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# Classical $\phi^6$-field theory in (1+1) dimensions. A model for structural phase transitions

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**Abstract.** The classical $\phi^6$ -field theory in (1+1) dimensions, is considered as a model for the first order structural phase transitions. The equation of motion is solved exactly; and the presence of domain wall (kink) solutions at and below the transition point, in addition to the usual phonon-like oscillatory solutions, is demonstrated. The domain wall solutions are shown to be stable, and their mass and energies are calculated. Above the transition point there exists exotic unstable kink-like solutions which takes the particle from one hill top to the other of the potential. The partition function of the system is calculated exactly using the functional integral method together with the transfer matrix techniques which necessitates the determination of the eigenvalues of a Schrödinger-like equation. Thus the exact free energy is evaluated which in the low temperature limit has a phonon part and a contribution coming from the domain wall excitations. It was shown that this domain wall free energy differs from that calculated by the use of the domain wall phenomenology proposed by Krumhansl and Schrieffer. The exact solutions of the Schrödinger-like equation are also used to evaluate the displacement-displacement, intensity-intensity correlation functions and the probability distribution function. These results are compared with those obtained from the phenomenology as well as the $\phi^4$ -field theory. A qualitative picture of the central peak observed in structural phase transitions is proposed.

**Keywords.** $\phi^6$-field theory; structural phase transitions; central peak; soft mode

## 1. Introduction

The structural phase transition (SPT) observed in ferroelectric crystals is usually associated with a soft phonon mode whose frequency decreases as the temperature is lowered towards its critical value ($T_c$) (Lines and Glass 1977). Besides the soft phonon mode a central peak near zero frequency is also observed in these transitions. The central peak is characterised by a negligible width and its strength grows as one approaches $T_c$ from above (Riste *et al* 1971; Shapiro *et al* 1972). Even though, some understanding of the soft mode has emerged the central peak phenomenon still remains a puzzle (Bruce 1978). Conventionally, in describing the SPT one takes recourse to two different types of models namely the order-disorder and the displacive transitions. Whereas in the former case the on-site energy of the atoms is much larger than the intersite coupling, in the latter case the reverse is true. However, lately it has been realized that both these transitions can occur within the same model (Bruce *et al* 1979). The major advancement in the understanding of SPT, and in particular the central peak phenomenon has emerged from one-dimensional model

calculations, as these provide a nonperturbative approach to strongly anharmonic systems. It may however be noted that these models do not show a phase transition at finite temperature.

The first significant calculation of this type was due to Krumhansl and Schrieffer (1975) (KS) who considered the $\phi^4$ field theory in (1+1) dimensions as a model for SPT. In particular they identified the kink solutions with domain walls and showed that the low temperature behaviour of the system is determined by both phonon and domain wall-like excitations. They also calculated the statistical mechanics of the system making use of the WKB approximation and found that at low temperatures the domain wall contribution to the free energy is exponentially small. In this model the domain wall solutions are identified with the central peak phenomena, however these exist only below the transition curve of the $\phi^4$ potential. Similar results have also been obtained by Varma (1976). Halperin and Varma (1976) applied the renormalization group technique to this model. Aubry (1976) performed molecular dynamics calculation for the $\phi^4$–field theory and showed the connection between the domain wall solutions and the peaks in the dynamical structure function. Further evidence in support of the connection between the domain walls or clusters and the central peak came from the molecular dynamics calculations of Schneider and Stoll (1975, 1976) in two dimensions; and the quantum mechanical calculation of Bishop *et al* (1976).

All these $\phi^4$ models exhibit second order phase transition for which it is well-known that the soft mode frequency goes to zero at transition point. However, experimental data on $SrTiO_3$ (Shapiro *et al* 1972) and other perovskites (see Halperin and Varma 1976 for references) indicate that the soft mode frequency does not vanish at $T_c$, which is indicative of a first order rather than a second order phase transition. With this in mind recently we (Khare and Behera 1980 hereafter referred to as I) have proposed an anharmonic oscillator model which exhibits first order phase transition, and applied it to SPT within the mean field approximation. In this paper we go beyond the mean field approximation by considering the $\phi^6$-field theory in (1+1) dimensions. A short account of this work is given in Behera and Khare (1979).

In § 2 we discuss the dynamics of the $\phi^6$–field theory. In particular we show that the exact solutions of the field equation are the Weirstrass' functions; Kink or domain wall solutions of finite energy are shown to exist below the phase transition point and their energy is calculated. Oscillatory solutions and the corresponding dispersion relations are also obtained. In addition to the kink solutions an exotic class of solutions of finite energy are shown to exist which take the particle from one hill top (maxima) of the potential to the other; as $x$ goes from $-\infty$ to $+\infty$. The physical interpretation of the kink and exotic solutions and their relevance to order-disorder and displacive phase transitions is discussed in § 3. § 4 is devoted to the calculation of the classical statistical mechanics of this system. We show that the classical partition function and the intensity-intensity correlation function can be calculated exactly below the transition point using the transfer matrix technique and the exact solution of a Schrödinger-like eigenvalue problem for the $\phi^6$ potential. The free energy is thus obtained exactly. Using the dispersion relations obtained in § 2, the phonon contribution to the free energy at low temperature is evaluated. The difference between the exact and phonon free energies is attributed to domain walls. Following KS the free energy of a system of non-interacting kinks is also estimated, and found to be exponentially small. In § 5 we calculate the displacement-displace-

ment, intensity-intensity correlations and the probability distribution functions. Finally we conclude by summarizing the results of the paper in § 6.

## 2. Dynamics of $\phi^6$–field theory

We consider the following model Hamiltonian for the one-dimensional lattice

$$H = \sum_i \left[\frac{1}{2} m \dot{\phi}_i^2 + V(\phi_i)\right] + \frac{1}{2} \sum_{i,j} C_{ij} (\phi_i - \phi_i)^2, \tag{1}$$

where the on-site potential is given by

$$V(\phi_i) = B \phi_i^2 + A \phi_i^4 + C \phi_i^6, \; C > 0, \tag{2}$$

and the last term in equation (1) describes the nearest neighbour coupling which is quadratic in $\phi$. The continuum limit of equation (1) will represent $\phi^6$-field theory and is given by

$$H = \int \frac{dx}{l} [\tfrac{1}{2} m (d\phi/dt)^2 + \tfrac{1}{2} m C_0^2 (d\phi/dx)^2 + V(\phi)], \tag{3}$$

where $l$ is the lattice constant and $C_0$ is the velocity of sound. Equation (3) can be easily converted to the standard field theory Lagrangian which is renormalizable in (1+1) dimensions. The on-site potential (equation (2)) whose average value essentially corresponds to the static free energy of the system exhibits a first order phase transition if

$$B > 0, \; A < 0 \text{ and } 0 < a \left(\equiv \frac{9BC}{2|A|^2}\right) < 3/2. \tag{4}$$

Under these conditions the potential (free energy) has three minima (which are essential for a first order phase transition) at

$$\phi = 0, \; (\phi_{\min}/\phi_0) = \pm \frac{1}{\sqrt{2}} \left[1 + \left(1 + \frac{2a}{3}\right)^{\frac{1}{2}}\right]^{\frac{1}{2}}, \tag{5}$$

with $\phi_0 = [2|A|/3C]^{\frac{1}{2}}$. The maxima of the potential occur at

$$(\phi_{\max}/\phi_0) = \pm \frac{1}{\sqrt{2}} \left[1 - \left(1 - \frac{2a}{3}\right)^{\frac{1}{2}}\right]^{\frac{1}{2}}. \tag{6}$$

The value of the potential at the extrema are ($\phi \neq 0$)

$$\left(V_{\substack{\max \\ \min}}/V_0\right) = \frac{1}{2}\left[(a-1) \pm \left(1 - \frac{2a}{3}\right)^{3/2}\right], \tag{7}$$

where $V_0 = (4|A|^3/27C^2)$. The potential for different values of $a$ is plotted in figure 1 of I. This being a one-dimensional model, in what follows we envisage a phase

transition in terms of the potential parameter $a$. It can be seen that at the first order phase transition point $a_c=9/8$, all the three minima of the potential are degenerate. While for $3/2 > a > a_c$ there are two degenerate local minima and an absolute minimum at $\phi=0$, for $0 < a < a_c$ there are two degenerate absolute minima and one local minimum (at $\phi = 0$). At $a = 3/2$ there is only one minimum at $\phi = 0$ and two points of inflation at $\phi=\pm(|A|/3C)^{1/2}$; while for $a > 3/2$ there is a single well. At and below $a=0$, the potential has a double well structure similar to the $\phi^4$-field theory. It may be worth mentioning that for

$$A > 0,\ C > 0, \tag{8}$$

this model exhibits a second order phase transition, the transition occurring at $B = 0$.

### 2.1. *Solutions of field equations*

The equation of motion for the field as obtained from equation (3) is

$$m\frac{d^2\phi}{dt^2} - m C_0^2\frac{d^2\phi}{dx^2} + 2B\phi - 4A\phi^3 + 6C\phi^5 = 0, \tag{9}$$

On substituting

$$\phi(xt) = f(x - vt), \tag{10a}$$

$$S = (x - vt)/\xi,\ \xi^2 = m(C_0^2 - v^2)/2B, \tag{10b}$$

in equation (9) we have

$$\frac{d^2f}{dS^2} - f + \frac{2|A|}{B}f^3 - \frac{3C}{B}f^5 = 0. \tag{11}$$

For $C = 0$, $A > 0$ and $B < 0$ this equation reduces to the well-known Ginzburg-Landau equation. It is instructive to compare (11) with the equation of motion for the corresponding single anharmonic oscillator (see equation (9) of I). As $s \to it$ equation (11) goes over to equation (9) of I; in other words the field dynamics is essentially equivalent to the particle dynamics in an inverted potential or equivalently in the Eucledian space. As we shall see this correspondence can be exploited for obtaining the various solutions of the non-linear field equation (11).

Equation (11) can be integrated to obtain

$$(df/dS)^2 - f^2 + \frac{|A|}{B}f^4 - \frac{C}{B}f^6 = \epsilon V_0, \tag{12}$$

where unlike the case of I, $\epsilon$ is an arbitrary constant and not the energy of the system. On further integrating (12) we have

$$S = \int^f \frac{df}{\left[\epsilon V_0 + f^2 - \frac{|A|}{B}f^4 + \frac{C}{B}f^6\right]^{1/2}} \tag{13}$$

We will consider the cases (a) $\epsilon \geqslant 0$, (b) $\epsilon < 0$ separately.

(a) $\epsilon \geqslant 0$: In this case (13) can be reduced to the form

$$-\left(\frac{2|A|\epsilon}{3aC}\right)^{\frac{1}{2}} S = \int_{\frac{1}{f^2}+\frac{aC}{2|A|\epsilon}}^{\infty} [d\eta/(4\eta^3 - g_2\,\eta - g_3)^{1/2}], \tag{14}$$

where
$$g_2 = \frac{3C^2}{|A|^2}\left(\frac{a^2}{\epsilon^2}+\frac{9}{\epsilon}\right), \tag{15a}$$

$$g_3 = -\frac{C^3}{|A^3|}\left(\frac{a^3}{\epsilon^3}+\frac{27}{2}\,\frac{a}{\epsilon^2}+\frac{27}{\epsilon}\right). \tag{15b}$$

The solutions of (14) can be expressed in terms of Weirstrass functions (Abramowitz and Stegun 1965).

$$1/f^2 = -\frac{aC}{2|A|\epsilon} + \wp\left[-\left(\frac{2|A|\epsilon}{3aC}\right)^{1/2} S,\ g_2,\ g_3\right] \tag{16}$$

This solution takes different forms for $\Delta \gtrless 0$, where $\Delta$ is defined by

$$\Delta \equiv g_2^3 - 27g_3^2 = \frac{16|A|^3}{V_0^3\epsilon^4}\left[-4\epsilon^2 + 4\epsilon(1-a) + \frac{a^2}{3}\left(1-\frac{8}{9}a\right)\right]. \tag{17}$$

(Equations (14)-(17) are analogous to the corresponding equations of I for $E < 0$). From (17) it follows that

(i) $a > 9/8$, $\Delta < 0$,

(ii) $a = 9/8$, $\Delta = 0$ at $\epsilon = 0$, $\Delta < 0$ otherwise,

(iii) $a < 9/8$, $\Delta > 0$ for $\epsilon < -(V_{\min}/V_0)$
$\Delta = 0$ for $\epsilon = -(V_{\min}/V_0)$
$\Delta < 0$ for $\epsilon < -(V_{\min}/V_0)$.

First let us consider the solutions for the case of $\Delta = 0$. For $a = 9/8$ ($\equiv a_c$) and $\epsilon = 0$, starting from (13) one finds two kink (domain wall) solutions (Khare 1979)

$$f^{(1)} = \pm\,(|A|/4C)^{1/2}\,[1 + \tanh S]^{1/2}, \tag{18a}$$

$$f^{(2)} = \mp\,(|A|/4C)^{1/2}\,[1 - \tanh S]^{1/2}. \tag{18b}$$

It follows from (18) that the width of these domain walls is $\Delta_d = 2\xi$. The solutions $f^{(1)\,(2)}$ have the property that as $S$ goes from $-\infty$ to $+\infty$, $f^{(1)}$ goes from 0 to

$\pm(|A|/2c)^{\frac{1}{2}}$ and simultaneously $f^{(2)}$ goes from $\mp\sqrt{(|A|/2c)}$ to 0; which are the three absolute minima of the potential. Hence in (18) the upper signs correspond to the kink (domain wall) solutions and the lower signs to antikink solutions. On the other hand for $a < 9/8$, and $\Delta = 0$ ($\epsilon = -V_{\min}/V_0$) there is only one domain wall solution, which is given by

$$f(S) = \pm\left[\frac{2|A|\epsilon}{3Ca\left(1+\frac{9\epsilon}{a^2}\right)^{1/2}}\right]^{1/2} \times \frac{\sin h\left(1+\frac{9\epsilon}{a^2}\right)^{1/4} S}{\left\{1+\frac{1}{3}\left(1-\left(1+\frac{9\epsilon}{a^2}\right)^{-1/2}\right)\sin h^2\left(1+\frac{9\epsilon}{a^2}\right)^{1/4} S\right\}^{1/2}}. \tag{19a}$$

As $S$ goes from $-\infty$ to $+\infty$, we again find that $f(S)$ goes from one absolute minimum to the other. The width of the domain wall in this case turns out to be

$$\Delta_d = 2\left(1+\frac{9\epsilon}{a^2}\right)^{-1/4}\xi. \tag{19b}$$

It can be easily checked that for $a = 9/8$, this reduces to $2\xi$.

In contrast to the case of $\Delta = 0$, for $\Delta \gtrless 0$ the solutions are oscillatory and can be expressed in terms of Jacobi-elliptic functions (Abramowitz and Stegun 1965). For $\Delta > 0$ the solution is given by

$$f(S) = \pm \frac{Sn\,[-y^{1/4}\,(2|A|\epsilon/3\,Ca)^{1/2}\,S\,|\,k]}{\left\{y^{1/2}+\left(e_3-\frac{Ca}{2|A|\epsilon}\right)Sn^2\,[-y^{1/4}\,(2|A|\epsilon/3\,Ca)^{1/2}\,S\,|\,k]\right\}^{1/2}} \tag{20}$$

where

$$e_3 = -\tfrac{1}{2}(k+1)\,[g_2/\,3(k^2-k+1)]^{1/2}, \tag{21}$$

$$k = \tfrac{1}{2}\,[1 \pm [3(g_2-y)/y]^{1/2}], \tag{22}$$

and $y$ is the real root of the cubic equation

$$y^3 - \frac{3}{2}g_2y^2 + \frac{9}{16}g_2^2\,y - \Delta/16 = 0. \tag{23}$$

The quantity $0 \leqslant k \leqslant 1$ measures the degree of anharmonicity of the oscillations. It can be checked that in case of extreme anharmonicity, ($k$=1) the solution (20) goes over to the kink solution given by (19). Using (10b) together with the fact that the $Sn$ function has a period of $4K(k)$ ($K(k)$ being the normal elliptic integral of the first kind), the dispersion relation for these oscillations can be written down as

$$\omega_q^2 \equiv v^2\,q^2 = C_0^2\,q^2 - \frac{\pi^2\,y^{1/2}\,|A|\,\epsilon\,B}{3\,Ca\,K^2(k)\,m}. \tag{24}$$

The frequency $\omega_q$ will only be real if

$$q \geqslant \left[\frac{\pi^2 y^{1/2} \,|A|\, \epsilon}{3\, C_0^2\, Ca\, K^2\,(k)}\, \frac{B}{m}\right]^{1/2}. \tag{25}$$

Similarly for $\Delta < 0$, the solution is

$$f(S) = \pm \frac{Sn\,[-y_1^{1/4}\,(2\,|A|\,\epsilon/3Ca)^{1/2}\, S\,|k]}{\left\{ y_1^{1/2}\, Cd^2\left[-y_1^{1/4}\,(2\,|A|\,\epsilon/3Ca)^{1/2}\, S|k\right] + \left(e_2 - \frac{aC}{2\,|A|\,\epsilon}\right)\right.}$$

$$\left. \times\, Sn^2\,[-y_1^{1/4}\left(\frac{2\,|A|\,\epsilon}{3\,Ca}\right)^{1/2} S\,|k\right]\Big\}^{1/2} \tag{26}$$

where $$e_2 = \left[\frac{g_2\,(1-2k)^2}{3\,(16k^2 - 16\,k + 1)}\right]^{1/2}, \tag{27}$$

$$k = \frac{1}{2}\left[1 - \frac{\sqrt{3}}{2}(1 + g_2/4y_1)^{1/2}\right], \quad 0 < k < \tfrac{1}{2}, \tag{28}$$

and $y_1$ satisfies the cubic equation

$$y_1^3 - \tfrac{3}{4}\, g_2\, y_1^2 + \Delta/16 = 0. \tag{29}$$

The dispersion relation for this case is the same as that given by (24) except for the fact that $y$ is replaced by $y_1$.

(b) $\epsilon < 0$ : In this case equation (13) can be reduced to the form

$$\left(\frac{2\,|A|\,|\epsilon|}{3a\,C}\right)^{1/2} S = \int_{-\frac{1}{f^2} + \frac{aC}{2\,|A|\,|\epsilon|}}^{\infty} \frac{d\eta}{(4\,\eta^3\, g_2'\,\eta - g_3')^{1/2}} \tag{30}$$

where $$g_2' = \frac{3\,C^2}{|A|^2}\left[\frac{a^2}{|\epsilon|^2} - \frac{9}{|\epsilon|}\right], \tag{31}$$

$$g_3' = -\frac{C^3}{|A|^3}\left[\frac{a^3}{|\epsilon|^3} - \frac{27}{2}\,\frac{a}{|\epsilon|^2} + \frac{27}{|\epsilon|}\right], \tag{32}$$

and one can define $\Delta'$ as

$$\Delta' \equiv g_2'^3 - 27\, g_3'^2 = \frac{16\,|A|^3}{V_0^3\,|\epsilon|^4}\left[-4\,|\epsilon|^2 + 4\,|\epsilon|\,(a-1) + \frac{a^2}{3}\left(1 - \frac{8a}{9}\right)\right]. \tag{33}$$

Again these equations compare with the corresponding equations for $E<0$ of I. The form of the solutions will depend on the value of $\Delta'$; which for

(i) $a>3/2 \quad \Delta'<0$

(ii) $a=3/2$ $\Delta'<0$, for $|\epsilon|>0$ but $|\epsilon| \neq \frac{1}{4}\,(\equiv V_{\text{infl}}/V_0)$

(iii) $3/2>a>9/8 \quad \Delta'<0$ for $(V_{\min}/V_0)>|\epsilon|>0$,
and $|\epsilon|>(V_{\max}/V_0)$; $\Delta'>0$ for $(V_{\min}/V_0)<|\epsilon|<(V_{\max}/V_0)$.

(iv) $a \leqslant 9/8$ $\Delta'>0$ for $(V_{\max}/V_0)>|\epsilon|>0$ and $\Delta'<0$ for $|\epsilon|>V_{\max}$.
Finally (v) $\Delta'=0$ at $|\epsilon|=(V_{\min/\max}/V_0)$.

For $\Delta'=0$ (case (v) there are two possibilities namely $g_2>0$, $g_3>0$ which happens at $|\epsilon|=(V_{\max}/V_0)$ and $g_2>0$, $g_3<0$ which is the case for $|\epsilon|=(V_{\min}/V_0)$ and hence is only possible for $3/2>a>9/8$. The solution for the former case can be written as

$$\frac{1}{f^2}=\frac{aC}{2|A||\epsilon|}\left[1+\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/2}\right]-\frac{\dfrac{3aC}{2|A||\epsilon|}\left(1-\dfrac{9|\epsilon|}{a^2}\right)^{1/2}}{\sin^2\left(1-\dfrac{9|\epsilon|}{a^2}\right)^{1/4}S}. \tag{33}$$

As is obvious from (33) for small $S$, $f(s)$ is imaginary, so that the solution in the present form is unphysical. However, if $s\to iS$, i.e. $v>C_0$, then the solution is acceptable and is given by

$$f=\pm\left[\frac{2|A||\epsilon|}{3Ca\left(1-\dfrac{9|\epsilon|}{a^2}\right)^{1/2}}\right]^{1/2}\frac{\sinh\left(1-\dfrac{9|\epsilon|}{a^2}\right)^{1/4}s}{\left\{1+\frac{1}{3}\left[1+\left(1-\dfrac{9|\epsilon|}{a^2}\right)^{-1/2}\right]\right.}$$

$$\left.\times\sinh^2\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/4}s\right\}^{1/2} \tag{34}$$

where $$s=iS=\frac{(x-vt)}{(v^2-C_0^2)^{1/2}}\sqrt{\frac{2B}{m}}. \tag{35}$$

This solution has the very interesting property that at $s=0$, $f(0)=0$ and as $s$ goes from $-\infty$ to $+\infty$, $f(s)$ goes from one hill top (maximum) of the potential to the other. Hence such a solution exists only for $3/2>a>0$. This again is a kink like localized solution and is very similar to the solutions as given in equations (29) of I. The physical interpretation of this solution will be discussed in the next section. As far as we are aware such localized solutions for the field theory are written down for the first time; and its interpretation deserves more attention.

For $a=3/2$ and $\Delta'=0$ ($g_2'=0$, $g_3'=0$), yet another interesting solution exists, for $v > c_0$, which is

$$f(s) = \pm \frac{s}{\left(\frac{9C}{|A|}\right)^{1/2} [1+\frac{1}{3}s^2]^{1/2}}, \tag{36}$$

having the property that at $s=0$, $f(0)=0$, while as $s$ goes from $-\infty$ to $+\infty$, $f(s)$ goes from $-(|A|/3C)^{1/2}$ to $+(|A|/3C)$ which are the points of inflation of the potential curve. This again is a kink like, sticking, localized solution. Equations (34) and (36) are the inverse of the instanton solutions obtained by going back from the Eucledian to the Minkowski space.

For the other case of $\Delta' = 0$ (where $g_3' < 0$) the solution can be written as

$$\frac{1}{f^2} = \frac{aC}{|2A||\epsilon|}\left[1-\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/2}\right] - \frac{\frac{3aC}{2|A||\epsilon|}\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/2}}{\sin h^2\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/4} S}. \tag{37}$$

As $S$ goes from $-\infty$ to $+\infty$, $f(S)$ goes from one local minimum of the potential to the other, but becomes unphysical around $S=0$. The situation can again be salvaged if $v > C_0$, in which case the solution reduces to an oscillatory form given by

$$f(s) = \pm\left[\frac{2|A||\epsilon|}{3Ca\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/2}}\right]^{1/2} \frac{\sin\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/4} s}{\left\{1+\frac{1}{3}\left[1-\left(1-\frac{9|\epsilon|}{a^2}\right)^{-1/2}\right]\right.}$$
$$\left. \times \sin^2\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/4} s\right\}^{1/2}. \tag{38}$$

and the dispersion relation is given by

$$\omega_q^2 \equiv v^2q^2 = C_0^2 q^2 + \left(1-\frac{9|\epsilon|}{a^2}\right)^{1/2} \frac{2B}{m}, \tag{39}$$

which is optical phonon-like.

For $\Delta' > 0$ the physical solution exists for $v > C_0$ and is oscillatory, given by

$$1/f^2 = \frac{aC}{2|A||\epsilon|} - e_3 + \frac{y_2^{1/2}}{S_c^2\left(-y_2^{1/4}\sqrt{\frac{2|A||\epsilon|}{3Ca}}\, s\,|\,1-k\right)} \tag{40}$$

where $e_3$, $k$ and $y_2$ are given by equations (21), (22) and (23) respectively with $g_2$, $g_3$, $\Delta$ replaced by the corresponding primed quantities. Equation (40) reduces to (37) for $k=0$. In this the dispersion relation becomes

$$\omega_q^2 \equiv v^2q^2 = C_0^2 q^2 + \frac{\pi^2 y_2^{1/2}|A||\epsilon|}{3CaK^2(k)} \frac{B}{m}. \tag{41}$$

Finally, for $\Delta' < 0$, the solution (with $v > C_0$) becomes

$$1/f^2 = \frac{ac}{2|A||\epsilon|} - e_2 + \frac{y_3^{1/2}\, nd^2\, [y_3^{1/4}\, (2|A||\epsilon|/3Ca)^{1/2}\, s\,|\,1-k]}{S_0^2\, [y_3^{1/4}\, (2|A||\epsilon|/3Ca)^{1/2}\, s\,|\,1-k]} \tag{42}$$

where again $e_2$, $k$ and $y_3$ are given by (27), (28) and (29) respectively with $g_2$, $g_3$, $\Delta \to g_2'$, $g_3'$, $\Delta'$. The dispersion relation for this case is the same as (40) with $y_2$ replaced by $y_3$.

## 3. Physical interpretation of the solutions

Here we shall discuss the properties of the various localized and oscillatory solutions obtained in the last section. The localized solutions are expected to be of finite energy. We shall also show that these solutions are stable against smooth, local but otherwise arbitrary perturbations of the dynamics because of topological charge conservation. The topological current can be defined as

$$j_\mu(x, t) = \epsilon_{\mu\nu}\, \partial_\nu f(x, t); \left(\binom{\mu}{\nu} = 0, 1\right) \tag{43}$$

where $\epsilon_{\mu\nu}$ is an antisymmetric tensor of rank two ($-\epsilon_{01} = -\epsilon_{10} = 1$, $\epsilon_{11} = \epsilon_{00} = 0$). Since by construction $\partial_\mu j_\mu = 0$, the corresponding topological charge

$$Q = \int_{-\infty}^{\infty} j_0(x, t)\, dx = [f(+\infty, t) - f(-\infty, t)], \tag{44}$$

is conserved, and will be nonzero for the localized solutions.

### 3.1 *Domain wall (kink) solutions*

**3.1a** *Domain wall energy:* We shall first calculate the domain wall energies associated with the solutions given by equations (18) and (19), which is given by (Bishop 1978)

$$E_D = \frac{C_0}{l}\left(\frac{2\,m\,B}{1 - v^2/C_0^2}\right)^{1/2} \int_{-\infty}^{\infty} ds\, (df/ds)^2 \equiv m_D^*\, C_0^2 \tag{45a}$$

$$= \frac{C_0}{l}\left(\frac{2m}{1 - v^2/C_0^2}\right)^{1/2} \int_{f_1}^{f_2} df\, [V(f) + \epsilon\, V_0]^{1/2} \tag{45b}$$

where $$m_D^* = \frac{1}{\xi l} \int_{-\infty}^{\infty} ds\, (df/ds)^2 \tag{45c}$$

is the domain wall mass. In deriving these equations use has been made of the fact that the energy is measured from the bottom (minima) of the well to which the par-

ticle is carried by the domain wall solutions as $S \to \pm \infty$. Using solutions (18a) and (18b) for the transition point ($a = 9/8$) equation (45a) yields

$$E_D = \frac{C_0}{l}(m/2)^{1/2}\frac{|A|^2}{8\,C^{3/2}}\Big/\left(1-\frac{v^2}{C_0^2}\right)^{+1/2} \equiv E_D^{(0)}\left(1-\frac{v^2}{C_0^2}\right)^{-1/2} \tag{46a}$$

and
$$m_D^* = \frac{1}{4}\,m\,\frac{1}{l\xi}\,(B/C)^{1/2}. \tag{46b}$$

On the other hand for $a < 9/8$, the solution (19) yields

$$E_D = \frac{C_0}{l}(m/2)^{1/2}\frac{|2|A|^2}{C^{3/2}}\left(1-\frac{v^2}{C_0^2}\right)^{-1/2} \times$$

$$\frac{\epsilon}{\sqrt{a}}\frac{F(3,\,5/2,\,11/4,\,\gamma)\;\Gamma(11/4)}{\left(1+\frac{9\epsilon}{a^2}\right)^{1/4}\left[1-\left(1+\frac{9\epsilon}{a^2}\right)^{-1/2}\right]^3\Gamma\left(\frac{5}{2}\right)\Gamma\left(\frac{1}{4}\right)} \tag{47}$$

where
$$\gamma = -\frac{\left[2\left(1+\frac{9\epsilon}{a^2}\right)^{1/2}+1\right]}{\left[\left(1+\frac{9\epsilon}{a^2}\right)^{1/2}-1\right]}, \tag{48a}$$

and the domain wall mass turns out to be

$$m_D^* = m\frac{1}{l\xi}(B/C)^{1/2}\,\frac{27\epsilon}{a^{3/2}}\,\frac{F(3,\,5/2,\,11/4;\,\gamma)\;\Gamma(11/4)}{\left(1+\frac{9\epsilon}{a^2}\right)^{1/4}\left[1-\left(1+\frac{9\epsilon}{a^2}\right)^{-1/2}\right]^3\Gamma(5/2)\;\Gamma(1/4)}, \tag{48b}$$

and $F$ is the hypergeometric function (Abramowitz and Stegun 1965).

3.1b *Topological charge:* The topological charges for these domain wall solutions as obtained from equation (44), (18) and (19) are given by

$$Q = \pm\,(|A|/2C)^{1/2} = \pm\,\phi_{\min} \text{ for } a_c = 9/8, \tag{49a}$$

and
$$Q = \pm\,2\,(|A|/3C)^{1/2}\left[1+\left(1-\frac{2a}{3}\right)^{1/2}\right]^{1/2} = \pm\,2\phi_{\min} \text{ for } a < 9/8. \tag{49b}$$

The $\pm$ signs correspond to the kink and antikink solutions respectively. It is worth noting that at phase transition point (equation (49a)) $Q$ is nothing but the order parameter for SPT, whereas for $a < 9/8$ it is twice the order parameter. It is needless to say that for $a > 9/8$, the order parameter vanishes which is also reflected in the absence of a kink solution. From (44b) we notice that as $a$ decreases from its critical value the order parameter increases reaching the maximum value of

$(2|A|/3C)^{1/2}$ at $a=0$, and on decreasing $a$ further its value decreases and asymptotically approaches the starting value of $(|A|2C)^{1/2}$.

3.1c *Stability analysis:* Let us now discuss the stability of the domain wall solutions (Aubry 1976). If a small perturbation is given to the system, then the static ($v=0$) domain wall solutions get modified as

$$f(x, t) = f_0(x) + f_1(x) \exp(-i\omega t),$$

which when substituted in the equation of motion (equation (9) and linearized yields the following eigenvalue equation for $f_1$;

$$\left[-C_0^2 \frac{\partial^2}{\partial x^2} + \frac{1}{m}(\partial^2 V/\partial f^2)_{f=f_0}\right] f_1(x) = \omega^2 f_1(x). \tag{50}$$

The stability of the solution $f_0(x)$ is guaranteed if $\omega$ is real. As is well-known $f_1^{(0)}(x) = (\partial f_0/\partial x)$ is an eigenfunction of (50) with $\omega^2=0$. If one can show that $f_1^{(0)}(x)$ is nodeless, (that is, it is the ground state of the system) then the stability of $f_0(x)$ is established. For our solutions (18a, b) and (19) $f_1^{(0)}(x)$ are given by

$$f_1^{(0)}(x) \propto [1 \mp \tanh(x/\xi_0)]\,[1 \pm \tanh(x/\xi_0)]^{1/2} \text{ for } a = 9/8 \tag{51a}$$

$$f_1^{(0)}(x) \propto \frac{\cosh\left(1+\frac{9\epsilon}{a^2}\right)^{1/4}(x/\xi_0)}{\left\{1+\frac{1}{3}\left[1-\left(1+\frac{9\epsilon}{a^2}\right)^{-1/2}\right]\sinh^2\left(1+\frac{9\epsilon}{a^2}\right)^{1/4} x/\xi_0,\right\}^{3/2}} \tag{51b}$$

for $a < 9/8$.

with $\xi_0=\xi$ ($v=0$), which are clearly nodeless; thereby establishing the stability of the domain wall solutions. It may be interesting to solve the Schrödinger-like equation (50) and see whether in addition to these translational modes (Goldstone modes) at $\omega=0$, other bound states exist. For the case $a=9/8$ (solution (18)) it is possible to do so (Khare 1979) and it turns out that there are no other bound states in the system. However, for $a<9/8$ (solution (19)) the effective potential is rather complicated, and we have not been able to solve equation (50).

3.2 *Exotic kink solutions*

Here we shall calculate the field energy and topological charge for the kink-like solutions given by equations (34) and (36) which take the particle from one hill top to the other as $s$ goes from $-\infty$ to $+\infty$. The field energy can be calculated from (45) with the modification that $S$ is replaced by $s$ and the factor $(1-v^2/C_0^2)^{1/2}$ by $(v^2/C_0^2-1)^{1/2}$; besides the energy is to be measured with respect to the maxima of the potential. The field energy thus obtained is given by

$$E_D' = \frac{C_0}{l}\sqrt{\frac{m}{2}}\frac{12|A|^2}{C^{3/2}}\left(\frac{v^2}{C_0^2}-1\right)^{-1/2} \times$$

$$\times \frac{|\epsilon| F(3, 5/2, 11/4, \gamma')}{\sqrt{a}\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/4}\left[1+\left(1-\frac{9|\epsilon|}{a^2}\right)^{-1/2}\right]^3} \quad \frac{\Gamma(11/4)}{\Gamma(5/2)\,\Gamma(1/4)}. \tag{52}$$

where
$$\gamma' = -\left[\frac{2\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/2}-1}{1+\left(1-\frac{9|\epsilon|}{a^2}\right)^{1/2}}\right]. \tag{53}$$

Similarly the field energy for the sticking solution (equation (36)) can be shown to be

$$E_D' = \frac{C_0}{l}\sqrt{\frac{m}{2}}\frac{\pi|A|^2}{12C^{3/2}}\left(\frac{v^2}{C_0^2}-1\right)^{-1/2}. \tag{54}$$

Thus solutions (34) and (36) are clearly finite but high energy solutions. The corresponding conserved topological charges for these two cases are given by

$$Q' = \pm 2\,(|A|/3C)^{1/2}\left[1-\left(1-\frac{2a}{3}\right)^{1/2}\right]^{1/2} \equiv 2\,\phi_{\max} \tag{55}$$

From (55) it is clear that the topological charge which only exists for $3/2 \geqslant a > 0$, has a maximum value of $2\,(|A|/3C)$ at $a=3/2$ and smoothly goes to zero as $a\to 0$. Since $\phi_{\max}$ is an unstable position for the particle $Q'$ cannot be identified with an order parameter. If one attempts a stability analysis for these exotic kink-like solutions, it is clear that they will be unstable. At this stage it is worth pointing out that the physical meaning of these solutions is somewhat obscure. We propose here the following tentative picture of the relevance of these solutions to the observed central peak in SPT. Even though these finite energy solutions are unstable, the existence of a conserved topological charge guarantees the meta stability of them; as a result the particle will spend a finite amount of time at the hill tops. As one approaches $a=9/8$ from above the height of the hill top decreases so that the probability of finding the particle there increases resulting in the appearance of fluctuating dipole moments which will show up as a central peak. For $a \leqslant 9/8$ this effect will be masked by the presence of the domain walls which act as a precursor to the Bragg peak below the phase transition (Bruce 1978).

### 3.3 *Oscillatory solutions*

The solutions (20), (26), (38), (40) and (42) being oscillatory are extended phonon-like solutions for the one-dimensional anharmonic linear chain. These are expected to have finite energy density. For the solutions (20) and (26) $v<C_0$ and the dispersion relations as given by (24) is acoustic but for the fact that it starts with a finite value of $q$. Unlike the Debye dispersion for the harmonic phonons, these anharmonic acoustic phonons do not have a linear dispersion. On the other hand for the solutions given by (38), (40) and (42) for which case $v>C_0$, the dispersion for this monoatomic anharmonic continuum chain is optic phonon-like, for the $\phi^4$-field theory a detailed analysis of the dispersion relations has been done by Aubry (1976), most of which will go through for this case as well. These dispersion relations will be used to calculate the phonon part of the free energy of the system in the next section.

## 4. Classical statistical mechanics of the system

In this section we shall carry out an exact evaluation of the classical partition function of the system. In the limit of weak interionic coupling the system can be approximated by an assembly of $N$ independent anharmonic oscillators (order disorder transition) and its thermodynamics can be calculated using the mean field approach. Such a calculation is attempted in I. However, this mean field approach suffers from the disadvantage that the dynamic information which depends on the interion displacements, (such as phonons) is lost. Hence we shall consider here the strong coupling limit (i.e. displacive transition) in calculating the classical partition function

$$Z = \int\int \delta p(x)\, \delta \phi(x) \exp\left[(-\beta H(\phi, p))\right] \equiv Z_p Z_\phi \tag{56}$$

where $\beta = (k_B T)^{-1}$, $H(p, \phi)$ is given by equation (3),

$$Z_p = \int \delta p(x) \exp\left(-\frac{\beta}{2m}\int \frac{dx}{l} p^2(x)\right) = (2\pi m k_B T)^{N/2} \tag{57}$$

and

$$Z(\phi) = \int \delta \phi(x) \exp\left\{-\beta \int \frac{dx}{l}\left[\tfrac{1}{2} m C_0^2 \left(\frac{d\phi}{dx}\right)^2 + V(x)\right]\right\}. \tag{58}$$

Equation (58) can be evaluated using the functional integral method together with the transfer matrix technique, as given by Scalapino *et al* (1972); which boils down to the solution of an eigenvalue equation and $Z_\phi$ becomes

$$Z_\phi = \sum_n \exp(-\beta N \epsilon_n) \cong \exp(-\beta N \epsilon_0). \tag{59}$$

The second step in (59) obviously follows in the thermodynamic limit. The quantities $\epsilon_n$ appearing in (59) are the eigenvalues of the Schrödinger like equation

$$\left[\frac{1}{2\beta}\ln\left(\frac{2\pi l^2}{\beta m C_0^2}\right) - \frac{1}{2m^*}\frac{\partial^2}{\partial \phi^2} + V(\phi)\right]\Psi_n(\phi) = \epsilon_n \Psi_n(\phi), \tag{60}$$

where

$$m^* = m\beta^2 C_0^2 / l^2, \tag{61}$$

is the temperature-dependent effective mass. Hence from (57) and (59) the free energy per unit length becomes

$$F/L = (\epsilon_0/l) - \frac{1}{2l\beta}\ln(2\pi m/\beta), \tag{62}$$

where the ground state eigenvalue $\epsilon_0$ is measured with respect to the absolute minima of the potential $V(\phi)$. For the $\phi^4$-field theory considered by KS, the non-existence of exact solutions of the eigenvalue equation (60) forced them to take recourse to the

WKB approximation for the calculation of the ground state eigenvalue. Fortunately in the present case (equation (2)) it is possible to find exact solutions to (60), which enables us to calculate the statistical mechanics of the system exactly. The knowledge of the eigenvalues $\epsilon_n$ and eigen functions $\Psi_n$ can also be used to calculate the displacement-displacement ($C_1(x)$) and intensity-intensity ($C_2(x)$) correlation functions (Scalapino *et al* 1972) which are given by

$$C_1(x) \equiv \langle \phi(x)\phi(0)\rangle = \sum_n |\langle \Psi_n | \phi | \Psi_0 \rangle|^2 \exp\left(-\frac{\beta x}{l}(\epsilon_n - \epsilon_0)\right) \quad (63a)$$

and

$$C_2(x) \equiv \langle \delta|\phi(x)|^2\, \delta|\phi(0)|^2\rangle = \sum_n |\langle \Psi_n | \delta|\phi|^2 | \Psi_0\rangle|^2 \exp\left(-\frac{\beta x}{l}(\epsilon_n - \epsilon_0\right) \quad (63b)$$

where $\delta|\phi(x)|^2 = |\phi(x)|^2 - \langle|\phi|^2\rangle$.

4.1. *Solution of the Schrödinger equation for the $\phi^6$ potential*

Singh *et al* (1978) have developed a general method for the solution of the Schrödinger equation for the $\phi^6$ potential (equation (2)) in terms of an infinite continued fraction expansion for the Green's function. In particular they showed that few of the exact solutions for this problem can be obtained provided the coefficients of the potential satisfy the condition

$$\left(\frac{A^2}{4C} - B\right) = (C/2m^*)^{1/2}\,(4n + 3 + 2q),\ n = 0, 1, 2, \quad (64)$$

with $q$=0(1) for even (odd) solutions. The right side of (64) being +ve, the condition implies that $A^2 > 4BC$, which in turn is satisfied only if a $a < 9/8$, that is below the phase transition point for $A < 0$. For this case the energy eigenvalues are given by

$$E_n = \frac{A}{2(2m^*C)^{1/2}}\,(4n + 1 + 2q), \quad (65)$$

which are +ve for $A > 0$ and −ve for $A < 0$ as expected. The corresponding eigenfunctions are given by

$$\Psi_n(\phi) = \exp(u(\phi))\,\psi_n(\phi), \quad (66)$$

where

$$u(\phi) = -\tfrac{1}{4}(2m^*C)^{1/2}\phi^4 + \frac{|A|}{4}(2m^*/C)^{1/2}\phi^2, \quad (67a)$$

and

$$\psi_n(\phi) = \sum_{v=0}^{n} b_v \phi^{2v+q}, \quad (67b)$$

is a polynomial in $\phi$. For the sake of completeness we list below the eigenvalues and eigenfunctions for the first few values of $n$, for the cases $A < 0$.

(i) For $n = 0$ and $q = 0$, the condition (equation (64)) becomes

$$a = \frac{9}{8}\,[1 + (9c/2m^*B^2)^{1/2}]^{-1} \equiv \frac{9}{8}\,(\alpha_0^0)^{-1}. \tag{68a}$$

The corresponding eigenvalue and eigenfunction are

$$E_0^0 = -\,(B/2m^*)^{1/2}\,(\alpha_0^0)^{1/2} \tag{68b}$$

and

$$\Psi_0 = b_0 \exp\,[-\tfrac{1}{4}\,(2m^*\,C)^{1/2}\,\phi^4 + (m^*B/2)^{1/2}\,(\alpha_0^0)^{1/2}\,\phi^2] \tag{68c}$$

$b_0$ being the normalization constant. Note that $\Psi_0$ has no nodes, hence $E_0^0$ is the ground state eigenvalue.

(ii) For $n = 0$, and $q = 1$, equations (64) to (67) reduce to

$$a = \frac{9}{8}\,[\,1 + (25C/2m^*\,B^2)^{1/2}]^{-1} \equiv \frac{9}{8}\,(\alpha_0^1)^{-1} \tag{69a}$$

$$E_0^1 = -\,3\,(B/2m^*)^{1/2}\,(\alpha_0^1)^{1/2} \tag{69b}$$

and

$$\Psi_1 = b_0\,\phi \exp\,(-\tfrac{1}{4}\,(2m^*\,C)^{1/2}\,\phi^4 + (m^*\,B/2)^{1/2}\,(\alpha_0^1)^{1/2}\,\phi^2] \tag{69c}$$

Since $\Psi_1$ has a node at $\phi = 0$ it corresponds to the first excited state but for a different potential as determined by (69a). Thus (68) and (69) are the ground and first excited states for two different potentials. For the case $A > 0$ these two solutions have been written down by Flessas (1979).

(iii) For $n = 1$, on the other hand there will be either two even solutions (i.e. ground state and second excited state) for $q = 0$ or two odd solutions (i.e. first and third excited states) for $q=1$. For the even solutions ($q=0$) equations (64) reduce to

$$a = \frac{9}{8}\,[\,1 + (49C/2m^*\,B^2)^{1/2}]^{-1} \equiv \frac{9}{8}\,(\alpha_1^0)^{-1}. \tag{70}$$

It can be seen from (67b), that for this case the eigenfunction involves an arbitrary constant, which can be determined by directly substituting (67b) into the differential equation for $\psi_n\,(\phi)$ (Singh *et al* (1978)). The energy eigenvalues are also determined from the same procedure (rather than from (65)) and are given by

$$E_1^0(\pm) = -\,(B/2m^*)^{1/2}\,[3\,(\alpha_1^0)^{1/2} \mp 2\,(\beta_1^0)^{1/2}] \tag{71a}$$

where

$$\beta_1^0 = [1 + \frac{9}{7}(49C/2m^*\,B^2)^{1/2}]. \tag{71b}$$

The corresponding eigenfunctions are

$$\Psi_{\binom{2}{0}} = b_0\,(1 + d_\pm^0\,\phi^2) \exp\,[-\tfrac{1}{4}\,(2m^*C)]^{1/2}\,\phi^4 + (m^*B/2)^{1/2}\,(\alpha_1^0)^{1/2}\,\phi^2 \tag{72a}$$

where $d_{\pm}^0 = (2m^*B)^{1/2}\,[(\alpha_1^0)^{1/2} \mp (\beta_1^0)^{1/2}$. (72b)

Since $\beta_1^0 > \alpha_1^0$, $d_{\pm}^0 < 0$, hence $\Psi_z$ has two nodes and $\Psi_0$ has no nodes. Thus the eigenvalues $E_1^0$ (—) and $E_1^0$ (+) correspond to the ground and second excited states respectively. It can be further checked that the eigenfunctions $\Psi_0$ and $\Psi_2$ are orthogonal to each other.

(iv) Finally for $n=1$, and $q=1$, the condition on the potential becomes

$$a = (9/8)\,[1 + (81C/2m^*B)^{1/2}]^{-1} \equiv (9/8)\,(\alpha_1^1)^{-1}, \tag{73}$$

and the corresponding eigenvalues and eigenfunctions can be written down as

$$E_1^1(\pm) = -(B/2m^*)^{1/2}\,[5(\alpha_1^1)^{1/2} \mp 2(\beta_1^1)^{1/2}] \tag{74a}$$

and $$\Psi_{\binom{3}{1}} = b_0\,\phi\,(1 + d_{\pm}^1\,\phi^2)\exp\,[-\tfrac{1}{4}\,(2m^*C)^{1/2}\,\phi^4 + (m^*B/2)^{1/2}\,(\alpha_1^1)^{1/2}\,\phi^2] \tag{74b}$$

where $\beta_1^1 = [1 + 5/3\,(81C/2m^*B^2)^{1/2}]$, (74c)

and $d_{\pm}^1 = (1/3)\,(2m^*B)^{1/2}\,[(\alpha_1^1)^{1/2} \mp (\beta_1^1)^{1/2}]$. (74d)

Again $\beta_1^1 > \alpha_1^1$, hence $d_+^1 < 0$, and $\Psi_3$ has two nodes where as $\Psi_1$, has only one node. Thus $E_1^1$ (—) and $E_1^1$ (+) correspond to the first and third excited states of the system.

The procedure can be generalized to $n=2$, 3, etc. and in each case only a certain number of eigenstates of the system are exactly determined, e.g., for $n=2$, either three lowest even states ($q=0$) or three odd states ($q=1$) will be determined exactly. The remaining infinite number of the eigenstates can only be calculated if one can solve for the infinite Hill determinant out of which the $3\times3$ determinant has been factorized out to give the three eigenstates mentioned above.

### 4.2 *Free energy*

The ground state eigenvalue $E_0^0$ (equation (68b)) of the Schrödinger-like equation together with (62) gives the exact free energy of the system. The ground state energy as obtained by (68b), however, has to be slightly modified on two counts: (i) the energy has to be measured with respect to the minima of the potential, which necessitates the substraction of the factor given by (7) from $E_0^0$; and (ii) the Schrödinger-like equation (60) has a constant factor on the left side which has to be further substracted from all the eigenvalues. Thus the modified ground state eigenvalue becomes

$$\epsilon_0 = -(B/2m^*)^{1/2}\,(9/8a)^{1/2} + (1/2C)^{1/2}\,(B/a)^{3/2}\,[1 - a + (1 - 2a/3)^{3/2}] - 1/2\beta\,\ln\,(2\pi l^2/\beta m C_0^2), \tag{75}$$

where $a$ is given by (68a). It is worth noting that both $a$ and $\epsilon_0$ have acquired temperature dependence through the effective mass $m^*$ which is proportional to $T^{-2}$

(equation (61)). Thus at $T=0$, $\epsilon=0$ and $a=9/8$, which in turn gives the first order transition point. The free energy per unit length as obtained from (62) and (75) is

$$F/L = -\frac{1}{l}(B/2m^*)^{1/2}(9/8a)^{1/2} + (1/l(2C)^{1/2})(B/a)^{3/2} \times \left[1 - a + \left(1 - \frac{2a}{3}\right)^{3/2}\right] + \frac{1}{\beta l}\ln\frac{\beta C_0}{2\pi l}. \tag{76}$$

It is interesting to note that the exact free energy thus obtained has no exponential tunnelling-like term obtained by KS. At low temperatures ($T\to 0$), (68a) can be approximated by

$$a \cong 9/8\ [1 - (9C/2m^* B^2)^{1/2}],$$

to lowest order in $T$. Note that neglecting the $T$-dependent term on the right side will violate the condition (equation (64)) on the potential. This demands that the free energy be evaluated upto terms of order $T^2$, thus reducing (76) to

$$F = Nk_BT(l/C_0)(2B/M)^{1/2}\ [1 + 3/8\ (2C/mB^2)^{1/2}(l/C_0)\ k_BT] + O(T\ln T). \tag{77}$$

On the other hand at high temperatures ($T\to\infty$) the free energy equation (76) goes as

$$F = Nk_B\frac{32}{27}\, l^{3/2}\, k_B^{1/2}\left(\frac{9\,C^{1/3}}{2mC_0^2}\right)^{3/4} T^{3/2}. \tag{78}$$

4.3 *Phonon free energy*

We shall now calculate the phonon contribution to the free energy assuming that the particles execute small amplitude vibrations about one of the absolute minima of the potential satisfying the condition (68a). For this purpose we expand

$$f = f_0 + \eta \quad \eta \ll f_0 \tag{79}$$

(where $f_0$ is given by (5)) which when substituted in (11) and terms to lowest order in $\eta$ are kept yields

$$\eta'' - D\eta = 0 \tag{80}$$

where

$$D = \frac{4|A|}{B} f_0^2 - 4 = \frac{6}{a}\left[1 + \left(1 - \frac{2a}{3}\right)^{1/2}\right] - 4. \tag{81}$$

In writing down (81) use is made of the fact that $f_0$ corresponds to the minima of the potential. Substituting for $a$ from (68a) and taking the low temperature limit the

constant $D$ turns out to be $[4 + 12(9C/2m^*B^2)^{1/2}]$. The dispersion for oscillatory solutions of (80) can be written down

$$\omega_q^2 \cong C_0^2 q^2 + \frac{8B}{m}[1 + 3(9C/2m^*B^2)^{1/2}] \tag{82}$$

It is interesting to note that the phonon frequencies acquire a temperature-dependent shift. Following the procedure outlined by KS (Appendix) the low temperature phonon free energy for the dispersion (82) can be evaluated to give

$$F_{\text{Vib}} = Nk_BT(l/C_0)\,(2B/m)^{1/2}\,[1 + \tfrac{9}{4}\,(2C/mB^2)^{1/2}\,(l/C_0)\,k_BT]. \tag{83}$$

4.4 *The domain wall energy*

On comparing the phonon free energy (equation (83)) with the total free energy of the system as given by (77) it is clear that the former is larger. Hence the difference between the two can be attributed to the domain wall excitations of the system, which is given by

$$F_D = F - F_{\text{Vib}} = -\frac{15}{4}N(k_BT)^2\,(l/C_0)^2\,\frac{1}{m}(C/B)^{1/2}. \tag{84}$$

In contrast to the result of KS the domain wall free energy rather than showing an exponential temperature dependence goes as $T^2$. Thus the domain wall contribution as it turns out from this exact calculation is much larger than that obtained by KS for the $\phi^4$-field theory. Equation (84) can be further used to estimate the splitting of the ground state energy level of the $\phi^6$ potential satisfying the condition (68a); which is

$$\Delta E_0 = 2\frac{|F_D|}{N} = \frac{15}{2}\,\frac{1}{m^*}(C/B)^{1/2}. \tag{85}$$

This result also differs considerably from that of the usual WKB tunnelling approximation which usually has an exponential form.

4.5 *Domain wall phenomenology*

We shall now calculate the free energy of a system of non-interacting domain walls distributed along the length ($L$) of a line; following phenomenology developed by KS. This domain wall free energy is given by

$$F_D = -k_BTn_s\left[1 + \frac{1}{2}\ln\left(\frac{2\pi k_BT}{d^2m_D^*}\right)\right]\exp(-E_{DP}/k_BT), \tag{86}$$

where $d$ is a normalization constant, $n_s = L/\Delta_d$, $\Delta_d$ being the domain wall width and $E_{DP}$ is the domain wall potential energy given by

$$E_{DP} = \tfrac{1}{2}\,m_D^*(2c_0^2 - v^2). \tag{87}$$

The domain wall mass for the solution (19) is given by (48b) and the corresponding domain wall width is given by (19b). Assuming that $v > c_0$, equation (86) together with (48b) and (19b) can be written as

$$F_D = -Nk_B T\,(l/2\xi_0)\left\{1+\frac{9}{2a^2}\left[1-a+\left(1-\frac{2a}{3}\right)^{3/2}\right]\right\}^{1/4} \times\left[1+\frac{1}{2}\ln\left(\frac{2\pi k_B T}{d^2 m_0^*}\right)\right]\exp\left(-m_D^* C_0^2/k_B T\right) \tag{88}$$

where $\xi_0 = \xi\,(v=0)$. In order to compare this with the domain wall free energy obtained from the exact calculations of (84), it is necessary to evaluate (88) satisfying the condition (68a) on the potential. Thus in the low temperature limit we get

$$F_D \cong -Nk_B T\,(l/2\xi_0)\left[1+\frac{9}{2}(C/2\,m^*\,B^2)^{1/2}\right] \times\left[1+\frac{1}{2}\ln\left(\frac{2\pi k_B T}{d^2 m_D^*}\right)\right]\exp\left(-m_D^* C_0^2/k_B T\right) \tag{89}$$

with
$$m_D^* = \frac{m}{\sqrt{2}\,l\xi_0}\,(B/C)^{1/2}\,(2m^*\,B^2/9C)\,\frac{F\,(3,\,5/2,\,11/4,\,\gamma)\,\Gamma\,(11/4)}{\Gamma\,(5/2)\,\Gamma\,(1/4)}, \tag{90a}$$

and
$$\gamma = -\,(2m^*\,B^2/9C)^{1/2}. \tag{90b}$$

The result of (89) is the same as that obtained from a WKB tunnelling approximation as has been shown by Polyakov (1977). The domain wall free energy (equation (89)) as well as the level splitting thus obtained decreases exponentially with decreasing temperature and is much smaller compared with the exact result of (84). This difference will be further reflected in the calculation of the correlation functions and correlation length as will be shown in § 5. Yet another difference between the exact and phenomenological calculations is the dependence of the free energy (level splitting) on the coefficient $C$ of the non-linear $\phi^6$ term in the potential. Whereas in (87) and (90) the domain wall potential energy has an inverse dependence on $C$, showing, its non-perturbative nature; (84) and (85) show that the exact $F_D$ and $\Delta E_0$ are proportional to $\sqrt{C}$.

It is further possible to calculate the domain wall free energy at the transition point ($a = 9/8$) from (86) together with (46) for the solutions (18); which is given by

$$F_D = -Nk_B T\,(l/2\xi_0)\,[1+1/2\,\ln\,(2\pi k_B T/d^2 m_D^*)]\,\times \exp\,[-1/4\,(mc_0^2/l\xi_0)\,(B/C)^{1/2}/k_B T].$$

For this case, exact evaluation of the domain wall free energy is not possible since the exact ground state eigenvalue of the Schrödinger-like equation (60) is not known. It is however important to note that unlike the $\phi^4$-field theory, in the case of the $\phi^6$-field theory not only that there exists a domain wall contribution to the free energy

below the transition point, but also at the transition point. The relevance of this in connection with the existence of the central peak above the phase transition point will be further discussed in the concluding section.

## 5. Calculation of correlation functions

We now proceed to calculate the equal time two-point, displacement-displacement and intensity-intensity correlation functions given by (63a) and (63b). At low temperatures, the sums over all states $n$ in (63) will be dominated by the two lowest states for which the matrix elements will have non-vanishing values. Thus (63) reduce to

$$C_1(x) = |\langle \Psi_1 | \phi | \Psi_0 \rangle|^2 \exp\,[-\beta\,(x/l)\,(\epsilon_1 - \epsilon_0)], \tag{92a}$$

and

$$C_2(x) = |\langle \Psi_2 | \delta | \phi |^2\, \Psi_0 \rangle/^2 \exp\,[-\beta\,(x/l)\,(\epsilon_2 - \epsilon_0), \tag{92b}$$

where $\Psi_0$, $\Psi_1$ and $\Psi_2$ are the ground, first and second excited states respectively. A knowledge of these states will permit us to calculate equation (92) exactly.

### 5.1 *Displacement-displacement correlation*

For the potential satisfying the condition (68a) the ground state is given by (68c). This is the only state known exactly for this case. However, the difference in the energy $\Delta E_0$ between the first excited state and the ground state is estimated from the domain wall energy and is given by (85). This allows one to obtain an estimate of the displacement-displacement correlation length, even though the exact evaluation of the matrix element is not possible. Equation (92a) together with (85) reduces to

$$C_1(x) = |\langle \Psi_1 | \phi | \Psi_0 \rangle|^2 \exp\,(-x/\lambda_c), \tag{93}$$

where

$$\lambda_c = \frac{4}{15}\,\frac{\xi_0^2}{l}\,(B^3/C)\,\frac{1}{k_B T}, \tag{94}$$

is the correlation length. It follows from (94) that $\lambda_c$ diverges only at $T=0$, rather slowly as $(T^{-1})$.

$C_1(x)$ can further be computed from the domain wall phenomenology following KS. For $a<9/8$, let us assume that at $x=0$, the particle has the displacement $\phi = \pm\,\phi_{\min}$ except for small phonon-like oscillations. But within a finite distance from $x=0$, say at $x$, the particle will encounter $n_w(x)$ domain walls each of which will flip the displacement from $\pm\phi_{\min}$ to $\mp\phi_{\min}$. This will provide the correlation between $\phi(0)$ and $\phi(x)$, which can be evaluated by assuming a Poisson distribution for $n_w(x)$ (see KS) to give

$$C_1(x) = \phi_{\min}^2 \exp\left(-2\,\frac{x}{\Delta_d}\right) \exp\,(-\beta E_{DP}) \equiv \phi_{\min}^2 \exp\,(-x/\lambda_c) \tag{95}$$

where

$$\lambda_c = \frac{\Delta_d}{2} \exp\,(-\beta E_{DP}), \tag{96}$$

and $\phi_{\min}$, $\Delta_d$ and $E_{DP}$ are given by equation (5), (19b) and (87) respectively. On substituting these in (96), and taking the low temperature limit $\lambda_c$ becomes

$$\lambda_c = \xi_0 \left[1 - \tfrac{3}{2} (9C/2m^*B^2)^{1/2}\right] \exp (\beta m_D^* C_0^2) \tag{97}$$

where $m_D^*$ is the domain wall mass given by (90). It follows from (97) that as $T \to 0$, $\lambda_C$ diverges exponentially. This rapid divergence of the correlation length is again in contrast with the algebraic temperature dependence of (94) obtained from the exact calculation.

### 5.2 *Intensity-intensity correlation*

As can be seen from (92b) the eigenfunctions and eigenvalues of both the ground and second excited states are necessary for the evaluation of $C_2(x)$. These are known for the potential satisfying the condition (70) and are given by (71) and (72). Hence $C_2(x)$ becomes

$$C_2(x) = |\langle \Psi_2 | \delta | \phi |^2 | \Psi_0 \rangle|^2 \exp \left(-\beta \frac{x}{l} [E_1^0(+) - E_1^0(-)]\right.$$

$$\propto \exp (-x/\lambda_C (I)), \tag{98}$$

where the intensity correlation length at low temperatures is given by

$$\lambda_C (I) = \frac{\xi_0}{2}\left[1 - \frac{9}{4}(l/\xi_0) (C/B^3)^{1/2} k_B T\right]. \tag{99}$$

Thus $\lambda_C (I)$ does not vanish at $T = 0$ but attains a constant value of $\xi_0/2$. At $T = 0$ the condition (70) on the potential reduces to $a = 9/8$ which is the transition point. Hence, the intensity fluctuations are strongly correlated at the transition point. This may be the evidence in support of the stabilization of the central peak to the Bragg peak at and below the transition. Further, with increasing temperature the correlation length decreases and goes to zero at

$$T = \frac{4}{9k_B} (\xi_0/l) (B^3/C)^{1/2}$$

where the intensity-intensity correlation vanishes. We are tempted to say that at this temperature the central peak first appears.

### 5.3 *The probability distribution function*

Recently Bruce *et al* (1979) have used the renormalization group approach to show that there is an intrinsic order-disorder nature associated with the cluster (domain wall) phenomenon in displacive phase transitions. This manifests itself in the appearance of two sharp peaks in the probability distribution function (PDF) calculated for the fixed point potential at the critical regime. The present model,

which utilizes the strong displacive nature, through the use of the functional integral and transfer matrix techniques, determines the partition function in terms of the ground state eigenvalue of the Schrödinger-like equation (60). Hence the PDF will be given by the ground state wave function and can be written as

$$P(\phi) = |\Psi_0|(\phi)|^2 \Big/ \int_{-\infty}^{+\infty} |\Psi_0|^2 \, d\phi, \tag{100}$$

where $\Psi_0(\phi)$ is given by (68c). Equation (100) in the limit of $T \to 0$ will give the value of the PDF in the critical regime since $T = 0$ corresponds to the transition point $a = 9/8$. It can be easily checked from equation (100) and (68c) that $P(\phi)$ has three points of extrema at

$$\phi = 0$$

and $$\phi = \pm \left[ \frac{B}{C} + \left( \frac{9}{2m^*C} \right)^{1/2} \right]^{1/4} \equiv \pm \phi_0'.$$

Out of these the point $\phi = 0$ is a minimum and the other two points $\phi = \pm \phi_0'$ are maxima. For low temperatures the value of $P(\phi)$ at $\pm \phi_0'$ is

$$P(\pm \phi_0') \propto \exp (m^* B^2 / 2C)^{1/2}$$

and that at $\phi = 0$ is $P(0) \propto 1$. Since $m^* \propto T^{-2}$, the PDF is strongly peaked at $\pm \phi_0'$ at low temperatures. This is in conformity with the result of Bruce *et al*; the only difference being that in their calculation $P(\phi)$ has a small peak at $\phi = 0$ too. Thus one can conclude that the present model too has an order-disorder component arising from the domain walls (clusters) of precursor order, which gives rise to a critically narrowing central peak.

## 6. Conclusion

In concluding we shall summarize the main results of the present paper. We have considered the $\phi^6$-field theory in (1+1) dimensions, as a model for first order structural phase transitions. The dynamics and thermodynamics of the model are studied exactly. It was shown that there exists exact solutions to the equation of motion which are expressible in terms of the Weirstrass functions. The equation of motion is reduced to a form similar to that of the single particle (Khare and Behera 1979) except for the fact that it now turns out to be in Eucledian space. In anology with the single particle equation it was shown that there exists oscillatory, travelling wave (phonon-like) solutions as well as domain wall (kink) solutions. Since the equation of motion in the Eucledian space is equivalent to that in the Minkowski space for an inverted potential, it is easy to see that the domain wall solutions exist only at and below the transition point. On the other hand above the transition point there can exist exotic kink-like solutions with $v > c_0$, which takes the particle from one hill top to the other of the potential. We have analysed in detail the characteristics of these domain wall and exotic kink solutions. While below the transition point

there is one domain wall solution which takes the particle from one absolute minima to the other, at the transition point there are two such solutions transferring the particle from first minima to the second and then from the second minima to the third. All these solutions are shown to carry a conserved topological charge. The stability analysis shows that the domain wall solutions are stable whereas the exotic kink solutions are not. The domain wall mass and energy for each of these solutions are calculated.

For the oscillatory solutions the dispersion relations are calculated; which for some solutions shows acoustic phonon-like behaviour, whereas for some others behaves optic phonon-like. These phonons acquire a shift in frequency because of anharmonicity.

On comparing our results with that of $\phi^4$ -field theory (considered by KS) we note that, in the latter case the domain wall solutions exist only below the transition point (in terms of the potential parameters). Since the domain wall solutions are relevant for the existence of a central peak in SPT, the existence of such a solution at the transition point in the present model, together with the fact that there exist local minima in the $\phi^6$-potential above the transition point makes it easier to understand the existence of the central peak above the transition point. We believe that even the exotic kink solutions play a role in the appearance of the central peak.

Next we proceeded to calculate the thermodynamics of the system. The calculation of the classical partition function was reduced to the evaluation of the eigenvalues of a Schrödinger-like equation, using the standard transfer matrix technique. Fortunately for us there exist exact solutions to the Schrödinger equation for the $\phi^6$-potential, provided the parameters of the potential are such that it corresponds to a point below the transition. This allows us to calculate the free energy of the system exactly. The low temperature limit of the free energy thus calculated does not have the usual exponential part, which was attributed to the domain walls when a WKB tunnelling approximation is used. This we believe is an important result which shows the difference between the exact and approximate calculations. Hence, unlike the result of KS for the $\phi^4$ -field theory, in the present calculation the domain wall energy evaluated from the exact calculation and the domain wall phenomenology does not agree. The functional integral approach is further used to calculate the displacement-displacement, and intensity-intensity correlation functions. It was shown that the correlation length calculated from the displacement-displacement correlation diverges at $T=0$, rather slowly, i.e. as $T^{-1}$; in contrast with the exponential divergence predicted by the approximate domain wall phenomenology. Similarly, the intensity-intensity correlation does have a correlation length which is finite at $T=0$. The probability distribution function was shown to have the two-peaked structure, indicating the presence of an order-disorder component arising from the domain wall (cluster) modes; within the displacive transition in conformity with the picture of Bruce *et al* (1979).

Finally, we would like to offer the following qualitative picture of the central peak. The $\phi^6$-potential above the transition point still has two local minima. Whenever the ground state energy lies above these local minima (which will happen at temperatures above the transition temperature), this state will be tunnel-split, which will contribute to the free energy. Thus there will be a pseudo-domain wall energy, even though above the transition point there are no domain wall solutions. This will result in the formation of the central peak. As one approaches the transition point,

the tunnelling probability will increase (because of the lowering of the local minima) resulting in an increase in the number of these pseudo-domain walls, and hence strengthening the central peak. The existence of domain wall solutions at and below the transition point, stabilises these clusters, which are precursors to the formation of the Bragg peak. Because of the emergence of the Bragg peak, it may be difficult to observe the central peak below the transition point. It is worth noting that such tunnell splitting above the transition point can never occur in the $\phi^4$ model since this model has no local minima. Thus the $\phi^6$ -model, while strengthening the picture of KS that the domain wall (cluster) excitations responsible for the central peak, provides a mechanism for its appearance above the transition point. Recently the critical behaviour of this $\phi^6$-model has been studied by Boyanovsky and Masperi (1980) using the block-spin renormalization group approach.

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