A Study of Tapping Mode Trajectories in an AFM

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Abstract

In an effort to aid in the understanding of the nonlinear dynamics of the trajectories followed by an Atomic Force Microscope (AFM), I have written an interactive java applet simulator using a simple inelastic billiard model developed by Cvitanović and Paškauskas. We study the trajectories followed by the tip of the AFM as a function of its physical parameters and initial conditions. The model represents the AFM as the addition of two harmonic oscillators vibrating independently in the vertical and horizontal planes. The moving surface imaged by the AFM is modeled as a time-periodic sinusoid. The attractors in this system can be strange attractors (recurrent and aperiodic), stable periodic trajectories, and possibly also attracting 2-tori. Once we have an idea of the nature of these attractors, we iterate points in their phase space vicinity to estimate their basins of attraction. We also study the basic topology of the various attractors produced in this system. The simulator is useful in developing intuition about the long term behavior of different AFM arrangements, and might also be helpful in developing new techniques for imaging clean periodic surfaces by atomic force friction microscopy. The program is open source, available on ChaosBook.org/extras.

I. INTRODUCTION

The Atomic Force Microscope has been invaluable in nanoscale surface imaging since its invention in 1986 by Binnig, Quate, and Gerber [**?**]. The apparatus consists of a cantilever mounted on a rigid structure with a fine tip (a few dozen atoms across) at its end. In the *tapping* mode, this tip is dragged across a surface with a given constant velocity, and the vibration due to coupling between the surface Van der Waals forces and oscillating modes of the cantilever that the AFM tip experiences as it travels along the surface is accurately detected by laser beam reflection off the cantilever. The AFM is capable of extremely high resolution surface imaging, down to individual atoms.

...Insert figure here...

The trajectories followed by the AFM in its tapping mode are, as yet, not fully understood, and are known to be chaotic. A better understanding of the AFM orbits would enable us to exert greater control over the AFM dynamics and should therefore facilitate an improvement in the efficiency of its operation.

The attractors observed in this system are often strange attractors, with dynamics recurrent (returns to a region of the phase space infinitely many times) and aperiodic ($f(t) = f(t + nT)$ is never satisfied $\forall n = 1, 2, ...$). I state this from observation only; actually proving this rigorously would be a very difficult undertaking [**?**]. We study these attractors, the conditions under which they exist, and their basins of attraction. We also study what happens immediately outside a basin of attraction.

II. MODEL

A. AFM: Free motion

We model the free motion of the AFM tip as a superposition of two harmonic oscillators vibrating independently in the vertical and horizontal planes. The two oscillators correspond to the cantilever oscillating in the vertical plane, rather softly, and the lateral vibration of the cantilever, which is relatively stiff. The equations of free motion for this very simplified model of the AFM are:

...Insert explanatory figure here with arrows indicating x- and y- motion, etc...

$$
\begin{aligned}
x(t) &= [x(t_0) - Vt_0]\cos(t - t_0) + p_x(t_0)\sin(t - t_0) + Vt \\
p_x(t) &= p_x(t_0)\cos(t - t_0) - (x(t_0) - Vt_0)\sin(t - t_0) \\
y(t) &= (y(t_0) - y_0)\cos(\epsilon(t - t_0)) + \frac{p_y(t_0)}{\epsilon}\sin(\epsilon(t - t_0)) + y_0 \\
p_y(t) &= p_y(t_0)\cos(\epsilon(t - t_0)) - \epsilon(y(t_0) - y_0)\sin(\epsilon(t - t_0))
\end{aligned} \tag{1}
$$

B. Reflection

In the billiard model of the tapping mode of an AFM, contact with the surface is assumed to be instantaneous, and microscopic friction effects are encapsulated in a *coefficient of restitution*, α. This parameter represents the ratio of the wall-normal velocity after reflection to the wall-normal velocity before reflection, and has a value between 0 and 1. Energy is lost during collision due to the transfer of the momentum of the AFM into surface vibrations (phonons); however, due to the fact that the surface is in motion (we assume that the AFM is in the rest frame), some energy is transferred back to the AFM. When the trajectory of the AFM intersects with the surface, the point of intersection needs to be calculated to a high degree of precision if the simulation is to be considered physically sound. Errors in unstable solutions are expected to grow exponentially. At present time, Newton's *bisection* method is used to ensure this precision. At the point of reflection, the new AFM dynamical equations are determined based on the "angle of incidence" of the trajectory at the surface. To determine exactly how the AFM will be reflected, we need to know the topography of the surface. In this model, the surface is assumed to be periodic, satisfying the general relation $f(x) = f(x + L)$, L being the period length of the function. We used a simple sinusoid for all of our simulations. The surface is described by the following set of equations:

$$
\begin{aligned}
y(x) &= A\sin(\frac{2\pi}{L}(x - pL)) && (2) \\
y'(x) &= A\frac{2\pi}{L}\cos(\frac{2\pi}{L}(x - pL)) && (3) \\
n_x(x) &= -\frac{y'}{(y'^2 + 1)^{\frac{1}{2}}} && (4) \\
n_x(x) &= \frac{1}{(y'^2 + 1)^{\frac{1}{2}}}, && (5)
\end{aligned}
$$

where n_x and n_y are the x- and y-components of the normal vector to the surface, respectively.

Upon reflection, the outgoing momentum is calculated as a function of the incoming momentum as:

$$\begin{pmatrix} p'_x \\ p'_y \end{pmatrix} = R \begin{pmatrix} p_x + V \\ p_y \end{pmatrix} - \begin{pmatrix} V \\ 0 \end{pmatrix},$$

where

$$R = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - (1+\alpha) \begin{pmatrix} n_x^2 & n_x n_y \\ n_x n_y & n_y^2 \end{pmatrix}$$

C. The System

The system that we simulate, then, is 5-dimensional, the five dimensions being:

x: horizontal AFM position (modulo L, the spatial period of the surface)
y: vertical AFM position
p_x: horizontal momentum
p_y: vertical momentum
t: time, scaled to the period of horizontal oscillation

There are three frequencies involved here, the vertical frequency of the AFM, ω_v, the horizontal frequency, ω_h, and the surface frequency, ω_s, relative to the AFM, which depends on the velocity with which the surface is being moved under the AFM. However, there are only two *independent* frequencies, so we normalize the surface frequency to 1 and represent the other frequencies in terms of this frequency, therby eliminating ω_s as a direct parameter. The physical values for these frequencies were obtained from Elisa Riedo's group at the picoForce Laboratory at Georgia Tech:

$$\omega_h = 442MHz$$
$$\omega_v = 35MHz$$

The AFM dimensions defined previously and the following parameters are used to completely define the system.

α: co-efficient of restitution in AFM-surface interaction
y_0: equilibrium point of vertical AFM oscillation
V: Shear velocity of the surface relative to the AFM
ϵ: Spring ratio of ω_v to ω_h

We assume some of these parameters to be constant in our simulations while we vary across the others. For example, it is reasonable to assume that α remains relatively constant across a surface. Certainly, there will be variation, and we know very little about the precise energy losses in this system, but it is safe to assume that for a locally homogenous surface, the variations in this parameter will be minimal. Other parameters that we take to be constant are y_0 and ϵ. The parameter t gives direction to the evolution of the system, but vanishes from the phase space when a mapping such as a Poincaré section is used. Therefore, we have a 4-dimensional phase space defined by x, y, p_x, and p_y.

III. THE SIMULATOR

I have written a Java simulator for the AFM impact oscillator system using the model described above. The advantages that such a simulator possesses over traditional C implementations are those of convenience and portability. When properly configured, it will be a very useful tool for conducting experiments in this system. The simulator has four major components:

1. AFM Animation: shows a rudimentary animation of what the actual AFM might look like as it maps the surface

2. $x(t), y(t)$: shows the trajectory over long periods of time

3. Phase space map (Stroboscopic or Poincaré section): plots (x, p_x) or (y, p_y) repeatedly either at a constant time interval, t_{strobe} (for stroboscopic map) or when a specific event happens, such as reflection off the surface (for Poincaré section)

4. Accumulated $x(t), y(t)$: gives a "long exposure" picture of the trajectory

A. Functionality

The simulator is currently still in a relatively inchoate state, and will likely experience significant revision and modification over the course of the next month or so. Some useful tools currently available include the *Select*, *Probe*, and *Get* functions.

The Select tool allows the experimenter to select a point in the visible phase space (in Window 3) which will represent the new initial conditions of the AFM, and the simulation will be restarted using these new values (the values will also be filled in in the Control Panel, so that interesting results may be recorded). The "invisible" phase space conditions (those 2 parameters that are not visible in the 4-dimensional phase space; only two parameters may be plotted at a time) will be reset to initial values used for the previous simulation.

The Probe tool is an extension of the Select tool. Rather than pick a single point, it allows the experimenter to pick a whole region of initial conditions across which the simulator will *scan*, outputting points to the map in a different color for each new set of initial conditions used. Currently, this function only scans across two parameter values. A combination of the Select tool, used in one half-space, and the Probe tool, used in the other half-space, will yield similar functionality.

The Get tool is available as a convenience to the experimenter who would like to see what is "really happening" at a particular observed point in time. In Window 2, if some interesting behavior is observed for some large t, rather than wait for the AFM animation to "catch up", the experimenter may use the Get function to tie the state of the animation window to the AFM at that value of t.

B. Interpreting Simulator Data

Remember to mention that t_{strobe} = total time to traverse a single period of the surface $= L/V$, $L = 1$ in our case. Also, how to convert this time unit into physically meaningful units (ms...).

IV. RESULTS

We found that for low values of the restitution coefficient α (whose true experimental value is, as yet, unclear), there is a prevalence of periodic-finding trajectories such as the one in figure 1 (see Appendix C for a method of obtaining a periodic point from such trajectories). At higher values of α, stable periodic orbits become increasingly rare, until beyond a certain value, it becomes impossible to find periodic points simply through observation and simulation.

Keeping all other values constant, there is a certain "critical value" of α below which an orbit tends to be a stable, attracting region, and above which the orbit yields a 2-torus or strange attractor. For the default values used in the simulator (see Appendix D), the critical value turned out to be around $\alpha = 0.6445$. At this value, an oval, quasiperiodic orbit, shown in Figure 3 below, was observed.

...Insert quasiperiodic orbit picture here...

FIG. 1: Quasiperiodic orbit for $\alpha = 0.6445$

The stable periodic attractor in Figure 1 was obtained using the same default values and a value of restitution below the critical value.

When the equilibrium point y_0 of vertical AFM oscillation was slightly raised from 0.0 to 0.1, it resulted in chaotic behavior, with the dynamics of the AFM becoming extremely unpredictable. However, although unpredictability will mean less control over imaging, it was observed that the AFM's chaotic motion yielded a "better," more balanced image of the surface than in other cases when the presence of an attractor caused the tip to land on the same region of the periodic surface on each bounce. y_0 can be raised in experiment by raising the AFM apparatus or in some way reducing the downward force on the AFM tip. Raising y_0 would also have the effect of reducing the vertical momentum at surface impact,

which should improve the useful lifetime of the AFM tip. Damage from collisions over time mean that the tip needs to be replaced periodically.

Increasing the shear velocity V had the effect of creating multiple attracting/ repelling points on the stroboscopic map (we only found repellors, but there is no reason to believe that attractors do not exist for high V). However, these should be interpreted as a single attractor/ repellor, rather than the multitude that they appear to be.

A. Conclusions

The AFM is a very rich system with widely varying behavior. For low values of the coefficient of restitution α, the system seemed predominantly stable. Stability in a system is good because it means that it can be more easily controlled, since the small variations that are likely to occur during experiment will not affect the behavior of the AFM. This system is inherently controllable for low restitution. For higher values of α, its dynamics are more unstable and less predictable, but chaotic orbits seemed to exhibit more "fairness" in surface imaging, when compared with stable attractive orbits, where interaction with the AFM was enjoyed only be a single region on the periodic surface.

V. FUTURE DIRECTIONS

With the implementation of a function to calculate the force experienced by the AFM tip at any instant, it will be possible to obtain a plot of the force in the system over time (force can be calculated simply as $F = \frac{dp}{dt}$). From this, one may extract data such as average force over N iterations, where 'N' may be specfied by the user. Since force in the AFM is measurable in the lab, it should be possible to test the predictions of this model against experiment, and therby determine the utility of the model. Also, if the model is found to be accurate, we can use it to estimate several features in the AFM system. For example, the energy losses in the system, quantified by the coefficient of restitution α, can be determined. One way to do this would be to determine force in the AFM over many iterations for different values of α in the simulator, and then compare this data with experiment to determine which value of α in the simulator corresponds to the real data.

Also, if the model is found to be effective in predicting the dynamics of the AFM, we

can use it to devise better algorithms for AFM use. For example, it is likely that one would like to minimize y-momentum during AFM operation because it reduces the velocity during impact with the surface (and hence reduces damage to the AFM tip), and also because one would like to spend more time interacting with the surface than hanging uselessly in the air. It might also be the case that, in order to improve imaging rate, the shear velocity V would need to be maintained at a relatively high value. However, for larger values of V, we lose surface resolution. This becomes a problem of optimization: an optimal trade-off between speed and resolution can probably be derived from extensive simulation.

...merge some of these appendices...

Appendix: How to use the simulator

Blue circle marks initial point. How to use tools. Click tool, then click map. Buttons control individual windows and there are global control buttons to control all four windows. How to use Probe.

Appendix: "Default" values used in the simulator

The default values used in the simulator were:

$$\alpha = 0.8$$
$$x = 0.018038553$$
$$y = 0.59851194$$
$$p_x = 0.0044457336$$
$$p_y = 0.045538494$$
$$y_0 = 0.0$$
$$V = 0.025836841$$

The above values are used as a physically realistic reference from which to start when varying parameters. They are within the range of values likely to be found in experiment.

Appendix: Sample Simulator Code (maybe structure of simulator? Class descriptions)

Give link to chaosbook.org/extras

Appendix: Finding periodic points in stable periodic-finding orbits

This section describes a method of using the simulator to obtain a periodic point when a stable periodic-finding orbit has been discovered. Such an orbit is characterized by "spiralling-in" of points in the phase space map (see Figure AX below).

First, one would have to zoom into the center of the spiral in the $x - px$ section of the map and select one of the points near the center. Then, one would have to switch to the $y - py$ section and repeat this procedure (Note: the "Clear" button is very useful here to determine where the point(s) of attraction lie(s).

If this is repeated a few times, getting closer and closer to the center of attraction each time, a periodic point can be obtained (since we are limited by machine precision, the "periodic point" will resemble a small circle of points at a magnification level of 10^{-14} or so).

Appendix: Some interesting results and the conditions that produce them

References

[1] P. Cvitanović et al. *Classical and Quantum Chaos*, 2005, e-book. http://chaosbook.org

[2] Binnig, Gerber, et. al. *Atomic Force Microscope*, 1986

...add more sources later...