Chapter 1

Introduction

Many processes of complex systems in condensed matter physics, optics and biological sciences can not be explained from simple linear theories [1]. The simplest but interesting example is that of a nonlinear pendulum [2]. In the exotic category, polaron motion [3–7], various ion pumps in living systems (of which proton pump is a prototypical example) [8–10], self-trapping phenomena [11–16], soliton formation in conducting polymers [17–19] (like polyacetylene), energy transport in the photosynthetic unit [20], pattern formation [21–23] and localized states (the number of which exceeds that of impurities [24–32,34]) etc. are, to say, a few examples. The richness in the behavior of systems operating in the nonlinear domain can be nicely illustrated by the simple nonlinear pendulum. Depending on the energy of the pendulum, it can go to the rotation from vibration separated by a separatrix [2]. So, it is natural than aberration that many unexplained rich behaviors of complex systems can be either explained or recovered through nonlinear theories. The nonlinearity in these systems can manifest in various forms through various interactions depending on the physics involved. It is worthwhile to mention that many nonlinear systems show transition from regular behavior to irregular (chaotic) behavior in their dynamics [35]. A simple but good example is the driven anharmonic oscillator [35]. Chaos is itself a big topic and finds tremendous application towards an understanding of the functioning of brain and heart where irregular dynamics can be controlled by applying a small electrical pulse. The nature of the pulse can be determined from the knowledge of chaotic regime and possible routes to Chaos [36].
Many simple but interesting nonlinear equations and models have been developed from time to time. The KdV and sine-Gordon (SG) equations, the Fermi-Pasta-Ulam (FPU) model, as also models based on the reaction diffusion mechanism, and the nonlinear Schrödinger equations are some of the examples [1,37] chosen here for elaboration for reasons as follows.

The KdV equation has a historical importance. The FPU and SG models deal with nonlinear lattices in condensed matter physics, the models based on the reaction diffusion mechanism are concerned with the pattern formation in chemical as well as biological systems, and the nonlinear Schrödinger equation (continuous as well as discrete version) is of great importance in condensed matter physics, optics, as well as in biological sciences.

John Scott Russell observed a smooth and well defined mass of water moving in a canal without changing its shape or dispersion. It was called a solitary wave. There was subsequently a gap of sixty years between Scott Russell’s observation and any theoretical treatment of the phenomenon. Despite some attempts by Scott Russell to guess at the analytical form of the wave profile, his observation went unexplained in his own lifetime. The initial theoretical explanation of Scott Russell’s observation had to wait till when two Dutch scientists, Kortweg and de Vries [38], derived their now famous equation for the propagation of waves in one direction on the surface of a shallow canal. If the canal has normal depth $l$ and $l + \eta$ ($\eta$ being small) represents the elevation of the surface above the bottom, the partial differential equation which governs the wave motion is:

\[
\frac{\partial \eta}{\partial t} = \frac{3}{2} \sqrt{\frac{g}{l}} \frac{\partial}{\partial x} \left( \frac{2}{3} \alpha \eta + \frac{1}{2} \eta^2 + \frac{1}{3} \sigma \frac{\partial^2 \eta}{\partial x^2} \right)
\] (1.1)

where $\sigma = l^3/3 - Tl/\rho g$, $\alpha$ is an arbitrary constant, $g$ is the gravitational constant, $T$ the surface tension and $\rho$ the density of the fluid. This is known as the Kortweg de Vries equation and usually abbreviated as KdV equation. After appropriate scalings the equation transforms to a more convenient form. Defining,

\[ \eta = 6\alpha u; \quad \xi = \left( \frac{2\alpha}{\sigma} \right)^{1/3} x; \quad \tau = \left( \frac{2\alpha^3g}{\sigma l} \right)^{1/3} t \] (1.2)

the eq. (1.1) looks as

\[ u_\tau + u_\xi + 12uu_\xi + u_{\xi\xi\xi} = 0 \] (1.3)
This nonlinear equation only could explain Scott Russell’s observation. Afterwards, Zabusky and Kruskal [39] found that when two or more KdV solitary waves collide they do not break up and disperse and therefore coined the name soliton for solitary waves. On the way of improvement of the theory, techniques like Inverse Scattering as well as Lax pair formalism came up and helped solving many nonlinear equations. References [1,37] can be consulted for further details.

One of the earliest models in field theory was the linear Klein-Gordon equation,
\[ \phi_{xx} - \phi_{tt} = m^2 \phi \]  
where \( \phi_{xx} \) and \( \phi_{tt} \) are double derivatives of the scalar field, \( \phi \), with respect to space and time respectively. \( m \) is the mass of the particle described by the scalar field, \( \phi \). Eq. (1.4) derives from the Lagrangian density:
\[ L = \frac{1}{2}(\phi_x^2 - \phi_t^2) + \frac{1}{2}m^2\phi^2 \]  
where \( \phi_x \) and \( \phi_t \) are the first derivative of \( \phi \) with respect to space and time respectively. Skyrme (1958) [40] proposed a nonlinear field theory which, for the scalar case and in one space dimension, reduces in simple terms to a nonlinear extension of the Lagrangian density. The \( \frac{1}{2}m^2\phi^2 \) term is replaced by its simple periodic extension \( \frac{1}{2}m(1 - \cos \phi)^2 \). The field equation now reduces to
\[ \phi_{xx} - \phi_{tt} = m^2 \sin \phi. \]  
This equation has subsequently become known as the sine-Gordon equation [1,37,41–43]. This nonlinear equation finds application in a number of physical systems (or reasonable approximate models). Several nice introductions to these applications are given by Barson, Esposite, Magee and Scott (1973) [44] and Scott, Chu and McLaughlin [45]. One physical model which leads to eq. (1.6) is the Frankel-Kentrova model. In this system a harmonic lattice of particles lie on a periodic potential. The \( j^{th} \) particle experiences a force,
\[ F_j = k(s_{j+1} + s_{j-1} - 2s_j) + A\sin(\frac{2\pi s_j}{\lambda}) \]  
where \( k \) is the force constant, \( \lambda \) is a constant, \( s_j \) is the location of the \( j^{th} \) particle and \( A \) is a constant. If \( m \) is the mass of each particle and we set \( \psi_i = \frac{2\pi s_i}{\lambda} \), Newton’s equations of motion of the \( j^{th} \) particle is given by
\[ m\frac{d^2\psi_j}{dt^2} = k(\psi_{j+1} + \psi_{j-1}) - T\sin(\psi_j) \]  
(1.8)
where $T = -\frac{2\pi A}{\chi}$. Now making the transition from the Lagrangian variable $\psi_j(t)$ to the Eulerian function $\psi(x, t)$ and using the scaled time $t' = \sqrt{\frac{T}{m}} t$, and the distance, so that 

\[
(\frac{\delta}{\delta t})(\psi_{j+1} + \psi_{j-1} - 2\psi_j) \rightarrow \psi_{xx},
\]

eq. (1.8) reduces to eq.(1.6). This equation gives soliton and multisoliton solutions. Some solutions are known as kink and others are known as antikink solutions. Kink and antikink solutions travel in opposite directions [41–43].

Another interesting model for nonlinear lattices is the Fermi-Pasta-Ulam (FPU) model [1,37,46]. It was presumed that the linear modes coupled by nonlinearity in nonlinear lattices share equal amount of energies among them and hence, equipartition theorem holds good for nonlinear lattices. Thus, FPU sought to investigate was not whether the system relaxes to equilibrium, but how long it takes for the relaxation to take place. To investigate the relaxation they studied the dynamics of several one dimensional lattices. The equation of motion for the displacement of the $k^{th}$ lattice point with the nearest neighbor interactions is given by

\[
\frac{d^2x_k}{dt^2} = F(x_{k+1} - x_k) - F(x_k - x_{k-1}), \quad k = 1, 2, \ldots, N
\]

(1.9)

where $x_k$ is the displacement of the $k^{th}$ particle of unit mass. They considered several forms of force, $F$, between particles. But strikingly, they found that for some cases, instead of getting distributed among all modes, the energy gets distributed only among a few modes and hence equipartition theorem does not hold good for all nonlinear systems. One of the consequences of the FPU investigation was to stimulate attempts to obtain analytical solutions for nonlinear lattice systems. A spectacular success of such searches was Toda’s discovery (1967) [47] that the rather unlikely looking potential

\[
V(r) = \frac{a}{b} \exp(-br) + ar, \quad (a \text{ and } b \text{ are constants})
\]

(1.10)
yields system of equation which can be solved exactly analytically for soliton. In Toda lattice, the equation of motion for the displacement looks like

\[
r_k'' = 2ae^{-br_k} - ae^{-br_{k+1}} - ae^{-br_{k-1}}
\]

(1.11)

The solution of this equation is given by

\[
e^{-\tau_k} - 1 = \beta^2 \text{sech}^2(\beta t + \alpha k)
\]

(1.12)
where $\beta = \pm \sinh(\alpha)$ and $\alpha$ is a constant. Large number of studies have been made on this. Furthermore, the quantum Toda lattice has become recent interest of research because it is fully solvable and it makes clear, how the low lying phonon-like modes go over to the soliton-like states [48].

We now discuss briefly about pattern formation in biological systems where nonlinearity plays an important role. The reliable development of highly complex organisms is an intriguing and fascinating problem. The genetic material is, as a rule, the same in each cell of an organism. How then do cells, under the influence of their common genes, produce spatial patterns? Simple models have been developed which describe the generation of patterns out of an initially nearly homogeneous state. They are based on nonlinear interactions of at least two chemicals and their diffusion, aptly called the reaction diffusion mechanism. There are applications to chemical reactions, animal coats and to the generation of polygonally shaped patterns. It is interesting to note that marine angelfish, pomacanthus, has stripe patterns which are not fixed in their skin. Unlike animal skin patterns, which simply enlarge proportionally during their body growth, the stripes of pomacanthus maintain the space between the lines by the continuous rearrangement of the patterns. Although the pattern alteration varies depending on the conformation of the stripes, a simulation program, based on the reaction diffusion mechanism, can correctly predict future patterns. This has sparked renewed interest in mathematical models (nonlinear) of pattern formation as well as the relationship of chemical patterns to the remarkably similar patterns observed in diverse physical and biological systems. Ref. [21–23] could be consulted for details on this.

Nonlinear dynamics has been invoked to understand the dynamics of living systems. A very good example is the understanding of proton pumps in living complex systems. Proton pumps play an important role in ATP synthesis and other biological activities, for example mobility [8–10]. It is noteworthy that the understanding of proton pumps and ATP synthesis brought two Nobel prizes. This is a vast and very active area of research and surely presents some of the greatest conceptual and analytical challenges in the field of nonlinear dynamics.

One further equation which deserves a special mention is the cubic nonlinear Schrödinger
(NLS) [49,50] equation. It takes the form

$$i \frac{\partial \phi}{\partial t} + \frac{\partial^2 \phi}{\partial x^2} + \chi |\phi|^2 \phi = 0$$

(1.13)

The name "Nonlinear Schrödinger" has been coined precisely because its structure is that of the Schrödinger equation with $\chi |\phi|^2$ acting as a potential although for most of the situations in which it occurs, it has no relation with the real Schrödinger equation other than in name. $\phi$ is a complex function and for this reason we would expect a traveling wave solution to have an oscillatory modulation. It is not difficult to show that a traveling wave solution of this equation subject to $\phi \to 0$ as $x \to \infty$ is

$$\phi = a \sqrt{\frac{2}{\chi}} \exp\left[\frac{1}{2}bx - \left(\frac{1}{4}b^2 - a^2\right)\text{sech}\left[a(x - bt)\right]\right]$$

(1.14)

where $a$ and $b$ are arbitrary constants. The sech shaped wave acts as an envelope to the oscillating part. The NLS equation plays an important role in the theory of the evolution of slowly varying wave trains, in stable weakly nonlinear systems and occurs in a whole series of physical situations including plasma physics and nonlinear optics and biology [51,52].

There exists an integrable version of discrete nonlinear Schrödinger equation, known as the Ablowitz-Ladik equation [53]. The Ablowitz-Ladik equation is given as

$$i \frac{dC_n}{dt} = -(C_{n+1} + C_{n-1}) - \lambda |C_n|^2 (C_{n+1} + C_{n-1}).$$

(1.15)

where $\lambda$ is a constant and $C_n$ is a complex function. This set of equations has infinite number of constants of motion and has been solved exactly by Ablowitz and Ladik using the Inverse Scattering technique [53]. But this integrable form of discretization does not occur in most of physically motivated models. Its importance lies in its yielding a solitonic solution. This equation has been further generalized and studied. For example, the set of equations considered by Bishop et al. [54] are given by

$$i \dot{C}_n = -(C_{n+1} + C_{n-1}) - [\mu (C_{n+1} + C_{n-1}) + 2 \nu C_n] |C_n|^2$$

(1.16)

where $n$ is the site index, and $\mu \geq 0$, $\nu$ are constants. Basically a nonintegrable term was added to the integrable Ablowitz-Ladik equation. The general properties of the localized states with an emphasis on the interplay of integrability and nonintegrability, discreteness,
and the continuum limit has been discussed. A particular set of localized solutions that have staggered form, i.e., the neighboring sites oscillates out of phase, has been studied thoroughly. These localized states arises only due to the discreteness. It does not have any counter part in the continuum limit. Takeno et al. [55] considered random site energy (diagonal) term to A-L equation, and showed how the solitonic profile can get destroyed as the width of the random site energy increases. On the other hand Vekhnenko and Gaididei [58] developed a perturbation theory for solitons using the Ablowitz Ladik equation as an unperturbed part. Within this framework, they also studied the dynamics of the intermolecular excitations interacting with acoustic phonons in a discrete molecular chain. They found soliton dynamics and also observed that the motion of the center of mass of the soliton is equivalent to the motion of the effective particle in a periodic potential with period equal to the lattice constant. Their findings have exact analogy with the dynamics of the simple nonlinear pendulam. Afterwards, the above mentioned perturbation theory with A-L equation as the unperturbed part was used to investigate analytically the intrinsic localized modes and its motion in the one dimensional anharmonic lattices [59]. Intrinsic localized modes are the vibrational localized modes [60,61] which appear in a perfect nonlinear lattice preserving the translational symmetry.

Direct discretization of the nonlinear Schrödinger equation given in eq. (1.13) is called discrete nonlinear Schrödinger equation and takes the form

\[ \frac{dC_n}{dt} = \epsilon_n C_n + V(C_{n+1} + C_{n-1}) + \chi |C_n|^2 C_n \]  

This set of equations can also be viewed as that describing the dynamics of an exciton in discrete geometries. It can be derived under the tight binding formalism. This set of equations or slightly modified form has been used thoroughly in different branches of science [11–16, 20, 62–72, 75–78]. \( C_n \) represents the probability amplitude of the exciton to stay at the \( n^{th} \) site of the system. This can be understood from the fact that the system described by this set of equations has a constant of motion given by \( \sum |C_n|^2 = \) const. \( V \) is the nearest neighbor hopping element. The nonlinear term in the equation originates from the physical fact that the exciton interacts with the lattice vibration. \( \chi \) is the interaction strength parameter. The equation is derived within an approximation, namely, the adiabatic approximation. It physically means that the oscillators are much
faster in motion compared to that of the exciton. The lattice oscillators are assumed to be Einstein oscillators and purely harmonic. The discrete nonlinear schrödinger equation has been used in Holstein model for describing polaronic motion in solids [3], in Davydov model for transport of vibrational energy in proteins [51], in model for nonlinear optical responses of superlattices [77] and models for nonlinear arrays of coupled wave guides [78]. This equation has also been used to model the energy transfer in photosynthetic unit [20]. The self-trapping is an interesting property of this equation. By self-trapping we mean the clustering of electronic probability on a single lattice site in solid state context and the trapping of power in a single wave guide in the context of optics problem. Because of the self trapping property, it has also been named as the discrete self trapping (DST) equation [12,14,79,80]. This will be discussed in detail in chapter 2.

One other important feature of the DNLSE is that this can yield stationary localized (SL) states. This is intricately related to the discretization and the consequent nonintegrability of the DNLSE [33]. To understand this we note that the continuous nonlinear Schrödinger equation is integrable and it yields soliton, multisoliton and multisoliton bound states [50]. The soliton solution of the DNLSE has also been investigated by a perturbative method [58,59]. The starting point of the approach is the Ablowitz-Ladik equation [53] which is discrete but integrable. It has been shown that from the DNLSE soliton in the form of a kink can be obtained under restrictive conditions. But mostly the solution has the center of mass of the soliton executing oscillatory motion [59]. This is due to the nonintegrability of the DNLSE. In the limit of small oscillation one obtains SL states. In other words, SL states are low energy excitations in the system described by the DNLSE in the quasicontinuum limit. On the other hand, stronger discretization destroys moving soliton altogether [59]. Hence SL states are the most prominent solutions of the equation. In the presence of gliding forces like applied electric field the SL state in the quasicontinuum limit can go to the finite oscillation state and finally to the moving soliton phase [33]. Hence the study of SL states is important for understanding transport properties of conducting polymers like trans-polyacetylene. The SL states might also play a relevant role in the nonlinear DNA dynamics [81] and in the energy localization in nonlinear lattices [54].

It is well known that localized states appear in linear systems due to static impurities
These linear impurities may be thought of different atoms present in a perfect lattice. The formation of localized states due to single, double and many linear impurities are studied in detail [82]. But the same due to the presence of nonlinear impurities are not well studied so far. It is also known that transport properties of a system is directly related to the existence of localized states therein. Again the kind of nonlinearity described in eq. (1.17) has its physical origin. But the lattice oscillators are assumed to be purely harmonic. On the other hand anharmonicity is also known to exist in physical systems and contributes to several phenomenon, e.g., thermal expansion, structural phase transition etc. So, it is necessary to consider a general kind of nonlinearity which takes care of both the harmonicity as well as the anharmonicity of the lattice sites. Taking this into account, one arrives at the general power law nonlinear Schrödinger equation given by

$$i\frac{dC_n}{dt} = \epsilon_n C_n + V(C_{n+1} + C_{n-1}) + \chi|C_n|^\sigma C_n.$$  

(1.18)

If $\sigma = 2$, the lattice oscillators are purely harmonic. Here $\chi$ is the nonlinear strength and $\sigma$ is the power of the nonlinearity. Different values of $\sigma$ represents lattice oscillators in different form of potential. Therefore, it is essential to study the formation of SL states due to the presence of power law nonlinear impurities in the linear systems. The appearance of stationary localized states (bound states) due to a single nonlinear impurity with $\sigma = 2$ was studied in one dimensional chain [26,34]. The nonlinear eigenvalue problem was treated fully analytically [107] through the Green’s function technique. It was found that there exists a critical value of the nonlinear strength ($\chi$) equal to 2 below which no bound state can appear whereas one bound state appears above that critical value. This is in contrast to the linear eigenvalue problem. The transmission [34, 73] due to a nonlinear impurity is always greater than that of the linear impurity. The density of states shows the formation of a discrete state for $\chi > 2$ at the expense of the continuous spectrum of the linear system. Below the critical value of $\chi$ the density of states remains unaffected even though the transmission decreases as the nonlinear strength increases. Then question arises, what happens due to the presence of a symmetric nonlinear dimer in an one dimensional perfect linear chain. The idea is that the impurities act as monomers if the nonlinear sites of the dimer are far apart in the chain. Thus, the critical value to get
a bound state will remain same as in the case of monomer. Furthermore, from Green’s function analysis it was found that one more bound state appears above a critical value of \( \chi \) approximately equal to 3.6 [34]. Then the arbitrary \( \sigma \) was also considered. But only the effect of a single power law nonlinear impurity in a one dimensional chain has been studied. An appropriate ansatz for the bound state was considered in this system. The ansatz for bound states due to a single impurity follows from the fact that the states in one dimension gets exponentially localized. Green’s function analysis can also be exploited to support the ansatz [30]. The phase diagram for stationary localized states due to a single power law nonlinear impurity embedded in an otherwise perfect linear lattice is also presented. This will appear again in chapter 3 as a special case of the problem we consider. The formation of SL states due to single nonlinear impurity has been studied in one, two as well as three dimensions [26–29, 34]. But for a full understanding of the formation of SL states due to nonlinear impurities, it is essential to study the formation of SL states due to various kinds of nonlinear impurities in various kinds of linear lattices. In our study, we consider two kinds of nonlinearities, namely, power law nonlinearity and rotational nonlinearity (see ref. [83]) respectively. Hosts that we consider are the one dimensional chain and the Cayley tree [84]. The reason behind the consideration of the Cayley tree as a linear host is to see the effect of connectivity on the formation of SL states. In other words we try to understand the effect of nonlinear impurities on the formation of SL states in one dimensional chain as well as the Cayley tree [25,30–32]. The SL states in translationally invariant nonlinear system has been investigated earlier but the study remained partial [85]. We, therefore, have taken up the system and recovered few more new possible SL states [24]. The fully nonlinear Cayley tree is also considered for the investigation of SL states [31]. For real systems it is possible that the exciton does not interact with all the lattice oscillators with equal strength. This introduces the inhomogeneity in the nonlinear system. For the simplest case we have considered a doubly periodic, fully nonlinear, one dimensional system.

In chapter 3 we consider the formation of SL states due to a single rotational as well as power law nonlinear impurity embedded in a Cayley tree, a symmetric rotational as well as power law nonlinear dimer embedded in a linear perfect chain. A model derivation of the generalized as well as the rotational nonlinear impurity is also presented in this
chapter [30].

In chapter 4 we complete the study of the formation of SL states in one dimensional chain due to a symmetric power law nonlinear dimer embedded in an otherwise perfect linear chain. The full phase diagram for SL states is presented here. We also study the effect of the asymmetric nonlinear dimer embedded in an otherwise perfect linear chain, on the formation of SL states [25,31].

The symmetric as well as asymmetric power law nonlinear dimer embedded in the Cayley tree is considered in chapter 5 to study the formation of SL states. A transformation is devised which reduces the Cayley tree into a one dimensional chain and makes the study easier [31,32].

The fully nonlinear systems are considered in chapter 6 to study the formation of SL states. Perfect as well as disordered nonlinear systems are studied and some discussions on the stability of the SL states are made in this chapter [24,31,32].

Finally, in chapter 7 we conclude about all of our findings.