summation is completed. It serves as a variational parameter for approximations, as will be seen in the following.

Terminating the above cumulant expansion at the first order, one arrives at the following approximate free energy [15, 16]:

$$F_1/k_BT = -\tfrac{1}{2}\sum_q \ln 2\pi G(q) + \tfrac{1}{2}\sum_q\left[\frac{G(q)}{G_0(q)} - 1\right] + N\frac{y_0}{k_BT}\left[1 - e^{-2\pi^2\bar{G}(0)}\right] \tag{6}$$

where $G_0^{-1}(q) \simeq q^2/K$ with $K = k_B T/2J$ and $\tilde{G}(r) = 1/N \sum_q G(q) e^{iqr}$.

In order to make the free energy (6) a good approximation to the true one of the sine–Gordon system, we resort to the variational method with respect to the Green function $G(q)$ in (6). Then, one obtains the following equation for $G(q)$:

$$G(q)^{-1} = G_0(q)^{-1} + (2\pi)^2 \frac{y_0}{k_B T} e^{-2\pi^2/N \sum_p G(p)} . \tag{7}$$

The solution to the above equation minimizes the approximate free energy (6). It is readily seen that the Green function should have the Ornstein–Zernike form $G(q) = K/(q^2+\xi^{-2})$. Since

$$\frac{1}{N}\sum_p G(p) = \frac{1}{N}\sum_p \frac{K}{p^2+\xi^{-2}} = \frac{K}{(2\pi)^2}\iint_{-\pi}^{\pi} \frac{d^2 p}{p^2+\xi^{-2}} \simeq \frac{K}{4\pi}\ln[(\pi\xi)^2+1] \tag{8}$$

one obtains from (7) the following equation for the correlation length ξ [16]:

$$(\pi\xi)^2 = \frac{J}{2y_0}[(\pi\xi)^2+1]^{\pi K/2} . \tag{9}$$

This equation shows a bifurcation around $K_c = 2/\pi$ and the critical behaviour for ξ is

$$\xi \sim \begin{cases} \infty & K > K_c \\ \exp\left[\dfrac{(\ln J/2y_0)/\pi}{K_c - K}\right] & K < K_c . \end{cases} \tag{10}$$

The critical exponent defined by $\xi \sim \exp[a(K_c - K)^{-\tilde{\nu}}]$ is $\tilde{\nu}_0 = 1$ [15, 16].

The above formalism is an EF theory and it is successful in understanding the essential singularity, or exponential singularity, of the correlation length in topological phase transitions [15, 16]. However, the value of critical exponent $\tilde{\nu}_0 = 1$ is different from the RG result $\tilde{\nu} = \frac{1}{2}$ [5, 7–9] which is supported by numerical simulations [11–13]. Therefore, it is important to investigate what will happen when one develops the above EF theory further to a series of approximations and whether it is possible to derive from them a non-classical exponent by means of Suzuki's CAM approach.

In order to show the difference between Saito's approximation reviewed briefly above and higher-order approximations, we present calculations for the second approximation in some detail.

We terminate the cumulant expansion (4) at the second order. The approximate free energy is then given by

$$\begin{aligned} F_2/k_B T = &-\frac{1}{2}\sum_q \ln 2\pi G(q) + \frac{1}{2}\sum_q \left[\frac{G(q)}{G_0(q)} - 1\right] + N\frac{y_0}{k_B T}[1 - e^{-2\pi^2 \tilde{G}(0)}] \\ &-\frac{1}{4}\sum_q \left[\frac{G(q)}{G_0(q)} - 1\right]^2 - \frac{N}{4}\left(\frac{y_0}{k_B T}\right)^2 \sum_r e^{-(2\pi)^2[\tilde{G}(0)-\tilde{G}(r)]} \\ &-2\pi^2 \frac{y_0}{k_B T} e^{-2\pi^2 \tilde{G}(0)} \sum_q G(q)\left[\frac{G(q)}{G_0(q)} - 1\right] . \end{aligned} \tag{11}$$

Instead of (7), we have in the present approximation the following self-consistency equation for the Green function $G(q)$ from the variational method:

$$\begin{aligned} &-\tfrac{1}{2}G^{-1}(q)\left[1 - \frac{G(q)}{G_0(q)}\right]^2 + 2\pi^2 \frac{y_0}{k_B T} e^{-2\pi^2 \tilde{G}(0)} \left\{2 - \frac{2}{N}\pi^2 \sum_p G(p)\left[1 - \frac{G(p)}{G_0(p)}\right]\right\} \\ &+\pi^2 \left(\frac{y_0}{k_B T}\right)^2 \sum_r e^{-(2\pi)^2[\tilde{G}(0)-\tilde{G}(r)]}(1 - e^{iqr}) = 0 . \end{aligned} \tag{12}$$

As in the first approximation, the solution $G(q)$ is also of the Ornstein–Zernike form $G(q) = x/(q^2 + \xi^{-2})$. However, the coefficient x of the Green function cannot be put as K in the present case. The third term in (12) yields a difference between x and K from its dependence on the wavenumber q. We remember that this term is derived from the second cumulant.

In order to clarify the relation between x and K, we bring $G(q) = x/(q^2 + \xi^{-2})$ into the above equation and put $\xi^{-1} = 0$ and $q \ll 1$. In this limit we obtain from (12)

$$-\frac{q^2}{2x}\left(1 - \frac{x}{K}\right)^2 + \frac{2q^2}{K} C_2(K)\left(\frac{y_0}{k_B T}\right)^2 = 0 \tag{13}$$

with

$$C_2(K) = \lim_{q\to 0} \frac{1}{q^2}\frac{\pi^2 K}{2} \sum_r \exp\left[-(2\pi)^2 \iint_{-\pi}^{\pi} \frac{d^2 p}{(2\pi)^2}\frac{K}{p^2}(1 - e^{ipr})\right](1 - e^{iqr}). \tag{14}$$

In the derivation of (13), we have neglected the difference between x and K in the third term of (12) since there is a prefactor of $(y_0/J)^2$ in that term and the difference only yields a higher-order correction. The discrepancy between x and K is then found to be

$$x = K - \sqrt{C_2(K)}\frac{y_0}{J} \tag{15}$$

from (13). Therefore, it is clarified that the square power of the small parameter y_0/J from the cumulants of orders higher than the first is necessary in order to derive the difference between x and K. It should be noticed that, although this discrepancy between K and x is proportional to the small parameter y_0/J, its contribution to the EF critical coefficient is significant since its derivative should be evaluated as shown in the following.

By putting $q = 0$ and taking $\xi^{-1} \ll 1$ in (12) we obtain the self-consistency equation for the correlation length near the critical point

$$\frac{\xi^{-2}}{x} = (2\pi)^2 \frac{y_0}{k_B T}\left[\frac{\xi^{-2}}{\pi^2 + \xi^{-2}}\right]^{\pi x/2}. \tag{16}$$

It is the same as (9) except for the replacement of K by x. As in the first approximation, the above equation bifurcates at $x_c = 2/\pi$,

$$\xi = \begin{cases} \infty & x > x_c \\ \dfrac{1}{\pi}\exp\left[\dfrac{(\ln J/2y_0)/\pi}{2/\pi - x}\right] & x < x_c. \end{cases} \tag{17}$$

The difference between x and K is once again neglected as a higher-order correction in the derivation of the coefficient on the right-hand side of (16). The integral

$$\frac{x}{(2\pi)^2}\iint_{-\pi}^{\pi} dq^2 \left[\frac{1}{q^2 + \xi^{-2}} - \frac{q^2}{(q^2 + \xi^{-2})^2}\right] \to \frac{1}{4\pi} \tag{18}$$

as $\xi^{-1} \to 0$ at $x = x_c = 2/\pi$ results in the very coefficient $(2\pi)^2 y_0/k_B T$ in (16) which is the same as the one in (9) for the first approximation. This invariance of the coefficient in the equation of the correlation length excludes the logarithmic dependence of the EF critical coefficient on the order of approximation and makes it possible to extrapolate the order of approximation to infinity, as will be revealed.

On the other hand, the difference between x and K has been kept in the exponent in (17) since the derivative of this difference with respect to K is necessary in the evaluation of the EF critical coefficient.

So long as the variational method is adopted, the critical exponent $\tilde{\nu}_0 = 1$ does not change even though the second-order cumulant is included. However, in order to explore fully the improvement of the EF approximation and to investigate the possibility of deriving the non-classical exponent from the present EF theory, we should compare the above two approximations in detail, namely we should study the coherent variances of the critical point and the EF critical coefficient [1]. For this purpose, we rewrite the singularity (17) of the correlation length in terms of K.

We first evaluate the critical point $K_c^{[2]}$ and $C_2(K_c^{[2]})$. Noting the asymptotic formula for the correlation functions at the critical point where $\xi^{-1}=0$

$$\iint_{-\pi}^{\pi} \frac{\mathrm{d}^2 p}{(2\pi)^2}\frac{K}{p^2}(1-\mathrm{e}^{\mathrm{i}pr}) \simeq \frac{K}{2\pi}\ln r + A \tag{19}$$

with $A=(\frac{3}{2}\ln 2+\gamma)/\pi^2$ and γ standing for the Euler constant, we have

$$C_2(K) = \frac{2}{\pi^2}\mathrm{e}^{-(2\pi)^2 A}\int_1^{\infty} r^{3-2\pi K}\mathrm{d}r \tag{20}$$

from (14). By bringing (15) into (20), we can determine $C_2(K)$ in terms of x. In particular, we have

$$\sqrt{C_2(K_c^{[2]})} = [\pi\mathrm{e}^{-(2\pi)^2 A}/4]^{1/3}\left(\frac{y_0}{J}\right)^{-1/3} \tag{21}$$

at the critical point $x_c = 2/\pi$. The critical point $K_c^{[2]}$ is then determined as

$$K_c^{[2]} = x_c + \sqrt{C_2(K_c^{[2]})}\frac{y_0}{J} \simeq \frac{2}{\pi} + 0.106\,838\,5\left(\frac{y_0}{J}\right)^{2/3} \tag{22}$$

in terms of (15).

It is interesting to notice that the discrepancy between x and K is linear with respect to the small parameter y_0/J off the critical region as in (15), while it is proportional to $(y_0/J)^{2/3}$ on the critical point. It will be revealed that the power of y_0/J in the relation between x_c and K_c varies according to the order of approximation.

We are now ready to transfer the parameter from x in (17) to K:

$$\xi = \begin{cases} \infty & K > K_c^{[2]} \\ \dfrac{1}{\pi}\exp\left[\dfrac{\bar{\xi}_2}{K_c^{[2]}-K}\right] & K < K_c^{[2]} \end{cases} \tag{23}$$

with the EF critical coefficient $\bar{\xi}_2$:

$$\bar{\xi}_2 = \frac{(\ln J/2y_0)/\pi}{\mathrm{d}x/\mathrm{d}K|_{K=K_c^{[2]}}} = \frac{(\ln J/2y_0)/\pi}{1-(y_0/2J)C_2'(K_c^{[2]})/\sqrt{C_2(K_c^{[2]})}}. \tag{24}$$

The derivative of $C_2(K)$ at the critical point with respect to K is also evaluated from (20) as

$$C_2'(K_c^{[2]}) = -\frac{\pi\mathrm{e}^{-(2\pi)^2 A}}{2K_c^{[2]}C_2(K_c^{[2]})(y_0/J)^2}. \tag{25}$$

It diverges as the small parameter y_0/J approaches zero. This is the origin of the anomalous variance of the EF critical coefficient in the present problem.

Incorporating (21) and (25) into (24), we arrive finally at the following simple expression for the EF critical coefficient:

$$\bar{\xi}_2 = \frac{2\ln J/2y_0}{3\pi}. \tag{26}$$

For comparison, we list the expressions for the critical point and the EF critical coefficient of the first approximation:

$$K_c^{[1]} = \frac{2}{\pi} \qquad \bar{\xi}_1 = \frac{2\ln J/2y_0}{2\pi} \tag{27}$$

and those of the second approximation:

$$K_c^{[2]} \simeq \frac{2}{\pi} + 0.106\,838\,5\left(\frac{y_0}{J}\right)^{2/3} \qquad \bar{\xi}_2 = \frac{2\ln J/2y_0}{3\pi}. \tag{28}$$

Therefore, the second cumulant yields the discrepancy between x and K as in (15), increases the critical point and reduces the EF critical coefficient.

In the present formalism, we can derive higher-order approximations by incorporating further high-order cumulants. Since the terms proportional to y_0/J produce the singularity and the terms proportional to the square power of y_0/J yield the discrepancy between x and K as revealed in the above arguments, it may be enough to pick up only the terms proportional to y_0/J and $(y_0/J)^2$ even in higher-order cumulants.

Within the approximation described above, the equation relating x and K is derived as

$$\frac{q^2}{2x}\left(1-\frac{x}{K}\right)^n = \frac{\pi^2(-K/2\pi)^{n-2}}{(n-2)!}\left(\frac{y_0}{k_BT}\right)^2\left(1-\frac{x}{K}\right)^{n-2} \times \sum_r e^{-(2\pi)^2[\tilde{G}(0)-\tilde{G}(r)]}[\tilde{G}(0)-\tilde{G}(r)]^{n-2}(1-e^{iqr}). \tag{29}$$

The factor $1/(n-2)!$ is the result of the cancellation between the factor $1/n!$ in the cumulant expansion (4) and the number $n!/2!(n-2)!$ of different ways to choose two vertices from a total of n, to establish the term $\exp\left(-(2\pi)^2[\tilde{G}(0)-\tilde{G}(r)]\right)$.

It is obvious from (29) that an approximation denoted by odd n is equivalent to the first approximation, since (29) has only the solution $x = K$ for odd n. Higher-order approximations are derived truncating the cumulant expansion (4) at orders of even numbers.

With the aid of the integral

$$\frac{1}{(2\pi)^2}\iint_{-\pi}^{\pi} dq^2 \frac{\xi^{-2m}}{(q^2+\xi^{-2})^{m+1}} \to \frac{1}{4m\pi} \tag{30}$$

as $\xi^{-1} \to 0$ for $m \geqslant 1$, we have been successful in showing that the self-consistency equation (16) for the correlation length remains the same within the approximation that the difference between x and K are neglected in the coefficient on the right-hand side of (16).

Noting the integral

$$\int_1^{\infty} r^{-1-\Delta}\ln^m r\,dr = \frac{m!}{\Delta^{m+1}} \tag{31}$$

we have obtained from (29)

$$\begin{aligned}\sqrt{C_n(K_c^{[n]})} &= \left(\frac{\pi^7\exp[-(2\pi)^2A]}{2^n\pi^{3n}}\right)^{1/(n+1)}\left(\frac{y_0}{J}\right)^{(1-n)/(1+n)} \\ C_n'(K_c^{[n]}) &= -(n-1)\sqrt{C_n(K_c^{[n]})}\left(\frac{y_0}{J}\right)^{-1}\end{aligned} \tag{32}$$

for the nth approximation with $n \geqslant 2$. These relations result in the following expressions for the critical point $K_c^{[n]}$ and the EF critical coefficient $\bar{\xi}_n$ for the nth approximation:

$$K_c^{[n]} = \frac{2}{\pi} + \left(\frac{\pi^7\exp[-(2\pi)^2A]}{2^n\pi^{3n}}\right)^{1/(n+1)}\left(\frac{y_0}{J}\right)^{2/(n+1)} \qquad \bar{\xi}_n = \frac{2\ln J/2y_0}{(n+1)\pi}. \tag{33}$$

Therefore, the EF critical coefficient $\bar{\xi}_n$ decreases systematically when the order of approximation n increases as seen in the second equation in (33).

Since $\bar{\xi}_n$ is defined by

$$\xi \sim \exp\left[\frac{\bar{\xi}_n}{(K_c^{[n]} - K)^{\tilde{\nu}_0}}\right] \tag{34}$$

the decreasing tendency of $\bar{\xi}_n$ suggests that the EF singularity is stronger than the true one. A systematic variance of the EF critical coefficient is related quantitatively to the true critical point K_c^* and the true exponent $\tilde{\nu}$ in the CAM scheme by

$$\bar{\xi}_n \simeq \mathcal{A}(K_c^* - K_c^{[n]})^{-\tilde{\nu}+\tilde{\nu}_0} \tag{35}$$

as reviewed briefly in section 1. Therefore, we are able to conclude $-\tilde{\nu} + \tilde{\nu}_0 > 0$, namely

$$\tilde{\nu} < 1\,. \tag{36}$$

This result is consistent with $\tilde{\nu} \simeq \frac{1}{2}$ by other methods [4, 5, 7–13].

Suppose that the expressions for $K_c^{[n]}$ and $\bar{\xi}_n$ in (33) are valid even for large value of n. Putting them into (35) and taking the limit $n \to \infty$, we arrive at

$$\tilde{\nu}_0 - \tilde{\nu} = 1 \qquad K_c^* = \frac{2}{\pi} + \frac{1}{2\pi^3} \tag{37}$$

and the amplitude $\mathcal{A} = 2\pi^2$. As $\tilde{\nu}_0 = 1$, the conclusion is as follows: $\tilde{\nu} = 0$, namely the essential singularity vanishes.

We notice, however, that in the present EF approximations we have treated only the terms proportional to y_0/J and $(y_0/J)^2$. The expressions for $K_c^{[n]}$ and $\bar{\xi}_n$ in (33) hold only up to a moderately large value of n of order of J/y_0, since terms proportional to y_0^m with $m > 2$ have been omitted, which may show an n-dependence of $n^{-\alpha}$ with α smaller than unity. Thus, in order to make conclusive estimation of the true critical exponent for the present topological phase transition by the CAM approach, terms proportional to higher powers of y_0/J in the cumulant expansion may be necessary. The improvement in this direction is beyond the content of the present paper and will be reported elsewhere.

3. KT transition in the *XY* model

The phase transition in the two-dimensional classical *XY* model

$$\mathcal{H}_{XY} = -\frac{J_{XY}}{2}\sum_{i,\delta}\cos(\theta_i - \theta_{i+\delta}) \tag{38}$$

is related to that in the crystal-surface system discussed in the preceding section [7, 10, 18, 16]. It is found by José *et al* [7] and Itzykson and Drouffe [10] that the spin–spin correlation function $\langle S(r_1)S(r_2)\rangle_{XY}$ in the *XY* model can be evaluated by the thermodynamic average of a set of variables $\{\eta_i\}$ defined in the dG system along a path from point r_1 to point r_2: $\eta_i = +1/-1$ if i site is a left/right neighbour of a site on the path and $\eta_i = 0$ otherwise. For simplicity, the path is chosen as the straight cut from r_1 to r_2. With this definition we have approximately [7, 16]

$$\langle\exp[\mathrm{i}(\theta_1 - \theta_2)]\rangle_{XY} \simeq \left\langle \exp\left[-\frac{1}{2K}|r_1 - r_2| + \frac{1}{K}\sum_i h_i(\eta_i^{\mathrm{l}} - \eta_i^{\mathrm{r}})\right]\right\rangle_{\mathrm{sG}} \tag{39}$$

where the thermodynamic average on the right-hand side is over the Hamiltonian (3) with $K = k_B T/2J = J_{XY}/k_B T_{XY}$. By rewriting the above equation into the following equivalent form:

$$\ln\langle\exp[\mathrm{i}(\theta_1-\theta_2)]\rangle_{XY} = -\frac{|r_1-r_2|}{2K} - \ln\left\langle\exp\left[-\frac{H_{sG}-H_e}{k_B T}\right]\right\rangle_e + \ln\left\langle\exp\left[-\frac{H_{sG}-H_e}{k_B T} + \frac{1}{K}\sum_i h_i(\eta_i^1-\eta_i^r)\right]\right\rangle_e \tag{40}$$

where the thermodynamic averages on the right-hand side are under Hamiltonian (5), we find that the correlation function can be evaluated by the following modified cumulant expansion:

$$\ln\langle e^{A+B}\rangle = \ln\langle e^B\rangle + \sum_{n=1}^{\infty}\frac{1}{n!}[(Ae^B)^n]_c \tag{41}$$

with $[Ae^B]_c = \langle Ae^B\rangle/\langle e^B\rangle, [(Ae^B)^2]_c = \langle A^2e^B\rangle/\langle e^B\rangle - \langle Ae^B\rangle^2/\langle e^B\rangle^2, [(Ae^B)^3]_c = \langle A^3e^B\rangle/\langle e^B\rangle - 3\langle A^2e^B\rangle\langle Ae^B\rangle/\langle e^B\rangle^2 + 2\langle Ae^B\rangle^3/\langle e^B\rangle^3$, etc. The transformation (40) for the correlation function makes it easier to construct approximations corresponding to those established in the preceding section and to use those results.

For simplicity, we concentrate our attention on the low-temperature phase of the *XY* model, since it corresponds to the rough phase of the sine–Gordon system where $\xi^{-1} = 0$. With some algebra one finds that the contribution from the nth cumulant for $n \geqslant 2$ is simply

$$\frac{(-1)^n}{n!K^2}\left(\frac{x}{k}-1\right)^n\sum_{k,l}(\eta_k^1-\eta_k^r)(\eta_l^1-\eta_l^r)\tilde{G}(r_k-r_l)\,. \tag{42}$$

We then derive from (40)

$$\ln\langle\exp[\mathrm{i}(\theta_1-\theta_2)]\rangle_{XY} \simeq -\frac{|r_1-r_2|}{2K} - \frac{1}{2K^2}\sum_{k,l}(\eta_k^1-\eta_k^r)(\eta_l^1-\eta_l^r)\tilde{G}(r_k-r_l) - \left(\frac{x}{K}-1\right)\frac{1}{2K^2}\sum_{k,l}(\eta_k^1-\eta_k^r)(\eta_l^1-\eta_l^r)\tilde{G}(r_k-r_l) \tag{43}$$

by omitting the higher orders of the difference between x and K in (42) for $n \geqslant 2$.

As far as the long-distance behaviour is concerned we have [7, 16]

$$\begin{aligned}\sum_{k,l}[\eta_k^1-\eta_k^r]\tilde{G}(r_k-r_l)[\eta_l^1-\eta_l^r] &\simeq -\iint \mathrm{d}r_k\,\mathrm{d}r_l[\Delta\tilde{G}(r_k-r_l)-\partial_\parallel^2\tilde{G}(r_k-r_l)] \\ &\simeq -\iint \mathrm{d}r_k\,\mathrm{d}r_l\Delta\tilde{G}(r_k-r_l)+2[\tilde{G}(r_1-r_2)-\tilde{G}(0)] \\ &\simeq -\iint \mathrm{d}r_k\,\mathrm{d}r_l[-K\delta(r_k-r_l)+\xi^{-2}\tilde{G}(r_k-r_l)]+2[\tilde{G}(r_1-r_2)-\tilde{G}(0)]\,.\end{aligned} \tag{44}$$

Thus, in the nth approximation the correlation function in the *XY* model assumes the following distance dependence at the corresponding critical point $K_c^{[n]}$:

$$\ln\langle\exp[\mathrm{i}(\theta_1-\theta_2)]\rangle_{XY} = -\frac{1}{2\pi K_c^{[n]}}\ln r \qquad r \gg 1 \tag{45}$$

where (19) is used. The square power of the difference between x and K has been neglected in the derivation of (45) from (43). Since there is no anomalous correction to the asymptotic formula (45) at all, the limit of the order of approximation $n \to \infty$ can be taken straightforwardly in the present case. Therefore, we arrive at the spin–spin correlation function

$$\langle S(r_1)S(r_2)\rangle_{XY} \sim |r_1 - r_2|^{-\eta_c} \tag{46}$$

with

$$\eta_c = \frac{1}{2\pi K_c^*} = \frac{1}{4 + 1/\pi^2} \tag{47}$$

for the XY model by incorporating K_c^* in (37) into (45). Our estimate of the critical exponent η_c is near to the RG value $\eta_c = \frac{1}{4}$ with a relative difference about 2.5%. The estimate made by Saito [16] from the first approximation is $\eta_c = \frac{1}{4}$.

It is readily seen that, for temperature $0 < T_{XY} \leqslant J_{XY}/k_B K_c^*$, the correlation function shows a power-law decay with respect to the distance. Thus, the present EF theory predicts correctly the absence of order parameter in the XY model [16].

Calculations have been carried out in the high-temperature phase in the higher-order approximations and we have found that the correlation length in the XY model ξ_M has the same singularity as that for the sine–Gordon system and we have obtained the following expression for the magnetic susceptibility:

$$\chi \sim \begin{cases} \infty & \text{for } K \geqslant K_c^* \\ \xi_M^{2-1/2\pi K_c^*} & \text{for } K < K_c^* \end{cases} \tag{48}$$

a result similar to that by Saito in terms of the first approximation [16]. The above critical behaviour is of course consistent with the results for the low-temperature phase.

4. Summary and discussion

We have studied Kosterlitz–Thouless-type transitions by means of a series of self-consistency approximations and Suzuki's coherent-anomaly method. We derive EF approximations by truncating the cumulant expansion of the free energy at successively higher orders and by the variational method. Although the variational principle cannot be proven generally, the present series of approximations are useful in the study of the true behaviour of the systems since higher-order cumulants are included one by one. The EF approximations yield the same essential singularity denoted by $\tilde{\nu}_0 = 1$ for the correlation length as first derived by Saito. However, we have discovered a systematic decrease in the EF critical coefficient $\bar{\xi}$ when the order of approximation increases. The origin of this coherent variance is the discrepancy between the coefficient of the variational Green function and the temperature, which comes from the second- and higher-order cumulants. Therefore, it is shown that besides the terms proportional to the small parameter y_0/J, which yield the phase transition and the EF essential singularity, the terms proportional to the square power of y_0/J are also of significant importance for the critical behaviour. The observed decrease in the EF critical coefficient implies that the true critical exponent is less than unity, $\tilde{\nu} < 1$, even within the scheme of EF theory. Terms proportional to higher powers of y_0/J may be necessary in order to derive numerical estimate for the true critical exponent $\tilde{\nu}$.

We have also investigated the critical phenomena of the two-dimensional XY model by using its relation with the sine–Gordon model. We have obtained an estimate $\eta_c = 1/(4 + 1/\pi^2)$ for the exponent of the spin–spin correlation function at the critical point. This value is close to the RG value $\eta_c = \frac{1}{4}$ with a relative difference about 2.5%.

The present approach is of theoretical importance for the study of topological phase transitions since an EF essential singularity is derived analytically and the investigation of the true singularity has been reduced to the discussion of the possible coherent anomaly in the argument of the exponential. Therefore, the ambiguity encountered in analyses of Monte Carlo data for finite-size systems in drawing a distinction between the power-law singularity and the exponential singularity is excluded.

As discussed by Saito, the present EF theory derives an exponential singularity only in two dimensions. Generally, an effective-field theory derived from the cumulant expansion and the variational method is important since it is able to provide the dependence of critical phenomena on the dimensionality of space. This aspect is also observed when this formulation is applied to the S^4 model. The results for the critical exponents in S^4 model are as following. There is no phase transition at all in dimensions lower than $d_l = 2$; in three dimensions we have a power-law singularity of the correlation length denoted by $\nu_0 = 1$ accompanied by a divergent critical coefficient; for dimensions higher than $d_u = 4$, $\nu = \frac{1}{2}$ with convergent critical coefficients. These results correspond to the fact that the lower and upper critical dimensions for the S^4 model are $d_l = 2$ and $d_u = 4$, respectively [20,21].

A further study taking into account the terms proportional to higher powers of y_0/J in the cumulant expansion for the KT transitions is now in progress. The detailed analysis and the CAM estimations of the critical point and the critical exponents will be reported in the near future.

Acknowledgments

I am indebted to Professor M Suzuki at University of Tokyo for drawing my attention to the present problem, his continuous encouragements, and critical reading of the manuscript. I am grateful to Professor S Miyashita at Kyoto University and Mr Y Nonomura at the University of Tokyo for useful discussions.

This study is financed in part by the Scientific Research Fund of the Ministry of Education, Science and Culture of Japan and supported in part by a grant from Iketani Science and Technology Foundation.

References

[1] Suzuki M 1986 *J. Phys. Soc. Japan* **55** 4205
Suzuki M, Katori M and Hu X 1987 *J. Phys. Soc. Japan* **56** 3093
[2] Hu X and Suzuki M 1990 *J. Phys. A: Math. Gen.* **23** 3051; 1988 *Physica* **150A** 310
Hu X, Katori M and Suzuki M 1987 *J. Phys. Soc. Japan* **56** 3865
Hu X and Suzuki M 1988 *J. Phys. Soc. Japan* **57** 791
[3] Suzuki M 1991 *Evolutionary Trends in Physical Science* ed M Suzuki and R Kubo (Berlin: Springer) and references therein
[4] Kosterlitz J M and Thouless D J 1973 *J. Phys.* C **6** 1181
[5] Kosterlitz J M 1974 *J. Phys.* C **7** 1046
[6] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
[7] José J V, Kadanoff L P, Kirkpatrick S and Nelson D R 1977 *Phys. Rev.* B **16** 1217
[8] Ohta T and Kawasaki K 1978 *Prog. Theor. Phys.* **60** 365
[9] Amit D J, Goldschmit Y Y and Grinstein G 1980 *J. Phys. A: Math. Gen.* **13** 585
[10] Itzykson C and Drouffe J M 1989 *Statistical Field Theory* (Cambridge: Cambridge University Press)
[11] DeLapp R G J and Batrouni G G 1988 *Phys. Rev. Lett.* **61** 1996
[12] Ding J Q and Makivić M S 1990 *Phys. Rev.* B **42** 6827
[13] Chui S T and Weeks J D 1976 *Phys. Rev.* B **14** 4978

[14] Swendsen R H 1977 *Phys. Rev.* B **15** 689
[15] Saito Y 1978 *Z. Phys.* B **32** 75
[16] Saito Y 1979 *Prog. Theor. Phys.* **62** 927
[17] Hu X 1993 *Prog. Theor. Phys.* **89** Prog. Lett. 545
[18] Villain J 1975 *J. Physique* **36** 581
[19] Nienhuis B 1987 *Phase Transitions and Critical Phenomena* ed C Domb and J L Lebowitz **11** (New York: Academic)
[20] Wilson K 1972 *Phys. Rev. Lett.* **28** 548
[21] Wilson K G and Kogut J 1974 *Phys. Rep.* C **12** 75