Simplified models for Intrinsic Localized Mode dynamics

Daniel Brake and Vakhtang Putkaradze

24 October, 2012

Project Overview

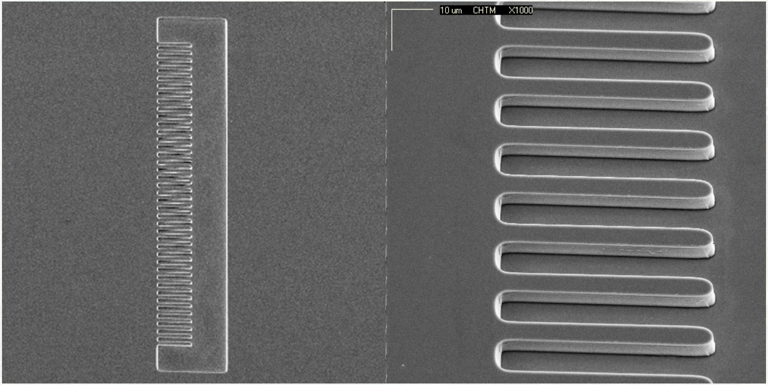
The main goal of the project is basic research for developing a single-molecule sensor.

- An array of crystals subjected to near-periodic motion will tend to vibrate somewhat coherently, especially if the driver is near a resonant frequency.
- Previous work has shown that coupled oscillators develop special waveforms known as Intrinsic Localized Modes (ILM).
- Defects in an oscillator array cause ILMs.
- Molecule attachment to pillar causes mass defect.
- If crystals are small enough, material will attach to pillars, and modify vibration.

This project received support from the Defense Threat Reduction Agency-Joint Science and Technology Office for Chemical and Biological Defense (Grant no. HDTRA1-10-1-0070).

Setup

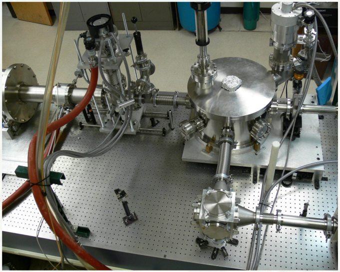
- GaAs Crystals, produced at UNM*



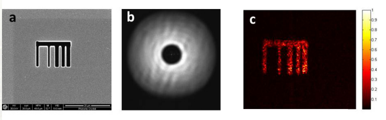
*Gunny Balakrishnan's group

Setup

- Experimental Setup at ERC*



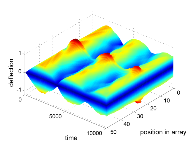
- Holography Results

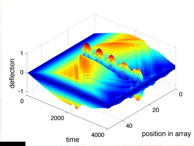


*Mario Marconi's group

- Can detect ILM's using EUV laser at ERC, near Laporte, using laser holography.
- Materials fabricated at CHTM in ABQ.
- Holography in this form uses a coherent beam of light with sufficient frequency to image an object. We can capture an essentially 3D image with a single 2D sensor, by:
  1. passing the laser through a splitter and suitable lens, then
  2. allowing it to pass back through itself, generating interference, and finally
  3. capturing it with a CCD camera.

What is an ILM?





Two main features of a wave form which is called a localized mode:

- Temporal *periodicity*,
- Spatial *localization* of energy.

Play

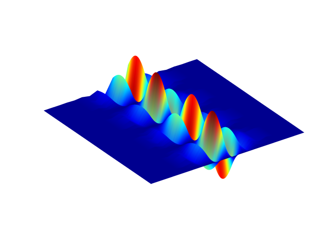
Deriving a Reduced System

To derive a reduced system, assume:

- Form for ILM, exponential in x, periodic in t, peak amplitude A.

$$u_n = A\exp(-\lambda|x(t) - n|)(-1)^n \sin(\omega t)$$

- Infinite array of pillars,
- Conservative system, no driving or dissipation.



ILM form

We will proceed through Hamiltonian Mechanics –

- Substitute ILM form into energies, collect, expand, etc.
- Write Laplacian, move into canonical variables, perform Legendre transform, write equations of motion.

Equations

$$
\begin{aligned}
\mathcal{H}_{\text{mono}} &= \mathcal{K}_{\text{mono}} + \mathcal{P}_{\text{mono}} \\
\mathcal{K}_{\text{mono}} &= \frac{1}{2}\sum_n \dot{u}_n^2 \\
\mathcal{P}_{\text{mono}} &= \frac{1}{2}\sum_n \left(\alpha_1 u_n^2 + \alpha_2 \left(u_n - u_{n-1}\right)^2\right) + \frac{1}{4}\sum_n \left(\beta_1 u_n^4 + \beta_2 \left(u_n - u_{n-1}\right)^4\right)
\end{aligned}
$$

$$
\begin{aligned}
\ddot{u}_n = &- \alpha_1 u_n - \alpha_2\big((u_n - u_{n-1}) + (u_n - u_{n+1})\big) \\
&- \beta_1 u_n^3 - \beta_2\big((u_n - u_{n-1})^3 + (u_n - u_{n+1})^3\big) .
\end{aligned}
$$

Hamiltonian Mechanics, Two Variables

Force $A = const$, let $x = x(t)$. First, write the kinetic and potential energies, $\mathcal{K}$, $\mathcal{P}$.

$$\mathcal{K} = \frac{A^2}{2}\frac{\omega + \frac{\lambda^2\pi}{\omega}\dot{x}^2}{1 - e^{-2\lambda}}\left(e^{-2\lambda(x-n_0+1)} + e^{-2\lambda(n_0-x)}\right),$$

$$\mathcal{P} = A^2\left(\frac{E_2}{2\xi_2} - (1+e^{-1})\frac{E_2}{\xi_2} + e^{-1}\right)$$
$$+ A^4\frac{3}{8}\left(\frac{E_4}{\xi_4} + (2 - 4e^{-\lambda} + 6e^{-2\lambda} - 4e^{-3\lambda})\frac{E_4}{\xi_4} - 4e^{-\lambda}E_2 + 6e^{-2\lambda}\right).$$

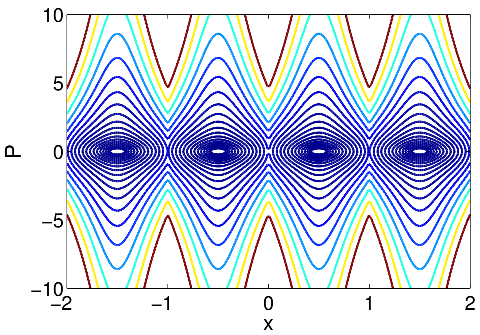
The Legendre transform gives the Hamiltonian $\mathcal{H}$ in terms of canonical variables:

$$\mathcal{H} = \mathcal{K} + \mathcal{P}.$$

A quick check confirms $\partial\mathcal{H}/\partial t = 0$, $\Rightarrow$ $\mathcal{H}$ is conserved.

Trajectories, Two Variables

Because $\mathcal{H}$ is conserved, paths are restricted to level sets of $\mathcal{H}$ in terms of x, P_x.



Notable properties:

1. Periodic Orbits,
2. Traveling trajectories,

- Defects raise or lower boundaries between wells,
- Essentially a pendulum.

Hamiltonian Mechanics, Four Variables

Now, both $A = A(t)$, $x = x(t)$. System will have four variables.

$$\dot{P}_x = -\left(\frac{1}{\Delta}\left(\frac{1}{2}\frac{\partial F_2}{\partial x}P_A^2 + \frac{1}{2}\frac{\partial F_1}{\partial x}A^{-2}P_x^2 - \frac{\partial F_3}{\partial x}A^{-1}P_A P_x\right) + A^2\frac{\partial c_2}{\partial x} + A^4\frac{\partial c_4}{\partial x}\right),$$

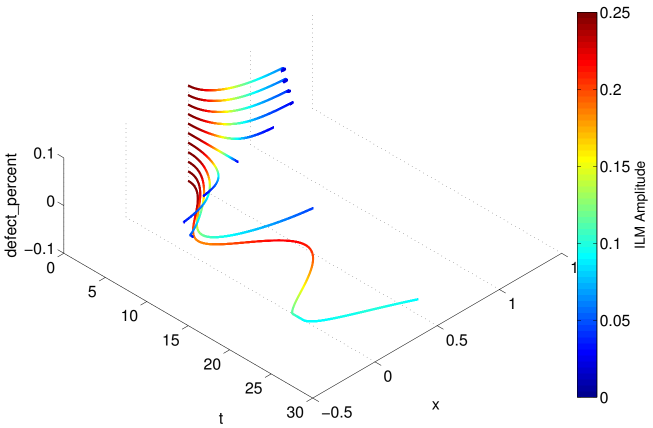
$$\dot{P}_A = -\left(-\frac{F_1}{\Delta}A^{-3}P_x^2 + \frac{F_3}{\Delta}A^{-2}P_A P_x + 2Ac_2 + 4A^3c_4\right),$$

$$\dot{x} = \frac{F_1}{\Delta}A^{-2}P_x - \frac{F_3}{\Delta}A^{-1}P_A,$$

$$\dot{A} = \frac{F_2}{\Delta}P_A - \frac{F_3}{\Delta}A^{-1}P_x.$$

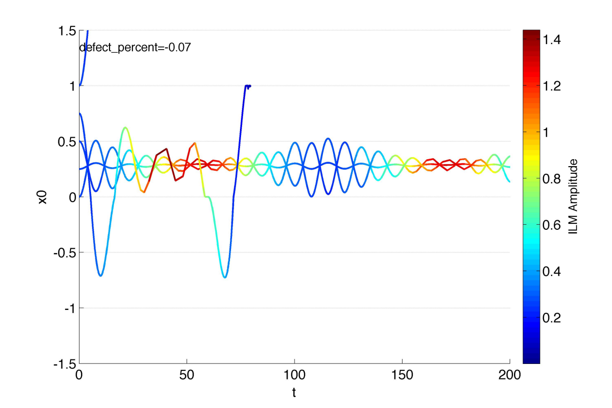
Many parameters to investigate.

Four-variable system, defect investigation



- With negative defect, ILM is initially attracted to defect.
- Positive defect, ILM it repelled from defect.

Various Initial Conditions



ILM is attracted to Defect location

Four-variable system, λ investigation

Four-variable system, varying λ.

Play

Summary

Conclusions

- Negative defect (reducing α_1) causes attraction toward the pillar,
- Positive defect (increasing α_1) causes repulsion away from the pillar.
- Bigger defect gives stronger attraction / repulsion.

Future work:

- Derive new reduced system for bidirectional oscillator array,
- Determine a scaling law for strength of attraction/repulsion as function of defect amplitude,