

Half-kink lattice solution of the ϕ^6 model

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Abstract. Investigation of a great number of physical systems shows that a scaled Landau free energy density of the form $F(\phi) = a/2\phi^2 - \frac{1}{4}\phi^4 + \frac{1}{6}\phi^6$ describes a first-order phase transition. To study the formation of static domain walls in these systems we include a spatial gradient (Ginzburg) term of the scalar order parameter ϕ . At the transition temperature (T_c) the potential has three degenerate minima corresponding to an asymmetric domain wall (i.e. a half-kink solution). We have obtained the associated kink lattice solution, its energy of formation and asymptotic kink–kink interaction. In addition, we report a ‘pulse’ lattice solution below T_c .

1. Introduction

Landau theory of phase transitions is remarkable in that, under simple assumptions that the order parameter is small and uniform near phase transition temperature (T_c), it yields a wealth of information about the phase transitions (Landau and Lifshitz 1958). Equilibrium thermodynamics is completely determined by the free energy function $F(T, \eta(x))$, where $\eta(x)$ is the local order parameter. F is a function that must be invariant under the symmetry group of the high temperature (parent) phase. Although the strict realm of the Landau theory is that of continuous transitions, the theory satisfactorily applies to most of the first-order transitions (Tolédano and Tolédano 1987). A 1D general expansion of free energy density for a first-order transition is given by:

$$F(\eta(x)) = \frac{A}{2}\eta^2(x) + \frac{B}{4}\eta^4(x) + \frac{C}{6}\eta^6(x) \quad (1)$$

where F is truncated after the sixth-order term and usually the coefficient of the second-order term (A) is temperature dependent. Note that an asymmetric double well [$F(\eta(x)) = \frac{A}{2}\eta^2(x) + \frac{B}{3}\eta^3(x) + \frac{C}{4}\eta^4(x)$] can also describe a first-order transition (Tolédano and Tolédano 1987, Sanati and Saxena 1998) but we will confine our discussion here only to the ϕ^6 model.

If $C = 0$, $A < 0$ and $B > 0$ then the Landau free energy density (equation (1)) represents a second-order phase transition, and if $B < 0$, $A > 0$ and $C > 0$, the Landau free energy density corresponds to a first-order phase transition. The latter free energy density has been used to explain many first-order phase transitions in different physical systems such as body-centred cubic (bcc) to hexagonal close-packed (hcp) reconstructive phase transitions in crystals (Lindgard 1991, Lindgard and Mouritsen 1986, Dmitriev *et al* 1991), ferroelectric transitions in materials (Lajzerowicz 1981) and copolymers (Furukawa 1989), smectic A to smectic C phase transitions in liquid crystals (Huang and Viner 1982), magnetoelastic transitions in Ni_2MnGa (Planes *et al* 1997, Sthur *et al* 1997) and field theoretic contexts (Makhankov 1990). The Landau free energy density F can be augmented by adding a term proportional to the square of

the order parameter gradient (i.e. Ginzburg term) which produces an energy cost for deviations from spatial uniformity such as in the presence of domain walls.

Although there are several studies on the static (kink and pulse) soliton lattice solutions of the ϕ^6 model and corresponding formation energies (Behera and Khare 1980, Falk 1983), (i) the soliton lattice solution and its energy of formation when the free energy density has three degenerate minima, and (ii) the ‘pulse’ lattice solution below T_c and associated energy of formation, have not been explicitly reported in the literature. We also present the asymptotic interaction between kink–kink (or pulse–pulse) for the four different types of domain walls. From the equilibrium condition, i.e. by solving the equation derived from the variation of the total free energy for physical parameters and boundary conditions corresponding to the triply degenerate case and below T_c , we find a half-kink lattice solution (domain wall array) and a pulse lattice solution, respectively. For these solutions we calculate the associated domain wall energy and asymptotic half-kink, anti-half-kink and pulse–pulse interactions. For the sake of completeness the other two solutions, namely the pulse lattice solution above T_c and the kink lattice solution below T_c with associated asymptotic interactions, are summarized in appendix A and B, respectively.

Our main motivation is to provide kink and pulse lattice solutions which can explain observed metastable (or stable) periodic microstructure in materials undergoing structural transitions. The half-kink lattice solution reported here corresponds to a coexisting periodic alternating array of parent and product phases at T_c . Specifically, it describes domain walls between (a) the cubic and tetragonal (or other low symmetry) phases in martensites and shape memory alloys such as NiTi (Falk 1983, Barsch and Krumhansl 1988), (b) paraelectric and ferroelectric phases in materials such as BaTiO₃, PbTiO₃ (Lajzerowicz 1981, Cao and Cross 1991) (c) paramagnetic and ferromagnetic phases in magnetoelastics, e.g. Ni₂MnGa (Planes *et al* 1997, Sthur *et al* 1997), etc. The kink lattice (appendix B) solution explains (stable) twinning in these materials at temperatures below T_c whereas the two types of pulse lattice solutions (section 5 and appendix A) describe metastable product and parent phases which may coexist under specific boundary conditions and materials processing.

2. Model

One can obtain the total free energy density by adding the Ginzburg term $F_G = \frac{G}{2}(\nabla\eta)^2$ to the effective Landau free energy density,

$$F_T = \frac{G}{2}(\nabla\eta)^2 + \frac{A}{2}\eta^2 - \frac{|B|}{4}\eta^4 + \frac{C}{6}\eta^6 \quad (2)$$

where the coefficient G in the Ginzburg term (in the crystallographic context) is proportional to the curvature of the phonon dispersion curve near the appropriate high symmetry point in the Brillouin zone for the material. However, in the field theoretic context $G = 1$.

Equation (2) contains four parameters; by scaling the energy and order parameter it can be reduced to a standard form with two control parameters a and g ,

$$\frac{F_T}{F_R} = \frac{g}{2}(\nabla\phi)^2 + \underbrace{\frac{a}{2}\phi^2 - \frac{\phi^4}{4} + \frac{\phi^6}{6}}_{F_L} \quad (3)$$

where

$$\phi_{(x)} = \left(\frac{C}{|B|} \right)^{1/2} \eta_{(x)} \quad F_R = \frac{|B|^3}{C^2} \quad g = \frac{GC}{B^2} \quad a = \frac{AC}{B^2}.$$

The scaled Landau free energy density F_L is plotted as a function of a in figure 1(a). The condition $\phi = 0$ corresponds to the parent phase and the other minima (if present) correspond to the product phase. There are several regimes depending on the parameter a ; the condition, $\partial F_L / \partial \phi = 0$ yields

$$\phi = 0 \quad \phi^2 = \frac{1 \pm \sqrt{1 - 4a}}{2}$$

then the following cases are possible:

(I) $a > \frac{1}{4}$, F_L has a real minimum at $\phi = 0$, only.

(II) $a = \frac{1}{4}$, F_L has a real minimum at $\phi = 0$, and two inflection points at $\phi = \pm\sqrt{2}/2$.

(III) $\frac{3}{16} < a < \frac{1}{4}$, F_L has a stable minimum at $\phi = 0$, two metastable minima at $\phi = \pm\sqrt{(1 + \sqrt{1 - 4a})/2}$, and two relative maxima at $\phi = \pm\sqrt{(1 - \sqrt{1 - 4a})/2}$ (figure 1(a)1). The pulse lattice (above T_c in appendix A) corresponds to this case.

(IV) $a = \frac{3}{16}$, F_L has three degenerate minima at values $\phi = 0$ and $\phi = \pm\sqrt{3}/2$ with $F_L = 0$ and two maxima at $\phi = \pm\frac{1}{2}$ (figure 1(a)2). This is the condition for the first-order phase transition and our main focus (half-kink lattice at T_c) here.

(V) $0 < a < \frac{3}{16}$, F_L has a metastable minimum at $\phi = 0$, and two stable minima at $\phi > \frac{1}{2}$ and $\phi < -\frac{1}{2}$, with two maxima $F_L > 0$ for ϕ in between (figure (a)3). The pulse lattice (below T_c reported in section 5) corresponds to this case.

(VI) $a \leq 0$, F_L has a maximum at $\phi = 0$ and two minima at $\phi \geq 1$ and $\phi \leq -1$ (figures 1(a)4 and 1(a)5). The kink lattice (below T_c reported in appendix B) corresponds to this case.

Domain walls exist in cases III–VI, since only in these regimes do parent and product phases or different product phases (twins) coexist. In the materials context the parameter a is determined from the experimental structural data (x-ray and neutron scattering) or from the thermodynamical quantities (specific heat and entropy).

3. Equilibrium conditions and total energy

From the variational derivative of the total free energy, one obtains the following static equilibrium condition:

$$\frac{\partial}{\partial x} \frac{\partial F_T}{\partial \phi_x} - \frac{\partial F_T}{\partial \phi} = 0. \quad (4)$$

By substituting the dimensionless equation (3) in (4), one obtains

$$g\phi'' - a\phi + \phi^3 - \phi^5 = 0. \quad (5)$$

We will show that the solutions of this differential equation for different physical parameters and boundary conditions (for cases III–VI) are quasi-one-dimensional static soliton-like domain wall solutions.

By substituting the solutions of equation (5) in

$$\frac{F_{total}}{F_R} = \int_{-\infty}^{\infty} \left(\frac{g}{2} (\nabla\phi)^2 + \frac{a}{2}\phi^2 - \frac{\phi^4}{4} + \frac{\phi^6}{6} - F_0 \right) dx \quad (6)$$

one can calculate the domain wall energy in each case with respect to some reference free energy density F_0 . However, one integration of equation (5) gives

$$\frac{g}{2} \left(\frac{d\phi}{dx} \right)^2 = \frac{a}{2}\phi^2 - \frac{\phi^4}{4} + \frac{\phi^6}{6} - f_0 \quad (7)$$

where f_0 is a constant of integration and determined by the boundary conditions imposed on the system. For physically admissible domain wall solutions f_0 ranges between the local

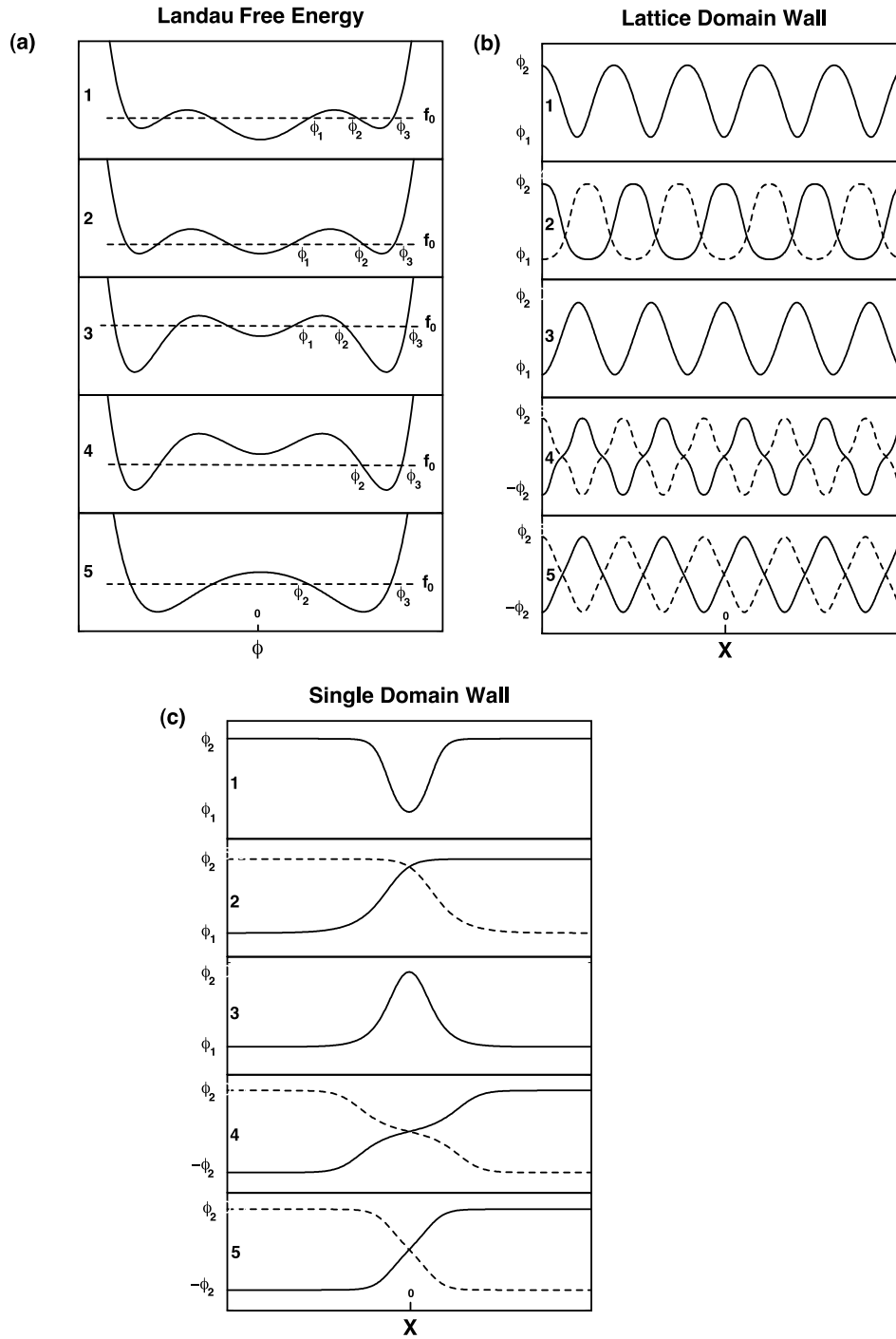


Figure 1. (a) The ϕ^6 potential for different temperatures. Case 1 is above T_c , case 2 is at T_c and cases 3–5 are below T_c . f_0 represents the constant of integration and ϕ_1 , ϕ_2 and ϕ_3 are values of the field ϕ where f_0 intersects the potential. (b) Corresponding kink and pulse lattice solutions. Dashed curves represent anti-kink lattice solutions. (c) Associated single kink and single pulse solutions. Dashed curves represent anti-kink solutions.

minimum and the local maxima (cases 1–3 in figure 1(a)), or between the global and the local minima (case 4 in figure 1(a)), or between the global minima and the local maximum (case 5 in figure 1(a)) of the potential. Using equation (7) and changing the variable of integration from x to ϕ , equation (6) transforms to

$$\frac{F_{total}}{F_R} = \sqrt{2g} \int_{\phi(-L)}^{\phi(L)} \left(\sqrt{\frac{a}{2}\phi^2 - \frac{\phi^4}{4} + \frac{\phi^6}{6} - f_0} \right) d\phi + \int_{-L}^L (f_0 - F_0) dx \quad (8)$$

where total free energy is evaluated for a finite length ($2L$) of the system. We will use equation (8) for evaluating the total energy of the lattice system.

4. Half-kink lattice solution and energetics

In this section we will calculate the half-kink lattice and single half-kink solutions for $a = \frac{3}{16}$ (case IV). We also present total energy of the kink lattice and asymptotic interaction between half-kink and anti-half-kink. For the sake of completeness the corresponding solutions for other cases are presented in appendices A and B.

4.1. Domain wall solutions

After two integrations, equation (5) leads to

$$x(\phi) - x_0 = \pm \sqrt{\frac{g}{2}} \int \frac{d\phi}{\sqrt{\frac{1}{6}\phi^6 - \frac{1}{4}\phi^4 + \frac{3}{32}\phi^2 - f_0}}. \quad (9)$$

For the boundary conditions $f_0 = \lim_{x \rightarrow \pm\infty} F_L$, $\lim_{x \rightarrow \pm\infty} \phi' = 0$ and the choice of origin $\phi(x_0) = 0$, two different lattice solutions are possible. The difference between these two solutions originates from the boundary conditions imposed on the system. These solutions are given by (using elliptic integrals in Byrd and Friedman (1954)) (figure 1(b)2)

$$\phi(x) = \frac{\pm\phi_1}{\sqrt{1 - \alpha^2 \operatorname{sn}^2\left(\frac{x-x_0}{\zeta}, k\right)}} \quad \alpha^2 = \frac{\phi_2^2 - \phi_1^2}{\phi_2^2} \quad (10)$$

$$\phi(x) = \frac{\pm\phi_2 \operatorname{dn}\left(\frac{x}{\zeta}, k\right)}{\sqrt{1 - \beta^2 \operatorname{sn}^2\left(\frac{x-x_0}{\zeta}, k\right)}} \quad \beta^2 = \frac{\phi_2^2 - \phi_1^2}{\phi_3^2 - \phi_1^2} \quad (11)$$

where

$$\zeta^2 = \frac{3g}{\phi_2^2(\phi_3^2 - \phi_1^2)} \quad k^2 = \frac{\phi_3^2(\phi_2^2 - \phi_1^2)}{\phi_2^2(\phi_3^2 - \phi_1^2)}$$

and sn , dn are Jacobi elliptic functions. This $\phi(x)$ is a periodic function with the period $2K(k)\zeta$. The physical meaning of equations (10) and (11) is that the order parameter $\phi(x)$ takes on two different values, ϕ_1 and ϕ_2 , alternatively as the coordinate x is varied. In other words equations (10) and (11) represent (dashed and solid curves in figure 1(b)2, respectively) an alternating array of parent and product phases (e.g. bcc–hcp interface at the transition temperature T_c). Because of the specific boundary conditions for evaluating the integral (9) to obtain the lattice solutions, equations (10) and (11) do not apply in the case $f_0 = 0$. Instead one must integrate (9) directly to find (figure 1(c)2)

$$\phi(x) = \sqrt{3} \left[4 + \exp\left(\mp \frac{x-x_0}{2\sqrt{g/3}}\right) \right]^{-1/2}. \quad (12)$$

Equation (12) represents an asymmetric half-kink soliton and its physical meaning is that the order parameter $\phi(x)$ takes on two different values, ϕ_1 and ϕ_2 , which in this case $\phi_1 = 0$ and $\phi_2 = \sqrt{3}/2$. In other words equation (12) represents a material sample consisting of parent and product phases separated by an asymmetric single domain wall.

4.2. Lattice and asymptotic half-kink/anti-half-kink interaction energies

Since the Landau free energy density has three degenerate minima the total free energy of the system for each lattice solution must be the same. By imposing the boundary conditions which lead to equations (10) or (11), the total energy for a finite length ($2L$) of the lattice is given by

$$\frac{F_{total}^{lattice}}{F_R} = \frac{n\sqrt{3}g}{8x} [(\phi_1^2\phi_2^2 - 8f_0)K(k) + x^2E(k)] \quad (13)$$

where $x^2 = \phi_2^2(\phi_3^2 - \phi_1^2)$ and $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kind, respectively, and n is the number of domain walls (i.e. the number of solitons or anti-solitons) in the system. Again, because of the specific boundary conditions, total lattice formation energy which was obtained in (13) does not apply for a single domain wall energy (classical mass of a half-kink). Instead one must integrate (6) directly with the solution in equation (12) to get

$$\frac{F_{total}^{half-kink}}{F_R} = \frac{3\sqrt{3}g}{64}. \quad (14)$$

The total free energy in each case is measured with respect to the minima of the system which in this case are equal to zero ($F_0 = 0$). To calculate the asymptotic interactions between half-kink and anti-half-kink one must expand equation (13) when $k \rightarrow 0$. However, there is no information about the explicit relation between ϕ_1 , ϕ_2 , ϕ_3 and k . Therefore, to calculate the interaction, we adopted the approach of Manton (1979) which is based on asymptotic expansion of a kink solution. Using this approach, the asymptotic interaction between half-kink and anti-half-kink is given by

$$U(s) = -\frac{3\sqrt{3}g}{256} \exp\left(-\frac{s}{2\sqrt{g/3}}\right) \quad (15)$$

where s is the distance between the half-kink and the anti-half-kink. As expected the interaction energy is an attractive and decays exponentially with increasing distance s .

5. Pulse lattice solution ($T < T_c$)

We consider here the case V of section 2, namely $0 < a < \frac{3}{16}$, $f_0 \geq F_0 = 0$. Apparently, Falk (1983) considered this case but obtained a solution which is appropriate to the case discussed in appendix A.

5.1. Domain wall solutions

The (nontopological) lattice (figure 1(b)3) solution is

$$\phi(x) = \frac{\pm\phi_2 dn\left(\frac{x}{\zeta}, k\right)}{\sqrt{1 - \beta^2 sn^2\left(\frac{x-x_0}{\zeta}, k\right)}} \quad (16)$$

$$\zeta^2 = \frac{3g}{\phi_2^2(\phi_3^2 - \phi_1^2)} \quad \beta^2 = \frac{\phi_2^2 - \phi_1^2}{\phi_3^2 - \phi_1^2} \quad k^2 = \frac{\phi_3^2(\phi_2^2 - \phi_1^2)}{\phi_2^2(\phi_3^2 - \phi_1^2)}.$$

This solution describes alternating parent (e.g. bcc) and product (e.g. hcp) phases with the parent phase at both the boundaries. The corresponding nontopological single domain wall (figure 1(c)3) solution, obtained in the limit $k \rightarrow 1$, is

$$\phi(x) = \frac{\pm\phi_2 \operatorname{sech} \frac{x-x_0}{\zeta}}{\sqrt{1 - \beta^2 \tanh^2 \frac{x-x_0}{\zeta}}} \quad (17)$$

where $\phi_1 = 0$ for a single domain wall. The physical meaning of this solution is that a narrow region of the product phase (hcp) is trapped between the parent (bcc) phase.

5.2. Lattice and single soliton energetics and asymptotic interaction:

The energy of formation for the pulse lattice is calculated to be

$$\frac{F_{total}^{lattice}}{F_R} = \frac{n\sqrt{3}g}{12x} \left[(12a\phi_2^2 - \frac{9}{4}\phi_2^2 + \frac{3}{2}\phi_1^2\phi_2^2 - 12f_0 - 24F_0)K(k) + \frac{3}{2}x^2E(k) - \beta x \left(12a - \frac{9}{4} \right) (K(k)E(\beta', k) - E(k)F(\beta', k)) \right] \quad (18)$$

where $x^2 = \phi_2^2(\phi_3^2 - \phi_1^2)$, $\beta' = \sin^{-1}(\beta/k)$ and $E(\beta', k)$ and $F(\beta', k)$ are incomplete elliptic integrals of the first and second kind, respectively. The energy of the single pulse soliton is

$$\frac{F_{total}^{pulse}}{F_R} = \frac{g\phi_3^2}{4\zeta} \left[(1 + \beta^2) - \frac{(1 - \beta^2)^2 \tanh^{-1} \beta}{\beta} \right]. \quad (19)$$

The asymptotic interaction between a pulse and an anti-pulse soliton can be calculated again using the approach by Manton (1979):

$$U(s) = -\frac{8g\phi_2^2}{\zeta(1 - \beta^2)} \exp\left(\frac{-2s}{\zeta}\right) \quad (20)$$

where s is the distance between the soliton and anti-soliton.

6. Conclusion

By augmenting the Landau free energy of the ϕ^6 model, which has been used to explain first-order phase transitions in physical systems, we explored a Ginzburg–Landau continuum model for the description of possible domain configurations created from the formation of low temperature (product) phase in the high temperature (parent) phase. From the nonlinear equations of equilibrium, the static domain wall and domain wall array (lattice) solutions were calculated both above and below as well as at T_c . From the lattice solutions, the kink and pulse-type soliton solutions were derived in the limit $k \rightarrow 1$. For each case, total energy for the lattice solution and asymptotic interaction energy between solitons in dilute (i.e. widely separated) limit were calculated. However, it is possible that the kink lattice solution at T_c and the pulse-lattice solution below T_c , considered here in detail, are contained in a disguised form in Behera and Khare (1980). In any event, our solutions are physically simpler for materials applications. Moreover, the (kink or pulse) lattice formation energy and the asymptotic soliton interactions were not calculated previously.

In certain first-order transitions, e.g. bcc to ω -phase transformation in elements Ti, Zr, Hf and their alloys (Sanati and Saxena 1998), a third-order term (η^3) is allowed by symmetry in the free energy. Thus, instead of a triple well, an asymmetric double-well free energy density [$F(\eta(x)) = \frac{A}{2}\eta^2(x) + \frac{B}{3}\eta^3(x) + \frac{C}{4}\eta^4(x) + \frac{G}{2}(\nabla\eta)^2$] is sufficient to describe the phase transition

and domain walls. For this case a kink lattice and two types of pulse-lattice solutions are presented in Sanati and Saxena (1998).

Note that we have considered only the static domain wall solutions here. Travelling domain wall solutions $\phi(x, t)$ are readily obtained from the static solutions $\phi(x)$ by boosting to velocity v via $x \rightarrow (1 - v^2)^{-1/2}(x - vt)$. The other important point is the stability of the solutions. The kink-type solutions are known to be linearly stable. The pulse-type solutions are known to be unstable in the field theoretic context (Makhankov 1990). Nevertheless, they could exist in real materials as long-lived metastable states by way of special sample preparation. In other words, there is a possibility that the system is trapped in a metastable minimum rather than the global minimum.

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Appendix A. $\frac{3}{16} < a < \frac{1}{4}$, $f_0 \geq F_0 > 0$ (case III of section 2)

The pulse lattice (figure 1(b)1) and single domain wall (pulse soliton, figure 1(c)1) solutions, their corresponding energies of formation and asymptotic interactions are summarized below. A detailed application of these solutions to martensitic structural transitions is considered by Barsch and Krumhansl (1988).

A.1. Lattice and single soliton solutions

The pulse-lattice solution above T_c is given by

$$\phi(x) = \frac{\pm\phi_1}{\sqrt{1 - \alpha^2 \text{sn}^2\left(\frac{x-x_0}{\zeta}, k\right)}} \quad (21)$$

where

$$\zeta^2 = \frac{3g}{\phi_2^2(\phi_3^2 - \phi_1^2)} \quad \alpha^2 = \frac{\phi_2^2 - \phi_1^2}{\phi_2^2} \quad k^2 = \frac{\phi_3^2(\phi_2^2 - \phi_1^2)}{\phi_2^2(\phi_3^2 - \phi_1^2)}.$$

The corresponding single pulse solution (in the limit $k \rightarrow 1$) is

$$\phi(x) = \frac{\pm\phi_1}{\sqrt{1 - \alpha^2 \tanh^2\left(\frac{x-x_0}{\zeta}\right)}} \quad (22)$$

where $\phi_2 = \phi_3 = \phi_0$.

A.2. Lattice and single soliton energetics and asymptotic interaction

The formation energy of the pulse lattice is

$$\frac{F_{total}^{lattice}}{F_R} = \frac{n\sqrt{3g}}{12x} \left[(12a\phi_1^2 - \frac{9}{4}\phi_1^2 + \frac{3}{2}\phi_1^2\phi_2^2 - 12f_0 - 24F_0)K(k) + \frac{3}{2}x^2E(k) \right. \\ \left. + \alpha x \left(12a - \frac{9}{4} \right) (K(k)E(\beta', k) - E(k)F(\beta', k)) \right] \quad (23)$$

where $x^2 = \phi_2^2(\phi_3^2 - \phi_1^2)$, $\beta' = \sin^{-1}(\alpha/k)$ and $E(\beta', k)$ and $F(\beta', k)$ are incomplete integrals of the first and second kind, respectively. The energy of the single pulse soliton is

$$\frac{F_{total}^{pulse}}{F_R} = \frac{g\phi_2^2}{4\zeta} \left[(3 - \alpha^2) - \frac{(3 + \alpha^2)(1 - \alpha^2)}{\alpha} \tanh^{-1} \alpha \right] \quad (24)$$

and the asymptotic pulse/anti-pulse interaction energy is

$$U(s) = -\frac{16g\phi_1^2\alpha^4}{\zeta(1 - \alpha^2)^3} \exp\left(\frac{-2s}{\zeta}\right) \quad (25)$$

where s is the distance between the soliton and anti-soliton.

Appendix B. $a < \frac{3}{16}$, $0 \geq f_0 \geq F_0$ (cases V and VI of section 2).

The kink lattice (figures 1(b)4 and 1(b)5) and single domain wall (kink soliton, figures 1(c)4 and 1(c)5) solutions, their corresponding energies of formation and asymptotic interactions are summarized below. Falk (1983) has discussed these solutions in detail. The solutions for cases V and VI are mathematically identical except that case V is associated with a triple-well kink while the case VI corresponds to a double-well kink.

B.1. Lattice and single soliton solutions

The kink lattice solution below T_c is given by

$$\phi(x) = \frac{\pm\phi_1\gamma sn\left(\frac{x}{\zeta}, k\right)}{\sqrt{1 - \gamma^2 sn^2\left(\frac{x-x_0}{\zeta}, k\right)}} \quad (26)$$

$$\zeta^2 = \frac{3g}{\phi_3^2(\phi_2^2 + \phi_1^2)} \quad \gamma^2 = \frac{\phi_2^2}{\phi_1^2 + \phi_2^2} \quad k^2 = \frac{\phi_2^2(\phi_3^2 + \phi_1^2)}{\phi_3^2(\phi_2^2 + \phi_1^2)}$$

The corresponding (symmetric) single kink solution (in the limit $k \rightarrow 1$) is

$$\phi(x) = \frac{\pm\phi_1\gamma \tanh\frac{x-x_0}{\zeta}}{\sqrt{1 - \gamma^2 \tanh^2\frac{x-x_0}{\zeta}}} \quad (27)$$

B.2. Lattice and single soliton energetics and asymptotic interaction:

The formation energy of the kink lattice is

$$\frac{F_{total}^{lattice}}{F_R} = \frac{n\sqrt{3g}}{6x} \left[-\left(\frac{3}{2}\phi_1^2\phi_2^3 + 12f_0 + 24F_0\right) K(k) + \frac{3}{2}x^2 E(k) - x \left(12a - \frac{9}{4}\right) (K(k)E(\beta', k) - E(k)F(\beta', k)) \right] \quad (28)$$

where $x^2 = \phi_3^2(\phi_1^2 + \phi_2^2)$, $\beta' = \sin^{-1}(\gamma/k)$ and $E(\beta', k)$ and $F(\beta', k)$ are incomplete integrals of the first and second kind, respectively. The energy of the single kink soliton is

$$\frac{F_{total}^{kink}}{F_R} = \frac{g\phi_1^2}{4\zeta} \left[\frac{3\gamma^2 - 1}{1 - \gamma^2} + \frac{1 + 3\gamma^2}{\gamma} \tanh^{-1} \gamma \right] \quad (29)$$

and the asymptotic kink/anti-kink interaction energy is

$$U(s) = -\frac{4g\phi_1^2\gamma^2(1 + \gamma^2)^2}{\zeta(1 - \gamma^2)^3} \exp\left(\frac{-2s}{\zeta}\right) \quad (30)$$

where s is the distance between the soliton and anti-soliton.

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