A Discussion of Research Activities With Delineation of Future Projects.

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I. INTRODUCTION

My research encompasses three seemingly different fields in Theoretical Physics. These are namely, (1) localization - delocalization of eigenstates in one-dimensional correlated disordered systems, (2) transport properties of conducting polymers, and (3) the study of systems, describable by discrete nonlinear Schrödinger equation (DNLSE) or by its standard variants, which include Ablowitz-Ladik nonlinear equation, modified Salerno equation (MSE) etc. These fields are, however, not as disparate or disjoint as it might appear. Their relationship and the logical follow up from one field to the other will be evident in the following discussion.

II. LOCALIZATION-DELOCALIZATION OF EIGENSTATES

We know that while perfect system is a phenomenon, impurity is the reality. Again, it is equally well known that transport and optical properties are directly related to the existence of localized states in the system. So, the study of formation of localized states due to linear as well as nonlinear impurities is an important and also an active area of research even today, in spite of its successful beginning in the late fifties by P. W. Anderson[1–3]. We note that in perfect systems, all states are extended, while localized states appear due to the presence of impurities in the system. Furthermore, according to Anderson's theorem, almost all eigenstates of one-dimensional linear disordered systems are exponentially localized.

Almost thirty years later in 1989 since the inception of the field, I in collaboration with Prof. D. H. Dunlap and Prof. P. Phillips wrote a very important paper in this field of localization of eigenstates. This paper appeared in Physical Review B[4]. We showed that in one-dimensional correlated disordered systems, it is indeed possible to have extended states without contradicting the basics of Anderson's theorem on localization. These extended states may give rise to anamoly in the transport properties of the system. This work subsequently gave birth to the now famous Random Dimer Model (RDM)[5, 6]. However, after the work of Dunlap, Wu and Phillips on RDM was published in 1990, an acrimonious controversy ensued. Consequently, my work on RDM and on one-dimensional extended correlated systems with my collaborators, Dr. P. K. Datta and Dr. D. Giri became extremely significant. We proved beyond doubt the merit and authenticity of the basic premises of

the RDM[7, 8]. Thereafter, we showed by studying the symmetric random trimer model (SRTM) that the merging of resonances can increase the width of the non-scattered states in one-dimensional correlated disordered systems. This paper, to our merits, is the first paper where the effect of resonance merging is studied . Another interesting fall out of this model is that it substantiates beyond any doubt by its own unambiguous scaling behavior of nonscattered states , the scaling behavior of nonscattered states in RDM[9, 10]. Furthermore, in these works, we introduced a simple but novel method for "Bandwidth Scaling Analysis". My this series of papers is so novel and so accurate in numerical analysis in liaison appropriate analytical approach , that these papers are used as bench-mark examples to study other related problems numerically. The third work in this category formulates this problem using the invariant measure method. This is the most natural linear extension of the field. For this purpose, the work of Bovier and Klein[11, 12] needed to be generalized. Obviously, the interest was to study one-dimensional extended correlated disordered systems analytically within the perturbation framework. This work appeared in J. Phys. A [13], and its abstract also appeared in Mathematical Review.

III. CONDUCTING POLYMERS

My second field of research deals with conducting polymers. The material importance of the field can be gauged from the vast literature it generated[14–18]. It is a field which synthesizes physics, chemistry, mathematics, and material science. In this field, we took interest in polythiophene (PT) and polyaniline (PAN). Both are exciting by their own merits. The basic aim was to understand the mechanism triggering the insulator to metal transition in these systems. There are two prominent schools of thought. One school thinks that the mechanism can be understood by considering these as archetype example of one-dimensional correlated disordered systems. The founding stone for this thought is the work of Wu and Phillips on polyaniline[19, 20]. Another school thinks that the transition occurs due to the spontaneous formation of a polaron lattice[18]. My work with Dr. Giri on PT reveals two interesting facets. In a published work in Phys. Rev. B , we showed that if the electron-lattice interaction is allowed to alter the site energies of the electron[21], the correlated disordered system model may not stand the scrutiny[22]. In another published work in J. Chem. Phys., it is shown that the boundary condition may play a crucial role in the

understanding of the mechanism[23].

In the case of polyaniline, Dr. Giri and I performed an extensive AM1 calculation to understand the structure of the neutral system as well as the system containing either a bipolaronic or a polaronic defect. The basic aim of the work was to understand comprehensively the reason, if any, for the formation of the polaron lattice. This work favors the polaron lattice theory. A part of the work is published in Theo. Chem. My other collaborators in this work were Dr. D. Majumdar and Prof. S. P. Bhattacharya of Indian association for The Cultivation of Science, Calcutta[24].

IV. DISCRETE NONLINEAR SCHRÖDINGER EQUATION

A. Small Polarons and Holstein Models

In continuation, we consider now another interesting as well as important aspect of physics of particle-phonon interaction [25–27]. Particles, like electron or quasiparticles like exciton and vibron can interact with phonon. This gives rise to another dressed quasiparticle, called polaron, as mentioned in the context of conducting polymers. Again, when the coupling with phonon increases, the polaron radius decreases and becomes of the order of the lattice constant of the crystal. Then, all momenta of the Brillouin zone contribute to the polaron wave function and the effective mass approximation cannot be applied. This regime occurs if the characteristic potential energy, E_p due to the local lattice deformation is comparable to or larger than the half bandwidth, D of the crystal. The strong coupling regime of the particle-phonon interaction with the dimensionless coupling constant, $\lambda = \frac{E_p}{D} \gg 1$ is called a small polaron.

The main features of the small polaron are revealed quite accurately in the simplest Holstein model consisting of only two vibrating molecular sites with a particle hopping between them. Even in this simple model, we can have two different situations, namely (i) nonadiabatic small polaron and (ii) adiabatic small polaron. In the first case, the lattice dynamics is significantly faster than the particle dynamics. In the second case, the situation is reversed. In both cases, hopping gets significantly reduced due to the interaction with phonon. In the language of effective mass, in the small polaron limit (SP), the effective mass of SP, m^* enhances exponentially as a function of the particle-phonon interaction parameter.

Furthermore, expectedly in the nonadiabatic limit, this mass enhancement of SP is larger than it is in the adiabatic limit. We note that in the zeroth order approximation, a crystal in the strong particle-phonon coupling limit can be considered a set of two level Holstein problem.

B. Many Small Polarons and Lang-Firsov Transformation

Consider now a many particle interacting system, interacting with one another and also with phonons in the system. Particles are assumed to hop from a site to another in the lattice. Consider again the strong coupling regime of particle-phonon interaction, $\lambda \rightarrow \infty$. In this limit, one can use the well known Lang-Firsov canonical transformation to partially diagonalize the relevant Hamiltonian[25, 28, 29]. This diagonalization is exact in the limit of no hopping or $\lambda = \infty$. We further note that the Lang-Firsov transformation is the displacement transformation for the multi-polaron system shifting ions to the new equilibrium positions. In a more general sense, it changes the boson vacuum. In the transformed Hamiltonian, both the hopping and the polaron-polaron interaction become dependent on phonon variables. Furthermore, the transformed Hamiltonian in zero order of hopping describes localized polarons and independent phonons which are vibration of ions relative to new equilibrium positions depending on the polaron occupation numbers.

When this transformed hopping term is averaged over the equilibrium phonon distribution, it shows dependence on the temperature as well as on phonon frequencies. In this order, we have a model in which a single Holstein polaron hops from a site to another with this averaged hopping. Of course, we also have the residual polaron-phonon interaction, described by H_{p-ph} and polaron-polaron interaction, H_{p-p}. In the limit of $\lambda \rightarrow \infty$, these extra terms in the total Hamiltonian give polaron band broadening, renormalization of phonon frequencies and scattering of polarons. The term, H_{p-ph} also gives negative contribution to the polaron self energy. So, the polaron energy is lowered and its effective mass increases.

C. Nonadiabatic Small polarons

We further note that there are systems in which the tunneling of the quasiparticle is inherently slow. A good example is this regard is the hopping of vibrons in α-helical pro-

teins. Of course, the application of Lang-Firsov transformations in this type of systems is reasonable. Also, increase in the temperature and/or the softening of phonons in the system can lead to extreme slowing down of the hopping. This situation can arise in high T_c oxides, in molecular solids like naphthalene, anthracene (in the crystallographic c′ direction) and in many biological systems having proton transport and energy transport. So, we can have systems having dynamics in the nonadiabatic limit. Consequently, the small polaron bandwidth will be smaller than the average phonon frequency. At high temperature, of course, polaron bandwidth will be quite narrow. Then, the prominent event will be the scattering of polarons by two phonons and multiphonons processes. This incoherent processes will lead to the thermally activated hopping of polarons from one localized state to another localized state. The dynamics can be described by a Master equation. On the other hand, if the temperature is not too high, scattering of polaron by two phonons and multiphonon processes can be ignored. So, there can be a coherent tunneling of polarons, even though the system is in the nonadiabatic limit. On the other hand, the self energy effect from H_{p-ph} and H_{p-p} will tend to trap the polarons.

This aspect is also nicely described by Holstein[30]. We already mentioned that the Lang-Firsov transformation is an exact transformation, and it makes the tunneling term in the tight binding formalism dependent on phonon variables. From the transformed Hamiltonian, it can be seen that there are possibilities of diagonal and nondiagonal tunneling of polarons, depending on the scattering of polarons by phonons. However, depending on the system, there will be a critical temperature below which coherent tunneling will be the dominant mode of transport. This is the regime which is of interest in my present research.

D. Alternative Approaches

This regime of transport of small polarons or transport below the critical can be treated classically in spite of the coherent nature of the tunneling. So, alternative descriptions of this dynamics, basing on discrete nonlinear Schrödinger equation (DNLSE) or its variants like Ablowitz-Ladik equation and Salerno equation, have emerged[31, 32]. In these descriptions, it is a single particle dynamics in the spirit of Hatree formalism[33]. The hopping is described by the usual tunneling of a small polaron. Mostly, nearest-neighbor hopping is considered. In a reasonable picture, two types of phonons are considered. One set of phonons dresses

the particle to form small polarons. The other set, being soft phonons, is treated classically by considering harmonic or anharmonic lattice vibrations. In quantum mechanical terms, this set of phonons are treated in the coherent state formalism. The lattice vibration is assumed to alter the site energy, or the hopping, or both. This causes the coupling of two dynamics. Since, the dynamics is in the nonadiabatic limit, the solution of the lattice dynamics is possible by ignoring the inertia of the elastic subsystems[34–36]. Its subsequent incorporation into the particle dynamics then leads to desired nonlinear equations. One such equation is, of course DNLSE. DNLSE is also a non-integrable standard discretization of the continuous integrable nonlinear Schrödinger equation[35]. A broader discrete nonlinear equation is obtained when the lattice dynamics is allowed to alter both the tunneling and site-energies. The following discussion is in the context of DNLSE.

V. SYSTEMS HAVING NONLINEAR IMPURITIES

When such strong interaction exists in domains, we get systems having domains of nonlinear impurities. Again, if we have anharmonic vibrations, we can have nonlinear impurities having power law structure[37]. These systems should also produce stationary localized states and in one-dimensional systems, these states should be exponentially localized. In this field, in my work in collaboration with Dr. B. C. Gupta, I considered first a one-dimensional perfect systems with two juxtaposed nonlinear impurities with power law structure. The power is denoted by a parameter σ. The strength of these impurities is denoted by χ_i $i = 1, 2$. It is found that this system has both stable and unstable stationary localized states. Furthermore, the phase diagram of stationary localized states in the $\chi - \sigma$ plane is found to be very rich, showing different regions containing different number of localized states. The maximum number of localized states is found to be six. In linear systems, we cannot have more than two localized states. Again, these are stable eigenstates. These results are published in Phys. Rev. B and Phys. Lett. A[38–40]. In another work, albeit not yet published, the effect of separation between two nonlinear impurities on the number of localized states is investigated[41].

Since, the standard DNLSE has same type of nonlinearity at all sites, it has the translational invariance. We note that linear systems with translational invariance does not produce any localized state. But, due to the nonlinearity, it can produce self-localized stationary

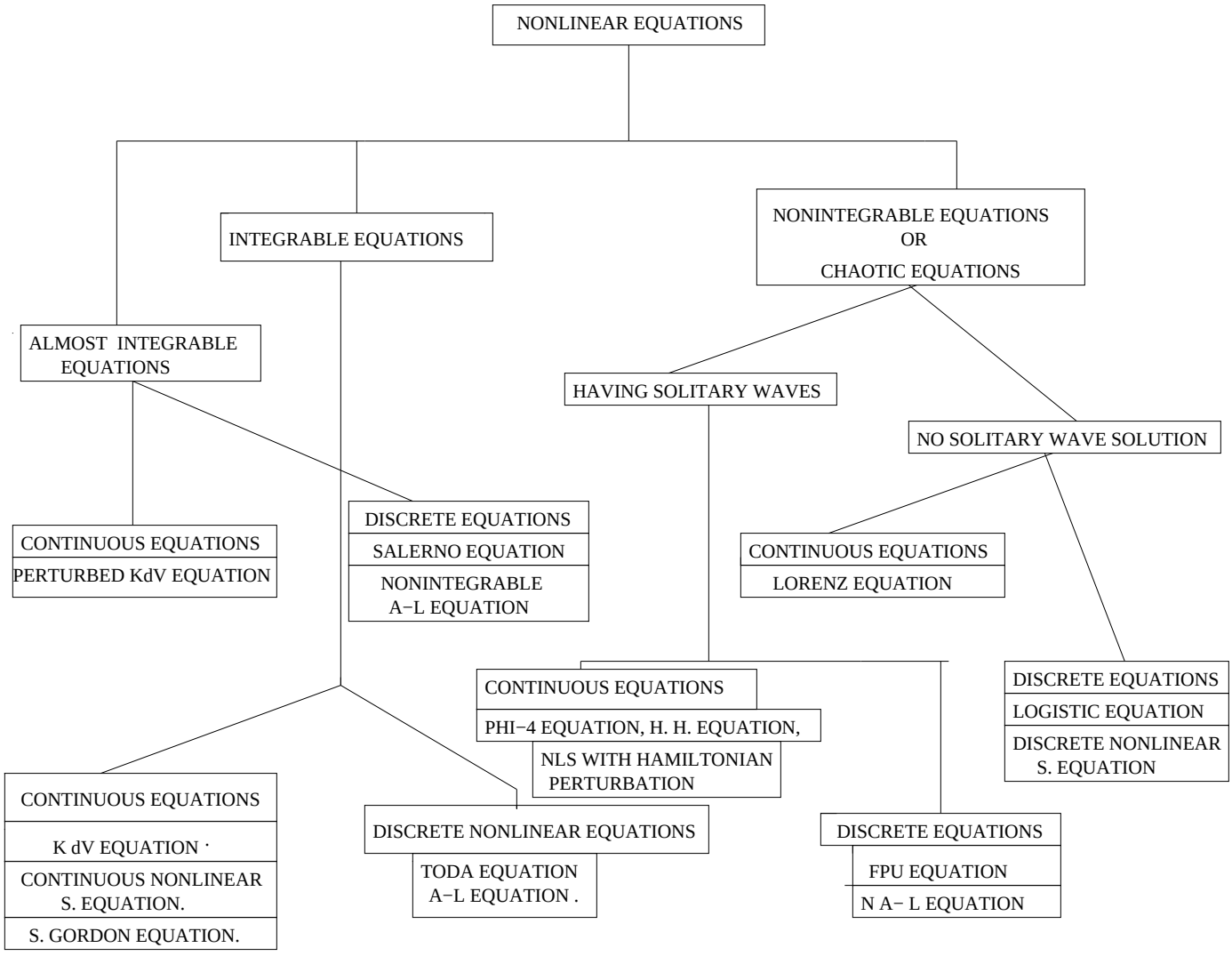
states or breathers. Breathers are spatially localized time periodic solutions of nonlinear equations[42–47]. It is further to be noted that the formation of breathers is enhanced by discreteness and lattice periodicity. As the type of breathers, that is investigated both in Cayley tree and in one dimensional system is stationary localized states of the system, these breathers are called trivial breathers. The formation of breathers is investigated using the mean field formalism. Importantly, for the Cayley tree an ingenious transformation is developed to transform the problem to an effective one dimensional problem with an extra bond (hopping) defect[48]. In this work, my collaborators were Dr. B. C. Gupta, and Mr. Ananda Mohan Ghosh. These works are published in J. Phys.: Condensed Matter[49] and in Eur. Phys. J. B [49].

VI. ALMOST INTEGRABLE NONLINEAR EQUATIONS

Nonlinear equations constitute a very big as well as a very important field of mathematics, with inherent application in in physical and biophysical problems. A not so precise flow chart of nonlinear equations is given here for better understanding of subsequent discussion. We note that "H. H. Equation" in this chart means the famouse "Hodgkin-Huxley equation".

Integrable nonlinear equations with single soliton and multisolitons solutions constitute a very rich facet, albeit not the only one, of nonlinear dynamics[31, 50]. These integrable equations can either be continuous or discrete. In the first category, we have the famous Korteweg-de Vries (KdV) equation. Another important examples are continuous nonlinear Schrödinger equation (CNLSE) and the famous Sine-Gordon (s-G) equation. In the other category, famous examples include Toda equation[51] and Ablowitz-Ladik equation[52]. We note in this context that Ablowitz-Ladik equation describes a Hamiltonian system with dynamics described by noncanonical variables[50]. However, a global transformation exists, which takes these noncanonical variables to canonical variables[53]. In case of integrable equations, there are two types of solitons. solitons that are formed due to acute balance between dispersion and nonlinearity are called dynamical solitons. Kdv solitons are dynamical solitons. On the other hand, solitons formed from the competition between nonlinearity and constraints arising arising topological invariants are called topological solitons. Kink and anti-kink solutions of s-G equation are examples of topological solitons [54, 55].

There is again a class of nonlinear equations that is as such not integrable, but in some



way similar to one of the known integrable equations. In other words, in the small perturbation limit, these equations are covered by KAM theorem [55]. A good example is Salerno equation[56]. In such a situation, soliton dynamics can be studied by one or the other prescribed perturbation methods[34]. So, one of my projects was to study soliton dynamics perturbatively of nonlinear equations that can arise in soft molecular chains due to interaction of excitation with acoustic phonon[36]. Soliton in soft molecular chains arising from above mechanism is generally referred to as Davydov's soliton. Soliton mechanisms have been proposed also in a number of biomolecular and molecular processes. One good example in the biological area is the attempt to explain the structural and dynamical flexibility of DNA by a soliton mechanism . However, most well studied of all is the problem of storage and transport of biological energy by Davydov's soliton in α-helical proteins. One of my

works in this field is the perturbative analysis of soliton dynamics. This has appeared in Phys. Rev. E[36]. The abstract of the paper is given below.

A. Abstract of the paper, Phys. Rev. E, 61, 5839 (2000)

Classical Ablowitz-Ladik type soliton dynamics from three closely related classical nonlinear equations is studied using a perturbative method. Model non-integrable equations are derived by assuming nearest neighbor hopping of an exciton(vibron) in the presence of a full exciton(vibron)-phonon interaction in soft molecular chains in general and spines of α-helices in particular. In all cases, both trapped and moving solitons are found implying activation energy barrier for propagating solitons. Analysis further shows that staggered and nearly staggered trapped solitons will have a negative effective mass. In some models the exciton(vibron)-phonon coupling affects the hopping. For these models, when the conservation of probability is taken into account, only propagating solitons with a broad profile are found to be acceptable solutions. Of course, for the soliton to be a physically meaningful entity, total nonlinear coupling strength should exceed a critical value. On the basis of the result, a plausible modification in the mechanism for biological energy transport involving conformational change in α-helix is proposed. Future directions of the work are also mentioned.

VII. A NEW CLASS OF NON-INTEGRABLE DISCRETE NONLINEAR EQUATIONS, HAVING SOLITARY WAVES

While working on this problem, I realized that a thorough mathematical analysis of a related nonlinear equation will be useful. This led me to propose a discrete nonlinear equation, which I called "N-AL" (nonintegrable Ablowitz-Ladik) equation. To understand the utility of this equation, I mention the following points.

One important field of study in nonlinear nonintegrable equations is whether or not solitary wave like solutions can exist in these equations. So, consider the NLS with an additional Hamiltonian perturbation that models a nonlinear interaction between Langmuir waves and electrons in plasma. It constitutes an interesting example of a continuous nonlinear nonintegrable equation, which can have solitary waves as well as periodic solutions, and

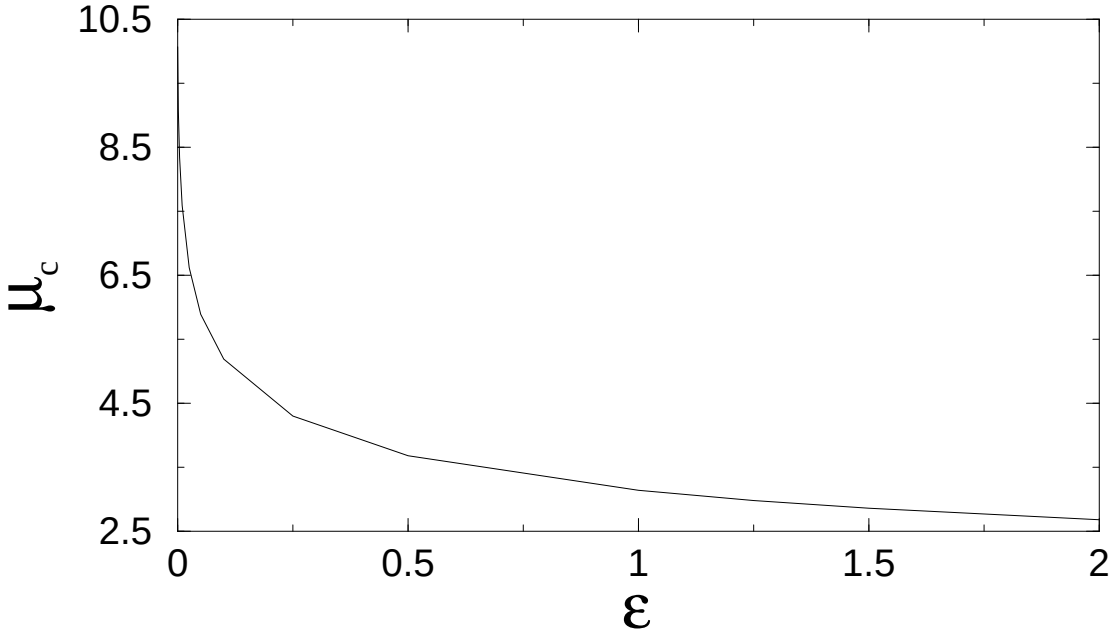


FIG. 1: This figure pertains to modified Salerno equation (MSE). It shows the dependence of the critical value of μ, $\mu_{\rm c}$ on the parameter, ϵ, which measures the strength of the nonintegrability term in MSE. Both $\mu_{\rm c}$ and ϵ are dimensionless. Ref. Phys. Rev. E, **61**, 5839 (2000).

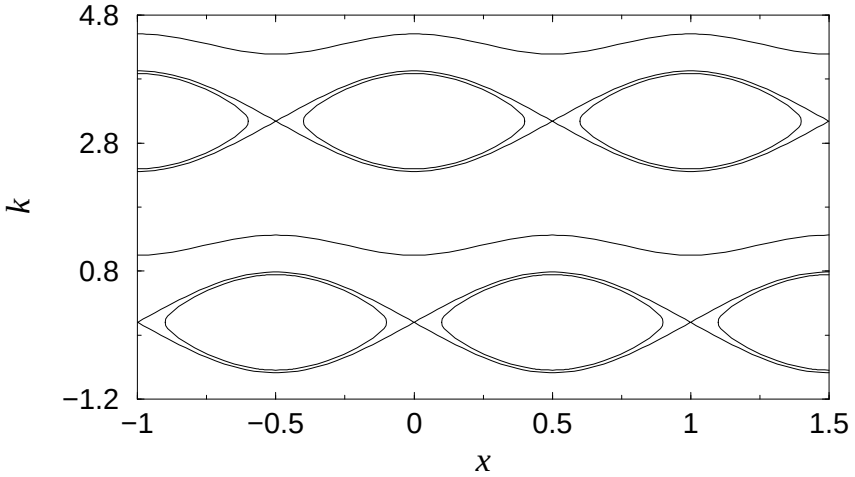


FIG. 2: Thess figures pertains to MSE, showing the dynamics of solitons in the (x, k) plane. $\epsilon = 1.0$, and $\mu_{\rm c} = \pi$. Since, $k_{\rm cr} = \frac{\pi}{4}$ as a choice, $\mu = 2.052$. So, $\mu < \mu_{\rm c}$. Ref. Phys. Rev. E, **61**, 5839 (2000).

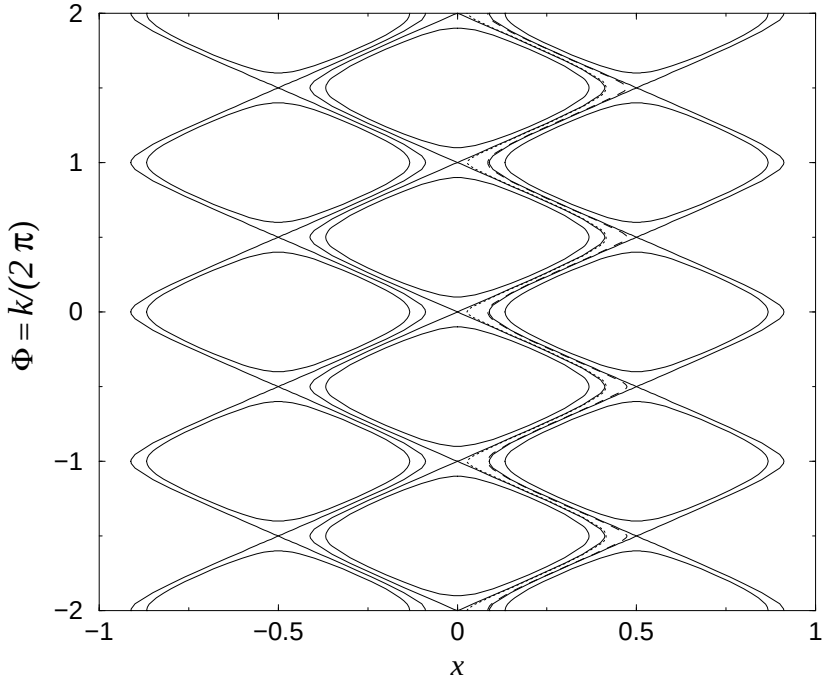


FIG. 3: This figure also pertains to MSE. However, for this figure $\mu = 3.2 > \mu_c$. Here $k = 2\pi\Phi$ to make the figure symmetrical. Two propagating modes in the Φ-direction are shown by broken curves. Again, all quantities are dimensionless. Ref. Phys. Rev. E, **61**, 5839 (2000).

recurrence. It is further observed by numerical analysis of the nonlinear equation that recurrence depends sensitively on initial conditions[57]. Contrary to the common belief, there are also nonintegrable discrete systems which possess exact solitary waves. Indeed, there is an existence theorem also[58].

The N-AL equation, that I proposed and studied to a certain extent, is an extended nonintegrable version of the ALDNLSE(Ablowitz-Ladik discrete nonlinear Scrödinger equation), which has a "tunable" nonlinearity in the intersite hopping term. At the same time, the form of nonlinearity is such that it can allow solitary wave like solutions. It is to be noted that my

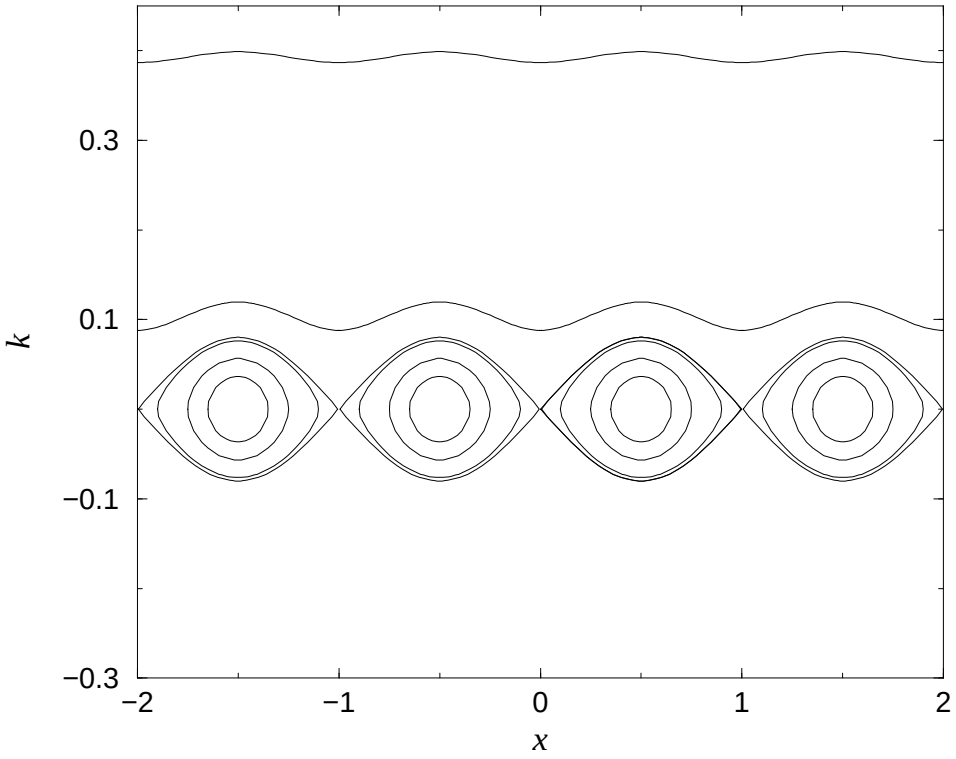


FIG. 4: This figure pertains to the model with sole off-diagonal coupling. It shows the phase diagram of the dynamics of solitons for in the x direction but for c = 1.2. $\mu_s = \sinh^{-1}(c) = 1.016$. All quantities are dimensionless. Ref. Phys. Rev. E, **61**, 5839 (2000).

case is not covered by the existence theorem, that I have already mentioned. Inasmuch as this nonlinearity is in the intersite hopping term, it serves two important purposes. First of all, this extra dispersive correction to the ALDNLSE will try to destroy the Ablowitz-Ladik (A-L) soliton by dispersion. So, by varying this term we can investigate the effect of dispersive imbalance on the maintenance of the moving solitonic profile. It is relevant at this point to note that both the IN-DNLS (describe later) and the MSE (modified Salerno Equation, a discrete nonlinear equation, that I also proposed) investigate the competition between the on-site trapping and the solitonic motion of the A-L solitons. In case of the MSE, it is found that the narrow A-L solitons, having width smaller than the critical width will get

pinned by the lattice potential[34, 36]. Similar results are obtained numerically from the IN-DNLS[53]. Secondly, since the extra dispersive term in the proposed equation breaks the integrability of the ALDNLSE, the dynamics of the A-L solitons will not be transparent to the lattice discreteness. So, along with the IN-DNLS and the MSE, this model also gives an opportunity to study further the effect of Peierls-Nabarro (PN) potential on the dynamics of solitons[53, 59]. My this work has appeared in J. Phys. A [60]. The abstract is given below.

A. Abstract of the paper, J. Phys. A : Math. Gen. 35, 8109-8133 (2002)

Schrödinger Hamiltonians with tunable nonlinearities is introduced, which includes the integrable Ablowitz-Ladik system as a limit. A new subset of equations, which are derived from these Hamiltonians using a generalized definition of Poisson brackets, and collectively referred to as the N-AL equation, is studied. The symmetry properties of the equation are discussed. These equations are shown to possess propagating localized solutions, having the continuous translational symmetry of the one-soliton solution of the Ablowitz-Ladik nonlinear Schrödinger equation. The N-AL systems are shown to be suitable to study the combined effect of the dynamical imbalance of nonlinearity and dispersion and the Peierls-Nabarro potential, arising from the lattice discreteness, on the propagating solitary wave like profiles. A perturbative analysis shows that the N-AL systems can have discrete breather solutions, due to the presence of saddle center bifurcations in phase portraits. The unstaggered localized states are shown to have positive effective mass. On the other hand, large width but small amplitude staggered localized states have negative effective mass. The collision dynamics of two colliding solitary wave profiles are studied numerically. Notwithstanding colliding solitary wave profiles are seen to exhibit nontrivial nonsolitonic interactions, certain universal features are observed in the collision dynamics. Future scopes of this work and possible applications of the N-AL systems are discussed.

VIII. FURTHER STUDIES ON BREATHERS

The study of energy localization in nonlinear lattices has become an important field of research in nonlinear dynamics in the past couple of decades[61]. In this context, the subject

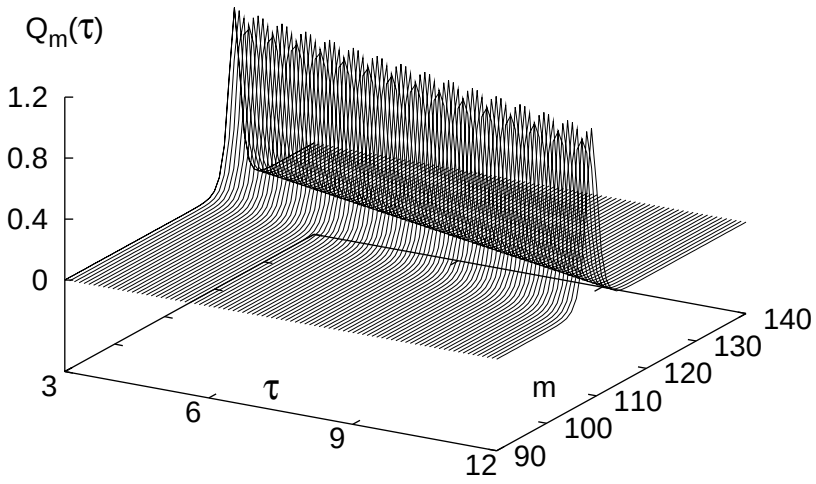


FIG. 5: The N-AL dynamics of an initial Ablowitz-Ladik soliton with $k = -\frac{3\pi}{4}$, Eq.(2.5). Furthermore, $l = 2$, $g_1 = 0.0$, $g_2 = 0.5$ and $\mu = 1.0$. The number of sites in the chain is 257 and the origin is taken at the center of the chain. Ref. J. Phys. A : Math. Gen. **35**, 8109-8133 (2002).

of intrinsic localized modes (ILM) has drawn a considerable attention as it offers appealing insights into a variety of problems ranging from the nonexponential energy relaxation[62] in solids, to the local denaturation of DNA double strands[63]. The subject is also an intense field of study in material science, and nonlinear optic applications[64, 65]. We note that ILMs can be formed in translationally invariant systems, and for this to happen, nonlinearity plays a crucial role.

There are two broad classes of intrinsic localizations in (1 + 1) dimensional nonlinear systems[66]. Shape preserving localized excitations are called dynamical solitons[31, 54, 55]. Breathers belong to the second category of ILM in nonlinear systems[54, 66]. Breathers are spatially localized time periodic solutions of nonlinear equations. They are characterized by internal oscillations[54, 66]. Again, by breathers we usually imply stationary localized excitations in nonlinear systems. However, under appropriate conditions, nonlinear systems may have moving breathers[54]. We again note that the formation of breathers is aided by lattice discreteness and lattice periodicity.

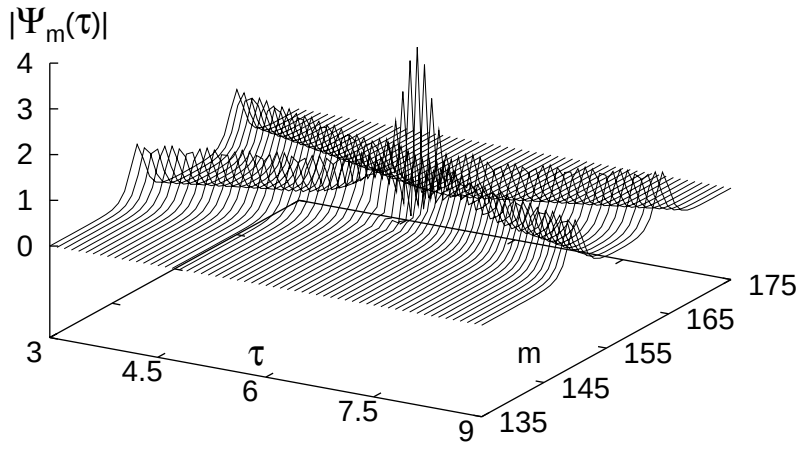


FIG. 6: The N-AL collision dynamics of two initial A-L pulses. $k_2 = -k_1 = \frac{\pi}{2}$. $l = 1$, $g_1 = 0.5$ and $\mu = 1.0$ as mentioned in the paper, J. Phys. A : Math. Gen. **35** 8109 (2002). The number of sites in the chain is 313 and the origin is taken at the middle of the chain.

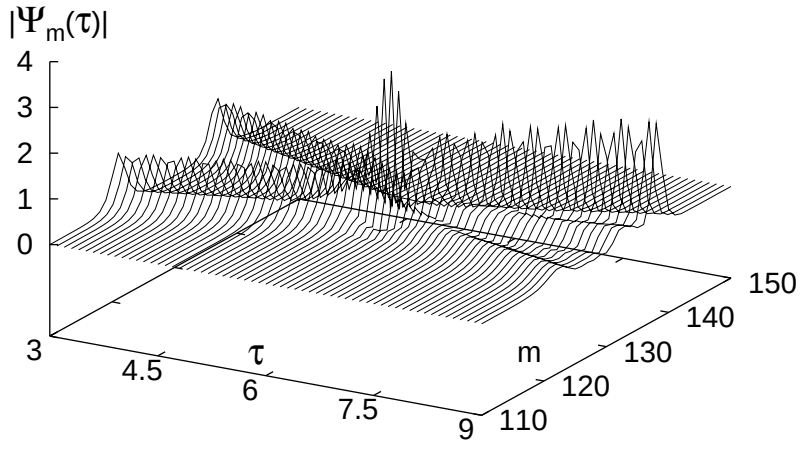


FIG. 7: The N-AL collision dynamics of two initial A-L pulses. $k_2 = -k_1 = \frac{\pi}{2}$. $l = 1$, $g_1 = 0.5$ and $\mu = 1.0$ as mentioned in the paper, J. Phys. A : Math. Gen. **35** 8109 (2002). The number of sites in the chain is 313 and the origin is taken at the middle of the chain.

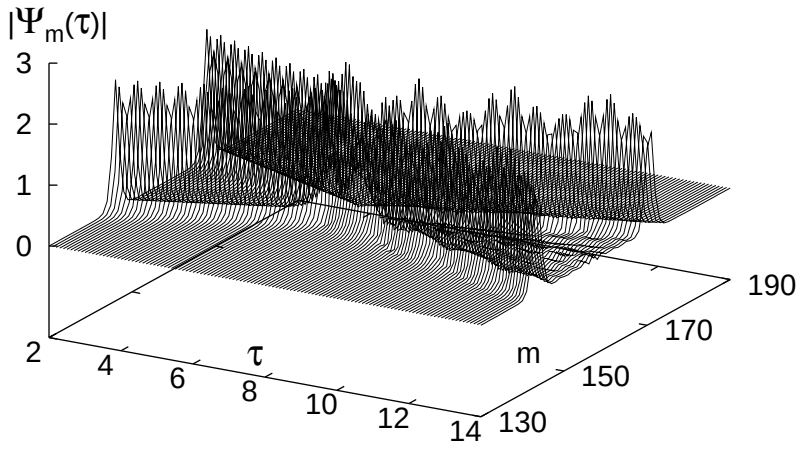


FIG. 8: The N-AL collision dynamics of two initial A-L pulses. $k_2 = -k_1 = \frac{3\pi}{4}$. $l = 2$, $g_1 = 0.0$, $g_2 = 0.5$ and $\mu = 1.5$ as mentioned in the above paper. The number of sites in the chain is 313 and the origin is taken at the middle of the chain. Ref. J. Phys. A : Math. Gen. **35** 8109 (2002).

IN-DNLS is a discrete nonlinear Schrödinger equation with tunable nonlinearity. In one extreme, it reduces to the integrable A-L equation and in the opposite limit, it is DNLSE. As this discrete equation is non-integrable in its general form, it is expected to form breathers. Though some studies were made in this direction, a systematic study of formation of breathers for systems described by this nonlinear equation was required. So, I studied this problem using discrete variational formulation. In this approach, we used the static form of A-L soliton, which is a breather as the ansatz. It is a very reasonable choice. Furthermore, in stead using Lagrangian for the formulation, it is shown that the standard Sturm-Liouville variational approach can be used to find the appropriate functional. A detailed analysis is presented in the following paper by me[67]. The abstract is given below.

A. Abstract of the paper, nlin.PS/0403060, International Journal of Mathematics and Mathematical Sciences, Vol. 2005, No. 4, 20 April 2005.

IN-DNLS, considered here is a countable infinite set of coupled one dimensional nonlinear ordinary differential difference equations with a tunable nonlinearity parameter, ν. This equation is continuous in time and discrete in space with lattice translational invariance and has global gauge invariance. When $\nu = 0$, it reduces to the famous integrable Ablowitz - Ladik (AL) equation. Otherwise it is nonintegrable. The formation of unstaggered and staggered stationary localized states (SLS) in IN-DNLS is studied here using discrete variational method. The appropriate functional is derived and its equivalence to the effective Lagrangian is established. From the physical consideration, the ansatz of SLS is assumed to have the functional form of stationary soliton of AL equation. So, the ansatz contains three optimizable parameters, defining width (β^{-1}), maximum amplitude and its position ($\sqrt{\Psi}$, x_0). Four possible situations are considered. An unstaggered SLS can be either on-site peaked ($x_0 = 0.0$) or inter-site peaked ($x_0 = 0.5$). On the other hand, a staggered SLS can be either Sievers-Takeno (ST) like mode ($x_0 = 0.0$), or Page(P) like mode ($x_0 = 0.5$). It is shown here that unstable SLS arises due to incomplete consideration of the problem. In the exact calculation, there exists no unstable mode. The width of an unstaggered SLS of either type decreases with increasing $\nu > 0$. Furthermore, on-site peaked state is found to be energetically stable. These results are explained using the effective mass picture. For the staggered SLS, the existence of ST like mode and P like mode is shown to be a fundamental property of a system, described by IN-DNLS. Their properties are also investigated. For large width and small amplitude SLS, the known asymptotic result for the amplitude is obtained. Further scope and possible extensions of this work are discussed.

IX. FUTURE PROJECTS

A. Further Study of N-AL Equation

Integrable nonlinear equations are characterized by their soliton and multisoliton solutions. Solitons also preserve their shape under collision. In that respect, solitons are like particles. Again, in the transport phenomena of energy, excitation, mass etc. solitons provide a nondispersive and nondissipative mechanism for transport[47, 68]. However, formation of

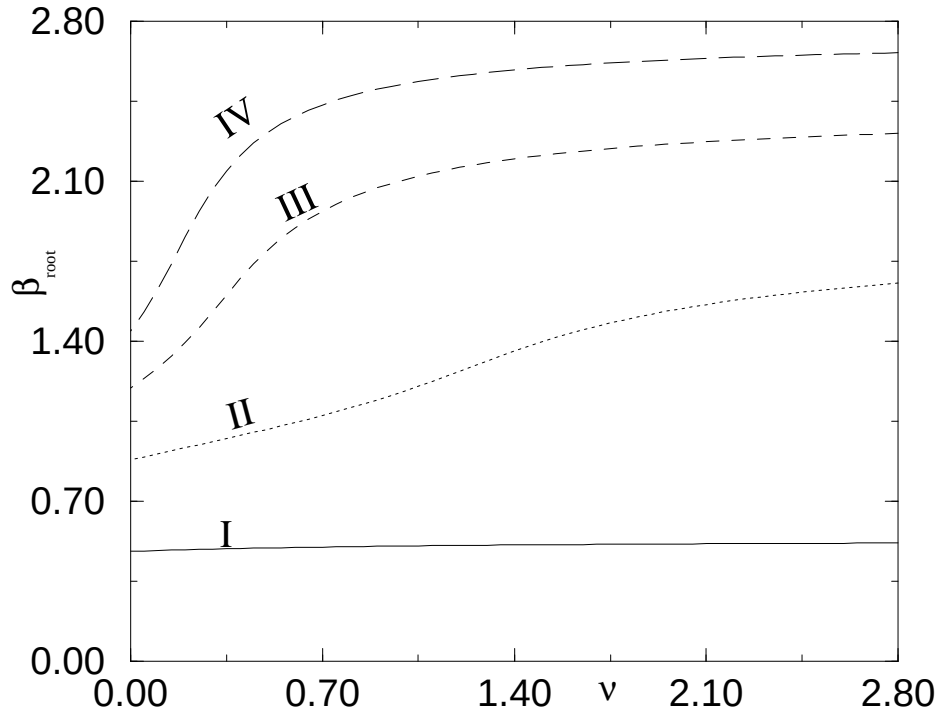


FIG. 9: This figure shows the variation of $\beta_{\rm root}$ as a function of the nonintegrability parameter, ν for various values of the parameter, a. It is obtained from the exact calculation. For this figure, $\tilde{\rm H}_0 = \text{constant},\ x_0 = 0.0,\ \text{and}\ \lambda = 1$. Curve I : $a = 0.5$, Curve II : $a = 1.0$, Curve III : $a = 1.5$, and Curve IV : $a = 2.0$. Ref. nlin.PS/0403060.

solitons in a physical system requires highly coherent dynamics of relevant dynamical variables of the system. Hence, in any physical system, occurrence of true solitons is not very likely. Take, for example KdV equation and KdV solitons. KdV solitons are obtained by assuming that the localized wave has small amplitude and large width. So, when it is said that transport in a physical system occurs by a soliton mechanism, implicitly or explicitly a time scale is attached. It means that below that time scale, the mechanism can be approximated by transport of solitons. So, if the relevant experimental time scale smaller than this time scale, we can talk of soliton mechanism.

On the other hand, solitary waves can be found in nonintegrable nonlinear equations[60]. Solitary waves are unstable under collision, and aloso produce fractal structure in the collision region[60, 69]. So, formation of solitary waves requires less constraint on the coherence of relevant dynamical variables. Now, if in a physical system scattering of solitary waves is not an important phenomenon, soliton mechanism, replaced by solitary wave can also

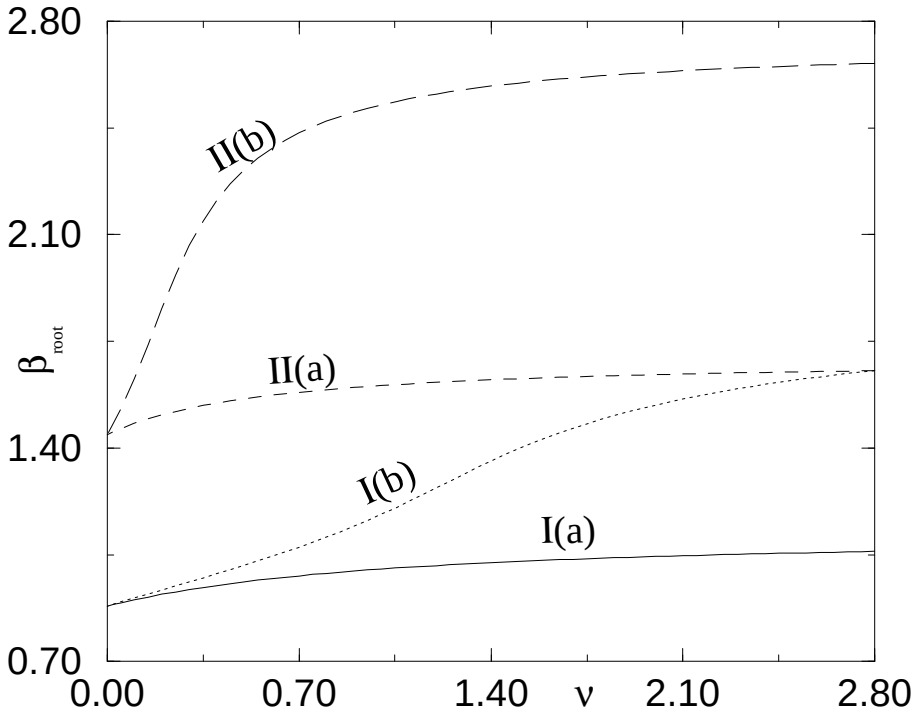


FIG. 10: This figure shows the variation of $\beta_{\rm root}$ as a function of the nonintegrability parameter, ν for two positive values of the parameter, a. This figure presents the exact solution for $\lambda = 1$. For Curves I(a) and I(b) $a = 1$, but $x_0 = 0.5$ and 0.0 respectively. For Curves II(a) and II(b) $a = 2.0$, but $x_0 = 0.5$ and 0.0 respectively. Ref. nlin.PS/0403060.

provide a nondispersive nondissipative mechanism for transport. In this context then, N-AL equation assumes much significance. Furthermore, I plan to give efforts to find other nonlinear equation, continuous as well as discrete to add to our understanding of nonlinear dynamics.

The existence of breathers in N-AL equation is found in my analysis[60]. So, a thorough analysis of breather formation in this equation is an important problem. Again, this equation, when studied for soliton solutions by perturbative methods, shows homoclinic orbits in the phase portrait. This indicates that the system may show chaotic dynamics[60]. As it describes a hamiltonian system, the bifurcation seen in the phase portrait as a function of the coupling parameter indicates destruction of one or more integral of motions. Since, the existence of a particular integral of motion is due to a certain symmetry of a system, a chaotic regime may emerge when the symmetry pattern of the system is changed[55]. In relation to "N-AL" equation, this is another aspect which I plan to pursue in the future.

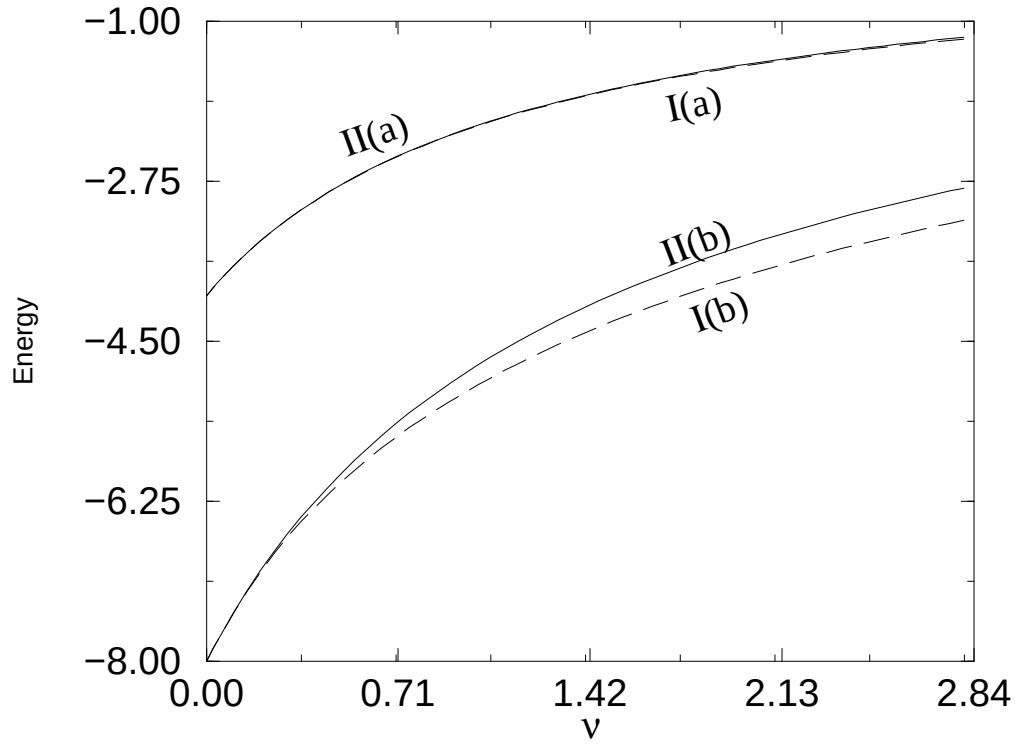


FIG. 11: This figure shows the variation of the energy of unstaggered stationary localized states as a function of ν for two values of a and for two permissible values of x_0. Of course, the result is obtained from the exact calculation with $\tilde{\mathrm{H}}_0$ = constant. For Curves I(a) and II(a) $a = 1.0$, but $x_0 = 0.0$ and 0.5 respectively. For Curves I(b) and II(b) $a = 2.0$, but $x_0 = 0.0$ and 0.5 respectively. Ref. nlin.PS/0403060.

Dynamics in nonlinear systems can also be effected by disorder and by stochastic forces. Therefore, the study of the effect of diagonal and off diagonal disorder also of stochastic forces on solitons and solitary waves and also on breathers constitute another important field of study. Some futurestudies in this direction with N-AL and IN-DNLS are also present in my scheme of things.

As I mentioned earlier that breathers can be formed in nonlinear Hamiltonian systems, described by discrete nonlinear equations, which show band structure in the linear domain[67]. Though breathers are stationary solutions, they can be made mobile by perturbation[70]. Furthermore, breather-breather interaction can also alter the transport properties of a system. In my plan of things, I would like to investigate these features of breathers, obtained from IN-DNLS, MSE and N-AL. Note that in all these equations there is a soliton stabiliz-

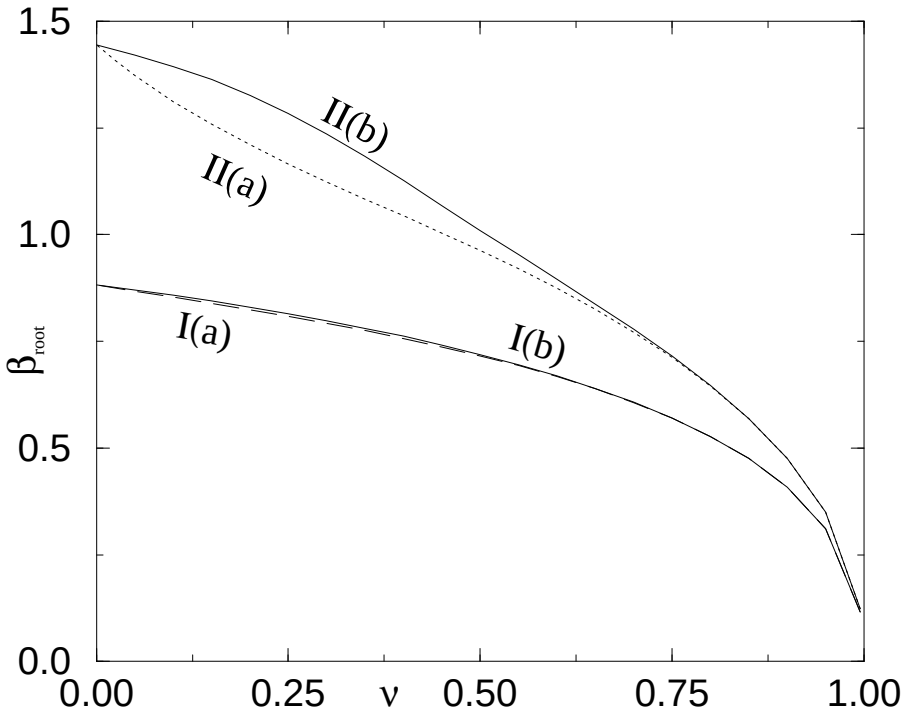


FIG. 12: This figure shows the variation of $\beta_{\rm root}$ as a function of the nonintegrability parameter, ν for $a = 1.0$ and 2.0, as obtained from the exact calculation. Since, $\lambda = -1$, these states are staggered stationary localized states. Curve I(a) : $a = 1.0$, and $x_0 = 0.0$. Curve II(a) : $a = 2.0$, and $x_0 = 0.0$. Curve I(b) : $a = 1.0$, and $x_0 = 0.5$. Curve II(b) : $a = 2.0$, and $x_0 = 0.5$. Ref. nlin.PS/0403060.

ing term. So, the structure of breathers, particularly trivial breathers may show structural stability in their transport under perturbation.

B. Soliton Transport in Molecular Solids

The prospect of field-effect transistors, FETs, made of easily processible thin organic films has stimulated considerable research effort. The most successful devices to date have been made of oligomeric rather than polymeric material, an outstanding one being α-sexithiophene, α-6T. The field-effect mobility of hole polarons in α-6T, measured in thin film transistors, can be well fitted by Holstein's small polaron theory[71]. The small polaron theory is also used to explain the mobilities of photoinjected electrons in Naphthalene[29]. Again, to explain almost-temperature-independent mobility above 100K for electrons in an-

thracene, naphthalene and in As_2S_3, Frölich large polaron theory is also developed. This theory is also reasonably successful[72].

We note that the bandwidth in the crystallographic c′ axis of these compounds is very narrow. So, the solitonic conduction along this axis can be investigated using the appropriate version of DNLSE[73]. It is going to be one of my major projects in future.

X. BIOLOGY AND NONLINEAR DYNAMICS

A rich domain of nonlinear dynamics is biology[74, 75]. In biology, we can find almost all possible nonlinear dynamics, starting from simple attracting fixed points to chaotic dynamics. The first important contribution to mathematical biology comes in 1952 from Hodgkin and Huxley[31]. They looked into the problem of electrical signal propagation on nerve axon of the giant squid[74]. In this context, they proposed effectively a fourth order nonlinear partial differential equation, which nicely modeled the problem. It is, however to be understood that in spite of its success, the Hodgkin-Huxley model is a mathematical model rather than a mathematical theory.

Another important field is the field of bioenergetics. Glycolysis, H^+-pumps and many other pumps like $Na^+ - K^+$- pumps, Ca^{+2}-pumps play very important roles in our biological activities. Glycolysis is shown to have oscillatory behavior and many studies have been done on this aspect of glycolysis. In general, the study of various oscillatory chemical reactions, though a very well-treaded field can still offer important insights into many biological phenomena. As I did some work on this in the context of H^+-pump, I am always fascinated by oscillatory chemical reactions. Definitely, I would like to study some aspects of those as when it appears appropriate.

An important as well as interesting problem in biology is the replication of DNA[76]. As DNA is a very complicated biological molecule, the problem at first sight appears hopeless. However, it is to be understood that not all degrees of freedom of DNA take part in the process. When the relevant degrees of freedom are properly understood and taken into account, the problem comes within the tractable regime[76]. Consider in this context Bishop-Peyrard model[63]. This is a very simple model. Still it is quite effectively in predicting DNA melting. In my subsequent studies, I plan to study this equation and its possible variants to understand relevant physical and biophysical problems. Consequently, higher order models

in the field DNA melting and transcription will be studied[76, 77].

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