Anharmonicity:Beyond MFT

Benny Wah

November 1, 2019

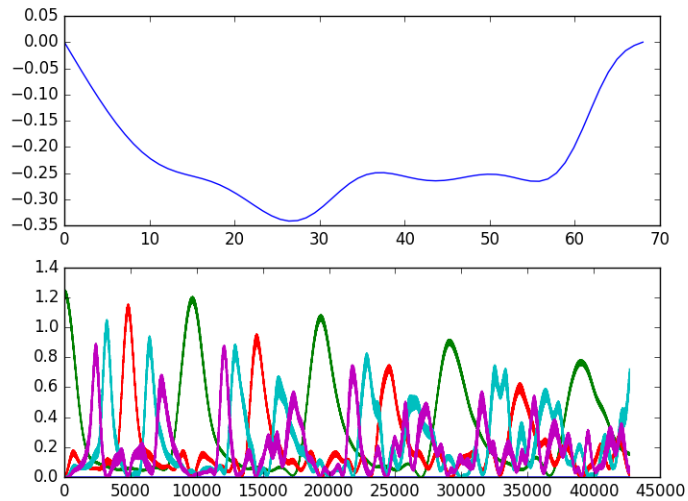
1 Introduction

From high-school to undergraduate classroom training in physics, the problems encountered are solvable by analytic attacks, boundary conditions and physically real impositions. These are due to the conditions of (1) linearity (2) harmonic hamiltonians which yield static coefficients in some orthogonal and complete basis (3) a sparse phase space in which all Lyapunov exponents are negative Among the non-analytically soluble classes of problems, there are chaotic systems which violate criterion (3), anharmonic hamiltonians which violate criterion (2) and systems whose dynamics are not factorizableinto linear equations violate criterion (1), not necessarily mutually exclusive of course.

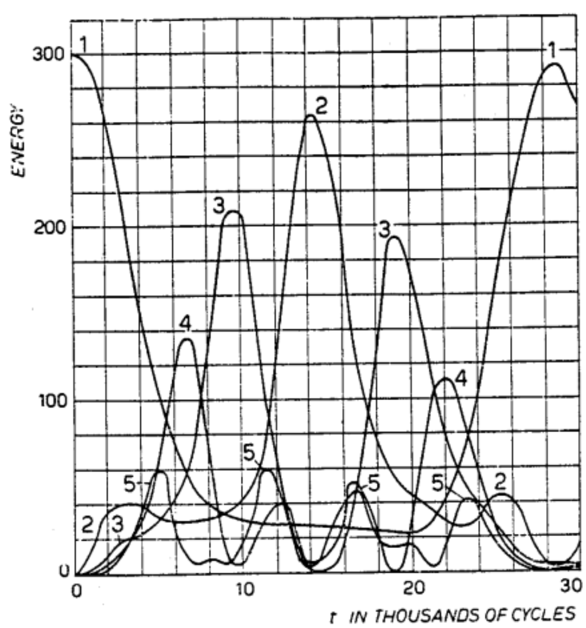
This article consists of personal thoughts on anharmonic class of systems.

Following the years of World War II, the advent of vacuum-tube computing allowed for virtual simulations. Among the first projects commissioned on the MANIAC I at Los Alamos laboratory was the "FPUT" problem concerning a non-linear oscillator. They included non-Hookean terms, such as a quadratic force, a cubic and a piece-wise linear force with differing slopes for differing regimes of displacements.

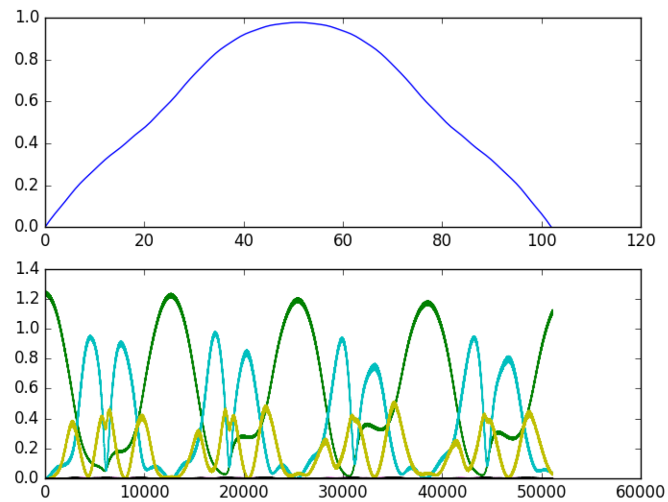
They used symplectic integrator, my suspiscion was leapfrog algorithm but cannot confirm as the authors have passed away and Mary Menzel (nee Tsingou) is quite old now, and was able to recover their results. For further reading on symplectic integrators, higher order versions of leapfrog are derivable through a detailed expansion via BCH formula as explained in Yoshida Haruo's article (Celestial Mechanics and Dynamical Astronomy 1993) A few are included below, one of which is leapfrog and the other using Ruth-Forest.

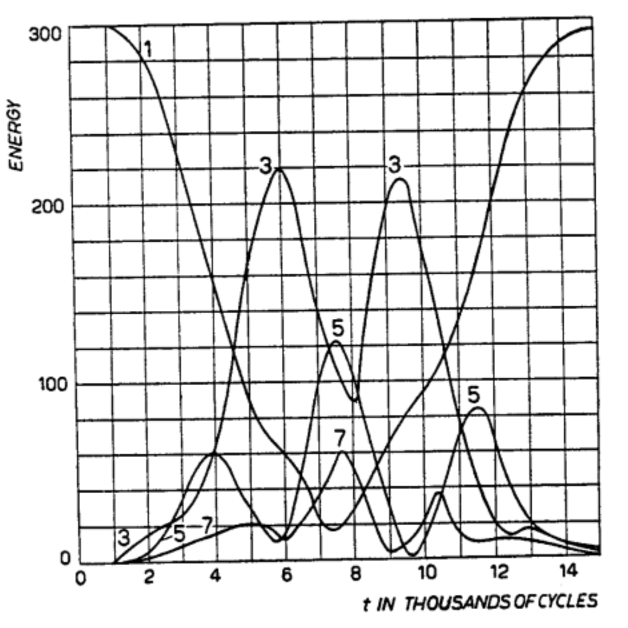


0.05
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
0
10
20
30
40
50
60
70
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
5000
10000
15000
20000
25000
30000
35000
40000
45000



ENERGY
300
200
100
0
0
10
20
30
t IN THOUSANDS OF CYCLES
1
2
3
4
5


1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
10000
20000
30000
40000
50000
60000


300
200
100
0
ENERGY
1
3
3
5
5
7
3
5
7
0
2
4
6
8
10
12
14
t IN THOUSANDS OF CYCLES

They initialized with low frequency sinusoidal displacement and so tracked the transfer between energies of Fourier modes. They measured the energies of the modes associated with the harmonic hamiiltonian, demonstrating that the remainder of the energy amounted to a few percent at the time.

The formulae for energy measurement are follows:

$$a_k = \sum_i x_i \sin \frac{ik\pi}{64} \tag{1}$$

$$E_{a_k} = \frac{1}{2}\dot{a}_k^2 + 2a_k^2(\sin \frac{\pi k}{128})^2 \tag{2}$$

They also observed the ”hyper-recurrence” seen above in the energetic mode distribution and concluded that non-linearity does not necessarily lead to thermalization or obey the ergodic hypothesis.

Using a discretized continuum of 64 slots along the oscillator. I attempted to recreate the above with discrete Fourier transform but always picked up a pre-factor (insert notes from home) and so discontinued efforts to derive the ”remianing few percent” of energy due to the anharmonic terms in the force law.

An analytic description with T-matrix methods and correctly treating the needed recursion relations was done by Joseph Ford [Equipartition of Energy for Nonlinear Systems, J. of Math. Physics (1961)] and the accepted solution from the community and by the only surviving author Mary in the follow-up published in the 90's.

2 Motivation

I will go on a brief side-bar here and so if disinterested, the reader can skip to the next section. The study of non-linear hamiltonians dates back to the beginning of the 20th century. Much of the world is not a problem that can be solved with analytic functions from an undergraduate textbook. Even in high-powered mathmatical formalisms, such as quantum field theory, anharmonic hamiltonians are not easily soluble if at all. Higher order terms and corrections are almost guaranteed to be tedious. Moreover, there are ultraviolet divergences introduced due to logarithmic integrals which were a subject of severe controversy when treated with various renormalization schemes. Even taking into account physical constraints such as Lorentz invariance, causality, etc it was not clear until Kenneth Wilson's numerically exact Renormalization Group technique (NRG) and his treatise that such schemes indeed stemmed from physical reality and not mathematical artefacts.

One of the consequences of this renormalization business is the scaling of interaction strength, so-called "coupling", with energy scales that leads to the notorious "Landau pole". Of course whatever Nature prescribed for our universe, there is no scientific reason to believe that all theories, or a complete theory, would be renormalizable and not subject to divergent couplings. Even in Wilson's treatment he asserts that a tremendous assumption is that the beta-functions, RG-flow in the stat. mech. community, are analytic. Therefore the phase transitions between physical theories of wordly phenomenon are of fundamental importance.

3 What to Do

Since running of the couplings necessitates logarithmic scaling, the range of anharmonic parameters that are computationally testable on a desktop workstation are limited. I have some preliminary results that suggest thermalization does occur for strong enough anharmonicity, but have not tested them. That is, the re-initialize the simulation from the ending configuration and calculate backwards time-wise in order to recover the initial pure sine mode.

As of currently, 3/2019, three things need to be accomplished:

(1) Analytically recreate the harmonic projections of the energy to each Fourier mode

(2) Implement above formula to see what happens to the remaining percent of energy, that is the Fourier components due to anharmonic terms

(3) Run the simulations backward to check energy conservation and rule out rounding errors

This will test the claims of non-ergodicity in this simple system and either confirm/reject Joseph Ford's theoretical results.

4 But why?

A few superficial contradictions have motivated me to study this.

(1) In Frölich coupling and microscopic BCS theory, they assume a harmonic bath of phonons due to the physically sound reasoning that low-energy fluctuations dominated the physics of superconductors.

However, (2) The phonons are due to lattice vibrations, which are typically ignored due to Born-Oppenheimer approximation. Although any small perturbation is automatically harmonic, in my opinion it remains to be seen whether any large coherence can arise from finer anharmonic terms

(3) In the case of type II superconductors, there is much discussion of the absence of isotope effect near optimal doping (Abrikosov claimed there was in fact a negative isotope effect upon Cu-substitution in YBCO) And so I assume there is some weak isotope-effect away from optimal doping. This suggests, in my view, that phononic distributions are important to the physics of type II and whatever enhances the T_c is cancelling the isotope effect. Whatever the mechanism, it is certainly much stronger.

Additionally, this study is very generalizable. Supposing that ionic vibration are a weak factor in the pairing of electrons, the mathematical study of coherent fluctuations and its measurable consequences is important in prediction of and understanding the mathematics of non-linearity that has correspondence principle to linear regime