Artificial Intelligence and Complex Dynamical Systems

Notes that are being progressively updated and follow approximately the Lecture plan

---

G. P. Tsironis
Department of Physics, Harvard University

9 May 2022

Contents

Introduction

Artificial Intelligence (AI) combines cognition with computers and makes autonomous dynamics possible. Complex Systems (CS) are hard to study yet comprise a realm that is both fundamental and useful. The combination of the two, i.e. AI and CS will lead perhaps to interesting scientific and practical developments in the years to come.

Artificial Intelligence

The advances on AI in the last decades are astonishing and they seem to have changed completely our way of living. From cell phones to banks, to security to social interactions, AI seems to play an increasing role to daily lives of billions of people around the world. On the other hand, it does no seem to have yet penetrated science in a similar profound way. Using Machine Learning (ML) in physics is relatively recent and certainly it does not appear to have blossomed yet. Why would one want to apply ML in physics? There are various levels to the answer of this question. Machine learning may provide methods for handling physical systems that are superior to traditional computational techniques. Having the code *learn* about the system instead of simply *modeling* the physical system of interest may led to serious simplifications in the actual representation of the physical system of interest. On a more fundamental level one may ask whether the system can actually modify itself through the (machine) learning process and acquire new features. This Darwinian-like approach is not unlike the mode of thinking, although much simper one, that we dedicate for nonlinear complex systems.

Complex systems

Ii is not very easy to define a ”complex system” since it depends also on the features we are focusing in. Is a piece of metal a complex system? If we look into the microscopic details of the metal we find that it comprises of a large number of atoms and its physical properties stem from the complicated dynamics of the constituent atoms and electrons. The detailed understanding of theses properties involves advanced theoretical and computational methods and many approximations. Yet, if we take this piece of metal and cut it in two halves, these two parts will retain essentially all properties of the original piece. Many of the functions of the metal do no depend on this process of halving; for instance if we use the metal as a wire, cutting in have does not change this feature.

Consider now a biological macromolecule such as a protein; it is also made of a large-yet not as large as the metal-number of atoms. The protein has many different physical and chemical properties that can be analyzed and understood through exact or approximate methods. These methods may be quite complicated, involved and cumbersome, but in many ways are similar to the methodology we apply to the metal. Yet, there is a significant difference with the metal, viz. the protein has a specific function within the cell. In fact the workings of the cell depends on the function of the proteins it includes. If we cut the protein in half, the protein ceases to function and through it the organization of the cell may become problematic. This property, viz. the loss of functionality when drastic changes are introduced characterizes complex systems as well as distinguishes them from the rest. The distinction is neither sharp nor well defined but nevertheless it easy to see when we encounter it. Although biology furnishes the archetypical complex systems, physical systems can also be complex. It appears that a necessary condition for complexity is the presence of some form of nonlinearity usually in the dynamical equations of motion. In fact, complex systems arise from nonlinear systems.

Nonlinear systems

Nonlinearity is ubiquitus in science and it would seem at first superfluous to reserve the term for an entire area of study. On the other hand, mathematical techniques that are based on linearity are so powerful and indeed useful that many times tend to overshadow and hide the role of nonlinearity. Linear algebra and linear differential equations are the ”bread and butter” of modern science and engineering. At the same time, Quantum Physics, the powerful intellectual creation of the twentieth century is "linear". If Quantum Mechanics that describes all physical processes in the world is linear, what is the reason to invoke "nonlinearity"? The answer is two fold. On one hand, linearity on the level of partial differential equations (pde's), such as the Schrödinger equation may hide nonlinearity at a different level expressed for instance through ordinary differential equations (ode's). This is particularly true when we consider interacting systems and a reduced representation where some, perhaps not so relevant, aspects of the problem are eliminated. The apparent linearity of the microscopic world and the Schrödinger equation may be transformed to nonlinearity at a more intermediate, "mesoscopic" level of description where multiple interactions are taken into account. In an simplistic form we may state that "Nonlinear = Linear + Mesoscopic".

Integrability and chaos

In this work we focus primarily on sets of differential equations, ode's and pde's. Integrability refers to the possibility of expressing the solutions of differential equations in terms of known functions. For example, in the case of the harmonic oscillator we have a second order linear ode that can be solved through trigonometric functions. This system is clearly *integrable*. In other cases the system is nonintegrable; for instance the famous Lorenz model:

$$\frac{dx}{dt} = \sigma(y - x) \tag{1}$$

$$\frac{dy}{dt} = x(\rho - y) - y \tag{2}$$

$$\frac{dz}{dt} = xy - \beta z \tag{3}$$

where $x,\ y,\ z$ are dynamic variables that depend on time t and $\sigma,\ \rho, \beta$ are system parameters. Edward Lorenz introduced this system in 1963 as a simplified model for meteorology and he showed that the system is *chaotic*. This means that the set of equations (1, 2,3) is nonintegrable, i.e. cannot be solved in terms of known functions. Furthermore, there is *sensitive dependence on initial conditions*, i.e. if we change slightly the initial state, the system wonders around in a completely different part of its state space. In chaotic systems the divergence of initially nearby trajectories takes place usually exponentially fast with a rate determined by the largest Lyapunov

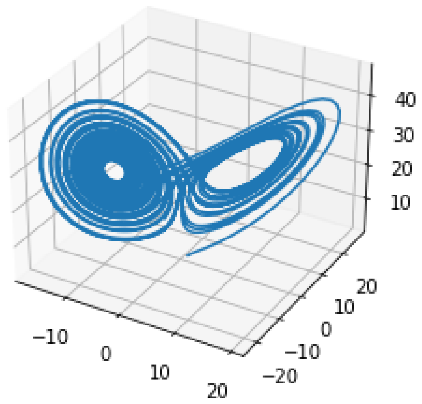

Figure 1: The Lorenz (strange) attractor is a surface with fractal Hausdorff dimension equal to 2.0627160, i.e. it slightly larger than 2. A trajectory that on this attractor moves continuously between the two lobes without a predictable character. In this figure $\rho = 28.0$, $\sigma = 10.0$ and $\beta = 8.0/3.0$

exponent. The Lorenz system generates for some parameters a *chaotic attractor*, i.e. a surface with a fractional dimension that has the shape of a butterfly and is called the *Lorenz attractor.* The shape is related the sensitive dependence on initial conditions and presented as the *Butterfly effect* where the flapping of the wings of a butterfly in Australia can change the weather and its prediction in ...Boston!

Chaotic systems are in many ways similar to stochastic systems where future evolution can be predicted only in a statistical sense. One interesting question for chaotic dynamical systems is thus the possibility to use machine learning in order to obtain a picture of their future evolution. In fact if ML can give a better forecasting horizon in problems such as weather prediction, a paradigmatic chaotic and complex problem, then its usefulness will prove to be significant in science as well.

Discrete Nonlinear Schrödinger Equation

The Discrete Nonlinear Schrödinger (DNLS) equation is a fundamental nonlinear equation that appears in many areas of physics. It is *discrete*, meaning mathematically that it comprises of multiple coupled ordinary differential equations. It is also *nonlinear*, with a specific type of nonlinearity and thus makes it a significant candidate equation for the study of complex systems with ML. It is also related to the *Schrödinger* equation, making it a significant equation for the study of fundamental processes although its scope goes much beyond these. In particular, the DNLS equation is a discrete version of the famous, continuous Nonlinear Schrödinger (NLS) that is one of the main pillars of Nonlinear Science. The NLS equation is one of the few fully integral nonlinear pde's that exist. We can apply the DNLS equation in at least three areas of physics, viz. condensed matter physics, optics and Bose-Einstein condensates (BEC). In condensed matter physics it models the propagation of an electron or, more generally an excitation, in a "discrete" medium consisting of atoms or molecules while the nonlinear term takes effectively into account the exciton-phonon interaction. In optics it describes photon propagation in coupled nonlinear fibers while in BEC systems the mesoscopic dynamics of the condensate. The form of the DNLS equation we will be using is the following:

$$i\hbar\frac{d\psi_n}{dt} = \epsilon_n\psi_n + V(\psi_{n+1} + \psi_{n-1}) - \chi_n|\psi_n|^2\psi_n \tag{4}$$

In the condensed matter interpretation we may think of an excitation that is hopping in a one-dimensional lattice with nearest neighbor interaction term V. The local site energy in each site is ϵ_n; this refers to a single energy state available for the excitation in each molecule where it moves. The basic unknown quantity $\psi_n \equiv \psi_n(t)$ is the probability amplitude to find the excitation at a given lattice site n. If the nonlinear parameter χ_n was equal to zero for all sites n, then Eq. (4) is nothing but the Schrödinger equation in the tight-binding approximation. For non-zero χ_n the DNLS equation becomes nonlinear and acquires entirely new properties that stem from the cubic nonlinear term.

The DNLS equation is fundamental in the understanding of complex nonlinear systems as it encompasses essentially all effects that stem from nonlinearity. For one and two degrees of freedom is integrable, for few degrees of freedom is chaotic while for very large, "infinite" degrees of freedom becomes integrable again in the form of the continuous NLS. In the intermediate range of many degrees of freedom we find both order and disorder. Order appears in the form of discrete breathers (of intrinsic localized modes) while disorder as spatiotemporal complexity. The study of the DNLS equation is both very interesting and exciting as its results apply in many areas of physics. Implementing machine learning methods to the DNLS equation and other nonlinear systems provides a new frontier for nonlinear science. We hope to learn how far we can go in the understanding of complexity with

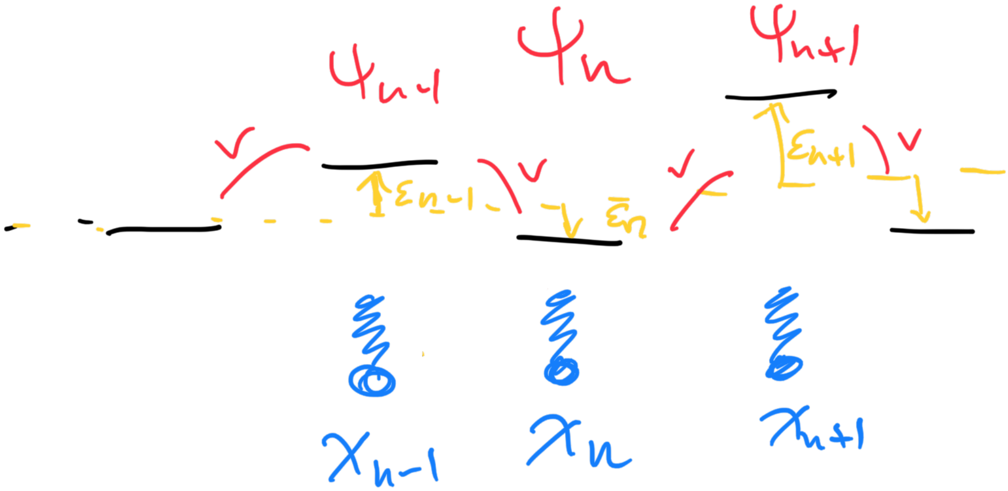

Figure 2: An excitation hopping from site to site with nearest neighbor matrix elements V, local site energies ϵ_n, and nonlinearity parameter χ_n.

these knowledge-based methods.

Chapter 1

Discrete Nonlinear Schrödinger Equation

The Discrete Nonlinear Schrödinger Equation (DNLS) or the Discrete Self-Trapping Equation (DST) and describes properties of chemical, condensed matter as well as optical or condensed systems where selftrapping mechanisms are present. These mechanisms arise either from strong interaction with the environment or genuine nonlinear properties of the medium. The DNLS equation was introduced in order to describe the dynamics of a set of coupled nonlinear anharmonic oscillators and understand nonlinear localization phenomena.[1] It can also be viewed as an equation describing the motion of a quantum mechanical particle interacting strongly with vibrations.[2] As noted in the Introduction, if $\psi_n(t)$ denotes the probability amplitude for the particle to be at site n at time t,the DNLS equation reads:

$$i\frac{d\psi_n}{dt} = \epsilon_n\psi_n + V(\psi_{n-1} + \psi_{n+1}) - \chi_n|\psi_n|^2\psi_n \tag{1.1}$$

where ϵ_n designates the local energies at cite n of a one dimensional crystal, V is the nearest-neighbor wavefunction overlap and χ_n is the nonlinearity parameter that is related to the local interaction of the particle with other degrees of freedom of the medium. For simplicity we will take $\hbar = 1$. We will start by considering a lattice where the nonlinearity is homogeneous throughout the system, viz. $\chi_n \equiv \chi$. This assumption will be lifted when need be.

An infinite, discrete set of equations, such as the one of the DNLS equation, is viewed in two different ways, either as a discretization of a corresponding continuous field equation, or an equation describing dynamics in discrete geometries. In the case of DNLS, the corresponding continuous field equation is the celebrated Nonlinear Schrödinger Equation. The present exposition will take the point of view that the DNLS equation represents dynamics in a discrete one dimensional lattice. We will therefore not relate properties of DNLS with the corresponding continuous NLS equation except when we discuss infinite degrees of freedom.

The DNLS equation has a long history; in its time independent form was first obtained by Holstein in his study of the polaron problem [3]. Subsequently derived in a fully time-dependent form by Davydov in his studies of energy transfer in proteins and other biological materials [4, 5, 6, 7]. Eilbeck, Lomdahl and Scott [1, 8, 9, 10] studied DNLS as a Hamiltonian system of classical oscillators, focussed on analytical and perturbative results and showed that bifurcations occur in the space of stationary states for different values of the nonlinearity parameter. These bifurcations in the discrete set of equations are associated with the nonlinearity induced selftrapping described by DNLS. In order to understand the dynamical properties of DNLS solutions, Kenkre, Campbell and Tsironis studied extensively the nonlinear dimer, the smallest nontrivial DNLS unit[2, 11, 12]. The latter proved to be completely integrable and from its complete solution a number of interesting properties of selftrapping were obtained. Additionally, the effects of nonlinearity on a variety of physical observables were studied leading to predictions for possible experiments [13, 14, 15].

In this first part of the exposition we will discuss some of the general properties of the discrete nonlinear Schrödinger equation both in small finite systems but also in longer extended chains. We will focus primarily to dynamical aspects of the DNLS solutions. These properties are pertinent to applications of DNLS in condensed matter physics as well as optics.

1.1 Motivation

We will now motivate a “derivation” of the DNLS equation in a condensed matter context. We start with the Hamiltonian:

$$\begin{aligned} H &= (K/2)\sum_n u_n^2 + (1/2)M\sum_n (du_n/dt)^2 + \sum_n \epsilon_n |n><n| \\ &\quad -J\sum_n [|n+1><n| + |n><n+1|] - A\sum_n u_n |n><n| \end{aligned} \tag{1.2}$$

This Hamiltonian represents an excitation moving in a one-dimensional crystal while interacting with local (Einstein-type) oscillators. In Eq. (1.2)

ϵ_n represents the local site energy at site n, J gives the magnitude of the wavefunction overlaps of neighboring sites, $|n>$ and $<n|$ are related to the probability amplitudes at site n whereas u_n is the displacement of the n-th local oscillator. The exciton-phonon coupling term is diagonal in the $|n>$ basis and depends only on local oscillator displacements.

Following Holstein [3], we neglect the kinetic energy terms and expand the time-dependent wave function as $|\psi>=\sum_p \psi_p|p>$, where the $|p>$ represent Wannier states. Inserting this into the time-dependent Schrödinger equation $i(d|\psi>/dt) = H|\psi>$, and using the orthonormality property for the $|p>$'s, we obtain:

$$\begin{aligned} i\frac{d\psi_n}{dt} &= (K/2)\sum_m u_m^2\psi_n + \epsilon_n\psi_n \\ &\quad -J[\psi_{n-1}+\psi_{n+1}] - Au_n\psi_n \end{aligned} \tag{1.3}$$

Next, we eliminate the vibrational degrees of freedom by imposing the condition of minimization of the energy of the stationary states [3]. Inserting $\psi_n \sim \exp[iEt]$ and using the normalization condition for the amplitudes ψ_p, $\sum_p |\psi_p|^2 = 1$, we get

$$\begin{aligned} E &= (K/2)\sum_n u_n^2 + \sum_n[\epsilon_n - Au_n]|\psi_n|^2 + \\ &\quad -J\sum_n(\psi_{n-1}-\psi_{n+1})\psi_n^* \end{aligned} \tag{1.4}$$

Imposing the extremum energy condition, i.e. $dE/du_n = 0$, we obtain $u_n = A|\psi_n|^2/K$. Inserting this back into Eq.(1.3), we get:

$$i\frac{d\psi_n}{dt} = (A^2/2K)\sum_p |\psi_p|^4 + \epsilon_n\psi_n - J[\psi_{n-1}+\psi_{n+1}] - (A^2/K)|\psi_n|^2\psi_n \tag{1.5}$$

This last step represents a departure from the Holstein adiabatic approach being valid only in the *opposite* limit, i.e. that where the vibrational degrees of freedom adjust rapidly to the excitonic motion. In this anti-adiabatic or *antiabatic* limit, it is still possible to retain the dynamics in the original Eq. (1.3). The quantity $(A^2/2K)\sum_p |\psi_p|^4$ represents the total vibrational energy. If we measure energies with respect to this background value, we arrive to an effective nonlinear equation for the amplitude $\psi_n(t)$:

$$i\frac{d\psi_n}{dt} = \epsilon_n\psi_n - J[\psi_{n-1}+\psi_{n+1}] - (A^2/K)|\psi_n|^2\psi_n \tag{1.6}$$

This closed nonlinear equation describes the effective motion of the "polaron" in the aforementioned antiabatic limit. The "time step" dt in the time derivative should be understood as short compared to the time scale of the "bare exciton motion" (proportional to $1/J$) but long compared to the fast vibrational motion (proportional to $1/K$). We conclude that the regime of validity of DNLS in the context derived above is in the range where $|J| << \hbar\Omega$, with Ω being the the frequency of the local Einstein oscillators.

Using $V = -J$ and $\chi = A^2/K$ we arrive at the form of the DNLS equation already stated, viz.

$$i\frac{d\psi_n}{dt} = \epsilon_n\psi_n + V[\psi_{n-1} + \psi_{n+1}] - \chi|\psi_n|^2\psi_n \tag{1.7}$$

1.2 Some General Properties of DNLS

In the previous section we showed how DNLS can be motivated in a solid-state context. In an optics context, DNLS describes wave motion in coupled nonlinear waveguides. When an electromagnetic wave is sent through a nonlinear waveguide coupled to other waveguides in its vicinity, ψ_n represents the amplitude coefficient in an expansion of the electromagnetic field in terms of the wave normal modes in the waveguide. Coupling causes power to be exchanged among the waveguides. The nonlinear nature of the materials in each waveguide (coupler) can cause a "trapping" of power in one of the waveguides. Selftrapping now happens in space rather than in time. These features can be exploited in the design of optical ultrafast switches with applications in optical computers [16, 17]. In order to address the optics problem we rewrite DNLS in a slightly different form. Let us define $\psi_n \equiv \tilde{c_n}$, $V \equiv -J$, $\tilde{\chi} \equiv A^2/K$ and consider the independent variable t not as time but the space variable in the direction of propagation. More importantly we must change the normalization condition to $\sum_p |\psi_p|^2 = P$, P being the total electromagnetic power injected into a waveguide system (recall that $P = 1$ in the exciton problem). The DNLS equation can then be written as:

$$i\frac{d\tilde{c_n}}{dt} = \epsilon_n\tilde{c}_n + V(\tilde{c}_{n-1} + \tilde{c}_{n+1}) - \tilde{\chi}|\tilde{c}_n|^2\tilde{c}_n \tag{1.8}$$

and

$$\sum_p |\tilde{c}_p|^2 = P \tag{1.9}$$

We note that whereas in the optics problem we are interested in the critical power P_{cr} that causes switching *in space*, in the condensed matter problem we focus on the critical nonlinearity χ_{cr} that causes selftrapping in time. We can show, however that the two problems are identical by simply rescaling the variables; defining $c_n = \tilde{c_n}/\sqrt{P}$ and $\tilde{\chi}P = \chi$ transforms Eq.(1.8) to

$$i\frac{dc_n}{dt} = \epsilon_n c_n + V(c_{n-1} + c_{n+1}) - \chi|c_n|^2 c_n \tag{1.10}$$

$$\sum_p |c_p|^2 = 1 \tag{1.11}$$

We note that the nonlinearity parameter χ in the equation where the total probability is normalized to one is equal to the nonlinearity parameter related to the optical nonlinearities (Kerr nonlinearity) and the total power injected in the system. Thus, for a system of weakly nonlinear couplers we need an increased input power to accomplish similar results. In addition to this property we observe that there are two conserved quantities, viz. the norm (total power) $\sum_n |c_n|^2$, and the energy H, with

$$H = \sum_n \epsilon_n |c_n|^2 + V\sum_n (c_{n-1} + c_{n+1})c_n^* - \frac{\chi}{2}\sum_n |c_n|^4 \tag{1.12}$$

Assuming now $\epsilon_n = \epsilon$ for all n and performing the transformation $c_n \to \exp(-i\epsilon t)c_n$, we can eliminate the “energy term” from the equation obtaining:

$$i\frac{dc_n}{dt} = V(c_{n-1} + c_{n+1}) - \chi|c_n|^2 c_n \tag{1.13}$$

This is the form of the DNLS equation we will be using when the molecular or optical units are identical.

Equation(1.13) represents two equations for $\mathrm{Re}(c_n)$ and $\mathrm{Im}(c_n)$, or equivalently for c_n and c_n^*; the equation for the latter is

$$i\frac{dc_n^*}{dt} = -V(c_{n-1}^* + c_{n+1}^*) + \chi|c_n|^2 c_n^* \tag{1.14}$$

In principle V and χ can have either sign depending on the physical problem at hand. For the exciton problem, χ must be positive [3], while V could have either sign. For the optics problem, the sign of V is related to the initial phase difference of the electric fields in different waveguides, while the sign of χ depends on the nonlinear optical response of the waveguide material. We will now show, however, that the transformation $(V, \chi) \to (-V, -\chi)$ does not affect the site probabilities $\rho_n \equiv c_n c_n^*$ (or the "transmission coefficient"). It is easy to see that the transformation $V \to -V$ and $\chi \to -\chi$ in Eqs.(1.13) and (1.14) turns the first equation into the second and viceversa. In other words, this transformation results in $c_n \to c_n^*$ and $c_n^* \to c_n$. As a result the site diagonal elements $\rho_n \equiv c_n c_n^* = |c_n|^2$ (site probability or "transmissivity") remain invariant under this sign exchange if, at the same time, the initial conditions are modified appropriately, viz. $c_n(0) \to c_n^*(0)$ and $c_n^*(0) \to c_n(0)$. Thus, for a complete parameter study it is sufficient to take $\chi > 0$ and consider the two possible signs of V. We will see that different signs lead in general to different physical behaviors for ρ_n. In what follows we normalize typically V to $|V| = 1$, and consider two types of boundary conditions, periodic and open. Also, as mentioned earlier, we consider only the special initial condition $c_n(0) = \delta_{n,1}$ corresponding to complete initial localization of the particle (or power) to the first site.

Chapter 2

The Degenerate Nonlinear Dimer

The simplest DNLS equation unit that can be analyzed is the degenerate dimer. This is constituted of two sites, 1 and 2 with the same energies that for convenience can be taken to be equal to zero, i.e. $\epsilon_1 = \epsilon_2 = 0$ and identical nonlinearity parameters, i.e. $\chi_1 = \chi_2 = 0$. The resulting equations are:

$$i\frac{d}{dt}\psi_1 = V\psi_2 - \chi|\psi_1|^2\psi_1 \tag{2.1}$$

$$i\frac{d}{dt}\psi_2 = V\psi_1 - \chi|\psi_2|^2\psi_2 \tag{2.2}$$

The set of Eqs. (—refDimer-1a,Dimer-1b) constitutes the degenerate nonlinear dimer. This is a unique system since it is the simplest DNLS unit that is actually fully integrable. As a result, many of the properties induced by nonlinearity in this equation can be understood from the degenerate dimer.

2.1 Bifurcation analysis

2.2 Density matrix equations

Since the nonlinear dimer equations are complex as well as nonlinear it is appropriate to turn them into a corresponding set of linear equations. The probability is normalized, i.e. $|\psi_1|^2 + |\psi_2|^2 = 1$ and, as a result, we expect the system of Eqs. (**??**) to reduce to three real ode's. A physically motivated way to proceed is through the density matrix; the latter is defined as $\rho_{mn} = \psi_m {\psi_n}^*$, where the star * denotes complex conjugation. For the nonlinear dimer the density matrix is a $2x2$ matrix where the diagonal elements denote occupation probabilities and the off-diagonal ones contain phase information. In order to turn Eqs. (**??**) into density matrix equations, we form the time-derivative of the (m, n) element of the density matrix for $m,\ n\ = 1,\ 2$ as $\dot{\rho}_m n = \dot{\psi}_m \psi_n^*$ and substitute the relevant terms on the RHS. We obtain

$$\dot{\rho}_{11} = iV(\rho_{12} - \rho_{21}) \tag{2.3}$$

$$\dot{\rho}_{22} = -iV(\rho_{12} - \rho_{21}) \tag{2.4}$$

$$\dot{\rho}_{12} = +iV(\rho_1 - \rho_{22}) + i\chi(\rho_{22} - \rho_{11})\rho_{12} \tag{2.5}$$

$$\dot{\rho}_{11} = -iV(\rho_{11} - \rho_{22}) + i\chi(\rho_{11} - \rho_{22})\rho_{21} \tag{2.6}$$

This set of equations is clearly nonlinear but some hints about the dynamics is already discernible. To expose this we may now introduce further a new set of variables, viz. $s = \rho_{11} + \rho_{22},\ p = \rho_{11} - \rho_{22},\ q = i(\rho_{12} - \rho_{21}),\ r = \rho_{12} - \rho_{21}$ that are linear combinations of the diagonal and off-diagonal matrix elements respectively. Simple algebra leads to

$$\dot{p} = 2Vq \tag{2.7}$$

$$\dot{q} = -2Vp - \chi pr \tag{2.8}$$

$$\dot{r} = \chi pq \tag{2.9}$$

This set of differential equations is much simpler; we may use Eq. (2.7) in Eq. (2.9) and obtain an equation for variables r and p as follows:

$$\frac{d}{dt}r = \frac{\chi}{2V}\frac{d}{dt}(p\dot{p}) \tag{2.10}$$

Equation (2.10) can be fully integrated since its RHS is proportional to the time derivative of p^2; it has the solution:

$$r(t) = (r_0 - \frac{\chi}{4V}p_0^2) + \frac{\chi}{4V}p^2 \tag{2.11}$$

where r_0 and p_0 are the initial values of these variables. To continue, we differentiate once Eq. (2.7), substitute $\dot{q}$ from Eq. (2.11) while replacing also the variable r with the value in Eq. (2.11). After these steps we arrive at the second order equation for the probability difference p:

$$\ddot{p} = -\left[(2V)^2 + 2V\chi r_0 - \frac{\chi^2}{2}p_0^2\right]p - \frac{\chi^2}{2}p^3 \tag{2.12}$$

We observe that Eq. (2.12) is an equation similar to Newton's second law of motion were the probability difference $p \equiv p(t)$ plays the role of the position of a particle; on the LHS we have the acceleration term while on the RHS the force that enables the motion. By multiplying both sides of Eq. (2.12) with $\dot{p}$ and integrating we obtain an "energy conservation equation" in the form

$$\dot{p}^2 + V(p) = E_0 \tag{2.13}$$

$$V(p) = \left[(2V)^2 + 2V\chi r_0 - \frac{\chi^2}{2}p_0^2\right]p^2 + \frac{\chi^2}{4}p^4 \tag{2.14}$$

$$E_0 = \dot{p}_0^2 + \left[(2V)^2 + 2V\chi r_0 - \frac{\chi^2}{2}p_0^2\right]p_0^2 + \frac{\chi^2}{4}p_0^4 \tag{2.15}$$

In order to gain further intuition in the nonlinear dimer dynamics it is judicious to study first the simpler case with perfectly localized initial conditions; i.e. $p_0 = 1$, $q_0 = r_0 = 0$.

2.2.1 Localized initial conditions

Effective classical particle motion

In this case the particle is placed completely initially on the first site while no complex phases are involved. The set of dynamic Eqs. (2.15,2.14,2.15) simplifies to:

$$\dot{p}^2 + V(p) = E_0 \tag{2.16}$$

$$V(p) = \left[(2V)^2 - \frac{\chi^2}{2}\right]p^2 + \frac{\chi^2}{4}p^4 \tag{2.17}$$

$$E_0 = (2V)^2 - \frac{\chi^2}{4} \tag{2.18}$$

where $\dot{p}_0 = 2Vq_0 = 0$. To simplify further the equations we rescale time to $\tau = 2Vt$ and introduce the variable $\zeta = \chi/4V$; we have

$$\left(\frac{dp}{d\tau}\right)^2 + V(p) = \epsilon_0 \tag{2.19}$$

$$V(p) = \left(1 - 2\zeta^2\right)p^2 + \zeta^2 p^4 \tag{2.20}$$

$$\epsilon_0 \equiv \frac{E_0}{(2V)^2} = 1 - \zeta^2 \tag{2.21}$$

We thus have the picture of a particle with mass equal to 2 that executes dynamics in a quartic potential. To make the representation simpler, it is preferable to absorb the nonlinear term $1-\zeta^2$ in the effective potential so that the effective initial energy is independent of ζ and equal to zero. We thus define

$$U(p) = V(p) + \zeta^2 - 1 \equiv \zeta^2 p^4 + \left(1 - 2\zeta^2\right) p^2 + \zeta^2 - 1 \tag{2.22}$$

With definition of Eq. (2.22) the conservation of energy for the effective particle becomes

$$\left(\frac{dp}{d\tau}\right)^2 + U(p) = 0 \tag{2.23}$$

We plot the effective potential $U(p)$ as a function of p for various nonlinearities ζ in Fig. (2.1); the horizontal line denotes the initial particle energy compatible with the localized initial conditions. Lets us follow the dimer dynamics through this potential picture. In the linear dimer for $\zeta = 0$ the potential is purely quadratic and a particle starting at $p_0 = 1$ simply performs oscillatory motion between the two extremes at $p = \pm 1$. The time dependent dynamics is purely trigonometric and the quantum particle simply oscillates completely between the two energy states available to if with period equal to $2VT = 2\pi$, i.e. $T = \pi/V$. Once ζ becomes non-zero the potential $U(p)$ starts deforming and becomes more shallow without however loosing the contact points at $p = \pm 1$ with the horizontal-constant energy-line. For small ζ's the dynamics is qualitatively similar to the linear motion, i.e. periodic dynamics between the two extremes. Since the potential is more shallow the kinetic energy at the bottom is smaller and, as a result, the dynamics becomes slower.

For the nonlinearity value $\zeta = 1/\sqrt{2} \approx 0.707$ the second derivative of $U(p)$ at $p = 0$ becomes zero and the bottom of the potential becomes flat, as in Fig. (2.1). It is clear that the particle dynamics is very slow for this value of nonlinearity as the particle crosses from positive to negative values of p. As ζ increases past this value, the quadratic term in the potential becomes negative and and a barrier develops at $p = 0$. The effective particle has to overcome this effective barrier- this means that the quantum particle dynamics becomes even slower as it tries to tunnel from the first site to the second one. The period thus of the periodic motion reduces as the nonlinearity value increases and actually becomes infinite at $\zeta = 1$. This marks the *self-trapping transition* where the quantum particle cannot cross completely to the second site and it simply reaches equipartition of probability. In the effective particle picture, the maximum of potential $U(p)$ at $p = 0$

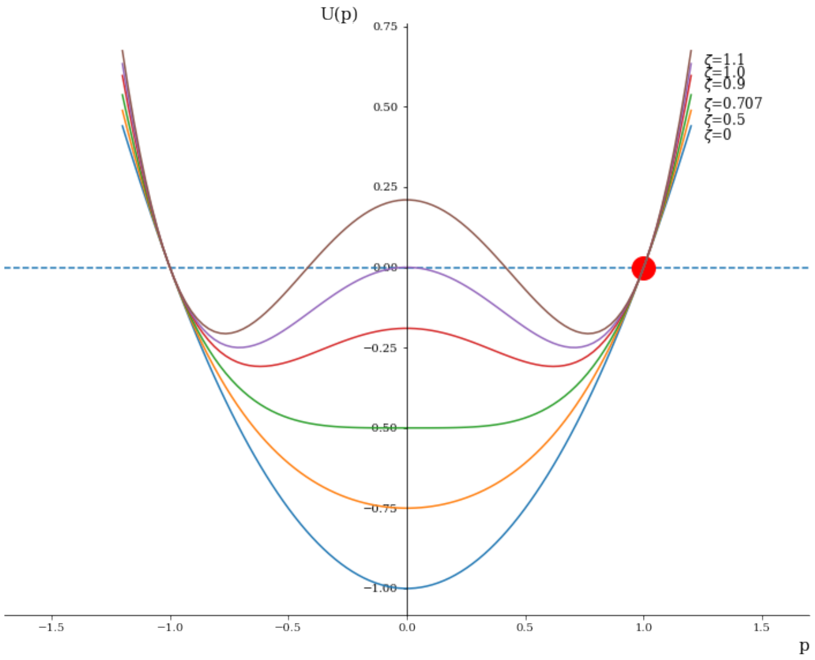

Figure 2.1: Effective potential motion for self-trapping with localized initial condition. On the abscissa the probability difference p, in the ordinate the effective potential $U(p) = V(p) + \zeta^2 - 1$. The horizontal line demarks the initial energy while the red bullet the initial state.

reaches the value "zero", i.e. $U(0) = 0$ and due to energy conservation the particle that starts from $p = 1$ can only reach asymptotically this maximum. The motion ceases to be periodic for this nonlinearity value and becomes hyperbolic. Further increase of ζ shifts the maximum $U(0)$ to] values than zero and the motion of the particle is again periodic yet incomplete. The quantum particle can reach over to the other side only partially to a degree that depends on the nonlinearity value. As nonlinearity increases without limit the particle localization on the initial site becomes more pronounced. The different regimes of the effective particle dynamics are portrayed in Fig. (2.1).

Exact time dependent solution

In order to obtain the exact time dependent solution one has to solve the differential Eq. (2.23) or Eq. (2.12) for the appropriate initial conditions. We can write formally the solution of the former as

$$\tau = \int_1^p \frac{dp'}{\sqrt{-U(p')}} = \int_1^p \frac{dp'}{\sqrt{-[\zeta^2 p^4 + (1 - 2\zeta^2)\, p^2 + \zeta^2 - 1]}} \tag{2.24}$$

We notice that by construction the values $p = \pm 1$ are roots of the potential $U(p)$; as a result we can express it in the simpler form

$$U(p) = (p^2 - 1)(\zeta^2 p^2 + 1 - \zeta^2) \tag{2.25}$$

Making the substitution $p = \cos\theta$ we have

$$\tau = \int_0^{\cos^{-1}\theta} \frac{-\sin\theta' d\theta'}{\sqrt{\sin^2\theta'(1 - \zeta^2 \sin^2\theta')}} = -\int_0^{\cos^{-1}\theta} \frac{d\theta'}{\sqrt{1 - \zeta^2 \sin^2\theta'}} \tag{2.26}$$

Equation (2.27) is simply the definition of an elliptic integral of the first kind-its inverse is a Jacobian elliptic function, specifically the Jacobian elliptic cosine. Finally,

$$p(t) = cn[\tau|\zeta] \equiv cn[2Vt|\frac{\chi}{4V}] \tag{2.27}$$

2.2.2 Weierstrass solution

Once we have understood the dimer selftrapping transition, it is instructive to express the degenerate dimer solution in terms of the Weierstrass elliptic function. In contrast to the Jacobi elliptic function approach, the

Weierstrass solution is not as intuitive; however teh method is more straightforward and produces additional insight. We write the energy Eqs. (**??**) as

$$\left(\frac{dp}{d\tau}\right)^2 = -\zeta^2 p^4 + \left(2\zeta^2 - 1\right) p^2 + 1 - \zeta^2 \equiv f(p) \tag{2.28}$$

and introduce the standard polynomial function $f(p)$ in the form

$$f(p) = a_0 p^4 + 4a_1 p^3 + 6a_2 p^2 + 4a_3 p + a_4 \tag{2.29}$$

where $a_0 = -\zeta^2,\ a_1 = 0,\ a_2 = 2\zeta^2 - 1,\ a_3 = 0,\ a_4 = 1 - \zeta^2$. The solution of Eq. (2.28) or, equivalently, Eq. (2.29) is generally

$$p(\tau) = p_{sr} + \frac{f'(p_{sr})}{4} \frac{1}{\wp(\tau; g_2, g_3) - \frac{1}{24} f''(p_{sr})} \tag{2.30}$$

where p_{sr} is a simple root of $f(p)$, primes denote differentiation wrt p while $\wp(\tau; g_2, g_3)$ is the Weierstrass elliptic function with invariants $g_2,\ g_3$. Using the simple root $p_{sr} = 1$ we have the explicit solution for the fully localized initial condition:

$$p(\tau) = 1 - \frac{1}{2} \frac{1}{\wp(\tau; g_2, g_3) + \frac{1+4\zeta^2}{12}} \tag{2.31}$$

The values of the invariants are given by the following general expressions:

$$g_2 = a_0 a_4 - 4a_1 a_3 + 3a_2^2 \tag{2.32}$$

$$g_3 = a_0 a_2 a_4 + 2a_1 a_2 a_3 - a_2^3 - a_0 a_3^2 - a_1^2 a_4 \tag{2.33}$$

that specialize presently as follows: or, finally

$$g_2 = -\zeta^2(1 - \zeta^2) + 3(\zeta^2 - 1)^2 = \tag{2.34}$$

$$4/3 * \zeta^4 - 4/3 * \zeta^2 + 1/12 \tag{2.35}$$

$$g_3 = -\zeta^2(2\zeta^2 - 1)(1 - \zeta^2) - (2\zeta^2 - 1)^3 = \tag{2.36}$$

$$8/27 * \zeta^6 - 4/9 * \zeta^4 + 5/36 * \zeta^2 + 1/216 \tag{2.37}$$

The modular discriminant $\Delta = g_2^3 - 27g_3^2$ has the following simple form:

$$\Delta = 1/16 * z^4 - 1/16 * z^2 = \frac{1}{16}\zeta^2(\zeta^2 - 1) \tag{2.38}$$

The conditions $\Delta \neq 0$ or $\Delta = 0$with $g_2 > 0$ and $g_3 > 0$ lead to periodic solutions for the dimer while $\Delta = 0$ with $g_2 \geq 0$ and $g_3 < 0$ to non-periodic ones.

The discriminant Δ determines the limiting behaviors of the full time dependence of the degenerate dimer. We have specific clear cases; when $\zeta = 0$ we obtain $\Delta = 0$ while $g_2 = 1/12 > 0$, $g_3 = 1/216 > 0$. This the case of the linear degenerate dimer with the known trigonometric time-evolution. The limiting form of the Weierstrass function is in this case

$$\wp(\tau, 1/12, 1/216) = -\frac{1}{12} + \frac{1}{4}\csc^2(\frac{\tau}{2}) \tag{2.39}$$

The second case where $\Delta = 0$ is for the value $\zeta = 1$, (assuming positive nonlinearity); for this value $g_2 = 1/12 > 0$ and $g_3 = -1/216 < 0$ leading to

$$\wp(\tau, 1/12, -1/216) = \frac{1}{12} + \frac{1}{4} csch^2(\frac{\tau}{2}) \tag{2.40}$$

Substituting these limiting forms back to the general solution of Eq(**??**) we have respectively:

$$p(\tau) = 1 - \frac{1}{2}\frac{1}{\wp(\tau; 1/12, 1/216) + \frac{1+4\zeta^2}{12}} = 1 - \frac{2}{\csc^2(\tau/2)} = 1 - 2\sin^2(\frac{\tau}{2}) = \cos(\tau) \tag{2.41}$$

and

$$p(\tau) = 1 - \frac{1}{2}\frac{1}{\wp(\tau; 1/12, -1/216) + \frac{1+5}{12}} = 1 - \frac{1}{1 + \frac{csch^2(\tau/2)}{2}} = \operatorname{sech}(\tau) \tag{2.42}$$

We observe that the limiting cases of pure trigonometric evolution for $\zeta = 0$ and hyperbolic one for $\zeta = 1$ are easily recovered.

The specifics of the Weierstrass-based time dependent solution can be analysed through the values of the pair $(g_3,\ \Delta)$; the latter controls also the half frequencies ω_1 and ω_3 of the fundamental parallelogram. Changes in the signs of g_3 and Δ reflect changes in the Weierstrassian dynamics and thus in the nonlinear dimer one. We notice four cases (Table 2)

ζ	g_3	Δ	ω_1	ω_3
$(0, \frac{\sqrt{2}}{2})$	+	-	Ω	$-\frac{\Omega}{2} + \Omega'$
$(\frac{\sqrt{2}}{2}, 1)$	-	-	$\lvert\Omega\rvert + i\frac{\Omega}{2}$	-i Ω
$(1, \frac{1}{2}\sqrt{\frac{3}{2}\sqrt{2}+2})$	-	+	$\lvert\omega'\rvert$	-iω
$(\frac{1}{2}\sqrt{\frac{3}{2}\sqrt{2}+2}, \infty)$	+	+	ω	ω'

Table 2

ζ	g_3	Δ	ω_1	ω_3
0	$\frac{1}{216}$	0	π	$i\infty$
$\frac{\sqrt{2}}{2}$	0	$-\ \frac{1}{64}$	$\frac{(4-4i)\Gamma\left(\frac{5}{4}\right)^2}{\sqrt{\pi}}$	$\frac{(4+4i)\Gamma\left(\frac{5}{4}\right)^2}{\sqrt{\pi}}$
1	$-\frac{1}{216}$	0	$-i\pi$	∞
$\frac{1}{2}\sqrt{\frac{3}{2}\sqrt{2}+2}$	0	$\frac{1}{512}$	$\frac{4\ 2^{3/4}\Gamma\left(\frac{5}{4}\right)^2}{\sqrt{\pi}}$	$\frac{4i2^{3/4}\Gamma\left(\frac{5}{4}\right)^2}{\sqrt{\pi}}$

The Weierstrassian analysis of the nonlinear dimer with localized initial condition reveals that for *four* distinct values of the nonlinearity parameter ζ we have changes in the characteristics of the motion. The values $\zeta = 0,\ 1$ coincide with the ones obtained from the Jacobian approach. The former corresponds to the linear dimer case while the latter signifies the location of the selftrapping transition. It is easy to check that for the value $\zeta = \sqrt{2}/2 \approx 0.707107$ the effective dimer potential becomes flat at $p = 0$ while for yet larger values a local maximum develops. The dimer motion becomes increasningly more sluggish, a tendency that will culminate at $\zeta = 1$ with the selftrapping transition. The characteristic value $\zeta = \frac{1}{2}\sqrt{2 + \frac{3}{\sqrt{2}}} \approx 1.015052$ occurs while the dimer is in the selftrapping regime-it demarks a change in the slope of the initial time-evolution. The role of these four special values of the nonlinearity parameter ζ is easier explored in phase space. In Fig. () we show the various regimes.

Bibliography

[1] J.C. Eilbeck, P.S. Lomdahl and A.C. Scott, Physica **16**D, 318 (1985).

[2] V.M. Kenkre and D.K. Campbell, Phys. Rev.B **34**,4959 (1986).

[3] T. Holstein, Ann. Phys. (Leipzig),**8**, 325 (1959).

[4] A.S. Davydov and N.I. Kislukha, Phys. Status. Solidi (B),**59**, 465 (1973).

[5] A.S. Davydov, J. Theor. Biol. **38**, 559 (1973).

[6] A.S. Davydov and N.I. KislukhaSov. Phys. JETP **44**, 571 (1976).

[7] A. S. Davydov, Sov. Phys. Rev. B**25**, 898 (1982).

[8] J.C. Eilbeck, P.S. Lomdahl and A.C. Scott, Phys. Rev. B **30**, 4703 (1984).

[9] A.C. Scott, P.S. Lomdahl and J.C. Eilbeck, Chem. Phys. Lett. **113**,29 (1985).

[10] A.C. Scott and J.C. Eilbeck, Chem. Phys. Lett. **132**,23 (1986).

[11] V.M. Kenkre, G.P. Tsironis and D.K. Campbell in *Nonlinearity in Condensed Matter'* , Eds. A.R. Bishop et al. Springer, 1987.

[12] G.P.Tsironis and V.M. Kenkre,Phys. Lett. A **127**,209 (1989).

[13] V.M. Kenkre and G.P. Tsironis,Phys.Rev.B **35**,1473 (1987).

[14] V. M. Kenkre and G. P. Tsironis, Chem. Phys. **128**, 219 (1989).

[15] G.P. Tsironis, Ph.D. Thesis, University of Rochester, New York, 1986.

[16] S.M. Jensen, IEEE J. Quant. Electron. vol QE-18,No 10,pp.1580-3 (1982).

[17] M. I. Molina and G. P. Tsironis, Physica D **65**, 267 (1993)

[18] J. D. Anderson and V. M. Kenkre, Phys. Stat. Solidi **55**, 1324 (1993).

[19] S. Wolfram, *Mathematica: A system for Doing Mathematics by Computer'*, second edition, Addison-Wesley, 1991.

[20] A. C. Scott, Physica Scripta **42**, 14 (1990).

[21] G. P. Tsironis, Phys. Lett. A **173**, 381 (1993).