Classical Statistical Mechanics of a Kink-Bearing Complex Scalar Field

Takashi MIYASHITA, Kazuo SASAKI and Toshio TSUZUKI

Department of Physics, Tohoku University, Sendai 980

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We investigate classical statistical mechanics of a kink-bearing complex scalar field of one dimension at low temperatures by means of both the transfer integral (TI) method and the ideal kink gas phenomenology. We calculate the free-energy density with the finite temperature corrections by the use of the TI method and reveal the Schottky-type anomaly of specific heat due to kinks. Next the free-energy density is re-calculated by means of the ideal kink gas phenomenology. Both theories give precisely the same expression at low temperatures, so that kinks and phonons are regarded as elementary excitations at low temperatures in the same manner as one-component scalar fields. Peculiar fluctuations inherent in our model make the temperature dependence of several kink-related physical quantities changed and they make the Schottky-type anomaly of specific heat conspicuous.

§ 1. Introduction

Recently statistical mechanics of kink-bearing non-linear fields of one dimension has been investigated actively. Particularly we have well-established notion for classical statistical mechanics of one-component scalar fields such as the sine-Gordon (SG) and the $\phi^4$ model. The notion is that the physical quantities such as the free-energy and the correlation functions of these systems are dominated by kinks and phonons at low temperatures.

From the experimental viewpoints, the SG model and $\phi^4$ model are applied to the quasi-one-dimensional magnets and ferroelectrics, respectively, and the analysis has been performed on this notion. As real physical systems are usually described by the multi-component fields, it is important to examine whether the notion is applicable also to multi-component fields.

In this paper we investigate, as a simple extension, classical statistical mechanics of a kink-bearing complex scalar field analytically in the sense of the low temperature expansion. Furthermore, we study peculiar fluctuations inherent in our model and its contribution to physical quantities. In § 2 we briefly explain our model Hamiltonian and its kink solutions. In § 3 we examine classical statistical mechanics by the use of the transfer integral (TI) method. We solve the two-dimensional pseudo-Schrödinger equation (continuum version of the TI equation) with the aid of separation of variables, "modified WKB method" and Green's functions. Our results are qualitatively different from those of Ref. 4). In § 4 we study the specific heat and kink-sensitive correlation.
length. In § 5 we consider the same problem by the use of the ideal kink gas phenomenology. We interpret the results obtained by the TI method from the physical viewpoints including interactions between kinks and phonons. Finally we summarize our conclusions and criticize the results of Ref. 4) in § 6.

§ 2. Model Hamiltonian and kink solutions

We consider the following discrete Hamiltonian defined on a one-dimensional lattice with lattice spacing $l$:  
\begin{align}
H &= \sum_{i=1}^{N} \left\{ \frac{1}{2} |\phi_i|^2 + \frac{1}{2l^2} (|\phi_{i+1} - \phi_i|^2 + V(|\phi_i|, \phi_i)) \right\}, \\
\phi_i &= |\phi_i| e^{i\phi_i}, \\
V(|\phi|, \phi) &= \frac{1}{4} (1 - |\phi|^2)^2 + \frac{1}{4} x|\phi|^2 \sin^2 \phi,
\end{align}

where $\phi_i$ is a complex scalar field at the $i$-th lattice point, $N$ is the number of lattice points, $LN=L$ is the system length and $x$ is a positive parameter. All of the above quantities are made to be dimensionless to simplify calculations. The discrete Hamiltonian (2.1) is rewritten in the continuum limit $l\to 0$ as  
\begin{equation}
H = \int dx \left\{ \frac{1}{2} |\phi|^2 + \frac{1}{2l} (|\phi_{x+1} - \phi_x|^2 + V(|\phi|, \phi)) \right\},
\end{equation}

where $x$ is the coordinate along the lattice, and the suffixes $t$ and $x$ of $\phi$ represent temporal and spatial derivatives respectively. The local potential $V(|\phi|, \phi)$ has two degenerate minima at $\phi = \pm 1$.

This system is reduced to the $\phi^4$ model in the limit $x\to \infty$, where it is described by the amplitude $|\phi|$ only, and to the SG model in the limit $x\to 0+$, where it is described by the phase $\phi$ only. In this way this model we consider hereafter is a kink-bearing complex scalar field which contains the well-known $\phi^4$ and SG models in the appropriate limits of parameter $x$.

As we see later, we have a crossover phenomenon from one model to another when we vary parameter $x$.  

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Fig. 1. The creation energies of the three classes of kinks at rest: $E_1(0)$, $E_3(0)$ and $E_3(0)$. For class-3 kink we can get $E_3(0)$ analytically only for $x=1/4$. For other $x$: $0 < x < 1$, $E_3(0)$ is obtained numerically.
Table I. The three classes of kink solutions and their properties.

<table>
<thead>
<tr>
<th>class</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>kink solution</td>
<td>( s = y(x - \nu t) )</td>
<td>( s = y(x - \nu t)^2 )</td>
<td>( s = y(x - \nu t)^3 )</td>
</tr>
<tr>
<td>( \xi(s) = \text{th} \frac{1}{2} s )</td>
<td>( \xi(s) = \text{th} \sqrt{2} s )</td>
<td>( \xi(s) = \text{th} \frac{1}{2} s )</td>
<td></td>
</tr>
<tr>
<td>( \eta(s) = 0 )</td>
<td>( \eta(s) = 0 )</td>
<td>( \eta(s) = 0 )</td>
<td></td>
</tr>
<tr>
<td>range of ( x )</td>
<td>all ( x &gt; 0 )</td>
<td>( 0 &lt; x &lt; 1 )</td>
<td>( x &gt; 1 )</td>
</tr>
<tr>
<td>trajectory</td>
<td>( \eta = 0, -1 &lt; \xi &lt; 1 )</td>
<td>( \xi^2 + \frac{\eta^2}{1 - x} = 1 )</td>
<td>( \left( \xi + \frac{1}{4} \right)^2 + \frac{\eta^2}{(2y^2/3)} = 1 )</td>
</tr>
<tr>
<td>creation energy</td>
<td>( E_1(x) = \gamma \frac{2\sqrt{2}}{3} )</td>
<td>( E_2(x) = \gamma \sqrt{2x \left( 1 - \frac{1}{2} x^2 \right)} )</td>
<td>( E_3(x) = \gamma \frac{9}{8} \sqrt{2} ) for ( x = 1/4 )</td>
</tr>
<tr>
<td>linear stability</td>
<td>stable for ( x &gt; 1 )</td>
<td>stable for ( 0 &lt; x &lt; 1 )</td>
<td>unstable for ( 0 &lt; x &lt; 1 )</td>
</tr>
<tr>
<td>note</td>
<td>( \phi^4 )-like topological kink</td>
<td>SG-like topological kink</td>
<td>non-topological kink</td>
</tr>
</tbody>
</table>

a) This interesting equality is satisfied for \( 0 < x < 1 \), but its meaning is not fully understood from the physical viewpoints so far. \(^{4,6}\)

If we write \( \psi = \xi + i\eta \), we get three classes of kink solutions from the continuum Hamiltonian (2·2). We summarize the properties of these kink solutions in Table I. \(^{4,7,8}\) In the case \( x > 1 \) the class-1 kinks (\( \phi^4 \)-like kinks) exist stably, but in the case \( 0 < x < 1 \) they become unstable and the class-2 kinks (SG-like kinks) emerge stably instead. Both kinks turn degenerate just at \( x = 1 \). Performing the linear stability analysis around the degenerate kinks at \( x = 1 \), we find that one of the small fluctuations of \( \eta \) is softened, that is, its frequency tends to zero (see the Appendix). Thus we conclude that this system has peculiar fluctuations at (and around) \( x = 1 \). We show in Fig. 1 the relationship between the creation energies of kinks at rest: \( E_1(0) \), \( E_2(0) \) and \( E_3(0) \). We see that \( E_1(0) \) and \( E_2(0) \) connect smoothly at \( x = 1 \).

§ 3. Transfer integral method

3.1. Formulation

Let us formulate exact classical statistical mechanics for the system governed by the discrete Hamiltonian given in Eq. (2·1). According to the well-established transfer integral (TI) method, \(^{3,6}\) the problem is reduced, in the continuum limit, to solving an eigenvalue problem of the following two-dimensional pseudo-Schrödinger equation: \(^{4}\)

\[
\left\{ -\frac{1}{2m} \left( \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right) + V(\xi, \eta) \right\} \Phi_n(\xi, \eta) = \epsilon_n \Phi_n(\xi, \eta), \tag{3·1a}
\]

\[
\sqrt{m} \equiv \beta. \tag{3·1b}
\]
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\[ V(\xi, \eta) = \frac{1}{4}(1 - (\xi^2 + \eta^2))^2 + \frac{1}{4} \chi \eta^2, \]  

(3.1c)

where \( \beta^{-1} = T. \) If we find eigenvalues of the ground state and the first excited state of Eq. (3.1a), \( \varepsilon_0 \) and \( \varepsilon_1 \) respectively, the free-energy density \( F \) and the kink-sensitive \( \xi - \xi \) correlation length \( \lambda \) are given by the following expressions:

\[ F = \frac{2}{\beta l} \ln \frac{\beta h}{l} + \varepsilon_0, \]  

(3.2)**

\[ \lambda^{-1} = \beta (\varepsilon_1 - \varepsilon_0). \]  

(3.3)

To fulfill an analytic calculation, we make a transformation from the Cartesian coordinates \((\xi, \eta)\) to the elliptic-polar coordinates \((u, v)\) in Eq. (3.1a), which is defined by

\[ \xi = \sqrt{\chi} \cosh u \cos v, \]  

(3.4a)

\[ \eta = \sqrt{\chi} \sinh u \sin v, \]  

(3.4b)

where \( 0 \leq u < \infty \) and \(-\pi < v \leq \pi\). Then Eq. (3.1a) is divided into the following two one-dimensional pseudo-Schrödinger equations if we assume a factorized form for the \( n \)-th eigenfunction \( \Phi_n(\xi, \eta) \) such as \( \Phi_n(\xi, \eta) = R_n(u) \chi_n(v) \):

\[ H(u; \varepsilon_n) R_n(u) = \Delta_n R_n(u), \]  

(3.5a)

\[ H(u; \varepsilon) = -\frac{1}{2m} \frac{d^2}{du^2} + \frac{1}{4} \left( (1 - \chi^2 \cosh^2 u)^2 - \frac{4 \varepsilon}{\chi} \cosh^2 u \right), \]  

(3.5b)

\[ H(v; \varepsilon_n) \chi_n(v) = -\Delta_n \chi_n(v), \]  

(3.5c)

\[ H(v; \varepsilon) = -\frac{1}{2m} \frac{d^2}{dv^2} + \frac{1}{4} \left( (1 - \chi \cos^2 v)^2 - \frac{4 \varepsilon}{\chi} \sin^2 v \right), \]  

(3.5d)

where \( \Delta_n \) stands for a separation constant. Thus we have to calculate eigenvalues, eigenfunctions and separation constants for the ground state \((n=0)\) and the first excited state \((n=1)\) in a self-consistent fashion.

3.2. "Modified WKB method"

According to the symmetry argument, it can be understood that \( \Phi_0 \) and \( \Phi_1 \) are even functions of both \( u \) and \( v \), and that \( \chi_0 \) is \( \pi \)-periodic while \( \chi_1 \) is \( \pi \)-antiperiodic: \( \chi_0(v+\pi) = \chi_0(v) \) and \( \chi_1(v+\pi) = -\chi_1(v) \). So it is sufficient to know \( \chi_0(v) \) and \( \chi_1(v) \) in the range \( 0 \leq v \leq \pi/2 \). Thus we impose on \( \Phi_0 \) and \( \Phi_1 \) the

\*\*\* T is dimensionless temperature.
\*\*\* h is dimensionless Planck's constant.
following boundary conditions (BC):

\[
R_0(\infty) = 0, \quad R'_0(0) = 0, \quad \chi_0'(0) = 0 \quad \text{and} \quad \chi_0\left(\frac{\pi}{2}\right) = 0
\]  

(3.6a)

for the ground state and

\[
R_1(\infty) = 0, \quad R'_1(0) = 0, \quad \chi_1'(0) = 0 \quad \text{and} \quad \chi_1\left(\frac{\pi}{2}\right) = 0
\]  

(3.6b)

for the first excited state. Note that both BC are different only in the condition on \( \chi \) at \( v = \pi/2 \).

The eigenvalues \( \epsilon_0 \) and \( \epsilon_1 \) are almost degenerate. The degeneracy is lifted slightly by the degenerate properties of the potential functions of Eqs. (3.5b, d) and the BC imposed above at \( u = 0 \) and \( v = \pi/2 \), if \( m \gg 1 \). So we write \( \epsilon_0 \) and \( \epsilon_1 \) as

\[
\epsilon_0 = \epsilon_0^{(0)} - \tau_0, \quad (\tau_0 \ll \epsilon_0^{(0)})
\]  

(3.7a)

\[
\epsilon_1 = \epsilon_0^{(0)} + \tau_1. \quad (\tau_1 \ll \epsilon_0^{(0)})
\]  

(3.7b)

Reflecting this fact we decompose \( \Delta_0 \) and \( \Delta_1 \) into

\[
\Delta_0 = \Delta_0^{(0)} - \delta_0, \quad (\delta_0 \ll \Delta_0^{(0)})
\]  

(3.8a)

\[
\Delta_1 = \Delta_0^{(0)} + \delta_1. \quad (\delta_1 \ll \Delta_0^{(0)})
\]  

(3.8b)

Quantities \( \epsilon_0^{(0)} \) and \( \Delta_0^{(0)} \) are determined self-consistently from Eqs. (3.5a, c) by requiring the BC only at \( u = \infty \) and \( v = 0 \):

\[
H(u; \epsilon_0^{(0)} R_0^{(0)}(u)) = \Delta_0^{(0)} R_0^{(0)}(u), \quad 0 \leq u < \infty,
\]  

(3.9a)

BC : \( R_0^{(0)}(\infty) = 0 \).  

(3.9b)

\[
H(v; \epsilon_0^{(0)} \chi_0^{(0)}(v)) = - \Delta_0^{(0)} \chi_0^{(0)}(v), \quad 0 \leq v \leq \frac{\pi}{2},
\]  

(3.9c)

BC : \( \chi_0^{(0)}(0) = 0 \).  

(3.9d)

where both \( R_0^{(0)}(u) \) and \( \chi_0^{(0)}(v) \) are nodeless in their defined regions. We use Eq. (3.9) as the auxiliary differential equations to solve the full problem later.

Let us solve the differential equation (3.9) by the use of the "modified WKB method". As we are interested in the low temperature region \( (1/\sqrt{m} = T \ll 1, \) so that \( T \ll E_K(0) \), we assume that \( \epsilon_0^{(0)}, \Delta_0^{(0)}, R_0^{(0)}(u) \) and \( \chi_0^{(0)}(v) \) have the following series expansion forms of the expansion parameter \( T \ll 1 \):

\[
\epsilon_0^{(0)} = \mu_1(x) T + \mu_2(x) T^2 + \cdots,
\]  

(3.10a)

\[
\Delta_0^{(0)} = \nu_1(x) T + \nu_2(x) T^2 + \cdots,
\]  

(3.10b)
Table II. Explicit forms of $\varepsilon^{(0)}$, $\Delta^{(0)}$, $R^{(0)}(u)$ and $\chi^{(0)}(v)$ in Eq. (3·10).

<table>
<thead>
<tr>
<th>$\varepsilon^{(0)}$</th>
<th>$\mu_1(x) = \frac{1}{2} \left( \sqrt{2} + \sqrt{x} \right)$</th>
<th>$\mu_1(x) = \frac{-1 + 2 + \sqrt{x}}{4(1 + \sqrt{x})}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta^{(0)}$</td>
<td>$\nu_1(x) = -\frac{1}{2} \sqrt{x}(1-x)$</td>
<td>$\nu_2(x) = \frac{1 + 5\sqrt{x}}{8(1 + \sqrt{x})}$</td>
</tr>
<tr>
<td>$R^{(0)}(u)$</td>
<td>$\sigma_0(u) = \frac{\sqrt{2}}{2} \left( \sqrt{x} \text{ si } u - \frac{1}{3}(\sqrt{x} \text{ ch } u)^3 \right)$</td>
<td>$\sigma_1(u) = -\ln\left((1 + \sqrt{x} \text{ ch } u)\sqrt{u + 1}\right)$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_2(u) = \frac{x(2 + \sqrt{x})\text{ si } u}{2\sqrt{x}(1 + \sqrt{x})}\text{ ch } u + (1 + \sqrt{x})(1 + 2\sqrt{x})$</td>
<td></td>
</tr>
<tr>
<td>$\chi^{(0)}(v)$</td>
<td>$\rho_0(v) = \frac{\sqrt{2}}{2} \left( \sqrt{x} \cos v - \frac{1}{3}(\sqrt{x} \cos v)^3 \right)$</td>
<td>$\rho_1(v) = -\ln\left((1 + \sqrt{x} \cos v)\sqrt{1 + \cos v}\right)$</td>
</tr>
<tr>
<td></td>
<td>$\rho_2(v) = \frac{x(2 + \sqrt{x})\cos^3 v + \sqrt{x}(2 + \sqrt{x})^2 \cos v + (1 + \sqrt{x})(1 + 2\sqrt{x})}{2\sqrt{2}\sqrt{x}(1 + \sqrt{x})\text{ ch } u} \left(\sqrt{\cos v + 1}\right)$</td>
<td></td>
</tr>
</tbody>
</table>

\[ R^{(0)}(u) = e^{(1/T)\sigma(u)} \sigma(u) = \sigma_0(u) + \sigma_1(u) T + \sigma_2(u) T^2 + \cdots \] \hfill (3·10c)*)

\[ \chi^{(0)}(v) = e^{(1/T)\rho(v)} \rho(v) = \rho_0(v) + \rho_1(v) T + \rho_2(v) T^2 + \cdots \] \hfill (3·10d)*)

Substituting these expressions into Eq. (3·9) and separating terms in different powers of $T$, we obtain hierarchy equations for $\sigma(u)$ and $\rho_1(v)$, where solutions can be found successively and analytically. The solutions contain the expansion coefficients $\mu_1(x)$ and $\nu_1(x)$ as parameters. They are uniquely determined by the condition that $R^{(0)}(u)$ and $\chi^{(0)}(v)$ are nodeless and never diverge in their defined regions. Thus we can determine $\varepsilon^{(0)}$ and $\Delta^{(0)}$ self-consistently. Explicit forms of $\varepsilon^{(0)}$, $\Delta^{(0)}$, $R^{(0)}(u)$ and $\chi^{(0)}(v)$ are summarized in Table II up to the second order of $T$.

3.3. Green's function method

We introduce the Green's functions $F(u, u')$ and $G(v, v')$ defined by

\[ \{ H(u; \varepsilon^{(0)} - \Delta^{(0)}) F(u, u') = \delta(u - u'), \quad 0 \leq u, u' < \infty \} \]

BC: $F(\infty, u') = 0,$ \hfill (3·11b)

\[ \{ H(v; \varepsilon^{(0)} + \Delta^{(0)}) G(v, v') = \delta(v - v'), \quad 0 \leq v, v' \leq \frac{\pi}{2} \} \]

BC: $G'(0, v') = 0,$ \hfill (3·11d)**)

*) If the expansion parameter $T$ is replaced by $h$, these expansions are the standard WKB method in quantum mechanics.

**) $G'(0, v') = \left[ \frac{d}{dv} G(v, v') \right]_{v=0}$.
where \( \delta(x) \) is the Dirac delta function. \( F(u, u') \) and \( G(v, v') \) defined above are expressed by the use of \( R^{(0)}_\theta(u) \) and \( \chi^{(0)}_\theta(v) \) as\(^{10}\)

\[
F(u, u') = 2m\theta(u' - u)R^{(0)}_\theta(u)R^{(0)}_\theta(u') \int_{u'}^u dx \frac{1}{(R^{(0)}_\theta(x))^2},
\]

\[
(3\cdot12a)
\]

\[
G(v, v') = -2m\theta(v - v')\chi^{(0)}_\theta(v)\chi^{(0)}_\theta(v') \int_{v'}^v dx \frac{1}{(\chi^{(0)}_\theta(x))^2},
\]

\[
(3\cdot12b)
\]

where \( \theta(x) \) is the Heaviside step function.

The eigenvalue equation (3·5) for the ground state is rewritten as

\[
\{H(u; \epsilon^{(0)}_\theta) - \Delta^{(0)}_\theta\} R_\theta(u) = - (\tau_\theta x \sin^2 u + \delta_\theta) R_\theta(u),
\]

\[
(3\cdot13a)
\]

\[
\{H(v; \epsilon^{(0)}_\theta) + \Delta^{(0)}_\theta\} \chi_\theta(v) = - (\tau_\theta x \sin^2 v - \delta_\theta) \chi_\theta(v).
\]

\[
(3\cdot13b)
\]

By the use of the Green's function (3·12), Eq. (3·13) is reduced to the following integral equations:

\[
R_\theta(u) = R^{(0)}_\theta(u) - \int_{-\infty}^{\infty} du' (\tau_\theta x \sin^2 u' + \delta_\theta) F(u, u') R_\theta(u'),
\]

\[
(3\cdot14a)
\]

\[
\chi_\theta(v) = \chi^{(0)}_\theta(v) - \int_{-\infty}^{\pi/2} dv' (\tau_\theta x \sin^2 v' - \delta_\theta) G(v, v') \chi_\theta(v').
\]

\[
(3\cdot14b)
\]

Those \( R_\theta(u) \) and \( \chi_\theta(v) \) automatically satisfy the BC \( R_\theta(\infty) = 0 \) and \( \chi_\theta(0) = 0 \). Imposing the remaining BC \( R_\theta'(0) = 0 \) and \( \chi_\theta'(\pi/2) = 0 \) and noticing \( R^{(0)}_{\theta'}(0) = 0 \), we get

\[
0 = - \int_{-\infty}^{\infty} du' (\tau_\theta x \sin^2 u' + \delta_\theta) F'(0, u') R_\theta(u'),
\]

\[
(3\cdot15a)
\]

\[
0 = \chi^{(0)}_{\theta'}(\frac{\pi}{2}) - \int_{0}^{\pi/2} dv' (\tau_\theta x \sin^2 v' - \delta_\theta) G'(\frac{\pi}{2}, v') \chi_\theta(v').
\]

\[
(3\cdot15b)
\]

Thus we obtain a set of Eqs. (3·14) and (3·15) to determine \( R_\theta(u) \), \( \chi_\theta(v) \), \( \tau_\theta \) and \( \delta_\theta \) self-consistently.

We can see that \( \tau_\theta \) and \( \delta_\theta \) are small like \( \exp(-E_K(0)/T) \) for \( T \ll E_K(0) \), if \( R_\theta \) and \( \chi_\theta \) are replaced by their leading terms of \( R^{(0)}_\theta \) and \( \chi^{(0)}_\theta \) in Eq. (3·15). Therefore we can get \( R_\theta \) and \( \chi_\theta \) with good accuracy by the iteration procedure in powers of \( \tau_\theta \) and \( \delta_\theta \) from Eq. (3·14). Substituting the resulting \( R_\theta \) and \( \chi_\theta \) into Eq. (3·15), we get a set of equations which determine \( \tau_\theta \) and \( \delta_\theta \) in the forms of double expansions with respect to \( t \) and \( \exp(-1/t) \), where \( t = T/E_K(0) \), as we have been able to obtain \( R^{(0)}_\theta(u) \) and \( \chi^{(0)}_\theta(v) \) in powers of \( t \).
3.4. Thermodynamic functions at low temperatures

Let us assume that the temperature is low enough to neglect the kink-kink interaction. This is equivalent to neglecting terms of order $\exp(-2/t)$. Replacing $R_0(u)$ and $\chi_0(v)$ by $R_0(0,u)$ and $\chi_0(0,v)$, we get the following expression for $\tau_0$ after some manipulations:

$$\tau_0 = N^{-1} \frac{1}{T^2} \int_0^{\pi/2} dv \left( \frac{1}{\chi_0(0,v)} \right)^2 \left[ \int_{\text{max}}^{\pi/2} dx \frac{1}{\chi_0'(x)^2} + \frac{1}{\chi_0'((\pi/2)) \chi_0'(\pi/2)} \right]$$

$$+ O(e^{-2t/\gamma}),$$

(3.16a)

$$N = \frac{\int_0^{\infty} dx \, sh^2 u [R_0(0,u)]^2 \int_{\text{max}}^{\pi/2} dx \frac{1}{\chi_0'(x)^2}}{\int_0^{\infty} dv \chi_0(0,v)^2 \int_{\text{max}}^{\pi/2} dv \chi_0'(v)^2},$$

(3.16b)

where $v_{\text{max}}$ is the maximum point between 0 and $\pi/2$ of the function $\rho_0(v)$ given in Table II.

The first excited state can be treated in the same manner. After all we obtain the following expression for $\tau_1$:

$$\tau_1 = N^{-1} \frac{1}{T^2} \int_0^{\pi/2} dv \chi_0(0,v)^2 \int_{\text{max}}^{\pi/2} dx \frac{1}{\chi_0'(x)^2} + O(e^{-2t/\gamma}).$$

(3.17)

From Eqs. (3.16) and (3.17) we obtain the full $t$ dependence of the prefactors of $\exp(-1/t)$ in $\tau_0$ and $\tau_1$ in powers of $t$.

Before proceeding such calculations, let us examine the mutual relation between $\tau_0$ and $\tau_1$ and their $x$ dependence. First we can obtain that

$$\int_{\text{max}}^{\pi/2} dx \frac{1}{\chi_0'(x)^2} = -\frac{1}{2} \frac{1}{\chi_0'((\pi/2)) \chi_0'(\pi/2)},$$

(3.18)

as the contribution to the integral comes from the region near $\pi/2$ mainly. We have proved the above equality using the first three terms of $\rho(v)$ which are given by Eq. (3.10d) and Table II. Thus we find an important relation $\tau_0 = \tau_1$ which means the symmetric splitting of $\epsilon_0$ and $\epsilon_1$ from $\epsilon_0^{(0)}$. Secondly the remaining integrals of $\tau_0$ and $\tau_1$ have different $t$ dependences according to the magnitude of $x$. We explain this as follows:

$$I \equiv \int_0^{\pi/2} dv \chi_0'(v)^2 = \int_0^{\pi/2} d\epsilon e^{(2iT)\rho_0(\epsilon)} e^{2\rho_1(\epsilon)} [1 + 2\rho_2(\epsilon) T + \cdots].$$

(3.19)
Under the low temperature condition \( T \ll 1 \), the contribution mainly comes from the vicinity of \( v=v_{\text{max}} \). Here we show the \( v \) dependence of \( \rho_0(v) \) for the three cases: (A) \( 0 < x < 1 \), (B) \( x = 1 \) and (C) \( x > 1 \) in Fig. 2. We find that as for (A) \( v_{\text{max}} = 0 \) and the maximum is quadratic, that as for (B) \( v_{\text{max}} = 0 \) but the maximum is not quadratic but quartic, and that as for (C) \( v_{\text{max}} = \cos^{-1}(1/\sqrt{x}) \) and the maximum is quadratic again. Consequently we conclude that \( \tau_0 \) (and \( \tau_1 \)) has the different asymptotic forms at low temperatures for the three cases.

After all we get the following asymptotic results for \( \tau_0 \) and \( \tau_1 \):

\[
\begin{align*}
\text{(A) } & \quad 0 < x < 1 \\
\tau_0 &= A_1(x) t^{1/2} e^{-1/t} [1 - A_2(x) t + O(t^2)] + O(e^{-2t}), \quad \text{(3.20a)*} \\
& \quad t \equiv T/E_2(0), \\
\text{(3.20b)}
\end{align*}
\]

\[
\begin{align*}
\text{(B) } & \quad x = 1 \\
\tau_0 &= B_1 t^{1/4} e^{-1/t} [1 - B_2 t^{1/2} - B_3 t - B_4 t^{3/2} + O(t^2)] + O(e^{-2t}), \quad \text{(3.20c)} \\
& \quad t \equiv T/E_{1,2}(0), \\
\text{(3.20d)}
\end{align*}
\]

| Table III. \( A_i(x) \), \( B_i \), and \( C_i(x) \) appearing in Eq. (3.20). |
|----------------------------------|--|
| \( A_1(x) = \frac{2}{\sqrt{\pi}} \left[ \frac{2}{3} \frac{x^2(1+\sqrt{x})^3(3-x)}{1-\sqrt{x}} \right]^{1/3} \) | \( A_2(x) = \frac{(8x^3 + 16x\sqrt{x} - 37x^2 + 7)(3-x)}{24(1-x)^2} \) |
| \( B_1 = 4 \left( \frac{2}{3} \right)^{1/4} \frac{1}{\pi} \Gamma \left( \frac{1}{4} \right) \) | \( B_2 = \frac{119}{96} \) |
| \( B_3 = \frac{1}{\sqrt{3}} \frac{503}{216\pi} \left( \Gamma(1/4) \right)^2 \) | \( B_4 = \frac{119}{96} \) |
| \( C_1(x) = \frac{4}{\sqrt{\pi}} \left[ \frac{2}{3} \frac{1}{\sqrt{x} - 1} \right]^{1/3} \) | \( C_2(x) = \frac{71x^2 + 60x\sqrt{x} - 130x - 84\sqrt{x} + 119}{72(x-1)^2} \) |

* Note that we should not use these expressions if \( x \) is extremely near 1 in the sense of \((1-x)^2/T \approx 1\).
(C) \( x > 1 \)

\[
\tau_0 = C_1(x) t^{\xi/2} e^{-\frac{1}{4t} \left[1 - C_3(x) t + O(t^2)\right]} + O(e^{-2t}), \quad (3\cdot20e)^*)
\]

\[
t = \frac{T}{E_1(0)}, \quad (3\cdot20f)
\]

\[
\tau_1 = \tau_0, \quad (3\cdot20g)
\]

where \( A_i(x), B_i, \) and \( C_i(x) \) are shown in Table III.

The temperature dependence of \( \tau_0 \) for (A) \( 0 < x < 1 \) and (C) \( x > 1 \) is completely the same as the case of one-component scalar fields (e.g., SG and \( \phi^4 \)).\(^{11)} \) While the \( T \) dependence of \( \tau_0 \) for (B) \( x = 1 \) is of a new type. It differs remarkably from that for (A) and (C). This is caused by the quartic maximum of \( \rho_0(v) \) near \( v_{\text{max}} \) and this is physically due to the fact that there appear peculiar fluctuations around the kink solution at \( x = 1 \), as explained in § 5.

By the use of the above results the free-energy density \( F \) and the kink-sensitive \( \xi \cdot \xi \) correlation length \( \lambda \) are written as

\[
F = F_0 + F_K, \quad (3\cdot21a)
\]

\[
F_0 = \frac{2}{\beta l} \ln \frac{\beta h}{l} + \epsilon_0^{(0)}, \quad (3\cdot21b)
\]

\[
F_K \equiv -\tau_0, \quad (3\cdot21c)
\]

\[
\lambda^{-1} = 2\beta \tau_0. \quad (3\cdot22)
\]

As we show later, \( F_0 \) and \( F_K \) are interpreted as the phonon part and the dressed kink part similar to the case of one-component scalar fields (e.g., SG and \( \phi^4 \)).\(^{3)} \) If we take such limit that \( x \to 0, \) or \( x \to \infty \) in Eq. (3\cdot21c), \( F_K \) is reduced

![Fig. 3(a) continued.](https://academic.oup.com/ptp/article-abstract/68/6/1880/1878622)
Fig. 3. Specific heats $C$ as functions of reduced temperature $t = T/E_k(0)$ for (a) $\kappa = 0.1$, (b) $\kappa = 1.0$ and (c) $\kappa = 10.0$. Here the harmonic phonon parts are subtracted from $C_0$. $t_m = 0.32$ for (a), $t_m = 0.20$ for (b) and $t_m = 0.26$ for (c).

exactly to the corresponding result for SG or $\phi^4$\textsuperscript{11)} respectively.

§ 4. Specific heat and $\xi$-$\xi$ correlation length

From the free-energy density Eq. (3·21) we get the specific heat $C$ per unit length\textsuperscript{11)}
\textbf{Statistical Mechanics of a Kink-Bearing Complex Scalar Field}

In Fig. 4, the $x$ dependence of the kink-sensitive $\xi-\xi$ correlation length $\lambda$ at the temperature $\beta E_1(0)=10.0$. The dashed line near $x=1$ is our interpolation.

\begin{equation}
C = C_0 + C_K,
\end{equation}

where $C_0$ corresponds to the phonon part and $C_K$ to the dressed kink part. We show the temperature and $x$ dependences of $C$, $C_0$ and $C_K$ in Figs. 3(a)~(c), where the harmonic phonon part $C_0^{(1)}$, given by

\begin{equation}
C_0^{(1)} = \frac{2}{l}, \quad \text{(the Dulong-Petit law)}
\end{equation}

is subtracted from $C_0$. From Figs. 3(a)~(c) we can understand that $C$ has an anomalous peak$^{19}$ at $t=t_m$ due to the kink excitation for all $x$, where $t_m=0.32$ for $x=0.1$, $t_m=0.26$ for $x=10.0$ and $t_m=0.20$ for $x=1$. Because the total kink (plus anti-kink) density $n(\beta)$, obtained in the next section by the use of the ideal kink gas phenomenology, has the maximum increase rate near $t=t_m$, we conclude that the peak of $C$ is interpreted as the \textit{Schottky-type anomaly} due to the kink excitation.$^{11}$ The reason why $t_m$ at $x=1$ is peculiarly lower than other cases is considered as follows: The thermally renormalized creation energy of kinks is considerably reduced by peculiar fluctuations as shown later, so that $t_m$ is lowered. Consequently we find that peculiar fluctuations make the anomalous specific heat, which exists for all $x$, more conspicuous.

We show the $x$ dependence of the kink-sensitive $\xi-\xi$ correlation length $\lambda$ given by Eq. (3·22) in Fig. 4. As $\ln \lambda$ is dominated by the creation energy of stable kinks at rest, we can point out that Fig. 4 resembles Fig. 1 that shows the $x$ dependence of $E_1(0)$ and $E_2(0)$.
§ 5. Ideal kink gas phenomenology

We now consider the phenomenological approach to classical statistical mechanics for the system governed by the continuum Hamiltonian given in Eq. (2.2). According to the ideal kink gas phenomenology by which we regard kinks and phonons as elementary excitations at low temperatures (i.e., \( t = T / E_K(0) < 1 \)) and disregard kink-kink interactions, the total kink density (kink density plus anti-kink density) \( n(\beta) \) is given by\(^3\)

\[
\eta(\beta) = a \frac{1}{h} E_K(0) \sqrt{\frac{2\pi}{\beta E_K(0)}} e^{-\beta E_K(0)} [1 + O(\beta E_K(0)^{-1})], \tag{5.1a}
\]

\[
E_K^*(\beta) = E_K(0) + \Sigma(\beta), \tag{5.1b}
\]

\[a = 1 \text{ for } x \geq 1 \quad \text{and} \quad a = 2 \text{ for } 0 < x < 1. \tag{5.1c}\]

\( \Sigma(\beta) \) is the change of the kink creation energy caused by fluctuations of the field around a kink at rest and is regarded as the self-energy of a kink at finite temperatures.\(^3\) Thus \( E_K^*(\beta) \) is considered as the thermally renormalized creation energy of a kink. \( a \) is the number of the homotopic variety of kink (anti-kink).\(^4\) By the use of the \( n(\beta) \), we get the total free-energy density \( F(\beta) \) as\(^3\)

\[
F(\beta) = F_0(\beta) - \frac{1}{\beta} \eta(\beta), \tag{5.2}
\]

where \( F_0(\beta) \) is the free-energy density due to phonons in the absence of kinks. \( F_0(\beta) \) is obtained for all \( x \) as (see the Appendix)

\[
F_0(\beta) = \frac{2}{\beta l} \ln \frac{\beta h}{l} + \mu_1(x) T + O(T^2). \tag{5.3}
\]

In the cases (A) \( 0 < x < 1 \) and (C) \( x > 1 \), we can apply the same method as in Ref. 3) to calculate \( \Sigma(\beta) \), as the fluctuations have finite frequencies.

First as for (C) we set \( E_K(0) = E_1(0) \) and the harmonic fluctuations around a class-1 kink at rest are obtained analytically (see the Appendix), so that we can proceed to calculate \( \Sigma(\beta) \).\(^\star\star\) \( \Sigma(\beta) \) has two origins:\(^3\) i) Due to kink-influenced phonon modes which have “phase-shift” interactions with kinks, ii) due to internal oscillation modes of kinks. Because \( \xi \) and \( \eta \) components of harmonic fluctuations around a kink in this case are completely independent of each other, \( \Sigma(\beta) \) is expressed as the sum of both components. After all we obtain the following results for \( \Sigma(\beta) \) (see the Appendix):

\(^\star\) The origin of the first order finite temperature correction of order \( \beta E_K(0)^{-1} \) is the same as the one-component fields.\(^{10}\)

\(^\star\star\) As for (A), on the contrary, the harmonic fluctuations around a class-2 kink at rest are not known analytically so far, so that we cannot calculate \( \Sigma(\beta) \) at present.
\[ \Sigma_t(\beta) = -\frac{1}{\beta} \ln(\beta h \sqrt{2}) - \frac{1}{\beta} \sigma_t, \quad \sigma_t = \ln 2\sqrt{3}, \quad (5.4a) \]

\[ \Sigma_\xi(\beta) = -\frac{1}{\beta} \sigma_\xi, \quad \sigma_\xi = \ln \left[ \frac{\sqrt{x} + 1}{\sqrt{x} - 1} \right]^{1/2}, \quad (5.4b) \]

\[ \Sigma(\beta) = \Sigma_t(\beta) + \Sigma_\xi(\beta) = -\frac{1}{\beta} \ln(\beta h \sqrt{2}) - \frac{1}{\beta} \sigma, \quad \sigma = \sigma_t + \sigma_\xi. \quad (5.4c) \]

The reason why \( \Sigma_\xi(\beta) \) does not have the term like \(-1/\beta \ln(\beta h \sqrt{2})\) is that \( \xi \) fluctuations have a translation mode, while \( \eta \) fluctuations do not. We have treated harmonic fluctuations by means of classical statistical mechanics. The condition under which we can treat them classically is given by

\[ \beta h \sqrt{2} \ll 1. \quad (5.5) \]

Thus we can conclude \( \Sigma(\beta) > 0 \) from Eq. (5.4c). Consequently we find that \( E_1^*(\beta) \) is larger than \( E_1(0) \). By the use of Eqs. (5.3) and (5.4) we get the following result which is the same as that of TI method:

\[ F(\beta) = \frac{2}{\beta} \ln \frac{\beta h}{l} + \mu_1(x) T + O(T^2) \]

\[ - C_1(x) t^{1/2} e^{-1/t} [1 + O(t)] + O(e^{-2t}), \quad (5.6a) \]

\[ t \equiv T/E_1(0), \quad (5.6b) \]

where \( \mu_1(x) \) and \( C_1(x) \) are the same quantities in \$3$. We can understand that \( F_\xi \) and \( F_K \) in Eq. (3.21) correspond to the phonon part and the dressed kink part (the kink dresses small fluctuations around it.)

Second, as for (B) \( x = 1 \) we set \( E_K(0) = E_{1,2}(0) \). We must treat a softened mode (peculiar fluctuations) carefully. If we write the canonical momentum and coordinate of this mode as \( P_1 \) and \( Q_1 \), we can understand the following situations by writing out the Hamiltonian for small fluctuations around a kink at rest (see the Appendix):

i) For \( x > 1 \), this mode is equivalent to a harmonic oscillator with finite frequency \( \omega_{s,1} \) which is given in Table IV.

ii) For \( x = 1 \), \( \omega_{s,1} \) becomes zero and then this mode is assumed to be a quartic oscillator, the effective Hamiltonian of which is given by

\[ H_1 = \frac{1}{2} P_1^2 + \frac{1}{4} a Q_1^4, \quad a: \text{constant.} \quad (5.7)^* \]

After treating this softened mode as above and other modes as harmonic, we get

---

* We do not have obtained yet the numerical factor "\( a \)" from the original Hamiltonian.
\[ \Sigma_\varepsilon (\beta) = -\frac{1}{\beta} \ln \beta^{1/4} - \frac{1}{\beta} \bar{\sigma}_{x} \quad \bar{\sigma}_x = \ln \left[ \frac{1}{\sqrt{2\pi}} \frac{\Gamma(1/4)}{a^{1/4}} \right] \]  
\[ \Sigma_\varepsilon (\beta) = \Sigma_\varepsilon (\beta) + \Sigma_\varepsilon (\beta) = -\frac{1}{\beta} \ln (\beta^{1/4} a^{1/2}) - \frac{1}{\beta} \bar{\sigma} , \quad \bar{\sigma} = \sigma_\varepsilon + \bar{\sigma}_x . \]  

If we compare Eq. (5.8b) with Eq. (5.4c), we find

\[ \Sigma(\beta)(x=1) < \Sigma(\beta)(x>1). \]  

Consequently we conclude that the thermally renormalized creation energy of a kink at \( x=1 \) is smaller than that at \( x>1 \). By the use of Eqs. (5.3) and (5.8) we get the following result which has the same temperature dependence as that of TI method:

\[ F(\beta) = \frac{2}{\beta t} \ln \frac{\beta h}{l} + \mu_1 (1) T + O(T^3) \]
\[ - 2^{-5/8} a^{1/4} B_1 t^{1/4} e^{-1/4} [1 + O(t^{1/2})] + O(e^{-2t}) , \]
\[ t \equiv T/E_{1,2}(0). \]

where \( \mu_1 (1) \) and \( B_1 \) are the same quantities in §3.

Thus we have succeeded in proving the equivalence between the TI method and the ideal kink gas phenomenology at low temperatures for the case of the present complex field.

### §6. Conclusion

We have first investigated classical statistical mechanics of a kink-bearing complex scalar field by the use of the TI method. We have calculated the free-energy density and the kink-sensitive correlation length exactly and analytically for all \( x \) in the sense of low temperature expansion. The "modified WKB method" and the Green's function method have been applied to estimate them. Next we have considered the same problem by the use of the ideal kink gas phenomenology regarding phonons and kinks as elementary excitations at low temperatures. We have interpreted the results obtained by the TI method from the physical viewpoints. In addition to the expressions of the free-energy density and the kink-sensitive correlation length, we have obtained the following:

1) Both methods give precisely the same result in the low temperature limit.

*) If \( a = 1/4\sqrt{2} \), both theories give the same result.
The term "low temperature" means finally that

\[ \hbar \omega_0 \ll T \ll E_K(0), \]  

(6.1)

where \( \omega_0 \) is the typical frequency of harmonic fluctuations. The temperature \( T \) is sufficiently lower than the static kink creation energy \( E_K(0) \) but higher than \( \hbar \omega_0 \) in order to be able to neglect the quantum properties of fluctuations. Consequently classical statistical mechanics of this complex scalar field is dominated by kinks and phonons at low temperatures as one-component fields.

2) This system has peculiar fluctuations at \( x = 1 \). This is a new phenomenon inherent in our model. According to the TI method we have found that the temperature dependence of kink-related physical quantities is different from that for \( x \neq 1 \). This difference is interpreted from the phenomenological viewpoints that peculiar fluctuations make the kink self-energy changed and be smaller than other cases. We expect that they play important roles also in the region \( (1 - x)^2 / T \ll 1 \).

3) Kink excitations cause the Schottky-type anomaly of specific heat for all \( x \). Peculiar fluctuations at \( x = 1 \) make it conspicuous.

Recently Takayama et al.\(^{17}\) and Sasaki et al.\(^{18}\) calculated specific heat of SG model up to order \( e^{-2t} \). They concluded that correction of order \( e^{-2t} \) is not quantitatively negligible. So we expect correction of order \( e^{-2t} \) is also important in this model especially near \( t = t_m \).

Now let us comment on the recent work of Trullinger et al.\(^{4,12,13}\) briefly. They got an asymmetric splitting of the ground state and the first excited state energies of the eigenvalue equations, that is, \( \tau_0 \neq \tau_1 \). We think their result was obtained by an inadequate use of the WKB method.\(^{16}\) They used WKB functions even in the region where the WKB approximation is invalidated. In contrast, if we use modified WKB method, there is no such ambiguity and we get \( \tau_0 = \tau_1 \), as shown in § 3. So there is no contribution to the free-energy from the non-topological kink in contrast with the result of Trullinger et al.\(^{4,12,13}\)

Finally as for the future problem, we are interested in the dynamics and the application to the real physical system of the present model.

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Appendix

Let us study small fluctuations of $\xi$ and $\eta$ around the static solutions $\xi^{(0)}(x)$ and $\eta^{(0)}(x)$, which are given in Table I, and their contributions to the kink self-energy. We expand $\xi$ and $\eta$ as

$$\begin{align*}
\xi(x, t) &= \xi^{(0)}(x) + \epsilon \tilde{f}(x, t), \\
\eta(x, t) &= \eta^{(0)}(x) + \epsilon \tilde{g}(x, t),
\end{align*}$$

(A.1a)

(A.1b)

where $\epsilon$ is an infinitesimal. Substituting them into Eq. (2.2) we get the following Hamiltonian for small fluctuations:

$$H = H^{(0)} + \epsilon^2 H^{(2)} + \epsilon^3 H^{(3)} + \epsilon^4 H^{(4)},$$

(A.2a)

$$H^{(0)} = E(0) = \int dx \left\{ \frac{1}{2} \left( \xi_x^2 + \eta_x^2 \right) + V(\xi^{(0)}, \eta^{(0)}) \right\},$$

(A.2b)

$$H^{(2)} = \int dx \left[ \frac{1}{2} \left( \pi_{\xi}^2 + \pi_{\eta}^2 \right) + \frac{1}{2} \left( \tilde{f}_x^2 + \tilde{g}_x^2 \right) \ight.$$  

$$\left. + \frac{1}{2} \left( 3\xi^{(0)2} + \eta^{(0)2} - 1 \right) \tilde{f}^2 + \frac{1}{2} \left( \xi^{(0)2} + 3\eta^{(0)2} \right) \right.$$

$$\left. + \left( \frac{1}{2} x - 1 \right) \tilde{g}^2 + 2\xi^{(0)}\eta^{(0)} \tilde{f} \tilde{g} \right],$$

(A.2c)

$$H^{(3)} = \int dx \left( \xi^{(0)} \tilde{f} + \eta^{(0)} \tilde{g} \right) \left( \tilde{f}^2 + \tilde{g}^2 \right),$$

(A.2d)

$$H^{(4)} = \int dx \frac{1}{4} \left( \tilde{f}^2 + \tilde{g}^2 \right)^2,$$

(A.2e)

where $\pi_{\xi} = \partial \tilde{f}/\partial t$ and $\pi_{\eta} = \partial \tilde{g}/\partial t$. $H^{(0)}$ is the creation energy $E(0)$ for rest solutions $\xi^{(0)}(x)$ and $\eta^{(0)}(x)$. $H^{(2)}$, $H^{(3)}$ and $H^{(4)}$ are the second order (harmonic), the third order and the fourth order Hamiltonians for small fluctuations. Assuming oscillating forms for $\tilde{f}(x, t)$ and $\tilde{g}(x, t)$ such that

$$\begin{align*}
\tilde{f}(x, t) &= f(x) e^{-i\omega t}, \\
\tilde{g}(x, t) &= g(x) e^{-i\omega t},
\end{align*}$$

(A.3a)

(A.3b)

we obtain the following coupled eigenvalue equations from $H^{(2)}$ that determine modes of harmonic fluctuations:

$$\begin{bmatrix}
f_{xx} \\
g_{xx}
\end{bmatrix} + \begin{bmatrix}
-1 + 3\xi^{(0)2} + \eta^{(0)2} & 2\xi^{(0)}\eta^{(0)} \\
2\xi^{(0)}\eta^{(0)} & \left( \frac{1}{2} x - 1 \right) + 3\eta^{(0)2} + \xi^{(0)2}
\end{bmatrix} \begin{bmatrix}
f \\
g
\end{bmatrix} = \omega^2 \begin{bmatrix}
f \\
g
\end{bmatrix},$$

(A.4)
If all of $\omega$ are real we can conclude that $\xi^{(0)}(x)$ and $\eta^{(0)}(x)$ are stable. We examine a few cases.

(i) Small fluctuations around a minimum of the local potential $V(\xi, \eta)$

We set $\xi^{(0)}(x)=1$ and $\eta^{(0)}(x)=0$, then we find $f$ and $g$ of Eq. (A·4) are not coupled with one another. We easily get the following results:

$$f_{k}(x)=\frac{1}{\sqrt{L}}e^{ikx}, \quad \omega_{f}(k)=\sqrt{k^{2}+2}, \quad Lk=2\pi n, \quad n=0, \pm 1, \ldots,$$

$$g_{k}(x)=\frac{1}{\sqrt{L}}e^{ikx}, \quad \omega_{g}(k)=\sqrt{k^{2}+\frac{1}{2}x}, \quad Lk=2\pi m, \quad m=0, \pm 1, \ldots,$$

where $\omega_{f}$ or $\omega_{g}$ is the eigenvalue of Eq. (A·4) for $f$ or $g$ respectively. We have assumed the periodic boundary condition. These modes are harmonic phonons. Their densities of states $\rho_{f}^{(0)}$ and $\rho_{g}^{(0)}$ are given by

$$\rho_{f}^{(0)}=\rho_{g}^{(0)}=\frac{L}{2\pi}.$$  (A·6)

$H^{(2)}$ in Eq. (A·2) is easily diagonalized by the use of the above complete sets $\{f(x)\}$ and $\{g(x)\}$ and reduced to the assembly of harmonic oscillators with frequencies $\{\omega_{f}\}$ and $\{\omega_{g}\}$. Neglecting the quantum properties of harmonic fluctuations, the free-energy density of harmonic phonons $F_{\theta}^{(0)}(\beta)$ is given by

<table>
<thead>
<tr>
<th>$f_{0}(x)$</th>
<th>$g_{0}(x)$</th>
<th>$f_{\pm 1}(x)$</th>
<th>$g_{\pm 1}(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-(3\sqrt{2})^{1/2}\text{sech}^{2}\frac{1}{\sqrt{2}}x$</td>
<td>$-(3\sqrt{2})^{1/2}\text{sech}^{2}\frac{1}{\sqrt{2}}x \text{sh} \frac{1}{\sqrt{2}}x$</td>
<td>$3\text{th}^{2}\frac{1}{\sqrt{2}}x-2k^{2}-3\sqrt{2}k\text{ th} \frac{1}{\sqrt{2}}x$</td>
<td>$3\text{th}^{2}\frac{1}{\sqrt{2}}x-2k^{2}-3\sqrt{2}k\text{ th} \frac{1}{\sqrt{2}}x$</td>
</tr>
<tr>
<td>$f_{k}(x)=\frac{1}{\sqrt{L}}e^{ikx}$</td>
<td>$g_{k}(x)=\frac{1}{\sqrt{L}}e^{ikx}$</td>
<td>$Lk+\delta_{s}(k')=2\pi n$</td>
<td>$\frac{Lk+\delta_{s}(k')}{2\pi}$</td>
</tr>
<tr>
<td>$\omega_{f}(k)=\sqrt{k^{2}+2}, \quad \omega_{g}(k)=\sqrt{k^{2}+\frac{1}{2}x}$</td>
<td>$\omega_{f}(k)=\sqrt{k^{2}+\frac{1}{2}x}, \quad \omega_{g}(k)=\sqrt{k^{2}+\frac{1}{2}x}$</td>
<td>$\delta_{s}(k')=2\pi\left</td>
<td>\frac{k'}{k}\right</td>
</tr>
</tbody>
</table>

* We can use classical statistical mechanics for $\beta h\sqrt{2}<1$ and $\beta h\sqrt{x/2}<1$. 

**Downloaded from https://academic.oup.com/ptp/article-abstract/68/6/1880/1878622 by guest on 06 December 2018**
\[ F_0^0(\beta) = F_{0,1}^0(\beta) + F_{0,2}^0(\beta), \]  
(A·7a)

\[ F_0^j(\beta) = \frac{1}{L} \int_{-\pi/L}^{\pi/L} dk \omega_j(k), \quad j = \xi \text{ or } \eta, \]  
(A·7b)

where \( \omega_j(k) \) is the discrete dispersion in contrast with continuum dispersion \( \omega_j(k) \) in Eq. (A·5). After calculating Eq. (A·7) and taking the continuum limit, we get the first two terms of Eq. (5·3). The third term of Eq. (5·3) is caused by the anharmonicity.

(ii) Small fluctuations around a class-1 kink at rest

We set \( \xi(0)(x) = \text{th}(x/\sqrt{2}) \) and \( \eta(0)(x) = 0 \), then we find \( f \) and \( g \) of Eq. (A·4) are not coupled with one another again. We get the result summarized in Table IV. We can find that \( \omega_{\eta,1} \), which is the frequency of the internal oscillations of \( \eta(0)(x) \), becomes zero just at \( x = 1 \) (peculiar fluctuations) and imaginary for \( 0 < x < 1 \). We conclude that the class-1 kink is stable only for \( x > 1 \).

In the case \( x > 1 \), \( H^{(2)} \) in Eq. (A·2) is diagonalized in the same way. The self-energy \( \Sigma(\beta) \) is given by

\[ \Sigma(\beta) = \Sigma_\xi(\beta) + \Sigma_\eta(\eta \beta), \]  
(A·8a)

\[ \Sigma_\xi(\beta) = \frac{1}{\beta} \mathcal{P} \int_{-\pi/L}^{\pi/L} dk \Delta \rho_j(k') \ln{\{\beta \hbar \omega_j(k')\}} + \frac{1}{\beta} \ln{\{\beta \hbar \omega_{\eta,1}\}}, \]  
(A·8b)

\[ \Delta \rho_j(k') = \frac{1}{2\pi} \frac{d \delta_j(k')}{dk'}, \quad j = \xi \text{ or } \eta, \]  
(A·8c)

where \( \delta_j(k') \) and \( \omega_{\eta,1} \) are shown in Table IV and \( \mathcal{P} \int \) means to take Cauchy's principal value. From Eq. (A·8) we obtain Eq. (5·4) similarly.

In the case \( x = 1 \) we get the same \( \Sigma_\xi(\beta) \) as Eq. (A·8b) as none of the \( \xi \)-fluctuations is softened. For the \( \eta \)-fluctuations we have to treat the softened mode separately from the non-softened modes. If we describe the softened mode by Eq. (5·7), we get

\[ \Sigma_\eta(\beta) = \frac{1}{\beta} \mathcal{P} \int_{-\pi/L}^{\pi/L} dk \Delta \rho_\eta(k') \ln{\{\beta \hbar \omega_\eta(k')\}} - \frac{1}{\beta} \ln{Z_1}, \]  
(A·9a)

\[ Z_1 = \frac{1}{\hbar} \int_{-\infty}^{\infty} dP_1 \int_{-\infty}^{\infty} dQ_1 e^{-\beta H_1} = \frac{\Gamma(1/4)}{2\sqrt{\pi}} \frac{1}{\beta^{3/4} \hbar a^{1/4}}, \]  
(A·9b)

where \( H_1 \) is given by Eq. (5·7). From Eq. (A·9) we obtain Eq. (5·8) similarly.

(iii) Small fluctuations around a class-2 or class-3 kink at rest

Because of \( \eta(0)(x) \neq 0 \) Eq. (A·4) is now coupled eigenvalue equation. Analytic solutions are not obtained so far. But the stability arguments of both kinks are performed by the numerical technique. As shown in Table I, the class-
2 kink is stable, but the class-3 kink is unstable. We believe that there must be one mode around a class-2 kink that is softened at $x=1$. If we could find analytic solutions of small fluctuations around a class-2 kink, we could obtain the free-energy density that is the same as Eq. (3.21) for $0<x<1$ in the same manner.

References

1) For a review, see for example, A. R. Bishop, J. A. Krumhansl and S. E. Trullinger, Physica 1D (1980), 1.
7) S. Sarker, S. E. Trullinger and A. R. Bishop, Phys. Letters A59 (1976), 255.