Modeling Atomic, Dynamical Friction Using an Inelastic Impact Oscillator

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July 26, 2004

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 [[1], [2]] for both engineers and physicists. For engineers, it has such applications as earthquake vibrations [3], articulated mooring towers [4], and engine rattling [5]. Fermi investigated the same system when dealing with cosmic rays impacting the atmosphere [6]. It also has been used to study more recent topics in physics such as granular media [7] 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 of mica. Consider a particle bouncing on a two-dimensional, infinitely long, infinitely dense table with a given periodic surface stucture. 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 [8] due to energy absorbtion into the surface, resisting the translational motion along the surface. Using more accurate tip-surface interaction models [cite papers here] is left for future study.

This model is important to study because of its inherent connection to microscopic friction. Although Tomlinson's model [9] is the most widely used for approximations to the FFT motion, our model more closely follows the more realistic Gyalog-Thomas model [10]. In this paper we study energy disapation in the regime where the tip is no longer dragging across the surface, but instead is bouncing along it. As we will show here, in certain velocity regimes the tip bounces chaotically off the surface.

The goal is to determine whether the chaotic bouncing can occur in the experimentally accessible parameter ranges and predict measurable observables

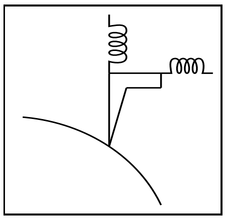

Figure 1: Simplified Friction Force Microscope

such as the mean kinetic friction. The chaotic behavior is most easily understood through the study of Poincaré maps as the velocity parameter is varied. The impact oscillator will be recast into a billiard system, a 3-dimensional Poincaré map will be constructed, and the linear stability of trajectories studied. The periodic orbit theory will be used to compute the coefficient of kinetic friction, with the suprising result that the coeffienct is a nonnegative fractal function of the FFM tip velocity.

This work will be a natural extension to the work done by Berg and Briggs [11], where 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

With the FFT arm velocity given by v_c, the vertical equilibrium point by y_e, potential by Φ, 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:

$$\begin{aligned} \Phi_x &= \frac{1}{2}k_x(x - v_c t)^2 \\ \Phi_y &= \frac{1}{2}k_y(y - y_e)^2 \end{aligned} \tag{1}$$

Neglecting gravity and coupling between horizontal and tensile motions, the forces on the particle are:

$$m\ddot{x} = -k_x(x + v_c t)$$
$$m\ddot{y} = -k_y(y + y_e)$$

So that the horizontal and vertical components of the trajectory are a linear superposition of two uncoupled harmonic motions,

$$x(t) = A_x \ \sin(\omega_x t - \Omega_x) + v_c t$$
$$\dot{x}(t) = A_x \ \omega_x \ \cos(\omega_x t - \Omega_x) + v_c \tag{2}$$
$$y(t) = A_y \ \sin(\omega_y t - \Omega_y) + Y_e$$
$$\dot{y}(t) = A_y \ \omega_y \ \cos(\omega_y t - \Omega_y) \tag{3}$$

where Ω_x, Ω_y are the initial phases, A_x, A_y are the oscillators' amplitudes and $\omega_i = \sqrt{\frac{k_i}{m}}$.

2.2 Atomic Surface

In the crudest approximation, we assume that the interaction between the FFM tip and the surface is instantanious (a hard billiard wall approximation). The particle is at a horizontal position x_i^+ with velocity v_i^+ and y_i^+ with velocity u_i^+ instantaneously after the impact with the surface, so the initial conditions for the i^{th} bounce are:

$$x(0) = x_i^+ = A_x \sin(-\Omega_x)$$
$$\dot{x}(0) = v_i^+ = A_x \ \omega_x \sin(-\Omega_x) + v_c$$
$$y(0) = y_i^+ = A_y \sin(-\Omega_y) + Y_e$$
$$\dot{y}(0) = u_i^+ = A_y \ \omega_y \sin(-\Omega_y)$$

Inserting these values into (2) and (3) we have an explicit formula for the FFT motion between the i^{th} and the $(i+1)^{th}$ impact.

$$x_i(t) = \frac{x_i^+}{\sqrt{1+(\frac{(v_i^+ - v_c)}{\omega_x x_i^+})^2}} \sin(\omega_x t + \tan^{-1}(\frac{x_i^+ w_x}{v_i^+ - v_c})) + v_c t \quad (4)$$

$$y_i(t) = \frac{y_i^+ - y_e}{\sqrt{1+(\frac{(u_i^+)}{\omega_y (y_i^+ - y_e)})^2}} \sin(\omega_y t + \tan^{-1}(\frac{(y_i^+ - y_e) w_y}{u_i^+})) + Y_e \quad (5)$$

$$t_{i+1} = \Delta t_i + t_i$$

2.3 Impact

We now consider the change in the tip motion due to instantaneous impact with the atomic surface. We model the atomic surface by a sinusoid:

$$C = A \ \sin(\frac{2\pi x}{a}) \ , \quad (6)$$

where A is the atomic height, and a is the lattice spacing. To see how the impact changes the velocity we use a rotation matrix aproach. We do this in a local reference frame. First, rotate the velocity by $\pi - \phi$, where ϕ is the angle of impact with respect to the normal to the surface. Apply the damping matrix, and finally rotate it back by the exit angle $\phi\prime$, which we calculate later.:

$$\begin{pmatrix} v_\perp^+ \\ v_{||}^+ \end{pmatrix} = \begin{pmatrix} \cos(\phi\prime) & \sin(\phi\prime) \\ -\sin(\phi) & \cos(\phi\prime) \end{pmatrix} \begin{pmatrix} \mu_k & 0 \\ 0 & -\gamma \end{pmatrix} \begin{pmatrix} -\cos(\phi) & -\sin(\phi) \\ \cos(\phi) & -\cos(\phi) \end{pmatrix} \begin{pmatrix} v_\perp^- \\ v_{||}^- \end{pmatrix} \quad (7)$$

In the simulation, $\mu_k = 1$. This leads us to the following transformation:

$$\begin{pmatrix} v_\perp^+ \\ v_{||}^+ \end{pmatrix} = \begin{pmatrix} \frac{\gamma}{\sqrt{\sin^2\phi + \gamma^2\cos^2\phi}} & 0 \\ \frac{(1-\gamma^2)\sin\phi}{\sqrt{\gamma^2 + \tan^2\phi}} & \sqrt{\sin^2\phi + \gamma^2\cos^2\phi} \end{pmatrix} \begin{pmatrix} v_\perp^- \\ v_{||}^- \end{pmatrix} \quad (8)$$

One approximation that is used is the coordinates of the tip-table impact is found by taking the intersection between two lines defined by the descrete points surrounding where the impact would actually happens. We have confindence in this approximation because it has been shown [12] that the full attractor will be explored.

2.4 Poincaré Map

There are two natural Poincaré maps for this problem. One is defined by the maximum height the ball reaches (zero vertical velocity). The coordinates for this plot will be the tip's longitudinal distance from last impact, its height from the surface, and the tips longitudinal velocity. The other Poincaré map of choice is similar to the one originally laid down by Birkhoff [cite his paper here] for billiard systems. The coordinates for this map are the distance along the surface from one impact to the next, the angle of impact, and the kinetic energy at impact.

[perhaps a few nice pictures here?]

2.5 Linear Stability

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2.6 The Elementary Domain

2.7 The Experimental Parameters

The simulation code to calculate the trajectories is given in Appendix A. The parameters chosen for the simulation are in accordance with what can be attainable in the laboratory and are summarized in table 1:

Table 1: Simulation and Labratory Parameters

Normal resonant freqency, free tip	$\omega_y = \sqrt{\frac{k_y}{m}} = 40\ kHz$
Normal spring rest point	$y_e = -0.05nm$
Longitudinal resonant freqency, free tip	$\omega_x = \sqrt{\frac{k_x}{m}} = 250\ kHz$
Arm Velocity	$v_c \in [1\ \frac{nm}{s},\ 50\ \frac{\mu m}{s}]$
Tip mass	$m = 408ng$
Mica lattice spacing	$a = 0.52nm$
Surface Amplitude	$ec = 0.05nm$

It is often more conveniant to work with dimensionless parameters. The most accessible experimental parameters in the lab are v_c and y_e. It follows that we use $v_c' \to \frac{v_c}{a*\omega_y}$ and $y_e' \to \frac{Y_e}{ec}$.

2.8 Dynamical Friction

Recall that the work, ΔW, required to move a box over a distance on a surface, Δs, is given by $\Delta W = F\Delta s$ where F is the frictional force. If we then say the box is being drug at constant velocity, the energy put into moving the box is given by $\Delta E_k = F\ v\ t$. A good judge of the average friction force on a macroscopic box is then $F = \lim_{t\to\infty} \frac{\Delta E_k}{v*t}$ We then consider the box on an atomic scale to be many of our particles, bouncing on the surface. We will find that the distance the box travels in some time t will be equivalent to the average distance the arm pulls one of our particles: $v_c t$. In our case, the kinetic energy loss (ΔE) only occurs at the impact due to the coefficient of restitution. The equation to find the long-time average change in energy over distance, and thereby the average friction, is then:

$$< F >= \lim_{t\to\infty} \frac{1}{v_c t} \sum_{k=1}^{N(t)} \Delta E_k \tag{9}$$

where N(t) is the number of bounces. Theory predicts that as v_c is varied within the acceptable values, one will find the average friction will not be smooth, but instead will have fractal properties. For certain arm velocities the system may exibit a high amount of friction, or it may have low friction. Numerical simulations seem to indicate that high amounts of friction happen at periodic orbits, whereas lower friction tends to occur when the impact oscillator is acting more chaotic. Consider that most of the energy is stored in the very stiff longitudinal spring (it has nearly 10 times the natural frequency then that of the vertical spring). If the impact happens just before the maximum peak of the surface, much energy will be lost due to the coefficient of restitution, and some energy will be transfered to the vertical height of the tip. This energy loss then shows up in the friction equation above. This is precisely what happens with the period one orbit as can be seen from the pictures below. If the ball is impacting at many other places along the surface, and not just near the peak, and these other places lose less energy, then the average loss of energy per impact is smaller than the period-one impacts. This results in a lower friction measurement for a chaotic orbit. The integer spacing between the peaks of the friction vs. velocity plot are due to orbits where the tip is going over 2, 3, etc. peaks of the surface before impacting it, but still has the essencial period-one behavior.

3 Conclusion

This paper explained a new model to connect studies in nanotribology to friction which happens in the macroworld. The model uses the well known impact oscillator to explain the behavior of a friction force microscope moving across a surface at such a velocity that the tip has no sliding motion but only bounces on the surface. The surface was modeled by a sinusoid and the energy loss at the surface was taken to be like that of a coefficient of restitution of a ball bouncing on a table. The energy loss per impact was summed over all impacts and divided by the distance the FFM arm moved. This equation was found by the typical energy definition of friction, which is the amount of work done to move an object a certain distance. A simulation was created to discover the wide variety of behavior associated with this model. We await experimental observations to confirm the theory.

Many advances in the theory are left to future study, such as what the actual coefficient of restitution of the tip-surface interaction actually is, or even if it is possible to model it this way. By using this model, we are ignoring any sort of surface defects, and any other energy losses due to thermal excitation. We will soon be applying other tools of chaos theory to investigate the system more.

A Art

[traj plot $g = 0.5$ $v_c = 16.3\mu m/sec$]

[poinImp plot $g = 0.5$ $v_c = 16.3\mu m/sec$]

[poiPeak plot $g = 0.5$ $v_c = 16.3\mu m/sec$]

[friction plot $g = 0.5$ $v_c = 16.3\mu m/sec$]

[parameter space plot $g = 0.5$ $v_c \in [0 : 50]\mu m/sec$]

[parameter space plot $v_c = 16.3$ $g\epsilon[0 : 1]$]

These pictures are found by running the simulation at the given parameters. The first image is a trajectory of a tip moving along the surface. The second is a Birkhoff Poincaré plot as explained above. The third is peak Poincaré plot. The forth is the friction found by using these parameters. The fifth is the friction force as velocity is varied from 0 to $50\mu m/sec$. The sixth is the friction force when the coefficient of resistution is varied from 0 to 1.

B 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
      parameter (dp=1100)
      real*8 :: wx,wy,vc,ye,g,muk,ec,tp,xa(3),ya(3),ta(3)
      real*8 :: vxi,vyi,xi,yi,t,vxt,vyt,taby,yin,xin
      real*8 :: xt, yt, pi, a, roo, rot, rtt
      real*8 :: phi,sf,dy,dt,xe,srt,nt,dsf,parisec
!     ****************
      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,*) ec
      read(5,*) a
```

```
      close(5)
!     ****************
      pi=4.d0*(datan(1.d0))
      dt=7000000.d0
      vxi=0.d0
      vyi=0.d0
      xe=0.d0
      xi=0.0d0
      yi=1.2d-10
      sf=0.d0
      srt=2*pi/a
      do i=1,2
       xa(i)=0.d0
       ya(i)=0.d0
       ta(i)=0.d0
      enddo
      xa(3)=xi
      ya(3)=yi
      ta(3)=ec
      open(unit=10, file='traj.txt',status='unknown')
      open(unit=20, file='phase.txt',status='unknown')
      do j=1, dp
      tp=dt
      i=1
      t=1.d0/tp
      flag=0
      do while (flag==0)
        call shift(xa,ya,ta)
        xt=(vxi-vc)/wx*dsin(wx*t)+(xi-xe)*dcos(wx*t)+vc*t+xe
        taby=ec*dcos(srt*xt)
        yt=vyi/wy*dsin(wy*t)+(yi-ye)*dcos(wy*t)+ye
```

```
xa(3)=xt
ya(3)=yt
ta(3)=taby
vxt=(vxi-vc)*dcos(wx*t)-(xi-xe)*wx*dsin(wx*t)+vc
vyt=vyi*dcos(wy*t)-(yi-ye)*wy*dsin(wy*t)
dy=yt-taby
if (dy.lt.0.d0) then
  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
  xin=parisec(xa,ya,ta)
  taby=ec*dcos(srt*xin)
  yin=taby
  dsf=dsqrt((xt-xin)**2+(yt-yin)**2)/dsqrt(vxt**2+vyt**2)
  t=t+dsf
  sf=sf+dsf
  vxt=(vxi-vc)*dcos(wx*t)-(xi-xe)*wx*dsin(wx*t)+vc
  vyt=vyi*dcos(wy*t)-(yi-ye)*wy*dsin(wy*t)
  xi=xin
  yi=yin
  xe=xe+vc*t
  phi=datan(-ec*srt*dsin(srt*xt))
  roo=muk*dcos(phi)**2-g*dsin(phi)**2
  rtt=muk*dsin(phi)**2-g*dcos(phi)**2
  rot=(g+muk)*dcos(phi)*dsin(phi)
  vxi=vxt*roo+vyt*rot
  vyi=vxt*rot+vyt*rtt
  if (j.ge.1000) then
  write(10,*) sf, xin, yin, taby
  write(20,*) xt-vc*t-xe, yt-ye, vxt-vc, vyt
  endif
```

```
        flag=1
        sf=sf+dsf  ! undiscretised time
      else
        i=i+1  ! time which is reset at each bounce
        t=t+1.d0/tp
        sf=sf+1.d0/tp
        if (j.ge.1000) then
        write(10,*) sf, xt, yt, taby
        write(20,*) xt-vc*t-xe, yt-ye, vxt-vc, vyt
        endif
      endif
    enddo
    enddo
    close(20)
    close(10)
    stop
    end
!
!     A subroutine to shift the array to hold the
!     last 3 points of x-position, y-position, and
!     table-position
!
      subroutine shift(x,y,s)
!
      integer :: i
      real*8 :: x(3),y(3),s(3)
!
      do i=1,2
      x(i)=x(i+1)
      y(i)=y(i+1)
      s(i)=s(i+1)
```

```
      enddo
      return
      end
!
!     A subroutine that finds the intersection
!     point of the two parabolas approximating
!     the ball and the table trajectories.
!
      function parisec(x,y,s)
!
      real*8 :: x(3),y(3),s(3),b(2),c(2),parisec
!
      b(1)=(y(3)-y(2))/(x(3)-x(2))
      c(1)=y(2)-b(1)*x(2)
      b(2)=(s(3)-s(2))/(x(3)-x(2))
      c(2)=s(2)-b(2)*x(2)
      parisec=(c(2)-c(1))/(b(1)-b(2))
      return
      end
```

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