In recent years one-dimensional field theoretic models exhibiting solitary wave solutions (kinks, solitons, nonlinear phonons) have played an important role in condensed matter physics. An example of such models is the nonlinear Klein-Gordon equation

\[ m \ddot{\phi}(x,t) - mC_0^2 \phi''(x) + \frac{dV}{d\phi} = 0 \]

This equation can be derived from a Hamiltonian which involves a kinetic term, a linear term and a nonlinear potential term \( V(\phi) \). In lattice dynamics application the Klein-Gordon equation corresponds to the continuum description of a monatomic chain of particles with nearest neighbour coupling \((\gamma)\) and a nonlinear onsite potential which can be described by the Hamiltonian

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

Here \( i, j \) denote lattice sites, \( \phi_i \), and \( \dot{\phi}_i \) are
from the symmetric phase (or the topologically disordered phase) at high temperatures to the topologically ordered phase at low temperatures. This cross over behaviour can be studied experimentally by measuring the thermodynamics quantities like specific heat, transport properties like magnetic susceptibility, electronic conductivity etc.

**Polyacetylene and charge density wave (CDW) transition**

An example of a quasi-one-dimensional system is polyacetylene, \((\text{CH})_x\) (Fig. 5.1). The pure material has one \(\pi\)- electron per \((\text{CH})\) group, that is it has a half filled band. It is known that (Peierls, 1955), due to electron-phonon interaction, a one-dimensional conductor with a partly filled band is unstable with respect to distortions of the lattice structure with wave vector \(\mathbf{Q} = 2\mathbf{k}_F\), where \(\mathbf{k}_F\) is the Fermi wave vector. As shown in Fig. 5.2 the electron spectrum develops an energy gap \(2\Delta\) at \(K = \pm \mathbf{k}_F\) and the materials became a semiconductor. In real space, the instability corresponds to setting up a charge-density-wave (CDW) in the electron density \(n(x)\) along the chain varying as

\[
\eta(x) = \eta_0 + \eta_0 \cos(Q + \phi)
\]

(5.3)

The oscillatory electron density modulation is balanced
Fig. 5.1. Polyacetylene \((\text{CH})_x\), (a) Trans \((\text{CH})_x\)
(b) Cis \((\text{CH})_x\).
Fig. 5.2. (a) Tight binding band for a perfect linear chain (b) the Peierl's distortion opens a gap $2\Delta$ at $\pm k_f$. 
by a periodic lattice distortions (PLD) and is described by an equation

\[ U_n = U_{n_0} + U \cos(\phi + \theta) \quad (5.4) \]

The CDW and PLD sustain each other and is usually termed as 'condensate'. It is to be noted that the CDW is tied to the PLD and not to the equilibrium positions of the underlying atoms or molecules. Here $\theta$ is the phase of the condensate which specifies its position relative to an external laboratory frame. A variation $\theta$ in phase translates the entire condensate over the distance

\[ \delta x = \frac{\delta \theta}{\nu} \]

It can be shown (Schrieffer, 1985) that the ground state energy of the system $E_0(u)$ is doubly degenerate. $E_0(u)$ is plotted in fig.5.3 and it has a maximum at $u = 0$, consistent with Peierl's instability. Because of the twofold degenerate ground state ($E(u_0) = E(-u_0)$), the system supports nonlinear excitations which act as moving domain walls separating regions having different ground states, usually termed as A phase ($+u_0$) and B phase ($-u_0$). Since these nonlinear excitations are shape-preserving excitations which alter the medium when they pass, these acts as topological solitons. A soliton corresponds to a field configuration which approaches the B phase for $N \to -\infty$ and the A phase as $N \to +\infty$ ($N$ being the number of monomers in $(CH)_x$) for an infinitely long chain. The displacement field can be written as
Fig. 5.3. Ground state energy $E_0$ as a function of the amplitude $u$. 
There is a preferred \( \xi \) of the soliton (over which \( u \) changes for \( -U_0 \) to \( +U_0 \) ) which minimizes the total energy. Numerical calculation shows that

\[
U_n = U_0 \tanh \frac{\eta a}{3} \tag{5.6}
\]

where \( \xi \approx 7a \), and \( a \) is the lattice constant (Su et al., 1979 and 1980).

It should be noted that such a lattice displacement pattern (eqn. (5.6)) can be obtained from the dynamics of a nonlinear monatomic chain (eqn. (5.2)) with a doubly degenerate \( \lambda \phi^4 \) onsite potential (eqn. (1.39)).

Order parameter and pinning of charge density wave

The order parameter of the CDW state is complex and we many defined it to be \( \psi = A \exp(\imath \phi) \), where \( A \) is the amplitude and \( \phi \), the phase of the CDW. In general both \( A \) and \( \phi \) may be functions of space and time. The behaviour of order parameter can be obtained from the Lagrangian density \( L(x,t) = L(\psi(x,t)) \). Usually the
low lying excitations of the condensate is dominated by deformation only in the phase $\phi$, as the deformation in amplitude needs more energy. By substituting into the Lagrangian the form of the order parameter $\psi(x,t) = A_0 \exp(i\phi(x,t))$, Rice et al (1976) obtained a '0 particle' model, which is a model of nonlinear phase deformations of weakly pinned CDW. The equation of motion for the phase is again the Klein-Gordon type (eqn. (5.1)) of nonlinear wave equation, where the potential $V(\phi)$ in this case is the pinning potential of the CDW wave (Lee et al, 1974 and Rice, 1978). Various factors responsible for pinning the CDW to the lattice are

1. the discreteness of the lattice, which gives rise to the commensurability pinning potential of the form

$$V(\phi) \propto (\frac{\Delta}{W})^M (1 - \cos M\phi)$$

where $\Delta$ denote the gap due to CDW transition and $W$ is the electronic bandwidth. This arise when the ratio of the linear chain reciprocal lattice vector $G$ and $Q$ is equal to integer $M$. (11) the interchain interaction, which gives rise to a pinning potential of the form

$$V_{12}(\phi) \propto \Delta_1 \Delta_2 \cos (\phi_1 - \phi_2)$$

where $\phi_1$ and $\phi_2$ are the phases of the CDW's on parallel chains, and (111) lattice defects, like presence of impurities, which gives rise to a pinning potential of the form

$$V(\phi) = \sum_i V_i \cos (Q\cdot x_i + \phi(x_i))$$

where $x_i$ denote locations of the impurities and $V_i$ the magnitude of the impurity potential. For more details on the
impurity pinning, see Chapter VI. With these pinning potentials, the equation of motion for the phase deformations is of the sine-Gordon type (eqn. (1.2)).

Beside polyacetylene \((\text{CH})_x\), there are other materials like organic conductor KCP \((\text{K}_2\text{P}_{4}\text{CN}_4\text{Br}_{0.3}\text{H}_{2.0})\), the organic charge transfer salt TTF-TCNQ (tetrathiofulvalene-tetracyanoquinodimethane) etc which also forms as an array of weakly coupled linear chains.

The Hamiltonian in eqn. (5.2) is also used as a standard model Hamiltonian (Krumhansl et al., 1975; Bruce, 1980) for systems which undergo a structural phase transition (SPT). In most of the models the onsite potential \(V(\phi_i)\) is taken to be of the \(\lambda \phi^4\) form (eqn. (1.39)). This onsite potential may be thought of as arising from an underlying sublattice of atoms which do not actively participate in the phase transition.

**Displacive and order-disorder structural phase transition**

The SPT are usually classified into two distinct types (a) the displacive transition and (b) the order-disorder transition. In a displacive SPT the atoms in the distorted phase are slightly displaced away from the equilibrium position of the high temperature phase. For example, Fig. 5.4
Fig. 5.4. Low temperature distorted phase of ferroelectric 
$\text{BaTiO}_3$. 

\[
\begin{array}{c|c|c}
\text{Ba} & 0 \\
\text{O} & 1 & 005 \\
\text{O} & 2 & 009 \\
\text{Ti} & 3 & 005 \\
\end{array}
\]
shows the low-temperature phase of BaTiO$_3$, in which the atoms are displaced away from the centro-symmetric positions at high temperature cubic phase. For this system Bersuker (1972) have shown that the oxygen-barium sublattice produces a double-well potential for this Titanium sublattice. In an order-disorder SPT as for example in NaN$_2$O$_2$ the transition is associated with an ordering of some variable which is disordered at high temperature phase. In the high temperature phase the triangular NO$_2$ groups have N-ions along either the positive or negative b-axis with equal probabilities, but below the transition point, the N-ions tend to align in the same direction, as shown in fig.5.5 (Hoshino et al., 1967). In NaN$_2$O$_2$ the energetically most favourable path of reorientation of an NO$_2$ group in the case of six nearest neighbour Na-atoms is describable in terms of a double-well potential.

In terms of the strength of the nearest neighbour interaction and the depth of the onsite double-well potential, one can also make a distinction between the two limiting types of SPT's. The order-disorder regime occurs when the nearest neighbour interaction energy is small compared with the single particle (onsite) potential barrier energy. The displacive regime occurs in the opposite limit where the intersite coupling dominates.
Fig. 5.5. The structure of ferroelectric NaNO$_2$. 
The SPT observed in ferroelectric crystals is usually associated with a soft phonon mode whose temperature dependence is approximately described by (Lines et al, 1977)

\[ \omega_F^2 = A (T - T_c) \]  

(5.7)

Besides the soft phonon mode a central peak near zero frequency is also observed in these transitions (Piste et al, 1971; Shapiro et al, 1972).

One-dimensional models of structural phase transition

The major advancement in the understanding of SPT, and in particular the central-peak phenomena have emerged from one-dimensional model calculations. Krumhansl and Schrieffer (1975) have used a \( \lambda \phi^4 \) field theoretic model for SPT. In this model the domain wall (kink) solutions are identified with the central peak phenomena. Halperin and Varma (1976) applied the renormalization group technique to this model. Aubry (1976) performed molecular dynamics calculations for the \( \lambda \phi^4 \)-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 have come
from the molecular dynamics calculations of Schneider and Stoll (1975, 1976) in two dimensions and the quantum mechanical calculations of Bishop et al. (1976).

All these models exhibit a 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) indicate that the soft mode frequency does not vanish at $T_c$, which is an indication of a first-order rather than second order phase transition. With this in mind, Behera and Khare (1980) used a $\phi^6$ field theoretic model to propose a qualitative picture of the central-peak phenomena. This is a model of first-order. SPT. Magyari (1981) has considered a model of one-dimensional chain with harmonic coupling between neighbouring lattice sites and a generalized onsite potential

$$ V(\phi) = C\phi^{2n+2} + B\phi^{n+2} + A\phi^2 + D $$

(5.8)

with adjustable nonlinearity for $n = 2, 4, 6, \ldots$. This potential has triply degenerate minima for

$$ B^2 = 4AC \quad \text{with} \quad A, C > 0 \quad \text{and} \quad B < 0 \quad (5.9) $$

and describes a first-order SPT. Solitary wave (kink) solutions are obtained in this model for $D = 0$. 
Buttner and Bilz (1978) have proposed a model of diatomic chain with two different masses, to describe the SPT in ferroelectric crystals. Recent interest in diatomic models for solids is largely due to the fact that many of the solids which undergoes a SPT (e.g. BaTiO$_3$, SrTiO$_3$, etc) have a diatomic structure along certain crystallographic directions. However in most of the studies the nonlinearity is introduced as anharmonic interactions between neighbouring atoms in the chain (Buttner et al., 1978). In other studies of nonlinear diatomic models, the nonlinearity is considered to be arising from shell-core interactions coupling electrons to alternate ions on a diatomic chain (Buttner et al., 1981). Henry and Oitmaa (1983) introduced a nonlinear diatomic model in which the nonlinearity is similar to that of Krumhansl and Schrieffer (1975) type, arising from a nonlinear onsite potential. The nonlinear onsite potential is considered to be a fixed external potential, arising from an underlying sublattice. Thus this diatomic model includes the sublattice as part of the vibrating complex.

It may be noted that these models do not show a phase transition at finite temperature. This is because in one-dimensional system true long range order is not possible at finite temperature. However in these models nonlinearity can be treated exactly and as a result interesting features like
domain wall solutions appears. It has been pointed out by many authors that, many statistical macroscopic properties of the systems are sensitive to these nonlinear excitations.

A model of first-order structural phase transition

We have (Dey, 1986) considered the potential in eqn. (5.8) for odd values of \( n (=1,3,5,\ldots) \) and have shown that this represents yet another model of a first order SPT at the transition temperature \( T = 0 \). In contrast to the case of even values of \( n (=2,4,6,\ldots) \) as considered by Magyari (1981), which has triply degenerate minima, the \( n=1,3,5,\ldots \) case has doubly degenerate minima for the condition given in eqn. (5.9). The potential for \( n = 1 \) case has been used (Viswanathan et al., 1979) to study the statistical mechanics of field theories with broken, global and local SU(3) gauge symmetries, where it has been shown that the presence of cubic term in the potential restores the symmetry by a first-order phase transition, rather than by a second order transition. The antisymmetric nature of the potential for odd values of \( n \) is particularly useful for describing the CDW transition in systems, where the gap appears in one particular direction. Solitary wave solutions (kink) are obtained for this potential, which are shown to be stable and represent the finite-energy solution
of the system. We have also extended the model (eqn. (5.8)) to the diatomic chain and have shown that, in the displacive phase transition limit the solitary-wave (kink) solutions exists for the potential for both the $n = 1, 3, 5, \ldots$ case and the $n = 2, 4, 6, \ldots$ case, satisfying the condition in eqn. (5.9). The solutions are again shown to be stable. The non-linear periodic solutions (non-linear phonons) are obtained for the case $n = 1$, as for $g^4$ onsite model (Henry et al., 1983), in this case the periodon solutions (solutions of discrete equations of motion (Buttner et al., 1981)) are also found to be analogous to the form of the non-linear periodic solutions. It is also shown that the solitary wave (kink) solutions exist even when a single-well potential is included on the atom of mass $M_2$ (Subbaswamy et al., 1978).

Monatomic chain with nonlinear onsite potential

First let us consider the case of a monatomic chain with the onsite potential represented by eqn. (5.8), for odd values of $n = 1, 3, 5, \ldots$. The system is illustrated in Fig. 5.6. The equation in which the first derivative of the potential \[
\frac{dV}{d\phi}
\] is set equal to zero has three different real roots, $\phi = 0$ is one, which corresponds to the equilibrium field configurations. The potential allows two stable and one unstable equilibrium field configurations.
Fig. 5.6. Nonlinear monatomic chain model for SPT (reproduced from Henry (1984)).
Thus from the topological point of view the potential (eqn. (5.8)) for odd values of $n$ never exceeds that of $\lambda \varphi^4$ theory. This is in contrast to the even $n(=2,4,6,\ldots)$ case as considered by Magyari (1981) where the potential allows three stable and two unstable equilibrium field configurations. It can be easily checked that the case for odd values of $n$ has doubly degenerate minima for the condition represented by eqn. (5.9), at

$$\phi = 0 \quad \text{and} \quad \phi = \left(\frac{2A}{|B|}\right)^{\frac{1}{n}} = \phi_0 \quad (5.10)$$

We consider $H$ (eqn. (5.2)) as the model Hamiltonian for the monatomic chain with the onsite potential given by eqn. (5.8). In the displacive regime of the SPT i.e.,

where

$$C_{ij} \phi_i^2 > \nabla (\phi_0) \quad (5.11)$$

the displacement field $\phi(x,t)$ does not alter greatly over a lattice spacing $a$ (i.e., the wavelength of the displacement pattern will be much greater than the lattice constant). So we can connect the displacements of the neighbouring atoms by a Taylor's series expansion and go over to the continuum limit of the Hamiltonian (eqn. (5.2)), which up to second order in $a$ is
\[ H = \int_{-\infty}^{\infty} \frac{dx}{\alpha} \left[ \frac{1}{2} m \left( \frac{\partial \Phi}{\partial t} \right)^2 + \frac{1}{2} mC_0^2 \left( \frac{\partial \Phi}{\partial x} \right)^2 + V(\Phi) \right] \]  

(5.12)

where \( C_0 \) is the velocity of sound \( \left( mC_0^2 = \gamma \alpha^2 = C_0 \alpha^2 \right) \).

The Euler-Lagrange equation of motion is given by

\[ m \left( \frac{\partial^2 \Phi}{\partial t^2} \right) = mC_0^2 \left( \frac{\partial^2 \Phi}{\partial x^2} \right) + \frac{dV}{d\Phi} = 0 \]

(5.13)

### Solitary wave (kink/antikink) solutions

For travelling wave solutions, we make a simple transformation

\[ \xi = \frac{(x-\nu t)}{\lambda} \]

(5.14)

The equation of motion then reduces to

\[ \left[ m \left( \frac{\nu^2 - C_0^2}{\lambda^2} \right) \right] \frac{d^2 \Phi(\xi)}{d\xi^2} = - \frac{dV}{d\Phi} \]

(5.15)

This equation can be readily integrated (See Chapter-II) to give the kink/antikink solutions (for \( D=0 \)) as

\[ \Phi_k = 2^{\frac{1}{n}} \Phi_0 \left( 1 \pm \text{tanh} \frac{\eta^3}{2} \right)^{\frac{1}{n}} \]

(5.16)

where we have put \( \lambda = m \left( \frac{C_0^2 - \nu^2}{2A} \right) \). The sign +
corresponds to kink and antikink solutions respectively.
As \( \xi \) varies from \(-\infty\) to \(+\infty\), \( \theta \) interpolates between 0 and \( \theta_0 \).

To check the linear stability of these solutions we write (see Chapter-IV)

\[
\dot{\Phi} = \Phi_k(\xi) + \Theta(\xi) \exp(-i\omega t)
\]  
(5.17)

which when substituted in the equation of motion (eqn.(5.13)) gives the stability equation in the form

\[
2A \Theta''(\xi) - 2\Im \omega \Theta'(\xi) + m \omega^2 \Theta(\xi) - V''[\Phi_k(\xi)] \Theta(\xi) = 0
\]  
(5.18)

as before the prime denote derivative w.r.t. the argument.
The solution of this equation for \( \omega = 0 \) is given by

\[
\Theta(\xi) = \Theta_0 \frac{d\Phi_k(\xi)}{d\xi}
\]  
(5.19)

where \( \Theta_0 \) is an arbitrary constant. Eqn.(5.7) then gives

\[
\Phi = \Phi_k(\xi + \Theta_0)
\]  
(5.20)

Thus the solution is a translation mode. The \( \omega = 0 \) mode is also nodeless (as can be seen from eqn.(5.16)) and thus represent the lowest energy solution of the excitation spectrum. This shows that the kink/antikink solutions (eqn.(5.16)) are stable.
Let us consider the potential (eqn. (5,8)) for $n = 1$ case in more detail. As mentioned earlier, this model has been used (Viswanathan et al., 1979) to study the statistical mechanics of field theories with various gauge symmetries. It can be used as a model of CDW transition also, beside other first-order SPT's. The stability equation for static case become

$$\left\{ \frac{d^2}{dk^2} + \left[ \frac{2}{A} m \omega^2 - (4 - 6 \text{sech}^2 k) \right] \right\} \phi(k) = 0$$

(5.21)

with $\phi_0 = \frac{m \phi_0^2}{2A}$ and $k = \frac{X}{2 \phi_0}$. This equation is of the same form as the stability equation of $\lambda \phi^4$ theory (Rajaraman, 1982). This is an Schrodinger-like eigenvalue equation. The complete eigenvalue spectrum consists of two bound states, for $\omega^2 = 0$ and $\omega^2 = \frac{3A}{2m}$, and a continuum for $\omega^2 = \frac{A}{2m} (4 + k^2)$ (See Chapter VI for more details on the excitation spectra for general value of $n$ of the potential). The energy of system (static) is finite and is given by

$$E = \int_{-\infty}^{\infty} \frac{dx}{\alpha} \left[ \frac{1}{2} m \phi_0^2 \left( \frac{\partial \phi}{\partial x} \right)^2 + A \phi^2 + B \phi^3 + C \phi^4 \right]$$

Using eqn. (5,16) it can be easily shown that

$$E = \frac{4A^3 \phi_0}{3B^2 \alpha}$$

(5.22)
which is same for both kink and antikink solutions. In Chapter-VI we study the excitation spectra of the kink/antikink solutions (eqn. (5,16)) for general value of and also the interaction of the kink with impurities (for \( n = 1 \) case).

**Diatomic chain with nonlinear onsite potential**

We now consider a diatomic chain with an onsite potential given by eqn. (5.8) on one of the species (say of mass \( M_1 \)) for both even and odd values of \( n \). The system is illustrated in Fig. 5.7. This is an extension of the monatomic chain model examined by Krumhansl and Schrieffer (1975), to include two types of atoms in the chain. As has been pointed out earlier, this represent a model for the first order displacive phase transition in ferroelectrics.

The Hamiltonian for the discrete lattice is taken to be (Henry et al, 1983)

\[
H = \sum_i \left[ \frac{1}{2} M_1 \dot{U}_i^2 + \frac{1}{2} M_2 \dot{V}_i^2 + \frac{1}{2} \gamma (U_i - V_{i-1})^2 + \frac{1}{2} \gamma (U_i - V_i)^2 + V(U_i) \right]
\]  

(5.23)

where \( U_i \) and \( V_i \) are the displacements of masses \( M_1 \) and \( M_2 \) respectively in the \( i \)th unit cell, \( \gamma \) is the
Fig. 5.7. Nonlinear diatomic chain model for SPT (reproduced from Henry (1984)).
harmonic force constant between neighbouring atoms and 
\( V(\mathbf{u}_i) \) is the onsite potential represented by eqn. (5.8).
The coupled equations of motion are given by
\[
\begin{align*}
M_1 \ddot{u}_n &= -\gamma \left( 2u_n - u_{n-1} - u_{n+1} \right) - V'(u_n) \\
M_2 \ddot{u}_n &= -\gamma \left( 2u_n - u_{n-1} - u_{n+1} \right)
\end{align*}
\] (5.24a, 5.24b)

We confine ourselves to the displacive regime of the phase transition i.e. where
\[
\gamma > \frac{|V(\phi_0)|}{\phi_0^2}
\] (5.25)

In this regime, we can use the Taylor's series expansion for the displacement field to go over to the continuum limit of the Hamiltonian \( H \) (eqn. (5.23)). Substituting
\[
\begin{align*}
u_i \rightarrow u(x,t) &\rightarrow u \\
\nu_i \rightarrow v(x+\frac{1}{2}a,t) &\rightarrow v + \frac{1}{2}a v' + \frac{1}{2} (\frac{1}{2}a)^2 v'' + \cdots \\
\nu_{i+1} \rightarrow v(x-\frac{1}{2}a,t) &\rightarrow v - \frac{1}{2}a v' + \frac{1}{2} (\frac{1}{2}a)^2 v'' - \\
\sum_i \rightarrow \int \frac{dx}{a}
\end{align*}
\] (5.26)

In the Hamiltonian \( H \) and retaining terms only up to \( a^2 \), we get the continuum limit of the Hamiltonian (Henry et al., 1983)
\[
H = \int \frac{dx}{a} \left[ \frac{1}{2} M_1 \dot{u}^2 + \frac{1}{2} M_2 \dot{v}^2 + \gamma (u-v)^2 + \frac{1}{4} \gamma a^2 uv' + V(u) \right]
\] (5.27)
where the prime denote \( \frac{\partial}{\partial x} \). The Euler-Lagrange equations of motion can be written as a coupled equation,

\[
\begin{align*}
\frac{1}{4} \gamma a^2 u'' + 2 \gamma u &= M_1 \ddot{u} + \frac{dV}{du} + 2 \gamma u \\
M_2 \ddot{u} + 2 \gamma u &= \frac{1}{4} \gamma a^2 u'' + 2 \gamma u
\end{align*}
\] (5.28)

**Solitary wave (kink/antikink) solutions**

We make the transformation \( S = x - ct \) and substitute \( u(x,t) = f(S) \) and \( U(x,t) = g(S) \). With this the coupled equations can be written as,

\[
\begin{align*}
\frac{1}{4} \gamma a^2 \frac{d^2 f}{dS^2} + 2 \gamma g &= M_1 c^2 \frac{d^2 f}{dS^2} + 2 \gamma f + \frac{dV}{df} \\
M_2 c^2 \frac{d^2 g}{dS^2} + 2 \gamma f &= \frac{1}{4} \gamma a^2 \frac{d^2 f}{dS^2} + 2 \gamma f
\end{align*}
\] (5.29)

For a particular velocity

\[
C = c_0 = \left( \frac{\gamma a^2}{4M_2} \right)^{\frac{1}{2}}
\] (5.30)

we get \( f(S) = g(S) \) (from the second equations of eqn. (5.29)). Substituting eqn. (5.30) in the first equation of eqn. (5.29) we get

\[
(M_1 - M_2) c_0^2 \frac{d^2 f(S)}{dS^2} + \frac{dV}{df} = 0
\]
Multiplying both side of this equation by $\frac{\partial f}{\partial s}$ and integrating w.r.t. s we get

$$\pm s = \left[ C_0^2 (M_1 - M_2)^\frac{1}{2} \int (I - 2V(s))^{-\frac{1}{2}} \right] dJ$$

(5.31)

where $I$ is an arbitrary constant of integration. For $I = 0$, $M_2 > M_1$, $D = 0$ and the condition in eqn. (5.9), we get the kink and antikink solutions ($\pm$ sign) as

$$U_k(x,t) = U_k(x,t) = 2^{\frac{1}{n}} U_0 \left[ 1 \pm \tanh \left( \frac{nS}{2\sqrt{3}K} \right) \right]^\frac{1}{n} ; \text{ for } n=1,3,5$$

(5.32a)

and

$$U_k(x,t) = U_k(x,t) = \pm 2^{\frac{1}{n}} U_0 \left[ 1 \pm \tanh \left( \frac{nS}{2\sqrt{3}K} \right) \right]^\frac{1}{n} ; \text{ for } n=2,4,6$$

(5.32b)

which represent two kink and two antikink solutions (See Chapter II) with

$$U_0 = \left( \frac{2A}{|B|} \right)^\frac{1}{n}$$

(5.33)

and

$$\delta_k = \left[ C_0^2 (M_2 - M_1)/2A \right]^\frac{1}{2}$$

(5.34)

It may however be noted that, as in the diatomic chain
model with $\lambda \phi^4$ onsite potential (Henry et al., 1983), there are no such pulse solutions (infinite energy solutions) for this potential (eqn. (5.8)) for both even and odd values of $n$. It may also be noted that, at velocities $C \neq C_0$ (eqn. (5.30)) and which are much lower compared to the velocity of sound in the lattice, one can also try to find a low-velocity kink and antikink solutions (Henry, 1984).

To check the stability of these solutions eqns. (5.32) we write

$$U(x,t) = U_K(s) + \Phi(s) \exp(-i\omega t)$$

(5.35a)

$$V(x,t) = V_K(s) + \Psi(s) \exp(-i\omega t)$$

(5.35b)

Substituting eqns. (5.35) in eqn. (5.28) and using eqn. (5.29) we get the coupled stability equations as

$$M_1 C^2 \phi''(s) - \frac{1}{4} \gamma a^2 \psi''(s) + 2i \gamma (\phi(s) - \psi(s)) + 2i M_1 \omega C \phi(s)$$

$$- M_1 \omega^2 \phi(s) + V' \left[U_K(s)\right] \phi(s) = 0$$

$$M_2 C^2 \psi''(s) + 2i M_2 \omega C \psi'(s) - M_2 \omega^2 \psi(s)$$

$$+ 2i \gamma (\psi(s) - \phi(s)) - \frac{1}{4} \gamma a^2 \phi''(s) = 0$$

(5.36)

where prime denote derivative w.r.t. the argument. It can be easily checked by direct substitution that the solution of this coupled equation for $\omega = 0$ is

$$\phi(s) = \phi_0 \frac{dU_K(s)}{ds}$$

(5.37a)
and

\[ \psi(s) = \psi_0 \frac{dU_k(s)}{ds} \]  

(5.37b)

with \( \phi_0 \) and \( \psi_0 \) as arbitrary constants. Eqns. (5.35) then implies

\[ U(x,t) = U_k(s) + \phi_0 \frac{dU_k(s)}{ds} \approx U(s + \phi_0) \]  

(5.38a)

and,

\[ U(x,t) = U_k(s) + \psi_0 \frac{dU_k(s)}{ds} \approx U(s + \psi_0) \]  

(5.38b)

to be the translation modes. These \( \omega = 0 \) modes are also nodeless as can be seen by taking derivatives of eqns. (5.32), and thus represent the lowest energy solutions of the excitation spectrum.

Nonlinear periodic solutions (nonlinear phonons)

Now we solve eqn. (5.29) for \( C \neq C_0 \) (eqn. (5.30)). We first decouple eqn. (5.29). From the second equation of eqn. (5.29) we have

\[ q''(s) = \frac{\frac{1}{4} \gamma a^2 \varepsilon'' + 2 \gamma f - 2 \gamma g}{M_2 C^2} \]

Substituting this in the first equation of eqn. (5.29) we get
\[ g(s) = \frac{M_1 M_2 c^4}{2\gamma (M_2 c^2 - \frac{1}{4} \gamma \alpha^2)} \frac{d^2 f(s)}{ds^2} + f(s) + \frac{M_2 c^2}{2\gamma (M_2 c^2 - \frac{1}{4} \gamma \alpha^2)} \frac{dv}{df}. \]  

(5.39a)

Eliminating \( 2\gamma \dot{q} \) term from the two equations in eqn. (5.29) we get

\[
\left( \frac{1}{4} \gamma \alpha^2 - M_2 c^2 \right) \frac{d^2 q}{ds^2} + \left( \frac{1}{4} \gamma \alpha^2 - M_1 c^2 \right) \frac{d^2 f}{ds^2} - \frac{dv}{df} = 0.
\]

Substituting eqn. (5.39a) in this equation and rearranging terms we get the equation for \( f(s) \) as

\[
\left( C_1 \frac{d^2 q}{ds^2} - C^2 \right) + 2\gamma \left( (M_1 + M_2) c^2 - \frac{1}{2} \gamma \alpha^2 \right) \frac{d^2 f}{ds^2} + M_2 c^2 \left( \frac{d^2 v}{ds^2} \right) + 2\gamma \frac{dv}{df} = 0.
\]

(5.39b)

Now for a particular velocity

\[
C = \left\{ \frac{\gamma \alpha^2}{4 (M_1 M_2)^{1/2}} \right\}^{1/2}
\]

(5.40)

eqn. (5.39b) becomes a second order differential equation which can be written in the form

\[
(M_1 + M_2) (C^2 - C_A^2) \frac{d^2 f}{ds^2} + \frac{M_2 c^2}{2\gamma} \frac{d^2 v}{ds^2} = 0.
\]

(5.41)

where \( C_A = \frac{\gamma \alpha^2}{2 (M_1 + M_2)} \). To solve eqn. (5.41) we
substitute (Henry et al., 1983)

\[ \frac{df}{ds} = \beta , \quad \frac{d^2f}{ds^2} = \beta \frac{d\beta}{df} \]

With this eqn., (5.41) can be written as

\[ \frac{d\beta}{df} = -\left[ \left( \frac{c^2 M_2 \frac{d^3V}{df^3} + 2 \frac{dV}{df} }{\alpha_0 \beta + c^2 M_2 \frac{d^2V}{df^2}} \right) \right] = - \frac{P(\beta, f)}{Q(\beta, f)} \]  

(5.42)

where \( \alpha_0 = 2 \left( (M_1 + M_2)(c^2 - c_0^2) \right) \). We now construct an exact differential

\[ \lambda P df + \lambda Q d\beta = 0 \]  

(5.43)

where \( \lambda \) is an integrating factor given by

\[ \lambda = \exp \left[ \int h(f) df \right] \]

with

\[ h(f) = \left( \frac{\delta P}{\delta \beta} - \frac{\delta Q}{\delta \beta} \right) / Q(\beta, f) \]

From eqn., (5.42) we get

\[ h(f) = \frac{c^2 M_2 \frac{d^3V}{df^3}}{\alpha_0 + c^2 M_2 \frac{d^2V}{df^2}} \]

so
\[ \lambda = \alpha_0 + c^2 M_2 \frac{d^2 V}{d \Omega^2} \quad (5.44) \]

If we define \( \psi(p, f) \) such that
\[ \frac{\partial \psi}{\partial f} = \lambda p \quad (5.45a) \]
\[ \frac{\partial \psi}{\partial p} = \lambda q \quad (5.45b) \]
then it follows from eqn. (5.43) that
\[ \psi(p, f) = 0 \quad (5.46) \]

From eqns. (5.42) and (5.45a) we get
\[ \psi = \alpha_0 c^2 M_2 p^2 \frac{d^2 V}{d \Omega^2} + 2 \delta \alpha_0 V + \frac{1}{2} c^4 M_2^2 p^2 \left( \frac{d^2 V}{d \Omega^2} \right)^2 \]
\[ + \gamma c^2 M_2 \left( \frac{d V}{d \Omega} \right)^2 + N(p) \]
which gives
\[ \frac{\partial \psi}{\partial p} = 2 \alpha_0 c^2 M_2 \frac{d^2 V}{d \Omega^2} + c^4 M_2^2 \frac{d^2 V}{d \Omega^2} \right) + \frac{d N(p)}{d \Omega} \quad (5.47) \]

where \( N(p) \) is some function of \( p \). Equating eqns. (5.47) and (5.45b) (with eqn. (5.42)) we get
\[ N(p) = \frac{b^2}{2} \left[ \lambda^2 - 2 \alpha_0 c^2 M_2 \frac{d^2 V}{d \Omega^2} - c^4 M_2^2 \left( \frac{d^2 V}{d \Omega^2} \right)^2 \right] - \frac{1}{2} \]
where $I$ is a constant of integration. Eqn. (5.46) then implies

$$\rho = \frac{\partial^2 r}{\partial S^2} = \frac{\{I-2\gamma C^2 M_2 (dV/df)^2 - 4\alpha_0 \gamma V\}^{\frac{1}{2}}}{(\alpha_0 + C^2 M_2 \frac{d^2 V}{df^2})}$$

which gives

$$S = \int \frac{(\alpha_0 + C^2 M_2 \frac{d^2 V}{df^2})}{\{I-2\gamma C^2 M_2 (dV/df)^2 - 4\alpha_0 \gamma V\}^{\frac{1}{2}}} \, df$$

(5.48)

It is very difficult to integrate eqn. (5.48) for the potential considered in eqn. (5.8) for any general value of $n$. However we have been able to obtain the result for a particular case of this potential, for $n = 1$, $A = C = 1$, $B = -2$, satisfying the condition in eqn. (5.9) for doubly degenerate minima. Substituting this form of the potential we get after some algebra

$$S = \int \frac{(\alpha_0 + 2C^2 M_2 - 12C^2 M_2 f + 12C^2 M_2 f^2)}{\{I-4\gamma f^2 (1-f^2) [(\alpha_0 + 2C^2 M_2 - 8C^2 M_2 f + 8C^2 M_2 f^2)^2]\}^{\frac{1}{2}}} \, df$$

which when integrated gives the non linear periodic solutions of eqn. (5.39b) for the particular value of velocity $C$ (eqn. (5.40)) as

$$f(S) = \frac{1}{2} (1 + f_0 \sin kS)$$

(5.49a)

where
From eqn. (5.39a) we get

\[ f_0 = \left[ 1 + \frac{2\alpha_0 + 2\gamma^2 M_2}{6\gamma C^2 M_2} \right] \frac{1}{2} \]

and

\[ k = \left( \frac{2\gamma}{q C^2 M_2} \right)^{\frac{1}{2}} \]

From eqn. (5.39a) we get

\[ q(s) = \frac{1}{2} + q_1 \sin kS + q_2 \sin k^2 S \]

(5.49b)

where

\[ q_1 = \frac{1}{2} \left( 1 - \frac{M_2 C^2}{2\gamma (M_2 C^2 - \frac{1}{4} \gamma \alpha^2)} \right) f_0 \]

and

\[ q_2 = \frac{M_2 C^2}{4\gamma (M_2 C^2 - \frac{1}{4} \gamma \alpha^2)} f_0^3 \]

It is interesting to note that with appropriate choice of amplitudes, these nonlinear periodic solutions (eqns. (5.49)) also solve the original coupled equations and motion (eqn. (5.29)) exactly. It can be checked by direct substitution of eqns. (5.49) in eqn. (5.29), that the appropriate amplitudes are given

\[ f_0 = \left\{ \left( \frac{3}{2\gamma} \right) \left[ \frac{1}{32} \gamma^2 C^4 k^4 - \frac{1}{8} \gamma^2 C^2 k^2 + \gamma (M_1 + M_2) \gamma C^2 k^2 \right. \right. \]
\[ \left. \left. - \frac{1}{4} M_2 C^2 k^2 - \frac{1}{2} M_1 M_2 C^4 k^2 \right] \right\} \frac{1}{2} \]

(5.50a)

\[ q_1 = \frac{3\gamma^2 C^2 k^2 q_2 - f_0 \left( \gamma^2 - \frac{1}{4} \gamma \sum C^2 k^2 \right)}{\left( \frac{1}{4} \gamma^2 C^2 k^2 - 2\gamma^2 \right)} \]

(5.50b)

and
where

\[ K = \left( \frac{2\gamma}{qC_2M_2} \right)^{\frac{1}{2}} \]  

(5.50d)

The solutions oscillate with frequency 

\[ \omega = \omega_K = \left( \frac{2\gamma}{qM_2} \right)^{\frac{1}{2}} \]  

Periodon solutions

It can be shown that solutions analogous to the nonlinear periodic solutions (nonlinear phonons) (eqns. (5.49)) also solve the discrete equation of motion (eqns. (5.24)) exactly. Those solutions of the discrete equations of motion are called 'periodon' solutions and are given by

\[ U_n = \frac{1}{2} \left[ 1 + F_0 \sin \left( \omega t - n\omega a \right) \right] \]  

(5.51a)

\[ U_n = \frac{1}{2} + g_1 \sin \left[ \omega t - (n+\frac{1}{2})\omega a \right] + g_2 \sin \left[ \omega t - (n+\frac{1}{2})\omega a \right] \]  

(5.51b)

The amplitudes can be obtained by direct substitution of these solutions in the discrete equations of motion (eqns. (5.24)) and these are given by

\[ F_0 = \left[ \frac{\frac{8}{3} \left\{ \left( \gamma - \frac{1}{2} - \frac{M_1}{2} \omega^2 \right) \left( M_2 \omega^2 \right) - 2\gamma^2 \cos^2 \frac{\pi n}{2} \right\}} {\left( M_2 \omega^2 - 2\gamma \right)} \right] \]  

(5.52a)
$G_1 = \frac{\gamma^2 \cos \frac{\theta}{2} F_0 - 6 M_2 \omega^2 \xi_2}{(2 \gamma^2 - M_2 \omega^2)} \quad (5.52b)$

and

$G_2 = \frac{F_0^3}{4 \gamma^2 \cos \left(\frac{3 \theta}{2}\right)} \quad (5.52c)$

where the frequency

$\omega = \left(\frac{2 \gamma^2}{M_2}\right)^{1/2} \quad (5.52d)$

An unusual feature of those nonlinear periodic solutions is that the amplitudes of these solutions are function of their frequency of vibration and hence the term 'periodon' solutions.

Subbaswamy and Mills (1978) have studied a similar diatomic model with an onsite potential on $M_2$ atoms, in connection with order-disorder types of SPT. We have generalised the Hamiltonian (eqn. (5.23)) to include a single-well onsite potential in the $M_2$ species. The model Hamiltonian in this case can be written as

$H = \sum_i \left\{ \frac{1}{2} M_1 \dot{u}_i^2 + \frac{1}{2} M_2 \dot{v}_i^2 + \frac{1}{2} \gamma (u_i - u_{i-1})^2 + \frac{1}{2} \gamma' (u_i - v_i)^2 
+ V(u_i) + U(v_i) \right\} \quad (5.53)$

In the displacive regime, the continuum coupled equations of motion can be written as (see eqn. (5.29))
\[
\frac{1}{4} \gamma^2 \frac{d^2 q}{ds^2} + 2 \gamma \frac{d q}{d s} = M_1 C^2 \frac{d^2 f}{d s^2} + 2 \gamma f + \frac{d V}{d f} \\
M_2 C^2 \frac{d^2 q}{d s^2} + 2 \gamma \frac{d q}{d s} = \frac{1}{4} \gamma^2 \frac{d^2 f}{d s^2} + 2 \gamma f - \frac{d U}{d q}
\]
(5.54)

where \( U(q) \) is a single well onsite potential (on the \( M_2 \) atoms) of the form
\[
U(q) = \frac{1}{2} \kappa A q^2
\]
(5.55)

Depending on the relative strengths of the coupling \( \gamma \) and the potential \( \infty \), two distinct ground state configurations are possible. In the order-disorder regime of this model (Subbaswamy et al., 1978), the ground states are \( u = u_0 \) and \( \varphi = 0 \). On the other hand in the displacive regime, where \( \frac{\gamma^2}{A} > \frac{\infty}{2} \), the ground states are as before \( u = \varphi = \pm u_0 \), as shown below.

For particular velocity
\[
C_\beta = \left( \frac{\gamma^2 \kappa^2}{4 M_2} \right)^{\frac{1}{2}}
\]
(5.56)

where
\[
\beta = \frac{(2 \gamma + \infty A)}{2 \gamma}
\]
(5.57)

the solutions of eqn. (5.56) can be written as
\[
\left\{ c^2 \left( M_1 - \frac{M_2}{\beta^2} \right) \right\}^{\frac{1}{2}} \int \frac{df}{\sqrt{K - 2V(f) - (2\gamma - 2\gamma \beta^{-1})f^2}} = \pm s
\]

(5.58a)

and

\[
\xi(s) = \beta^{-1} \xi(s)
\]

(5.58b)

for \( M_1 \beta^2 < M_2 \). For the potential in eqn. (5.8) we can integrate eqn. (5.57a) to get the kink and antikink solutions as

\[
U(x,t) = \xi(s) = (\xi \beta)^n \left[ 1 \pm \tanh \left( \frac{n \xi \beta}{2 \beta} \right) \right]^{\frac{1}{n}} \text{ for } n = 1, 3, 5 \ldots
\]

(5.59a)

\[
= \pm (\xi \beta)^n \left[ 1 \pm \tanh \left( \frac{n \xi \beta}{2 \beta} \right) \right]^{\frac{1}{n}} \text{ for } n = 2, 4, 6 \ldots
\]

(5.59b)

for the condition

\[
B^2 = \frac{4C(A + \gamma - \gamma \beta^{-1})}{|B|}
\]

(5.60)

and where

\[
\xi = \frac{A + \gamma - \gamma \beta^{-1}}{|B|}
\]

(5.61a)

\[
\beta = \left[ \frac{c^2 \left( \frac{M_2}{\beta^2} - M_1 \right)}{\left( 2A + 2\gamma - 2\gamma \beta^{-1} \right)} \right]^{\frac{1}{2}}
\]

(5.61b)

Note that, for \( \alpha = 0, \beta = 1 \) (eqn. (5.57)) this above condition (eqn. (5.60)) for the existence of kink/antikink solutions reduces to the condition (eqn. (5.9)) for the
degenerate minima of the potential $V(f)$ (eqn. (5.8)). Also for $\alpha = 0$, these results reproduce the earlier obtained results (eqns. (5.32)).

It may however be noted that in this case the nonlinear periodic solutions (for $n=1$) of the form of eqns. (5.49a) and (5.49b) do not solve the equations of motion with an on site potential on the $M_2$ species. This is because of the presence of the cubic term in the potential for $n = 1$ case. This is in contrast to the case of $\lambda \Phi^4$ on-site potential (Henry et al., 1983), where the nonlinear periodic solutions for $\alpha = 0$ also solve the equations of motion for $\alpha \neq 0$, with an appropriate change of amplitudes.

**Conclusion**

In conclusion we summarise the main results of this Chapter. We considered the dynamics of nonlinear monatomic and diatomic chains with degenerate on site potential, which serves as a model for SPT in ferroelectrics, CDW transition etc. We have shown that the nonlinear on site potential considered by us (eqn. (5.8)) have doubly degenerate minima for $n = 1, 3, 5, \ldots$ and represent a model for first-order phase transition at $T = 0$. This is in contrast to the case where $n = 2, 4, 6, \ldots$ considered by
Magyari (1981) which represent triply degenerate minima. We have obtained kink and antikink solutions for this potential for a monatomic chain. The solutions are shown to be stable, having finite energy (shown for the case where \( n=1 \), but can easily be generalised for other values of \( n \)). The solutions resemble the domain wall solutions of K-dV like equations with higher order nonlinearity as obtained by us (see Chapter-II). The solitary wave solutions (antikink/kink) are also found for the diatomic chain for \( M_2 \rangle M_1 \) and the stability of these solutions examined. The pulse solutions for \( M_1 \rangle M_2 \) as obtained for the case of the \( \lambda \phi^4 \) onsite potential (Henry et al., 1983) does not exist here. The nonlinear-periodic and periodon solutions are also obtained for the special case of the potential where \( n=1, A=C=1, B=-2 \). These nonlinear periodic solutions represent the high energy phonons. It is also shown that the kink/antikink solutions are retained even if a single-well onsite potential of the form \( U(\phi) = \frac{1}{2} \alpha C A \phi^2 \) is included on one species of atoms along with the nonlinear onsite potential \( \nabla(\phi) \) on other species of the diatomic chain. However, in this case the solutions in the form of periodic solutions for \( \alpha = 0 \), do not satisfy the equations of motion with \( \alpha \neq 0 \). This is in contrast to the case of the \( \lambda \phi^4 \) on-site potential (Henry et al., 1983). In the
next Chapter we analyse the excitation spectrum of these kink/antikink solutions in more detail and use the results to calculate the kink impurity interaction in the chain.
References


Rajaraman, R (1982) in 'Solitons and Instantons' North Holland-Amsterdam


Shapiro, S.M.; Axe, J.D; Shirane, G and Riste, T (1972) Phys. Rev. B6, 4332

