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# Classical $\phi^6$-field theory in (1+1) dimensions 2. Proof of the existence of domain walls above the transition point

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**Abstract.** The existence of a domain wall-like contribution to the free energy above the first order phase transition point is demonstrated for a system described by the $\phi^6$-field theory in (1+1) dimensions.

**Keywords.** $\phi^6$-field theory; domain walls; structural phase transition.

## 1. Introduction

In an earlier paper (Behera and Khare 1980a; hereafter referred to as I) the dynamics and thermodynamics of the $\phi^6$-field theory in (1+1) dimensions were extensively studied. The use of the $\phi^6$-field theory as a model for first order structural phase transitions (see I and the references therein) was also discussed. Of particular importance to the problem of structural phase transitions is the existence of domain wall-(kink) like solutions, which are responsible for the occurrence of the central peak phenomena. It was shown that these domain wall solutions exist below the transition point ($a < 9/8$, notations are same as in I), the latter being determined by the parameters of the $\phi^6$-potential. However, the exact evaluation of the free energy of the system in this regime revealed that the tunnelling-like contribution expected for the domain wall free energy is absent *i.e.* identifying the domain wall free energy as the exact free energy minus the phonon part, it was found to be large and proportional to $T^2$ instead of $\exp(-\text{const}/T)$. In the concluding section of I, it was conjectured that the presence of local minima in the $\phi^6$-potential, above the transition point, *i.e.* $9/8 < a < 3/2$, will lead to the existence of a tunnelling-like contribution to the free energy which can explain the experimentally observed central peak in ferroelectrics at temperatures above $T_c$. The purpose of the present paper is to prove this conjecture.

The plan of the rest of the paper is as follows. In § 2 an upper bound to the ground state energy eigenvalue of the corresponding Schrödinger equation (see I) for the $\phi^6$-potential will be calculated for $a > 9/8$. This will then be used to calculate the free energy using equation (62) of I, and the existence of a domain wall-like contribution will be demonstrated. The concluding § 3 is devoted to the discussions of the results.

## 2. Calculation of free energy above the phase transition point

It was shown in I that the evaluation of the free energy of the system reduces to the solution of an equivalent eigenvalue problem given by (some of the essential results of I are reproduced for the sake of completeness)

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

where the temperature-dependent effective mass is

$$m^*=m\beta^2C_0^2/l^2;\quad \beta=(k_BT)^{-1}, \tag{2}$$

and the potential is given by

$$V(\phi)=B\phi^2-|A|\phi^4+C\phi^6,\ C>0. \tag{3}$$

The free energy of the system can be written in terms of the ground state eigen value $\epsilon_0$ as

$$F=N\epsilon_0-Nk_BT\ln(2\pi m/\beta)^{1/2}. \tag{4}$$

In I, equation (1) was solved exactly for the case $a(\equiv 9BC/2|A|^2)<9/8$ when certain constraints on the coupling constants $A$, $B$, $C$ are satisfied. We now show that for $a>9/8$ (*i.e.* above the phase transition point) even though the ground state energy cannot be calculated exactly, stringent upper and lower bounds on it can be obtained. Let us first notice that if

$$B=\frac{|A|^2}{4C}+3(C/2m^*)^{1/2}, \tag{5}$$

or equivalently

$$a=\frac{9}{8}\left[1-\left(\frac{9C}{2m^*B^2}\right)^{1/2}\right]^{-1}>9/8, \tag{6}$$

then the Hamiltonian of equation (1) can be written as

$$H=A^*(\phi)A(\phi)+\frac{1}{2}\left(\frac{2B}{m^*}\right)^{1/2}\left[1-\left(\frac{9C}{2m^*B^2}\right)^{1/2}\right]^{1/2}+\frac{1}{2\beta}\ln\left(\frac{2\pi l^2}{\beta m C_0^2}\right), \tag{7}$$

$$\text{where } A(\phi)=\frac{1}{(2m^*)^{1/2}}\frac{d}{d\phi}+\frac{|A|}{(C)^{1/2}}\phi-C^{1/2}\phi^3. \tag{8}$$

Hence the ground state energy

$$\epsilon_0 \geqslant \frac{1}{2}\left(\frac{2B}{m^*}\right)^{1/2}\left[1-\left(\frac{9C}{2m^*\,B^2}\right)^{1/2}\right]^{1/2}+\frac{1}{2\beta}\ln\left(\frac{2\pi l^2}{\beta m\,C_0^2}\right)$$

where the equality holds if and only if the solution $\psi(\phi)$ of the equation

$$A(\phi)\,\psi(\phi)=0, \tag{9}$$

is square integrable. The solution $\psi(\phi)$ which we normalise by

$$\psi(\phi)=\exp\left[-\frac{|A|}{4}\left(\frac{2m^*}{C}\right)^{1/2}\phi^2+\frac{(2m^*\,C)^{1/2}}{4}\phi^4+\frac{|A|^2}{16\,C}\left(\frac{2m^*}{C}\right)^{1/2}\right], \tag{10}$$

is however not square integrable and hence

$$\epsilon_0 > \frac{1}{2}\left(\frac{2B}{m^*}\right)^{1/2}\left[1-\left(\frac{9C}{2m^*B^2}\right)^{1/2}\right]^{1/2}+\frac{1}{2\beta}\ln\left(\frac{2\pi l^2}{\beta mC_0^2}\right). \tag{11}$$

However, since $\psi(\phi)$ obeys

$$\psi(\phi=\pm(|A|/2C)^{1/2})=1, \qquad \left.\frac{d\psi}{d\phi}\right|_{\phi=\pm(|A|/2C)^{1/2}}=0. \tag{12}$$

Hence following Herbst and Simon (1978, 1979) we can obtain a lower bound on $\epsilon_0$ *i.e.* we have the following stringent upper and lower bounds on it

$$0<\epsilon_0-\frac{1}{2}\left(\frac{2B}{m^*}\right)^{1/2}\left[1-\left(\frac{9C}{2m^*B^2}\right)^{1/2}\right]^{1/2}-\frac{1}{2\beta}\ln\left(\frac{2\pi l^2}{\beta mC_0^2}\right)<N_1$$
$$\times\exp\left[-N_2\frac{|A|^2}{16C}\left(\frac{2m^*}{C}\right)^{1/2}\right]. \tag{13}$$

In order to determine the constants $N_1$ and $N_2$, the trial function is chosen to be

$$\psi(\phi)=\begin{cases}\exp\left\{-a\left[\phi+\left(\frac{|A|}{2C}\right)^{1/2}\right]^2\right\}, & \phi<-\left(\frac{|A|}{2C}\right)^{1/2}\\ \exp\left[-\frac{|A|}{4}\left(\frac{2m^*}{C}\right)^{1/2}\phi^2+\frac{(2m^*C)^{1/2}}{4}\phi^4+\frac{|A|^2}{16C}\left(\frac{2m^*}{C}\right)^{1/2}\right], & -\left(\frac{|A|}{2C}\right)^{1/2}<\phi<\left(\frac{|A|}{2C}\right)^{1/2}\\ \exp\left\{-a\left[\phi-\left(\frac{|A|}{2C}\right)^{1/2}\right]^2\right\}, & \phi>\left(\frac{|A|}{2C}\right)^{1/2},\end{cases} \tag{14}$$

so that the boundary conditions are satisfied at $\phi = \pm(|A|/2C)^{1/2}$ and $\alpha$ is the variational parameter. On minimising the energy with the trial function (14) and after some complicated algebra one gets

$$E_0 = \frac{1}{2}\left(\frac{2B}{m^*}\right)^{1/2}\left[1-\left(\frac{9C}{2m^*B^2}\right)^{1/2}\right]^{1/2} + \frac{3}{\sqrt{\pi}}\frac{2B}{m^*}\left[1-\left(\frac{9C}{2m^*B^2}\right)^{1/2}\right]\frac{(2m^*)^{1/4}}{C^{3/4}}$$

$$\times \exp\left[-\frac{|A|^2}{8C}\left(\frac{2m^*}{C}\right)^{1/2}\right] \tag{15}$$

or

$$\epsilon_0 = E_0 - \frac{1}{2\beta}\ln\left(\frac{2\pi l^2}{\beta m C_0^2}\right). \tag{16}$$

In evaluating equation (15), it has been assumed that $C$ is small. On evaluating the free energy from equation (4) (using equation (2)) in the limit of $T \to 0$ yields;

$$F = Nk_BT\frac{l}{C_0}\frac{1}{2}\left(\frac{2B}{m}\right)^{1/2}\left[1-\frac{1}{2}\left(\frac{9C}{2mB^2}\right)^{1/2}\frac{l}{C_0}k_BT\right]$$

$$+N(k_BT)^{3/2}\frac{3}{\sqrt{\pi}}\left(\frac{l}{C_0}\right)^{3/2}\frac{(2m)^{1/4}}{C^{3/4}}\frac{2B}{m}\left[1-\left(\frac{9C}{2mB^2}\right)^{1/2}\frac{l}{C_0}k_BT\right]$$

$$\times \exp\left[-\left(\frac{|A|^2}{8C}\left(\frac{2m}{C}\right)^{1/2}\frac{C_0}{l}\right)\Big/k_BT\right] - Nk_BT\ln\left(\frac{2\pi l}{\beta C_0}\right) \tag{17a}$$

$$\equiv F_{\text{osc.}} + F_{\text{tunn.}} + O(T\ln T) \tag{17b}$$

## 3. Conclusion

It is clear from (17) that the free energy has a part corresponding to phonons and a part corresponding to tunnelling or domain walls. The domain wall contribution ($F_{\text{tunn}}$) has a structure similar to that obtained by Krumhansl and Schrieffer (1975) (KS) in the case of the $\phi^4$-field theory. The domain wall contribution vanishes either as $T\to 0$ or as $C\to 0$. This suggests that for $a > 9/8$, i.e. above the phase transition point, there exists a domain wall contribution to the free energy. However, such a contribution does not appear below the phase transition point ($a<9/8$) as was demonstrated by an exact calculation in § 4·2 of I.

In order to compare the oscillatory part of the free energy ($F_{\text{osc}}$) as given by equation (17) with that of the phonons, one can estimate the later following KS. In doing so one has to note that $\phi = 0$ corresponds to the absolute minimum of the potential, hence for small oscillations around $\phi=0$. Linearisation of the equation of motion (equation (11) of I), yields the phonon dispersion to be

$$\omega_q^2 = C_0^2 q^2 + (2B/m), \tag{18}$$

which is the same as that of the $\phi^4$ theory of KS. Thus the phonon free energy becomes

$$F_{osc} = N k_B T \frac{l}{C_0}\frac{1}{2}(2B/m)^{1/2} + \ldots . \tag{19}$$

which is the same as that of equation (17) for $T \to 0$. On the other hand if one assumes small oscillations around one of the local minima $\phi = \pm (|A|/2C)^{1/2}$, then following the procedure of I, the phonon free energy can be written as ($T \to 0$)

$$F_{osc} = N k_B T \frac{l}{C_0}\left(\frac{2B}{m}\right)^{1/2}\left[1 - \frac{3}{2}\left(\frac{9C}{2mB^2}\right)^{1/2}\frac{l}{C_0} k_B T\right], \tag{20}$$

which is much larger than the $F_{osc}$ given by equation (17). This is physically reasonable because it costs more energy to make the particles oscillate about the local minima, which are higher in energy than the absolute minimum of the potential at $\phi = 0$.

Finally it is worth pointing out that, proceeding as in § 2 it is easy to show that, for

$$a = \frac{9}{8}\left[1 + \left(\frac{9C}{2m^* B^2}\right)^{1/2}\right]^{-1} < 9/8;$$

the Hamiltonian of the system can be written as

$$H = A^*(\phi)\, A(\phi) - \tfrac{1}{2}\left(\frac{2B}{m^*}\right)^{1/2}\left[1 + \left(\frac{9C}{2m^* B^2}\right)^{1/2}\right]^{1/2},$$

where $$A(\phi) = -\frac{1}{(2m^*)^{1/2}}\frac{d}{d\phi} + \frac{|A|}{2\sqrt{C}}\phi - \sqrt{C}\,\phi^3,$$

so that $$E_0 = -\tfrac{1}{2}\left(\frac{2B}{m^*}\right)^{1/2}\left[1 + \left(\frac{9C}{2m^* B^2}\right)^{1/2}\right]^{1/2}.$$

thereby the result obtained in I is reproduced.

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