Modeling Atomic, Dynamical Friction Using an Inelastic Impact Oscillator

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Abstract

Kinetic friction experienced by the tip of a Friction Force Microscope (FFT) is modeled by a 2-dimensional impact oscillator. We derive the equations of motion and linearized stability matrix to study the dynamics of a tip being pulled across a 1-dimensional periodic atomic "washboard" at constant velocity. For experimentally realistic parameter values the tip can bounce chaotically. We apply the periodic orbit theory in these chaotic regimes to evaluate the kinetic friction coefficient, and compare the result with numerical simulations.

1 Introduction

An impact oscillator is a system which has a forcing function driving a particle to repeatedly impact a solid barrier. The impact oscillator has been an important system to study for both engineers and physicists. For engineers, it has such applications as earthquake vibrations [1], articulated mooring towers [2], and engine rattling [3]. Fermi investigated the same system when dealing with cosmic rays impacting the atmosphere [4]. The impact oscillator is also ideal for studying the dynamics of a disapative chaotic system. It is conceptually easy to understand, yet there is still much to investigate.

Here we shall study a particular type of impact oscillator which models the motion of a friction force microscope tip (FFT) over a clean atomic surface. Consider a particle bouncing on a two-dimensional, infinitely long, infinitely dense table with a given periodic surface. The FFT is moving in a harmonic potential due to a combination of a vertical and a horizontal spring. The horizontal potential is translating at a fixed velocity, v_c. The tip is assumed to bounce off the surface with a fixed coefficient of restitution, resulting in energy loss at each collision. There may also be energy loss tangent to the surface [5] due to some energy absorbtion into the surface, resisting the translational motion along the surface.

This model is important to study because of its inherent connection to microscopic friction. Although Tomlinson's model [6] is the most widely used for approximations to the FFT motion, our model more closely follows the more realistic Gyalog-Thomas model [7]. In this paper we study the regime in which the FFT moves across a surface with a velocity large enough to bounce chaotically off of it.

The goal is to determine whether the chaotic bouncing can occur in the experimentally accessible parameter ranges. We will do this by studying the bifurcations that take place as the parameters are varied. The most convenient variable parameter is the FFT arm velocity. The impact oscillator will be recast into a billiard system, a 3-dimensional Poincaré map will be constructed, and

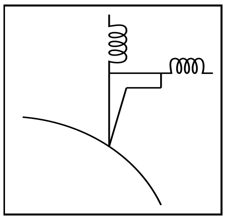


Figure 1: Simplified Friction Force Microscope

the linear stability of trajectories studied. The periodic orbit theory will be used to compute the statistical diffusion, yielding a value for kinetic friction. A few additional facets to play with will be using a Poincaré map defined by the maximum height the ball reaches (zero vertical velocity) versus the previous maximum height. This work will be a natural extension to the work done by Berg and Briggs [8].

The ultimate goal is to understand the impact system well enough to be able to compute the coefficient of kinetic friction using periodic orbit theory.

2 Inelastic Impact Oscillator

2.1 Above the Table

We model the atomic surface by a sinusoid

$$C = A \ \sin(\frac{2 \ \pi \ x}{a}) \ , \tag{1}$$

where A is the atomic height, and a is the lattice spacing. With the FFT arm velocity given by v_c, the vertical equilibrium point by Y_e, potential by U, with spring constants k_x, k_y, and mass m, the potential of the free FFT, not in contact with the surface is given by given by:

$$\begin{aligned} U_x &= \frac{1}{2}k_x(x - v_c t)^2 \\ U_y &= \frac{1}{2}k_y(y - Y_e)^2 \end{aligned} \tag{2}$$

Neglecting gravity, the forces on the particle while above the table are given by:

$$m\ddot{x} = -k_x x + k_x v_c t$$
$$m\ddot{y} = -k_y y + k_y Y_e$$

It follows that the horizontal and vertical components of the trajectory are given by the two oscillations

$$x(t) = A_x \ \sin(\omega_x \ t) + B_x \ \cos(\omega_x \ t) + v_c t$$
$$\dot{x}(t) = A_x \ \omega_x \ \cos(\omega_x \ t) - B_x \ \omega_x \ \sin(\omega_x \ t) + v \tag{3}$$
$$y(t) = A_y \ \sin(\omega_y \ t) + B_y \ \cos(\omega_y \ t) + Y_e$$
$$\dot{y}(t) = A_y \ \omega_y \ \cos(\omega_y \ t) - B_y \ \omega_y \ \sin(\omega_y \ t) \tag{4}$$

The particle is at a position x_i with velocity v_{xi}^+ and y_i with velocity v_{yi}^+ instantaneously after the impact with the surface, so the initial conditions for the i^{th} bounce are:

$$x(0) = x_i = B_x$$
$$\dot{x}(0) = v_{xi}^+ = A_x \ \omega_x + v_c$$
$$y(0) = y_i = B_y + Y_e$$
$$\dot{y}(0) = v_{yi}^+ = A_y \ \omega_y$$

Inserting these values into (3) and (4) we have an explicit formula for the FFT motion between the i^{th} and the $(i+1)^{th}$ impact.

$$x_i(t) = \frac{(v_{xi}^+ - v_c)}{\omega_x} \ \sin(\omega_x t) + x_i \ \cos(\omega_x t) + v_c t \tag{5}$$
$$y_i(t) = \frac{v_{yi}^+}{\omega_y} \ \sin(\omega_y t) + (y_i - Y_e) \ \cos(\omega_y t) + Y_e \tag{6}$$
$$t = \Delta t_i + t_i$$

2.2 Impact

We now consider the change in the tip motion due to instantaneous impact with the table. Let ϕ be the angle of the line perpendicular to the curvature of the table, with respect to the x-axis. First rotate the axis counter-clockwise by an angle $\phi - \frac{\pi}{2}$. Then apply the two damping effects at impact: one due to a coefficient of restitution of the particle, γ, and the tangential damping due to thermal excitation, μ_k. These will show up as $v_y^{'+} = -\gamma\ v_y^{'-}$ and $v_x^{'+} = \mu_k\ v_x^{'-}$. We then rotate the coordinates back clockwise by the same angle. This gives the following transform:

$$\begin{pmatrix} v_x^+ \\ v_y^+ \end{pmatrix} = \begin{pmatrix} \sin(\phi) & \cos(\phi) \\ -\cos(\phi) & \sin(\phi) \end{pmatrix} \begin{pmatrix} \mu_k & 0 \\ 0 & -\gamma \end{pmatrix} \begin{pmatrix} \sin(\phi) & -\cos(\phi) \\ \cos(\phi) & \sin(\phi) \end{pmatrix} \begin{pmatrix} v_x^- \\ v_y^- \end{pmatrix} \quad (7)$$

In the simulation, $\mu_k = 1$ and γ is taken to be nearly 1. This leads us to the following transformation:

$$\begin{pmatrix} v_x^+ \\ v_y^+ \end{pmatrix} = \begin{pmatrix} -\gamma\ \cos^2(\phi) + \sin^2(\phi) & -(1+\gamma)\ \cos(\phi)\ \sin(\phi) \\ -(1+\gamma)\ \cos(\phi)\ \sin(\phi) & -\gamma\ \sin^2(\phi) + \cos^2(\phi) \end{pmatrix} \begin{pmatrix} v_x^- \\ v_y^- \end{pmatrix} \quad (8)$$

This transform could also be found by noting that $\vec{p}^{'} = \vec{p} - (1+\gamma)(\vec{p}\dot{\vec{n}})\vec{n}$, where $\vec{n}$ is a unit vector in the direction tangent to the curve. If we then set $\vec{n}_x = \cos(\phi)\vec{e}_x$ and $\vec{n}_y = \sin(\phi)\vec{e}_y$, we retrieve the same set of equations.

2.3 Linear Stability

All the necessary tools are in our bag to find the linear stability matrices of our system. There are two types of linear stability matrices to find. The first is for the motion while the particle is in transit above the table, which will be referred to as $\mathcal{J}_T$. The second describes the instantaneous change of linear stability at impact, called here $\mathcal{J}_R$. The latter shall be described first, as it requires intuition, rather than mathematical rigger.

The foundations for the theory to follow are based on the principles defined here. The particle has a coefficient of restitution, $\gamma <= 1$ which is the factor by which the velocity is damped normal to the surface. Let the phase coordinates be chosen as $\vec{x} = (x', z, p_x', p_z)$. For ease of calculations, the mass is set equal to 1. Let $x' = x - v_c\ t$, with x as defined above, putting us in the frame of the moving support. Let $z = y - Y_e - T$, where z is then the height above the table, with respect to the equilibrium of the FFT. v_x; v_z are their respective momenta.

As the simplest example, consider a flat, motionless table, and two particles bouncing vertically off of it. There is a variation of position along the flow, normal to the flow, and there is also a small variation of their velocities along the flow. The first particle impacts the table at some time τ_1, and slows down to a velocity $v_z^+ = -\gamma v_z^-$. The second particle continues at v_z^- until it impacts the table at time τ_2, slowing down to $v_z^+ = -\gamma v_z^-$. We now know $\delta v_z^+ = -\gamma \delta v_z^-$. The difference in time,

$$\Delta\tau = \tau_2 - \tau_1 = \frac{\delta z^-}{\delta v_z^-}$$

Which implies

$$\delta z^+ = \frac{\delta z^-}{\delta v_z^-} * \delta v_z^+$$

but since $\delta v_z^+ = -\gamma \delta v_z^-$, we have $\delta q_z^+ = -\gamma \delta q_z^-$.

Now take the particles to impact the table at some angle ϕ. We take the velocity tangent to the surface to remain constant. Because the velocity stays in the same direction and the ordering of two nearby points remains the same, the matrix equation is given by:

$$\begin{pmatrix} \delta x^+ \\ \delta v_x^+ \\ \delta z^+ \\ \delta v_z^+ \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -\gamma & 0 \\ 0 & 0 & 0 & -\gamma \end{pmatrix} \begin{pmatrix} \delta x^- \\ \delta v_x^- \\ \delta z^- \\ \delta v_z^- \end{pmatrix}$$

the linear stability matrix for reflection off a flat table at some angle ϕ is then given by:

$$\mathcal{J}_R = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -\gamma & 0 \\ 0 & 0 & 0 & -\gamma \end{pmatrix}$$

Note that the Hamiltonian of a particle attached to a spring in the y and x directions, yet uncoupled is given by:

$$\mathcal{H}_x = \frac{p_x^2}{2m} \;+\; \frac{1}{2}m\omega_x^2(x - v_c\ t)$$
$$\mathcal{H}_y = \frac{p_y^2}{2m} \;+\; \frac{1}{2}m\omega_y^2(y - Y_e)$$

Transforming these to the coordinates designated above, the solution to our equations of motion are:

$$\begin{aligned}
x^- &= x^+ \cos(\omega_x t) + \frac{v_x^+}{\omega_x}\sin(\omega_x t)\\
v_x^- &= -\omega_x x^+ \sin(\omega_x t) + v_x^+ \cos(\omega_x t)\\
z^- &= z^+ \cos(\omega_y t) + \frac{v_z^+}{\omega_y}\sin(\omega_y t) - A\sin(\frac{2\pi}{a}(x^- + v_c t)\\
v_z^- &= -\omega_y z^+ \sin(\omega_y t) + v_z^+ \cos(\omega_y t) - \frac{2*\pi*A}{a}((v_x^- + v_c)\cos(\frac{2\pi}{a}(x^- + v_c t))
\end{aligned}$$

Taking the infintesimal variations, setting m=1, with τ as the time of flight, and small angle approximations then gives:

$$\begin{aligned}
\delta x^- &= \delta x^+ \cos(\omega_x \tau) + \delta v_x^+ \frac{\sin(\omega_x \tau)}{\omega_x}\\
\delta v_x^- &= -\omega_x \delta x^+ \sin(\omega_x \tau) + \delta v_x^+ \cos(\omega_x \tau)\\
\delta z^- &= \delta z^+ \cos(\omega_y \tau) + \delta v_z^+ \frac{\sin(\omega_y \tau)}{\omega_y} - \frac{2*\pi*A}{a}(\delta x^+ \cos(\omega_x \tau) + \delta v_x^+ \frac{\sin(\omega_x \tau)}{\omega_x})\\
\delta v_z^- &= -\omega_y \delta z^+ \sin(\omega_y \tau) + \delta v_z^+ \cos(\omega_y \tau) - \frac{2*\pi*A}{a}(-\omega_x x^+ \sin(\omega_x \tau) + v_x^+ \cos(\omega_x \tau))
\end{aligned}$$

This implies a transit linear stability matrix like:

$$\mathcal{J}_T = \begin{pmatrix}
\cos(\omega_x\ \tau) & \frac{\sin(\omega_x\ \tau)}{\omega_x} & 0 & 0\\
-\omega_x\ \sin(\omega_x\ \tau) & \cos(\omega_x\ \tau) & 0 & 0\\
-\frac{2\pi A}{a}\cos(\omega_x\ \tau) & -\frac{2\pi A}{a}\frac{\sin(\omega_x\ \tau)}{\omega_x} & \cos(\omega_y\ \tau) & \frac{\sin(\omega_y\ \tau)}{\omega_y}\\
\frac{2\pi A}{a}\ \omega_x\ \sin(\omega_x\ \tau) & -\frac{2\pi A}{a}\cos(\omega_x\ \tau) & -\omega_y\ \sin(\omega_y\ \tau) & \cos(\omega_y\ \tau)
\end{pmatrix}$$

Note that taking ω_y and ω_x to be very small (i.e. free particles) this reduces to a nice free particle stability matrix. Also note that for $v_c = 0$ and $\gamma = 1$ the determinant of the linear stability matrices are 1.

Another possibility of phase coordinates is to choose $x = (q_{||}, q_T, p_{||}, p_T)$. For ease of calculations, the mass is set equal to 1. The variation is then given by $\delta x = (\delta q_{||}, \delta q_T, \delta v_{||}, \delta v_T)$, where $\delta q_{||}$ is the variation along the flow, δq_T is the variation normal to the flow, and $\delta v_{||}, \delta v_T$ are their respective momenta.

Recall the analysis of the first example of a ball impacting a motionless flat table. Now take the particles to impact the table at some angle ϕ. From simply geometry we see that

$$\frac{\Delta z}{\sin(\phi)} = \frac{\delta q_T^-}{\sin(\frac{\pi}{2} - \phi)} = \frac{\Delta x}{\sin(\frac{\pi}{2})}$$

which implies that $\Delta z = \delta q_T^- \ \tan(\phi)$. Now

$$\delta q_{||}^+ = \frac{\Delta z \ (\delta v_{||}^- - \delta v_{||}^+)}{\delta v_{||}^-} = \Delta z \ (1-\gamma) = \delta q_T^- \ (1-\gamma) \ \tan(\phi)$$

Which gives:

$$\delta q_{||}^+ = \gamma \delta q_{||}^- + \delta q_T^- \ (1-\gamma) \ \tan(\phi)$$

The linear stability matrix for reflection off a flat table at some angle ϕ is then given by:

$$\mathcal{J}_R = \begin{pmatrix} \gamma & 0 & (1-\gamma)\tan(\phi_k) & 0 \\ 0 & \gamma & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

More analysis is left for future study.

2.4 The Elementary Domain

A nice elementary domain is always an important tool for cyclists, if it can be found. It is an axiom of this project that the surface is periodic. This allows for a natural elementary domain to be defined as follows: let the table to be the bottom boundary, and let one atomic period be bounded by two energy conserving walls. Consider the table composed of a sinusoid, as in 1. The elastic walls will then be placed at $x^{'} = 0$ and π. There will be no boundary at the top. This setup will have the same dynamics as that of the original system. See 2. Sadly, because there are springs working in each direction, there are no pruning rules for this setup.

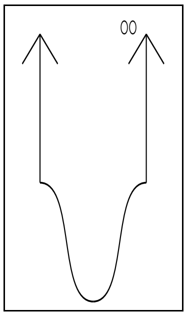


Figure 2: The Elementary Domain

2.5 The Simulation

The simulation code for the trajectories is given in Appendix A. The parameters chosen for the simulation are in accordance with what can be attainable in the laboratory. The natural frequency for the vertical spring is $\omega_y = \sqrt{\frac{k_y}{m}} = 35\ KHz$, the horizontal spring's natural frequency is $\omega_x = \sqrt{\frac{k_x}{m}} = 442\ KHz$.. The FFT arm is bounded between $1\ \frac{nm}{s}\ <\ v_c\ <\ 50\ \frac{\mu m}{s}$. The mass of the tip is $m = 408ng$.

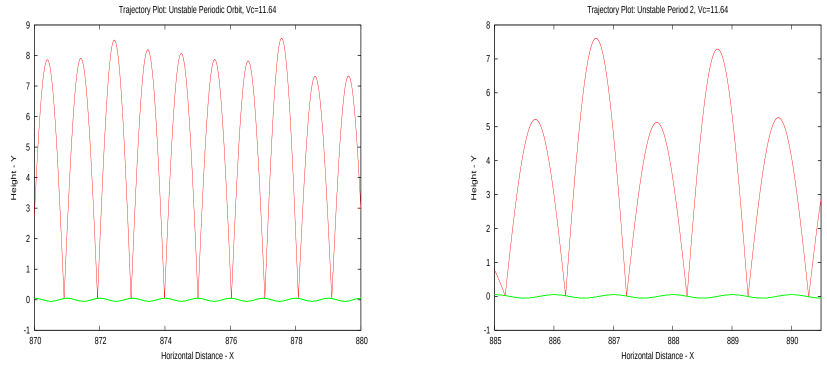


Figure 3: (a) Unstable 1-Cycle (b) 2-Cycle

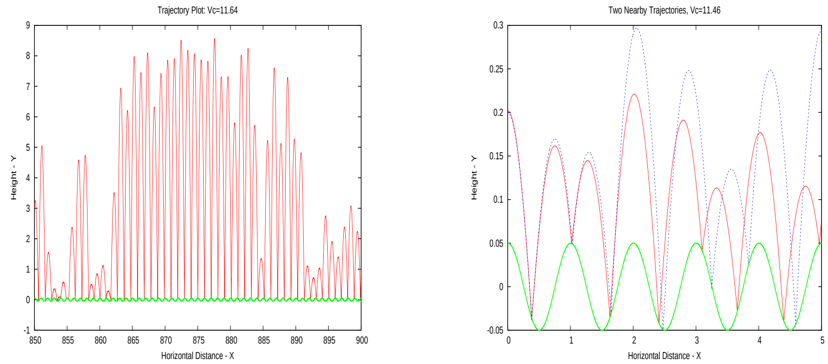
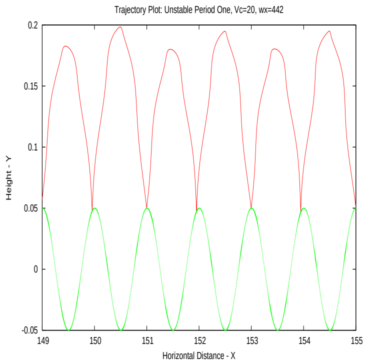


Figure 4: (a) Long-Term Dynamics (b) Rapid Separation



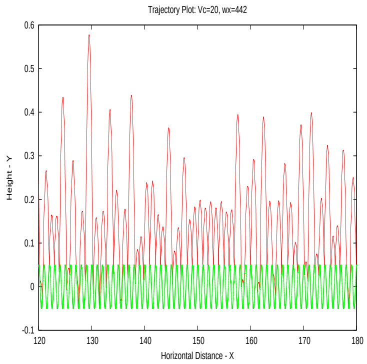


Figure 5: (a) Unstable 1-Cycle (b) Long-Term Trajectory

The first set of pictures are taken with $\omega_x = \text{inf}$, $\gamma = 1$, which is a constrained particle. The arm velocity is at 11.64 $\frac{\mu m}{s}$. The first three are of the trajectory and its unstable cycles, the fourth is of two nearby conditions with $x_0 = 0, y_0 = 0.2, v_{x0} = 0, v_{y0} = 0$ and $x_0 = 0, y_0 = 0.202, v_{x0} = 0, v_{y0} = 0$.

The next set of pictures are taken with $\omega_x = 442KHz$, $\gamma = 0.9$. Note the behaviour becomes vastly more complex. The first pictures describe the same plots as above but with $v_c = 20\frac{\mu m}{s}$. The fifth and sixth pictures are of the Poincaré sections when $v_y = 0$ and when the ball impacts the table, respectively.

A Source Code

```
      program trajImpOsc
!
!     ****************
!     This program is the main part to calculate the trajectories of a
!     ball bouncing off a table with some periodic defect.  The ball
!     loses energy due to friction and the coefficient of restitution,
!     and gains energy from a constant drift velocity and a spring system.
!     ****************
      integer :: i,j,dp,flag,k
      parameter (dp=1000)
      real*8 :: wx,wy,vc,ye,g,muk,amp,tp
      real*8 :: vxi,vyi,xi,yi,t,vxt,vyt,taby
      real*8 :: xt, yt, pi, a, roo, rot, rtt
      real*8 :: phi,sf,dc,dy,dt,xe,srt
!     ****************
      open(unit=5,file='traj.inp',status='unknown')
      read(5,*) wx
      read(5,*) wy
      read(5,*) ye
      read(5,*) vc
      read(5,*) g
      read(5,*) muk
      read(5,*) amp
      read(5,*) a
      close(5)
!     ****************
      pi=4.d0*(datan(1.d0))
      dt=7000.d0
      vxi=0.d0
```

```
vyi=0.d0
xe=0.d0
xi=0.d0
yi=0.2d0
sf=0.d0
srt=2*pi/a
open(unit=10, file='traj.txt',status='unknown')
open(unit=20, file='phase.txt',status='unknown')
open(unit=30, file='eqs.txt',status='unknown')
do j=1, dp
tp=dt
i=1
t=2.d0/tp
flag=0
do while (flag==0)
  xt=(vxi-vc)/wx*dsin(wx*t)+(xi-xe)*dcos(wx*t)+vc*t+xe
  yt=vyi/wy*dsin(wy*t)+(yi-ye)*dcos(wy*t)+ye
  vxt=(vxi-vc)*dcos(wx*t)-(xi-xe)*wx*dsin(wx*t)+vc
  vyt=vyi*dcos(wy*t)-(yi-ye)*wy*dsin(wy*t)
  taby=amp*dcos(srt*xt)
  dy=yt-taby
  if (abs(dy).lt.0.00001d0) then
    xi=xt
    yi=taby
    xe=xe+vc*t
    dc=-amp*srt*dsin(srt*xt)
    phi=datan(-1.d0/dc)
    if (phi.lt.0.d0) phi=phi+pi
    write(30,*) "y=",(dc),"*x+",yi-dc*xi, 180.d0*phi/2.d0*pi
    roo=(g+muk)*dcos(phi)**2
    rtt=(g+muk)*dsin(phi)**2
```

```
    rot=(g+muk)*dcos(phi)*dsin(phi)
    vxi=vxt-roo*vxt-rot*vyt
    vyi=vyt-rot*vxt-rtt*vyt
    if (j.gt.899) then
    write(10,*) sf, xt, yt, taby
    write(20,*) xt, yt, vxt, vyt
    endif
    flag=1
    sf=sf+1.d0/tp  ! undiscretised time
  elseif (dy.lt.0.d0) then
     k=k+1
     i=i-1  ! time which is reset at each bounce
     t=t-1.d0/tp
     sf=sf-1.d0/tp  ! time which is not reset
     tp=tp*2.d0
  else
     i=i+1  ! time which is reset at each bounce
     t=t+1.d0/tp
     sf=sf+1.d0/tp
     if (j.gt.899) then
     write(10,*) sf, xt, yt, taby
     write(20,*) xt, yt, vxt, vyt
     endif
  endif
enddo
enddo
close(30)
close(20)
close(10)
stop
end
```

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