Simplified models for Intrinsic Localized Mode dynamics

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Abstract—We discuss possible application of Intrinsic Localized Modes (ILM) in nano pillar arrays to sensing. When a molecule attaches to a pillar, it causes a change in the pillar's natural frequency. The idea of the method is to use ILMs to detect this defect in the array. We outline some difficulties posed by visualization of nanoscale vibrations. As a first step in theoretical understanding of ILM dynamics in the presence of defects, we use variational models to derive simplified equations of motion for ILMs.

1. Introduction

Intrinsic Localized Modes (ILMs) occurs in a wide variety of systems of coupled nonlinear oscillators. ILMs were first discovered in [1, 2], and since then the existence of ILMs as been demonstrated in a wide variety of physical experiments and models, and for a variety of of nonlinearities – see *e.g.* [3]. The most common apparatus for the study of ILM is the micromechanical array [4, 5, 6, 7, 8, 9]. Additionally, many different forms of ILM have been investigated, such as 'twisted un/staggered modes' [10] and 'bright compact breathers' [11]. Furthermore, there has been considerable investigation in the theoretical analysis and practical applications of these structures, at both the microscopic and macroscopic scales. We refer the reader to the exhaustive review article [6] which discusses ILM history, experiments and theory in detail.

There has been substantial interest in application of resonators to sensing. Previous studies employing micromechanical cantilevers for use in sensing have monitored frequency shift upon attachment of particles or molecules [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22]. It has been demonstrated that micro- and nano mechanical sensors can afford single molecule, or even atom, sensitivity, achieved by producing a very high Q-factor resonator and measuring frequency shift upon attachment of a particle. The use of multiple resonators has been suggested for multi-channel sensing applications [23]. However, as far as we are aware, there has not been any work on single molecule detection utilizing the amplitude of oscillations of nano mechanical arrays, although these ideas have been tested on the micro scale, see *e.g.* [7]. The scaling of ILM-based sensors to nanoscale presents several challenges, the most important being impossibility of visualization of motion using any light of near-visible spectrum. We refer the reader to our recent paper [24] for the discussion of challenges of nanoscale dynamics, methods of solutions and some theory behind visualization of the dynamics of nano pillar arrays.

One of the most crucial parts of the sensor based applications of ILMs is the analysis of defect pinning for ILMs. A molecule attached to a resonator in an array introduces a localized impurity in the array. As the detailed direct analysis of the ILM dynamics with impurity is seemingly impossible to track analytically, in this manuscript we shall concentrate on the derivation of approximate methods of analysis. Our methods are based on the variational approach which has been successfully applied to *e.g.*, the Discrete Nonlinear Schrödinger equations with impurity [25]. We show that while there are some differences with that system, in general one can demonstrate the defect influence on ILM using variational methods.

2. Derivation of Equations

For the purpose of this manuscript, we shall only consider one dimensional deflection of oscillators. As we discuss in [24], to accurately model nano mechanical arrays, one needs to consider two dimensional vibrations, but this is left for future consideration. For now, define u_n be the deflection of the nth pillar. In order to use the variational approach, we define the kinetic and potential energies

$$\mathbb{K} = \frac{1}{2}\sum \dot{u}_n^2 \tag{1}$$

$$\mathbb{P} = \sum_n \frac{\alpha_1}{2}u_n^2 + \frac{\alpha_2}{2}\left(\nabla_n u\right)^2 + \frac{\beta_1}{4}u_n^4 + \frac{\beta_2}{4}\left(\nabla_n\right)^4 \tag{2}$$

where we have defined the discrete gradient $\nabla_n f := f_n - f_{n-1}$. The equations of motion are Hamiltonian,

with $\mathbb{H} = \mathbb{K} + \mathbb{P}$. Defining the canonical pair (p_n, u_n), and doing Legendre transform of the Lagrangian $L = \mathbb{K} - \mathbb{P}$, we see that the momenta are simply $p_n = \dot{u}_n$. The Hamiltonian equations of motion are

$$\begin{aligned} \dot{u}_k =& p_k \\ \dot{p}_k =& -\alpha_1 u_k - \alpha_2\big(\nabla_k^2 u\big) - \beta_1 u_k^3 - \beta_2 \nabla_k (\nabla_k u)^3 \end{aligned} \quad (3)$$

For a simplified theory of ILM motion, let us first consider an ILM of the following approximate form:

$$u_n = A(t)\exp(-\lambda|n - x(t)|)(-1)^n \cos(\omega t). \quad (4)$$

If x is an integer or half-integer, (4) is an accurate approximation of either Sievers-Takeno [1] or Page [2] type. If x is an arbitrary real number, shape (4) should approximate the intermediate form of ILM.

We will consider two particular cases. First, $x(t)$ is assumed to depend on time, but the amplitude A of ILM is fixed. As we show, this leads to rather simple, but perhaps too simplistic to accurately describe complex behavior of solutions to (3). We continue by allowing $A(t)$, to vary with time, which can lead to more realistic behavior.

3. Simplistic Consideration

We shall consider the solution (4) with $A(t) := A =$const and $x(t)$ varying with time. While the practical value of this method may be limited, it allows complete analytical solution of the problem and thus is interesting from at least the pedagogical point of view. Substituting (4) into (1,2) and averaging over a period $T = 2\pi/\omega$, we see that the two-variable kinetic and potential energies, respectively $\overline{\mathbb{K}}_2$ and $\overline{\mathbb{P}}_2$, are approximated as:

$$\overline{\mathbb{K}}_2 = \dot{x}^2 f(x)\,, \quad \overline{\mathbb{P}}_2 = g(x)\,, \quad (5)$$

where $f(x)$ and $g(x)$ are periodic functions of x with period 1, with discontinuities at integer values of x. An example of these functions with $A = 1$ is presented on Figure 1. We do not present explicit expression for $g(x)$ here as it is quite cumbersome.

The reduced averaged Lagrangian is then $\overline{L}(x, \dot{x}) = \frac{1}{2}\dot{x}^2 f(x) - g(x)$. The generalized momentum is $p = \partial L/\partial \dot{x} = \dot{x} f(x)$, so the generalized velocity is expressed as $\dot{x} = p/f(x)$. The reduced Hamiltonian H_0 is then given by

$$H_0 = \frac{p^2}{2f(x)} + g(x) \quad (6)$$

The equations of motion are then:

$$\dot{x} = \frac{\partial H_0}{\partial p} = \frac{p}{f(x)} \quad (7)$$

$$\dot{p} = -\frac{\partial H_0}{\partial x} = \frac{p^2}{2f(x)^2} f'(x) - g'(x) \quad (8)$$

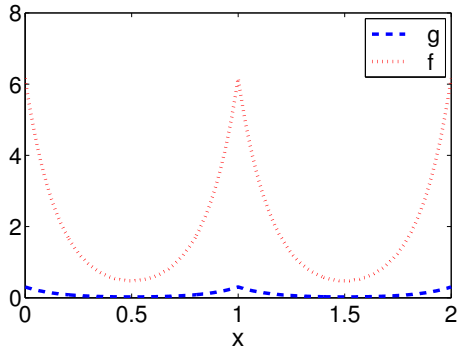

Figure 1: Example plots of f (dashed) and g (dotted) for the simple 2D system. Both are periodic with period 1, corresponding to normalization of distance between pillars on the array.

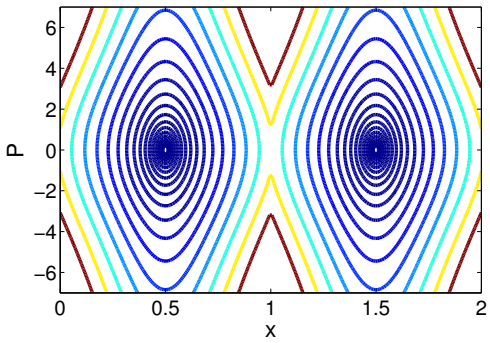

Figure 2: Level sets of the Hamiltonian (6). Trajectories are either oscillatory or escaping.

From (6) we conclude that in the (p, x) plane, the solution is given by the level curves $\frac{p^2}{2f(x)} + g(x) =$const; the speed of trajectory along these curves is given by (7,8). In practice, and as seen in Figure 2 the only possible solutions for $x(t)$ and $p(t)$ are either oscillatory or escaping trajectories.

4. Coordinate-Amplitude approach

To make the approximate system more realistic, we now consider the case when both the coordinate $x(t)$ and amplitude $A(t)$ in (4) are allowed to vary. Proceeding similarly to the previous case, the reduced averaged kinetic and potential energies are now given by

$$\overline{\mathbb{K}}_4 = F_1(x)\dot{A}^2 + F_2(x)\dot{x}^2 + F_3(x)\dot{A}\dot{x} \quad (9)$$

$$\overline{\mathbb{P}}_4 = g(x, A)\,, \quad (10)$$

where $F_i(x)$ are some functions of x, similar to $f(x)$ in (5). By computing the Lagrangian and proceeding in the standard way to compute generalized momenta

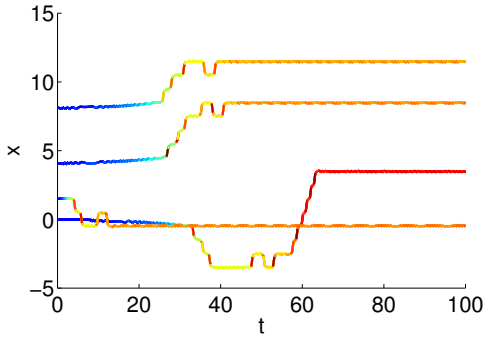

Figure 3: Four example paths of ILM across infinite oscillator array, changing only initial position; all other parameters remain fixed. The change of ILM position appears chaotic. The ILMs travel through the array, eventually pinning on or halfway between pillars. The color of each path indicates the amplitude A, with darker blue being smaller, and red being larger.

P_x, P_A, we see that

$$P_x = F_2\dot{x} + F_3\dot{A}\,, \quad P_A = F_1\dot{A} + F_3\dot{x}\,. \tag{11}$$

Defining $\Delta = F_1F_2 - F_3^2$, the Hamiltonian is

$$H_4 = \frac{1}{\Delta}\left(\frac{F_1}{2}P_x^2 + \frac{F_2}{2}P_A^2 + F_3P_AP_x\right) + g\,. \tag{12}$$

Again omitting cumbersome expressions for $g(x, A)$ and with $\xi_{i,x} = \frac{\partial F_i/\Delta}{\partial x}$, $\xi_{i,A} = \frac{\partial F_i/\Delta}{\partial A}$, the Hamiltonian equations for the canonically conjugated (x, p_x, A, p_A) are:

$$\begin{aligned}
\dot{x} &= \frac{F_1P_x - F_3P_A}{\Delta}\,,\ \dot{A} = \frac{F_2P_A - F_3P_x}{\Delta} \qquad (13)\\
\dot{P}_x &= -\xi_{1,x}P_x^2 - \xi_{2,x}P_A^2 - \xi_{3,x}P_AP_x - \frac{\partial g}{\partial x}\\
\dot{P}_A &= -\xi_{1,A}P_x^2 - \xi_{2,A}P_A^2 - \xi_{3,A}P_AP_x - \frac{\partial g}{\partial A}
\end{aligned}$$

The term Δ is homogeneous degree 2 in A, implying that the system (13) has a singularity at $A = 0$. Despite this singularity, simulation of the reduced system (13) is reasonably well behaved. Examples are given in Figure 3, in which four initial x values are plotted, with all other system parameters remaining fixed. In all shown cases, the ILM travels across the array in what appears to be a chaotic fashion before becoming pinned at either a pillar, or halfway between two pillars.

Solving the system (13) for equilibria solutions, one derives the steady solution $(\tilde{x}, \tilde{A}, \tilde{P}_x, \tilde{P}_A) = (x_0, 0, 0, 0)$ which actually indicates that no ILM is present. However, $\tilde{A} = 0$ indicates that the ILM has vanished, so this is a degenerate solution. When the system reaches $\tilde{A} = 0$, the momentum diverges to compensate for the vanishing amplitude. Continuation through this singularity does not appear to be possible. This degenerate solution seems to appear seldom in simulations; the detailed reason for this behavior will be explained later.

In order to understand the effect of defects on ILMs, the equations above can be modified to take into account a pillar which has a different parameter value than the rest of the array. For example, change in k_0-th pillar's mass under attachment affects α_1 at that pillar, so we modify α_1 at the location k_0 by a defect α_D. The result of this is the addition of the term $D = A^2/2\alpha_D \exp(-2\lambda|x - k_0|)$ to g in (12). This procedure introduces a force acting on an ILM. In general, one thus concludes that a defect affects ILM through the force that is exponentially decaying with the distance between ILM and the defect. In the following work, we will present a detailed analysis of the defect pinning or repulsion for ILM, which is made possible through this procedure.

5. Conclusion

In this paper, we have derived an approximate variational approach that is capable to describe moving ILMs as well as influence of defects on ILM motion. Only the derivation is presented here, detailed analysis of the system will be addressed in our future work. We believe that such approximate methods are highly useful in analysis of ILM dynamics and subsequent sensor applications.

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