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Approximate ILM dynamics in DNA models

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Abstract—We investigate the existence of Intrinsic Localized Modes (ILMs) in nonlinear one-dimensional Klein-Gordon chains. We use the Lagrangian averaging approach parameterizing ILM by several slow-varying variables, and apply the averaging directly in the action principle. Our preliminary studies yield results for ILM dynamics in accordance with those obtained by other methods.

1. Introduction

Since the pioneering paper by Sievers and Takeno in 1988 [1], there has been extensive work on the existence and stability properties of Intrinsic Localized Modes (ILM). These modes are characterized by localized vibrations in a lattice and are due to both the nonlinearity and discreteness of the system. Several approaches have been used to investigate the existence of ILMs in various systems that support them. In [2] a one-dimensional lattice with nearest-neighbor purely anharmonic (quartic) interactions was considered. It was noted that a large family of time periodic solutions can be found with an ansatz $u_n(t) = (-1)^n \phi_n U(t)$, describing standing oscillations. In [3] the existence of ILMs was proved in nonintegrable generic one-dimensional Hamiltonian lattices. In the same work, a class of Fermi-Pasta-Ulam (FPU) chains was considered in more detail. A map of the Fourier coefficient of the ILM was analyzed, with the ILM corresponding to homoclinic points in the phase space of this map. More recently, in [4] discrete breathers in diatomic FPU type lattices were shown to exist and their stability was analyzed. Their existence was proved by continuation of periodic solutions from a homogeneous lattice potential. In [5] the existence of breathers in diatomic FPU lattices was proved via a discrete spatial centre manifold reduction.

Variational approaches have been used to find soliton solutions in the context of the discrete Nonlinear Schrödinger equation [6, 7]. According to the variational principle, an ansatz with a finite number of parameters is substituted into the Lagrangian whose critical points correspond to the solutions of the dynamic equation of the system. In the context of nonlinear Klein-Gordon lattices, which is the focus of this work, a mathematical proof of breather existence in Klein-Gordon chains was given in [8] for small coupling in a general class of oscillator networks. The existence of solutions of fixed period was formulated as a problem of finding zeros of an operator in a Banach space using the implicit function theorem and then it was proved that they decay exponentially in space. In [9] the existence of multi-breathers was proved in the case of weak coupling using as starting point the limit where the oscillators are not coupled and the periodic solutions can be found by phase portrait techniques. Then, these trivial solutions were continued as a function of the small coupling constant using the implicit function theorem. In [10] small Hamiltonian perturbations of Hamiltonian oscillator networks were considered and an effective Hamiltonian on the submanifold of periodic orbits was introduced. The critical points of the effective Hamiltonian subject to the action (which is preserved) correspond to exact periodic solutions. The linearization of the effective Hamiltonian about the critical points gives the linearized dynamics of the full system to leading order in the perturbation.

In this contribution we investigate the existence of ILMs in a Klein-Gordon chain with a Morse onsite potential and interactions beyond the nearest neighbor. The choice of the Morse potential has applications to DNA [11, 12] while longer range interactions are believed to more accurately represent the dynamics of DNA [13, 14]. We will follow a method suggested originally in [15] for a different system of coupled oscillators.

2. Localized solutions of lattice systems

2.1. General considerations

We shall first consider a rather general system described by a Lagrangian L of coupled nonlinear oscillators with the state described by the variables $\mathbf{x} = (x_1, \dots x_N)$, *i.e.*, $L = L(\mathbf{x}, \dot{\mathbf{x}})$. The Euler-Lagrange equations are derived from the minimal action principle $\delta S = \delta \int L dt = 0$, leading to

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{x}}} - \frac{\partial L}{\partial \mathbf{x}} = 0\,. \tag{1}$$

Suppose we wish to find the localized solutions that are approximated by a set of parameters $\mathbf{Q} = (Q_1, \dots, Q_m)$, *i.e.*, $\mathbf{x} = \mathbf{x}(\mathbf{Q}, t)$. The length of vector $\mathbf{Q}$, *i.e.*, the number of parameters, is assumed to be much smaller than the dimension of $\mathbf{x}$. We shall assume that the parameters $\mathbf{Q}$ can depend on the slow time variable $\tau = \epsilon t$ with $\epsilon \ll 1$, as well as fast time t, and being periodic in t with the period 2π.

There are several approaches to this multi-scale problem. One approach would be to average (1) over one fast period directly. This averaging, usually done in the Hamiltonian counter-part of (1), has a long and storied history. It is particularly useful in the context of averaging for perturbed Hamiltonian systems [16], which addresses small perturbations to an *integrable* Hamiltonians. On the contrary, the Lagrangian averaging approach outlined here seeks to find slow changes of time-periodic solutions to non-integrable Hamiltonians by averaging directly in the action principle first. While being less rigorous in nature, at least at this point, in nevertheless allows useful insights in ILM behaviour. This approach is also easy to generalize to include multiple parameters. The disadvantage of this approach, on the other hand, is the appearance of artificial singularities in the equations when some of the parameters reach a critical value; for ILM, such a singularity is manifested when the amplitude of ILM reaches zero.

Let us denote the average Lagrangian as $\bar{L}$ as follows:

$$\overline{L}(\mathbf{Q},\mathbf{Q}') = \frac{1}{2\pi}\int_0^{2\pi} L\Big(\mathbf{x}(Q(\epsilon t),t),\dot{\mathbf{x}}(Q(\epsilon t),t),t\Big)\mathrm{d}t\,, \qquad (2)$$

where $\mathbf{Q}' := d\mathbf{Q}/d\tau$. We then seek to minimize the action

$$\delta\overline{S} = \delta\int \overline{L}(\mathbf{Q},\mathbf{Q}')\mathrm{d}\tau = 0 \qquad (3)$$

This approach can be justified by the following rather simple consideration, which is also useful for understanding its limitations. Formally, we can write the action as

$$S = \int_0^\infty L\mathrm{d}t = \sum_{n=0}^{\infty}\overline{L}(\epsilon n) \simeq \epsilon\int_0^\infty \overline{L}(\tau)\mathrm{d}\tau\,. \qquad (4)$$

Does it mean that whenever $\delta S = 0$, we also have $\delta\overline{S} = 0$? Unfortunately not, since it depends on the variations we choose. In the general variational principle $\delta S = 0$ the variation $\delta\mathbf{x}$ is chosen arbitrary. However, since $\overline{S}$ depends on the parameters $\mathbf{Q}$ and their time derivatives, the variations $\delta\mathbf{Q}$ are chosen arbitrarily, which means that $\delta\mathbf{x}$ has to be of a certain shape. For the case considered here, taking $\delta\mathbf{Q}$ arbitrary means that $\delta\mathbf{x}$ follow from the ILM ansatz, *i.e.* have to be localized about the center in a particular way. Thus, we can make the following statements about the limitations of the method considered here:

1. If the averaged system describing localized solutions is unstable, the full system is also unstable.
2. If the averaged system is stable, no information about the full system can be inferred.
3. Slowly varying solutions of the averaged system will likely have nearby solutions of the full system, but the method gives no information about their stability.

With these cautionary remarks in mind, let us proceed to investigate the slow dynamics of parameters $\mathbf{Q}(\tau)$. The standard Euler-Lagrange approach gives

$$\delta\overline{S} = 0 \quad\Leftrightarrow\quad \frac{d}{d\tau}\frac{\partial\overline{L}}{\partial\mathbf{Q}'} - \frac{\partial\overline{L}}{\partial\mathbf{Q}} = 0\,. \qquad (5)$$

It is also useful to rewrite the equations of motion in the Hamiltonian form as follows. Define the generalized momenta $\mathbf{P}$ and the corresponding Hamiltonian $\overline{H}$ as

$$\mathbf{P} = \frac{\partial\overline{L}}{\partial\mathbf{Q}'}\,, \quad \overline{H} = \mathbf{P}\cdot\mathbf{Q}' - \overline{L}(\mathbf{Q},\mathbf{Q}')\Big|_{\mathbf{Q}'=\mathbf{Q}'(\mathbf{P},\mathbf{Q})}\,. \qquad (6)$$

We shall note that our approach does not involve friction. For systems where friction and forcing is important, for example, nano resonator arrays [17], this method needs to be modified. Alternatively, we refer the reader to Van der Pol approach developed in [18]. It is important to note that our method is approximate, but valid for arbitrary amplitude, and should be understood as complimentary to the finite amplitude expansion method developed in [19].

2.2. Applications to DNA models

Let us now proceed to discuss a concrete example of that is related to ILM motion, namely, a dynamical DNA model. The system is written as follows. Let us approximate the dynamics of molecules in a DNA chain $i = (1,2,\ldots,N)$ by a scalar variable u_i, and take $\mathbf{x} = (u_1,\ldots,u_N)$. The Lagrangian is [13, 14]

$$L = \frac{1}{2}\dot{u}_n^2 - \sum_{i=1}^{3} W_i\Big(u_n,u_{n+i}\Big) - V(u_n)\,, \qquad (7)$$

where $V(x) = D(e^{-ax}-1)^2$ is the onsite Morse potential, having a single minimum at the origin, depth D and width a^{-1}. The harmonic couplings with the first, second, and third neighbors are given by

$$W_i(x,y) = \frac{k_i}{2}(x-y)^2,\ \ 1\le i\le 3, \qquad (8)$$

with coupling strengths k_i, $1\le i\le 3$. The full Euler-Lagrange equations (1) give

$$\ddot{u}_n + V'(u_n) + \sum_{i=1}^{3}\frac{\partial W_i(u_n,u_{n+i})}{\partial u_n} + \sum_{i=1}^{3}\frac{\partial W_i(u_n,u_{n-i})}{\partial u_n} = 0. \qquad (9)$$

2.3. Static ILMs as approximate localized solutions

Let us show how to use Lagrangian averaging techniques to describe approximate dynamics of ILM formation in (9). Consider the case of static ILM with ansatz

$$u_n(t) = A(-1)^n e^{-\lambda|x_0-n|}\sin\omega t. \qquad (10)$$

Here, the parameters have the following meaning

- u_n is the deflection of the oscillator;
- A is the amplitude of the peak;
- λ is the sharpness of the ILM;
- x_0 is the center of the ILM (not necessarily an integer, time independent);
- ω is the temporal period;
- n_0 is the oscillator left of x_0, *i.e.* $n_0 \le x_0 \le n_0+1$.

If a particular static ILM exists, the amplitude A, width λ and the frequency ω are chosen dynamically, and thus should be considered as unknowns. We shall investigate the cases where $\mathbf{Q}$ has dimension 1, by taking $\mathbf{Q}$ to be one

of the parameters (A, λ, ω) and allow it to change with time while others are being fixed. We shall call this case the one-parameter model; because of the Hamiltonian structure of the system, it can be solved analytically. Next, we shall investigate the case when two parameters of the triple (A, λ, ω) are allowed to vary and one remains fixed, there are three possible combinations, namely $\mathbf{Q} = (A(t), \lambda(t))$, $\mathbf{Q} = (A(t), \omega(t))$ and $\mathbf{Q} = (\omega(t), \lambda(t))$. Finally, the most general case is that of the three parameter model $\mathbf{Q} = (A(t), \lambda(t), \omega(t))$. For the case of briefness and because of space limitation, we will sketch the solution and outline some results, with the full paper following these proceedings expanding on this topic.

3. One-parameter models

We shall only outline the computations for $\mathbf{Q} = A(t)$. The other cases when $\mathbf{Q} = \omega(t)$ and $\mathbf{Q} = \lambda(t)$ are considered similarly, but the formulas are considerably more complex. We start with computing the kinetic energy as $K = \frac{1}{2}\sum_{n=-\infty}^{+\infty} \dot{u}_n^2$. with u_n given by (10), and setting $x_0 = 0$. After some algebra, the kinetic energy averages to

$$\overline{K} = \frac{1}{2} F_0(x_0, \lambda)\Big(A'^2(\tau) + \omega^2 A^2(\tau)\Big), \quad \text{where} \tag{11}$$

$$F_0(x_0, \lambda) := \frac{e^{-2\lambda(x_0 - n_0)} + e^{-2\lambda(n_0 + 1 - x_0)}}{2(1 - e^{-2\lambda})}\,. \tag{12}$$

Next, we average the potential energy

$$\Pi = \sum_{n=-\infty}^{+\infty} V(u_n) + \sum_{i=1}^{3} \frac{k_i}{2}(u_n - u_{n-i})^2 \tag{13}$$

using the ansatz (10). After some tedious calculations we arrive to the following expression:

$$\overline{\Pi} = \frac{A^2(t)}{2} \sum_{n=1}^{3} k_n[4F_0 - 2(-1)^n e^{-n\lambda}(2F_0 + n)] + \overline{V}(A) \tag{14}$$

Averages of the Morse potential can be computed exactly in terms of modified Bessel functions $I_0(x)$ as

$$\overline{V}(A) = D\Big(I_0(2aA) - 2I_0(aA) + 1\Big). \tag{15}$$

Note that for large A, the Bessel function and hence $\overline{V}(A)$ increase exponentially. Thus, the averaged Lagrangian for the system $\mathbf{Q} = A(t)$ is

$$\overline{L} = \frac{1}{2} F_0 A'^2 - \Big(\overline{\Pi}(A) - \omega^2 F_0 A^2 + \overline{V}(A)\Big) \tag{16}$$

The generalized momentum is then simply $P_A = A'/F_0$ and the motion is Hamiltonian with the generalized coordinates (A, P_A) and Hamiltonian

$$\overline{H}_A = \frac{P_A^2}{2F_0} + \Big(\overline{\Pi}(A) - \frac{\omega^2}{2} F_0 A^2 + \overline{V}(A)\Big) := \frac{P_A^2}{2F_0} + U(A)\,, \tag{17}$$

where the term in the parentheses in (17) denoted as $U(A)$ is the effective potential energy. According to the general considerations, the $A = 0$ critical point is unstable if $U''(0) < 0$. The solutions in the (A, P_A) plane are generated by $\overline{H}_A$ =const, and since $\overline{V}(A)$ increases exponentially with A, they are all bounded. Since $\overline{V}''(0) = Da^2 = \omega_0^2$, the base frequency of a single oscillator, the condition for instability is given by

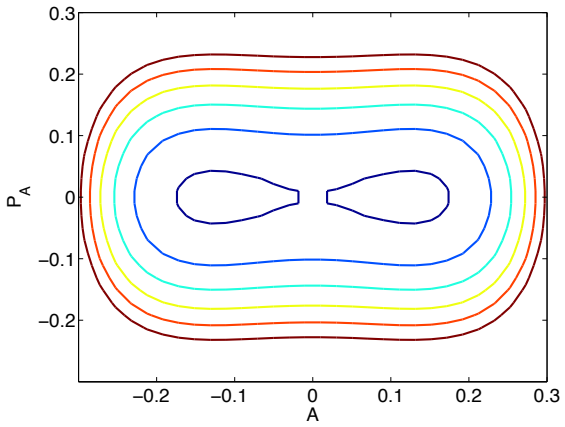

Figure 1: Level sets computed with the Hamiltonian for values of parameters: $k_1 = 0.025$, $k_2 = 0.05$, $k_3 = 0.05$, $x_0 = 0$, $D = 0.05$, $a = 5$, $\omega = 0.9\omega_0 \simeq 1.42$ and $\lambda = 2$.

$$\omega^2 F_0 > \sum_{n=1}^{3} k_n[4(1 + e^{-\lambda})F_0 - (-1)^n e^{-n\lambda}] + \omega_0^2\,. \tag{18}$$

However, we need to remember that for ILMs, ω and λ are not independent but are chosen dynamically, and are not known *a priori*. The only physical restriction is that the frequency of ILM has to be less than the natural linear frequency of a single oscillator ω_0. In Figure 1 we present an unstable case for a particular case with physical parameters chosen to coincide with those in [13, 14]. As we see, a small perturbation will make the ILM grow to a finite value and experience a long-term dynamics similar to that of a pendulum. Interestingly, this pendulum-like motion is in agreement with recent results for ILM dynamics obtained by a combination of numerical and analytical methods [20].

4. A summary of two parameter case studies

We now consider the ansatz

$$u_n(t) = A(\tau)(-1)^n e^{-\lambda(\tau)|x_0 - n|} \cos \omega t, \quad \text{or} \tag{19}$$

$$su_n(t) = A(\tau)(-1)^n e^{-\lambda|x_0 - n|} \cos \omega(\tau) t\,. \tag{20}$$

Using general considerations in Sec. 2.1, and taking $\mathbf{Q} = (A, \lambda)$ in the first case and $\mathbf{Q} = (A, \omega)$ in the second case, we can write the Hamitonian equations for the canonical variables $(\mathbf{P}, \mathbf{Q})$. The formulas are unfortunately too complex to be presented here, but we outline the general feature of the system. As it turns out, the solution of the generalized momenta $\mathbf{P}$ in terms of generalized coordinates $\mathbf{Q}'$ possesses a singularity (vanishing determinant) at $A = 0$, $\lambda = 0$ and $\omega = 0$. Ideally, a solution would remain bounded and non-singular for all $\tau > 0$, however, we have yet failed to find these solutions. This may not be a problem in view of general considerations presented in Sec. 2.1, since the full solution does not have to follow the averaged solution for all $\tau > 0$, and only the instability of $A = 0$ is relevant.

In what follows, we shall investigate the system (19), the system (20) is studied in a similar way. For any $\lambda_0 > 0$,

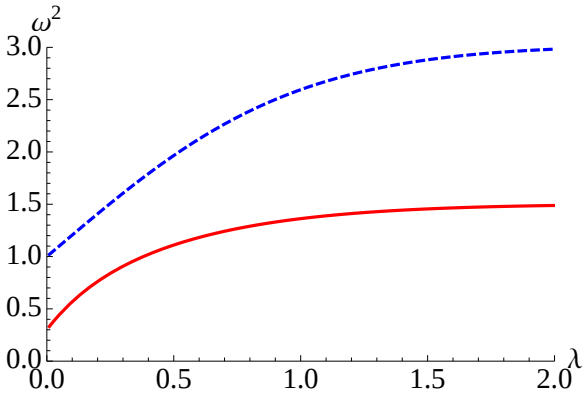

Figure 2: Stability boundary for ω^2 obtained from equations (18) (solid red line) and (21) (dashed blue line).

$(A = 0, \lambda = \lambda_0)$ is a steady state. To linearize about this state, we posit $A(\tau) = \delta A_1 e^{\mu}\tau$, $\lambda = \lambda_0 + \delta\lambda_1 e^{\mu\tau}$ and assume $0 < \delta \ll 1$, taking only the linear terms in δ. The dispersion relation, arising from the condition that nontrivial solutions (A_1, λ_1) exist, depends only on μ^2 because of the time reversal symmetry, and is in fact full square of an affine function of μ^2. Thus, the only way the instability can occur is for μ to cross zero, which happens when

$$\begin{aligned} &e^{8\lambda_0}\left(\omega^2 - 2\left(k_1 + k_2 + k_3\right)\right) - 4e^{7\lambda_0}k_1 + e^{4\lambda_0}\left(k_1 - 4k_2\right) \\ &+2e^{5\lambda_0}\left(k_1 - 4k_3\right) + 6e^{3\lambda_0}k_3 - e^{6\lambda_0}\left(k_1 - 5k_2 + k_3\right) \\ &+k_3 - e^{6\lambda_0}\left(e^{2\lambda_0} - 1\right)\omega_0^2 + e^{2\lambda_0}k_2 = 0 \end{aligned} \tag{21}$$

(This formula was obtained using the symbolic package *Mathematica*). While this expression is considerably more algebraically complex than (18), it shares similar features, being linear in the coefficients k_i and frequencies ω_0^2 and ω^2. In the future, we shall investigate the correspondence of the instability boundary obtained from different models. In Figure 2, we plot the stability boundaries for the values of ω obtained from (18) and (21). As expected, the one-parameter model over-estimates the stability region.

5. Conclusions

In this paper, we have outlined some preliminary studies for simplified Lagrangian-averaged models for the theory of ILM motion. These models are applicable to a wide range of ILM motion and, in general, have a potential to capture the full dynamics quite well. However, more studies of the long term dynamics of the simplified models obtained by these methods are necessary for further applications, which will be undertaken in our future studies. Here, we concentrated mostly on ILM emergence, also of particular interest are propagating ILMs and pinning on defects. In future work we will consider the minimum number of parameters necessary for a quantitatively accurate description of ILM formation.

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References

[1] A. J. Sievers and S. Takeno. Intrinsic localized modes in anharmonic crystals. *Phys. Rev. Lett.*, 61(8):970–973, Aug 1988.

[2] Y. Kivshar. Intrinsic localized modes as solitons with compact support. *Physical Review E*, 48:R43–R45, 1993.

[3] S. Flach. Existence of localized excitations in nonlinear hamiltonian lattices. *Physical Review E*, 51:1503–1507, 1995.

[4] K. Yoshimura. Existence and stability of discrete breathers in diatomic fermi-pasta-ulam type lattices. *Nonlinearity*, 24:293–317, 2011.

[5] G. James and P. Noble. Breathers in diatomic fermi-pasta-ulam lattices. *Physica D*, 196:124–171, 2004.

[6] D. J. Kaup. Variational solutions for the discrete nonlinear schrödinger equation. *Math. Comput. Simulations*, 69:322–333, 2005.

[7] C. Chong, R. Carretero-Gonzalez, B.A. Malomed, and P.G. Kevrekidis. Variational approximations in nonlinear schrodinger lattices with next-nearest-neighbor couplings. *Physica D*, 240:1205–1212, 2011.

[8] R.S. MacKay and S. Aubry. Proof of existence of breathers for time-reversible or hamiltonian networks of weakly coupled oscillators. *Nonlinearity*, 7:1623–1643, 1994.

[9] S. Aubry. Breathers in nonlinear lattices: Existence, linear stability and quantization. *Physica D*, pages 201–250, 1997.

[10] T. Ahn, R. S. MacKay, and J. A. Sepulchre. Dynamics of relative phases: generalized multibreathers. *Nonlinear Dynamics*, 25:157–182, 2001.

[11] M. Peyrard and A. R. Bishop. Statistical mechanics of a nonlinear model for dna denaturation. *Phys. Rev. Lett.*, 62:2755–2758, 1989.

[12] T. Dauxois. Dynamics of breather modes in a nonlinear "helicoidal" model of dna. *Phys. Lett. A*, 159:390–395, 1991.

[13] Z. Rapti. Stationary solutions for a modified peyrard-bishop dna model with up to third-neighbor interactions. *European Physical Journal E*, 32:209–216, 2010.

[14] Z. Rapti. Multibreather stability in discrete klein-gordon equations: Beyond nearest neighbor interactions. *Phys. Lett. A*, 377:1543–1553, 2013.

[15] D. Brake and V. Putkaradze. Reduced systems for intrinsic localized modes on an infinite oscillator array. *NOLTA*, 2013.

[16] V. I. Arnold, V. V. Kozlov, and A. I. Neishtadt. *Mathematical Aspects of Classical and Celestial Mechanics, 2nd ed.* Springer, 1997.

[17] Daniel Brake, Huiwen Xu, Andrew Hollowell, Ganesh Balakrishnan, Chris Hains, Mario Marconi, and Vakhtang Putkaradze. Intrinsic localized modes in two-dimensional vibrations of crystalline pillars and their application for sensing. *Journal of Applied Physics*, 2012.

[18] T. Ikeda and Y. Harata. Intrinsic localized modes in nonlinear discrete mechanical systems, ENOC 2011.

[19] M. Barbi, S. Cocco, M. Peyrard, and S. Ruffo. A twist opening model for dna. *Journal of Biological Physics*, 24:97, 1999.

[20] M. Kimura, Y. Matsushita, and T. Hikihara. A numerical study on parametric resonance of intrinsic localized modes in coupled cantilever arrays, NOLTA 2012.