Analysis of periodic solutions in tapping-mode AFM: An IQC approach

A. Sebastian, M. V. Salapaka
Department of Electrical and Computer Engineering
Iowa State University
Ames, IA 50014
USA

Abstract

The feedback perspective with the cantilever viewed as a linear system and the tip-sample interaction appearing as a nonlinear feedback is useful in analyzing AFM (Atomic Force Microscope) dynamics. Conditions for the existence and stability of periodic solutions for such a system when forced sinusoidally are obtained. These results are applied to the case where the AFM is operated in the tapping-mode. The near sinusoidal nature of periodic solutions is established by obtaining bounds on the higher harmonics. The concept of Integral Quadratic Constraints (IQC) is widely used in the analysis.

1 Introduction

The atomic force microscope (AFM) has contributed significantly to a variety of engineering and scientific areas. Over the years a wide range of imaging modes of operation have emerged. The tapping-mode is one of the most widely used modes in AFM operation. Many of the drawbacks of the original contact-mode imaging are overcome in this mode. In this mode, a micro-cantilever is forced sinusoidally thus inducing a periodic oscillation of the cantilever. The sample properties are inferred by analyzing the changes in the cantilever's oscillations due to the interaction between the sample and the cantilever tip.

The interaction between the tip and the sample is highly nonlinear. In the contact-mode operation the tip moves over a short range of tip-sample interaction making linear approximations valid for analysis. But in tapping-mode, the tip moves over a long range of tip-sample potential making a linear model of the interaction inadequate. Even the existence of chaotic behavior is established for models of tip-sample interaction [1].

Under these circumstances, the questions on the existence and stability of periodic solutions for tapping-mode dynamics are very relevant. Once the existence and stability are established, the questions on the near sinusoidal nature of the periodic solution become relevant. It is experimentally observed that when the tip-sample offset is relatively large, the periodic solution is almost sinusoidal. The almost-sinusoidal nature of cantilever oscillation is made use of in identifying tip-sample interaction forces [2] and in obtaining analytical expressions for frequency shift [3], [4]. Hence obtaining magnitude bounds on the higher harmonics is of great importance.

In Ref. [2], the cantilever in the presence of the sample was modeled as a linear system in feedback with a nonlinear system. The linear system models the micro-cantilever and the nonlinear system models the tip-sample interaction forces. The study of inter-connection of linear systems with nonlinear systems is a classical area in control and dynamical systems. Such systems with bounded energy input are particularly well studied (see Ref. [5], Ref. [6], Ref. [7]). But this theory doesn't account for the analysis of systems which have periodic inputs. However in this paper, we have shown that ideas from these classical approaches can be extended to the study of periodically forced feedback inter-connection of linear and nonlinear systems. Specifically the existence and stability of periodic solutions are explored. Other approaches towards establishing the existence of periodic solutions involve the use of describing functions and fixed point theorems (See Ref. [8] and Ref. [9]).

Results from Ref. [10] are used to prove the near sinusoidal nature of cantilever oscillations. Bounds are obtained on the higher harmonics. If the bounds are very small compared to the magnitude of the first harmonic then the periodic solution has to be near sinusoidal. No prior assumptions are made on the magnitude of higher harmonics in this derivation.

In the next section the cantilever dynamics is introduced. The state space formulation of cantilever dynamics will be used in most part of the paper. In section 3 criteria for existence and stability of periodic solutions are developed. Assumptions are made on the nature of tip-sample interactions. Also the problem of obtaining bounds on the higher harmonics is reduced to the problem of solving a linear matrix inequality. In section 4, the results of the previous section are applied to a cantilever model obtained experimentally.

2 Tapping-mode AFM dynamics

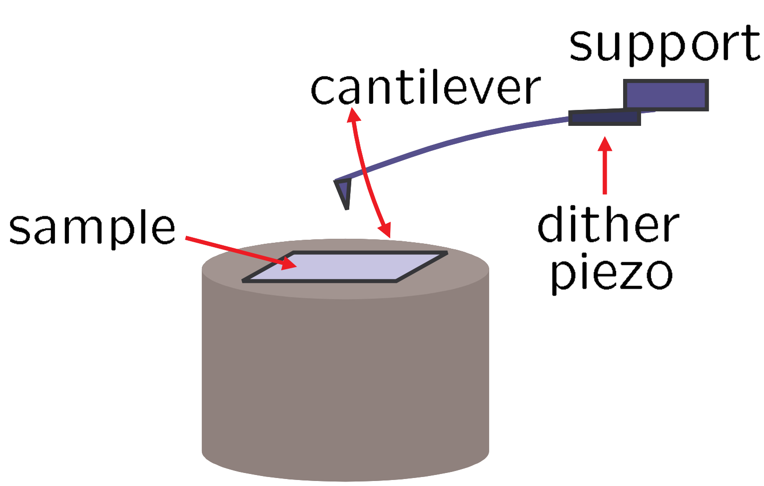

Figure 1: Schematic of the micro-cantilever in tapping-mode AFM.

In the tapping-mode operation of an AFM a dither piezo attached to the substrate that forms the support of the cantilever is forced sinusoidally (see figure 1). As the cantilever oscillates it interacts with the sample. A linear model can explain the cantilever dynamics fairly accurately whereas the tip-sample interaction is highly non-linear.

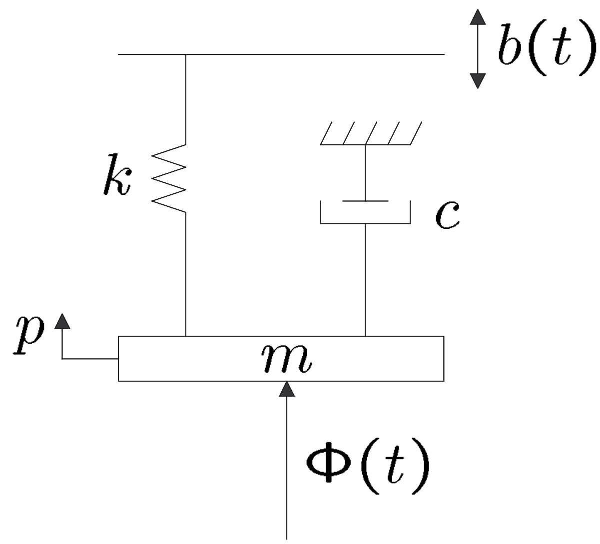

Figure 2: Second order model for the cantilever. m is the mass, k the spring constant and c the damping coefficient. $p(t)$ corresponds to the instantaneous position of the cantilever tip. Φ corresponds to the tip-sample interaction.

A spring-mass system (see figure 2) is commonly used to model the cantilever. The dynamical equation for the displacement of the cantilever is then given by,

$$m\ddot{p} + c\dot{p} + kp = kb(t) + \Phi(t) \tag{2.1}$$

where m, c and k are the effective mass, the viscous damping coefficient and the spring constant respectively of the free cantilever. Φ is the force on the cantilever due to the sample and b describes the displacement of the base of the cantilever. $p(t)$ is the instantaneous position of the cantilever tip measured from it's equilibrium position. Equation (2.1) can be recast as,

$$\ddot{p} + 2\xi\omega_0 + \omega_0^2 = g(t) + \phi(p) \tag{2.2}$$

Here $\omega_0 = \sqrt{k/m}$, $2\xi\omega_0 = c/m$, $g(t) = kb(t)/m$ and $\phi = \Phi/m$. Note that the tip-sample interaction is assumed to be a static nonlinear function of $p(t)$. The system described by (2.2) can be viewed as an inter-connection of a linear system and a nonlinear system as depicted in Figure 3. Here $G(s) = \frac{1}{s^2+2\xi\omega_0 s+\omega_0^2}$.

For the analysis in the next section, a state space formulation of (2.2) is useful. The position and velocity of the cantilever tip are chosen to be the state variables. Let $x_1 := p$,

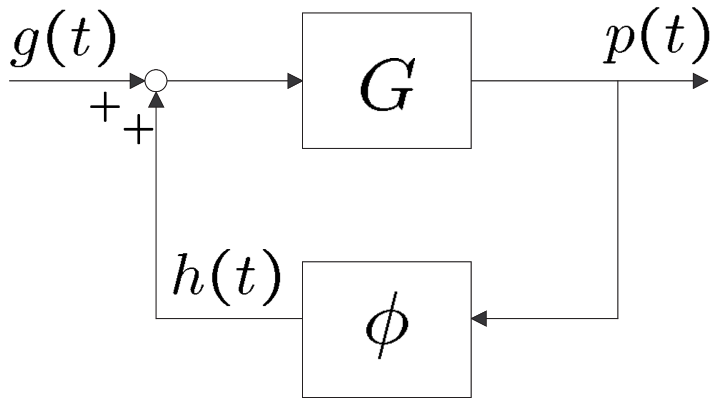

Figure 3: The feedback perspective of tapping-mode AFM dynamics. G corresponds to the linear cantilever model. ϕ is a static nonlinear model for the tip-sample interaction.

$x_2 := \dot{p}$ and $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$. Equation (2.2) can be written as,

$$\begin{aligned} \dot{x} &= Ax + B(\phi(y) + g(t)) \\ y &= Cx \end{aligned} \tag{2.3}$$

where, $A = \begin{pmatrix} 0 & 1 \\ -\omega_0^2 & -2\xi\omega_0 \end{pmatrix}$, $B = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $C = \begin{pmatrix} 1 & 0 \end{pmatrix}$. x is called the state variable, y is the output and g is the input.

Note that instead of the second order model, a higher order model can be used for the cantilever. The dynamical equation governing the motion of the tip can still be cast as (2.3). The state vector x no longer being two dimensional is the only difference.

3 Analysis

3.1 Existence and stability of periodic solutions

In this section the existence and stability of periodic solutions are established for the system described by Equation (2.3). This problem is of great theoretical interest with ramifications for the study of periodic orbits in general.

When the cantilever is not forced ($g(t) = 0$), $x = 0$ is clearly an equilibrium point for (2.3). This corresponds to the case where the cantilver tip is at it's equilibrium point and it's velocity is zero. The first step is proving the exponential stability of the equilibrium point $x = 0$ in the absence of forcing. $x = 0$ is said to be globally exponentially stable if $\exists\ \beta > 0, \epsilon > 0$ such that $\|x(t)\| \leq \beta e^{-\epsilon(t-t_0)}\|x(t_0)\|$ for any $x(t_0)$. This means the cantilever tip will approach the equilibrium point at an exponential rate if perturbed from that point. If the cantilever is fairly stiff (which is usually the case with tapping-mode AFM), it seems reasonable to assume that the equilibrium point of the cantilever tip is exponentially stable.

Unlike the traditional Lyapunov function based methods[11], the problem of proving the global exponential stability is approached in the framework of Integral Quadratic Constraints. For this the notions of input-output and input-state L_2 stability are defined next.

Definition 3.1. *(2.3) is said to be input-output L_2 stable if there exists a $K > 0$ such that $\int_0^T |y(t)|^2 dt \leq K \int_0^T |g(t)|^2 dt$ for all $T > 0$, for all $g \in L_2$ for any solution of (2.3) with $x(0) = 0$.*

Input-output stability ensures that the energy of the output is less than a constant times the energy of the input. In the following stronger notion of input-state stability the energy of the state is bounded by a constant multiple of the input energy.

Definition 3.2. *(2.3) is said to be input-state L_2 stable if there exists a $K > 0$ such that $\int_0^T |x(t)|^2 dt \leq K \int_0^T |g(t)|^2 dt$ for all $T > 0$, for all $g \in L_2$ for any solution of (2.3) with $x(0) = 0$.*

From the stronger notion of input-state L_2 stability the exponential stability of the equilibrium point $x = 0$ can be concluded. The input-state L_2 stability of (2.3) can be proven using the notion of Integral Quadratic Constraints (IQC). The following definition is needed before introducing the stability result.

Definition 3.3. *ϕ is said to satisfy the IQC defined by $\Pi = \begin{pmatrix} \Pi_{11} & \Pi_{12} \\ \Pi_{21} & \Pi_{22} \end{pmatrix}$ if*

$$\int_{-\infty}^{\infty} \begin{pmatrix} \hat{y}(j\omega) \\ \hat{\phi(y)}(j\omega) \end{pmatrix}^* \Pi(j\omega) \begin{pmatrix} \hat{y}(j\omega) \\ \hat{\phi(y)}(j\omega) \end{pmatrix} \geq 0 \tag{3.4}$$

for all $y \in L_2$.

In the above definition $\hat{y}$ corresponds to the Fourier transform of y. Π is usually called the *multiplier* that defines the IQC. For a nonlinear system which doesn't have the notion of frequency response, the IQC is a convenient way to capture the input-output energy relation over the frequency spectrum. There are quite a few IQCs available in literature[7] which use certain structural information of the nonlinearity ϕ.

Assume that $\Pi_{11} \geq 0$ and $\Pi_{22} \leq 0$. From the stability theorem[7], the input-output L_2 stability of (2.3) can be concluded if,

- the IQC defined by Π is satisfied by ϕ.
- $\exists\ \epsilon > 0$ such that $\begin{pmatrix} G(j\omega) \\ 1 \end{pmatrix}^* \Pi(jw) \begin{pmatrix} G(j\omega) \\ 1 \end{pmatrix} \leq\ -\epsilon$ for all $\omega \in R$

It is easy to show that input-state L_2 stability follows if Π is satisfied by ϕ and $\exists\ \epsilon > 0$ such that

$$\begin{pmatrix} (j\omega I - A)^{-1}B \\ I \end{pmatrix}^* \tilde{\Pi}(jw) \begin{pmatrix} (j\omega I - A)^{-1}B \\ I \end{pmatrix} \leq\ -\epsilon I \forall \omega \tag{3.5}$$

where $\tilde{\Pi} = \begin{pmatrix} C^T\Pi_{11}C & C^T\Pi_{12} \\ \Pi_{21}C & \Pi_{22} \end{pmatrix}$.

The problem of establishing the global exponential stability of $x = 0$ for (2.3) is reduced to finding an appropriate Π such that (3.5) is satisfied. This can be further reduced to the problem of solving linear matrix inequalities using the Kalman-Yakubovic-Popov Lemma [7]. Software tools are available to solve this problem [12].

If $x = 0$ is proved to be a globally exponentially stable equilibrium point of the unforced (2.3), the converse Lyapunov theorem could be invoked to obtain a C^k function W and constants α, β, γ, $\mu > 0$ such that,

$$\alpha\|x\|^2 \leq W(x) \leq \beta\|x\|^2 \tag{3.6}$$

$$\|\frac{dW(x)}{dx}\| \leq \mu\|x\| \tag{3.7}$$

$$\tag{3.8}$$

Also the theorem states that $W(x)$ when evaluated along the trajectories of the unforced (2.3) will satisfy,

$$\frac{d}{dt}W(x) = \frac{dW}{dx}(Ax + B\phi(Cx)) \leq -\gamma\|x\|^2 \tag{3.9}$$

$W(x)$ was obtained for the unforced system. The same $W(x)$ is used for the forced system using the fact the periodic forcing is magnitude bounded. If $\dot{W}(x)$ is evaluated along the trajectories of 2.3 with $g(t) \neq 0$ and $g(t) \leq M < \infty$,

$$\begin{aligned} \frac{d}{dt}W(x) &= \frac{dW}{dx}(Ax + B\phi(Cx) + Bg(t)) \\ &= \frac{dW}{dx}(Ax + B\phi(Cx)) + \frac{dW}{dx}Bg(t) \\ &\leq -\gamma\|x\|^2 + |\frac{dW}{dx}||Bg(t)| \\ &\leq -\gamma\|x\|^2 + \mu\|x\||B|M \\ &= -\gamma a(x) \end{aligned}$$

where $a(x) = \|x\|^2 - \frac{\mu|B|M}{\gamma}\|x\|$. $a(x)$ is a continuous function of x. Also there exists $\xi > 0$ such that $a(x) > 0$ for $|x| \geq \xi$. From (3.6) as $|x| \to \infty$, $W(x) \to \infty$. In short we have found a C^k function $W(x)$ for (2.3) such that

- $W(x) \to \infty$ as $|x| \to \infty$
- There exists $\xi > 0$ and a continuous function $a(x) > 0$ for $\|x\| \geq \xi$ such that for any solution $\|x(t)\| \geq \xi$, $\frac{d}{dt}(w(x(t)) \leq -a(x(t))$.

Hence there is a closed and bounded invariant set, F for (2.3), any solution of (2.3) reaches F and (2.3) has a solution $x_0(t) \in F$ bounded for $-\infty < t < \infty$ [13].

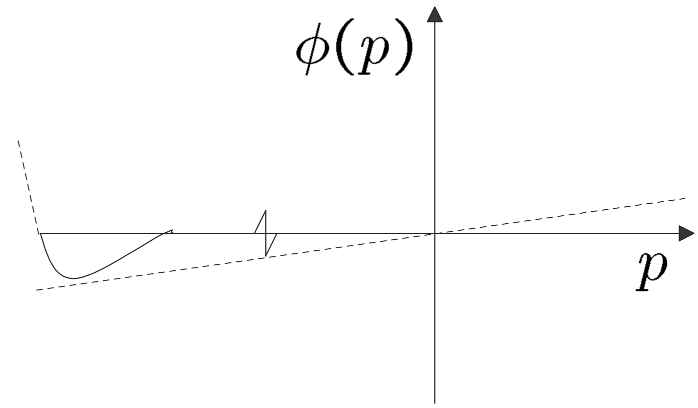

Figure 4: A typical tip-sample interaction for AFM is depicted. If the attractive forces (negative) alone are considered $\phi(p)$ can be assumed to satisfy (3.10) with an appropriate k_{sec}.

A typical graph of ϕ is shown in Figure 4. If only the attractive region is considered then there exists a k_{sec} such that,

$$0 \leq y\phi(y) \leq k_{sec}y^2 \tag{3.10}$$

With this sector condition, ϕ can be shown to satisfy the IQCs defined by

$$\Pi(\eta) = \begin{pmatrix} 0 & j\omega\eta + k_{sec} \\ j\omega\eta + k_{sec} & -2 \end{pmatrix}$$

where $\eta \in R$. If some $\Pi(\eta)$ satisfies (3.5), then (2.3) has a bounded solution $x_0(t)$ defined on $-\infty < t < \infty$. Also since g is periodic with period T, it can be shown that $x_0(t)$ is T periodic if some $\Pi(\eta)$ satisfies (3.5). Thus we have developed a criterion for the existence of periodic solutions for (2.3).

To establish the stability of $x_0(t)$ further development is needed. If the more stringent assumption of ϕ being monotonic non-decreasing is made, a condition for stability can be derived. Let,

$$0 \leq \frac{\phi(y_1) - \phi(y_2)}{y_1 - y_2} \leq k_{sl} \text{ for } y_1 \neq y_2. \tag{3.11}$$

From (3.11), it's clear that (3.10) is satisfied with $k_{sec} = k_{sl}$. Assume that the existence of a solution $x_0(t)$ is established as before. Let $x(t)$ be another solution of (2.3). Let $\tilde{x}(t) := x(t) - x_0(t)$. From (2.3) we arrive at,

$$\dot{\tilde{x}} = A\tilde{x} + B\tilde{\phi}(t, \tilde{y}), \ , \tilde{y} = C\tilde{x} \tag{3.12}$$

where $\tilde{\phi}(t, z) := \phi(z + y_0(t)) - \phi(y_0(t)$.

The global exponential stability of $\tilde{x} = 0$ of (3.12) implies the stability of the solution $x_0(t)$ of (2.3). The exponential stability of (3.12) can be established in the same way as it was done for (2.3) in the absence of $g(t)$. It is easy to verify that $\tilde{\phi}$ also satisfies the condition (3.10) with $k_{sec} = k_{sl}$. But unlike ϕ, $\tilde{\phi}$ is time-varying. Hence $\Pi(\eta)$ with $\eta \neq 0$ may not be satisfied by $\tilde{\phi}$. But $\Pi(\eta)$ with $\eta = 0$ which corresponds to $\Pi_{sl} = \begin{pmatrix} 0 & k_{sl} \\ k_{sl} & -2 \end{pmatrix}$ is satisfied by $\tilde{\phi}$. By the previous methodology if (3.5) is satisfied then we can conclude the exponential stability of $x_0(t)$. The stability of $x_0(t)$ implies $x_0(t)$ is unique. Since $g(t) = g(t+T)$, $x_0(t+T)$ is also a solution of (2.3). But uniqueness of solutions implies, $x_0(t) = x_0(t+T)$. Hence we could conclude the existence and stability of a T periodic solution for (2.3). Π_{sl} could give conservative results. But using additional properties of $\tilde{\phi}$, one could get less conservative IQCs. Having developed a paradigm for the existence and stability analysis of periodic orbits for (2.3), we move on to the study of near sinusoidal nature of the periodic solutions.

3.2 Bounds on the harmonics of periodic solutions

One of the elegant features of the tapping-mode dynamics is the near sinusoidal nature of the periodic orbits. Various attempts have been made to prove the smallness of the higher harmonics. We argued hueristically in Ref. [2] that the low pass characteristics of the cantilever subsystem leads to a near sinusoidal periodic orbit. But it is also necessary to characterize the response of ϕ to the periodic solution. The nonlinear interation force (which is also periodic) should not have large magnitude higher harmonics. The Integral Quadratic Constraints introduced earlier can be used to quantify the higher harmonics of the interaction force in terms of the harmonics of cantilever oscillation. It appears intuitive if we note that an IQC acts as a generalized "frequency response" for the nonlinearity. In this approach we are not making any prior assumptions on the smallness of the higher harmonics. This approach is better than in Ref. [14] where the author evaluates the interation forces only for the first harmonic which is equivalent to making a prior assumption on the sinusoidal nature of the periodic solution. Also in our method no analytical models are used for the interaction force.

Bounds are obtained on the higher harmonics using the above arguments. If the bounds are significantly smaller than the first harmonic, then it can be concluded that the periodic solution is almost sinusoidal. The following theorem is a modified version of one appearing in Ref. [10].

Theorem 3.1. *In Figure 2 let* $g(t) = g_1 e^{j\omega_0 t} + g_{-1} e^{-j\omega_0 t}$, $p(t) = \sum p_k e^{jk\omega_0 t}$ *and* $h(t) = \sum h_k e^{jk\omega_0 t}$. *If*

1. *ϕ satisfies the IQC defined by Π*

2. $\begin{pmatrix} G(jk\omega_0) \\ 1 \end{pmatrix}^* \Pi(jk\omega_0) \begin{pmatrix} G(jk\omega_0) \\ 1 \end{pmatrix} \leq -\epsilon$ *for all* $|k| \neq 1$.

Then for $|k_0| \neq 1$, *the bound* $|p_{k_0}| < \beta |g_1|$ *holds for all* β *that together with some* $\tau > 0$

satisfies the inequality

$$0 > \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\beta^2 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \tau \begin{pmatrix} K_1 & L_1 & 0 \\ L_1^* & M_1 & 0 \\ 0 & 0 & K_{k_0} \end{pmatrix} \tag{3.13}$$

where

$$\begin{pmatrix} K_k & L_k \\ L_k^* & M_k \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ G^{-1}(jk\omega_0) & -1 \end{pmatrix}^* \Pi(jk\omega_0) \begin{pmatrix} 1 & 0 \\ G^{-1}(jk\omega_0) & -1 \end{pmatrix}$$

For each higher harmonic of $p(t)$, we can solve the Linear Matrix Inequality (LMI) given by (3.13), and get β. β multiplied by the magnitude of forcing will be the upper bound for this harmonic. The bounds on the higher harmonics can also be used to assess the limitations on how well the tip-sample potential can be characterized.

The results from this section are used to analyze the data obtained from an experiment.

4 Application

An atomic force microscope (Multi-mode, Digital Instruments, Santa Barbara, CA) was operated in tapping mode. A silicon cantilever $225\mu m$ in length was used. The cantilver model was obtained to be $G(s) = \frac{1}{s^2+2\xi\omega_0 s+\omega_0^2}$ where $\xi = 0.0038$ and $\omega_0 = 0.4642\mu s^{-1}$. The sinusoidal forcing $g(t) = \gamma\cos(\omega_0 t)$ where $\gamma = 0.0393 nm\mu s^{-2}$. Corresponding to this forcing the amplitude of the cantilever oscillation in the absence of sample was $24nm$. Note that the cantilever oscillation will be sinusoidal in the absence of sample. ϕ corresponds to the tip-sample interaction forces.

Using the identification paradigm developed in Ref. [2], the slope of ϕ in the attractive region was estimated to be ω_a^2 where $\omega_a = 0.3029\omega_0$. It is reasonable to assume that ϕ satisfies the sector condition, (3.10) with $k_{sec} = \omega_a^2$. In fact this is a rather conservative estimate of ϕ. As we could see from Figure 3, because of the relatively large offset between the tip and the sample, a much smaller k_{sec} could satisfy the condition (3.10). Note that we are dealing only with attractive tip-sample interaction forces.

From the above discussion ϕ satisfies the IQCs defined by $\Pi(\eta) = \begin{pmatrix} 0 & j\omega\eta + \omega_a^2 \\ j\omega\eta + \omega_a^2 & -2 \end{pmatrix}$, where $\eta \in R$. For $\eta = 0.2$ it can be shown that the condition (3.5) is satisfied by $\Pi(\eta)$. This proves the existence of a $\frac{2\pi}{\omega_0}$ periodic solution for (2.3).

To test for the stability of the periodic solution, stronger assumptions are needed on ϕ. The attractive region is assumed to be long enough so that ϕ is monotonic. Also from the earlier estimation, (3.11) is satisfied by $k_{sl} = \omega_a^2$. The stability criterion developed in the previous section with the IQC defined by $\Pi = \begin{pmatrix} 0 & k_{sl} \\ k_{sl} & -2 \end{pmatrix}$ is not met with $k_{sl} = \omega_a^2$. If $\omega_a \leq 0.123\omega_0$, then the stability criterion is met. It is seen that stability of periodic solutions can be rigorously established using this Π only for weak interaction forces. Neverthless, the existence of a less conservative Π satisfying the stability criterion cannot be ruled out.

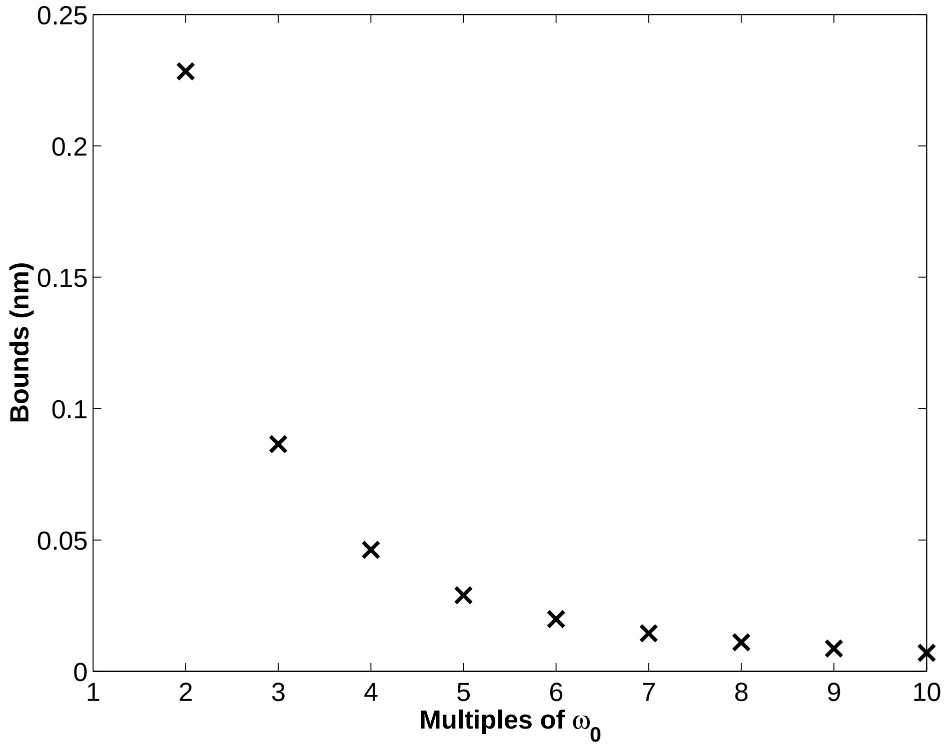

Figure 5: The higher harmonics are bounded by $\approx 0.22nm$ which is very small compared to the free oscillation amplitude of $24nm$. This proves the almost-sinusoidal nature of the cantilever oscillation.

Assuming the existence of a periodic solution, bounds are obtained on the higher harmonics using subsection 3.2. Since ϕ satisfies the IQCs defined by $\Pi(\eta) = \begin{pmatrix} 0 & j\omega\eta + \omega_a^2 \\ j\omega\eta + \omega_a^2 & -2 \end{pmatrix}$ it can be shown that the following is true.

$$0 \leq \sum \begin{pmatrix} p_k \\ h_k \end{pmatrix}^* \Pi(\eta) \begin{pmatrix} p_k \\ h_k \end{pmatrix} \tag{4.14}$$

The results obtained by applying theorem 3.1 using $\Pi(0.2)$ is depicted in Figure 5. The free oscillation amplitude of the cantilever was $24nm$. The bound on the magnitude of the second harmonic is $0.22nm$ which is very small compared to $\approx 24nm$. This conclusively proves that the cantilever oscillations are almost sinusoidal in nature.

5 Conclusion

The feedback perspective towards the analysis of tapping-mode dynamics is introduced in this paper. The cantilever sample system is viewed as a feedback inter-connection of a linear system with a nonlinear system. Stability analysis of such feedback inter-connections is extended to incorporate sinusoidal forcing. An Integral Quadratic Constraint (IQC) based approach is developed to establish the existence and stability of periodic solutions for the tapping-mode dynamics. It is possible to arrive at conditions on tip-sample interaction which ensure the existence and stability of periodic solutions. The experimentally observed, near sinusoidal nature of periodic solutions is proven by obtaining bounds on the higher harmonics. The analytical tools developed in this paper can be applied on a very general class of tip-sample interaction forces. This enables the study of complex interactions without the need for analytical models of the interaction potential.

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