Proceedings of the
44th IEEE Conference on Decision and Control, and
the European Control Conference 2005
Seville, Spain, December 12-15, 2005

Harmonic Bounds in Atomic Force Microscopy

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Abstract— **The paper addresses the problem of evaluating magnitude bounds on higher harmonics of the periodic tip oscillation in an Atomic Force Microscope (AFM). The suggested approach considers a class of nonlinearities well suited to the tip-sample interaction in AFMs, and reduces the bounding problem to an optimization problem. For a relaxation of the problem a solution in a closed form is provided and reduces the conservativeness of estimates existing in literature.**

I. Introduction

In recent years there has been a considerable progress in nanotechnology particularly propelled by instruments capable of providing atomic resolution. The Atomic Force Microscope (AFM) is one of the most widely employed instruments of this kind [1]. It can work in many different operating modes; however, in this paper, we limit ourselves to the study to the so-called "tapping" or "dynamic" mode. In such an operating mode, the AFM cantilever is periodically forced by a piezo placed under its support inducing a periodic oscillation that is naturally influenced by the interaction forces between the cantilever tip and the sample. The topography is inferred by slowly moving the cantilever along the sample surface by means of a piezoactuator and by measuring the magnitude and phase of the first harmonic of the cantilever deflection through an optical lever method as shown in Figure 1a. Towards this aim, the quasi-sinusoidal nature of cantilever oscillation is exploited. The

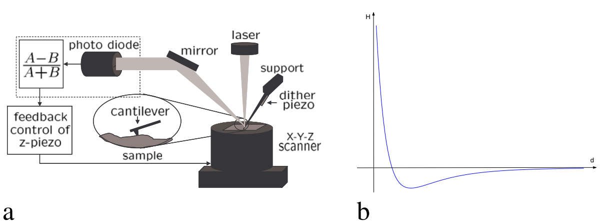

Fig. 1. (a) A typical setup of an AFM is shown. The dither piezo forces the cantilever to oscillate at its resonance frequency with certain magnitude. The deflection of the cantilever is registered by the laser incident on the cantilever tip, which reflects into a split photo-diode. The xyz-piezo scanner is used to position the sample. The deflection signal is fedback to the z-piezo to track the sample profile. The xy-piezo moves the sample in a raster scanning pattern during imaging.
(b) Qualitative behaviour of the interaction force F between the AFM tip and the sample as a function of the relative distance d. The force is strongly repulsive for small values of d while it is weakly attractive for large ones, converging to 0 as d approaches $+\infty$

quasi-sinusoidal nature of the oscillation is also employed in identifying tip-sample interaction forces [2] and in obtaining analytical expressions for frequency shifts [3], [4]. In most of the analytical studies it is assumed that the higher harmonics are small and the oscillation is assumed to be sinusoidal. Such an assumption is reasonable when large amplitude oscillations are envolved. However, the dynamic mode AFM scheme is increasingly being used in operating conditions

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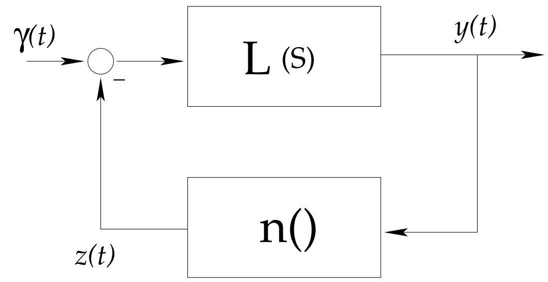

Fig. 2. AFM model in a Lur'e form

where a pure sinusoidal assumption becomes unreasonable. For example, there are proposed studies on using higher modes of AFM for imaging where evidently the higher harmonic study becomes important. Furthermore, in many high resolution studies it becomes important to study how much energy is coupled to the higher harmonics in schemes where only the first mode is utilized to explore the dynamics[5]. Hence estimating magnitude bounds on the higher harmonics is of great importance.
Upper bounds are the focus of this study since they allow to evaluate the distortion of the tip oscillation. However, lower bounds are useful since they provide an estimate on the conservativeness of the upper bounds. In [6] upper bounds on higher harmonics have been provided considering an AFM described by a Lur'e system [7] under the assumption that the tip never enters the repulsive potential. A sector nonlinearity is used to model the tip-sample interaction. Obtained bounds reveal to be relatively conservative because the shape of the tip-sample interaction can be only partially represented by a sector nonlinearity. In this paper, we similarly assume that the tip never enters the repulsive zone and we consider again a model in a Lur'e form. However, the nonlinearity describing the interaction is assumed to be zero when the tip-sample distance is greater than a fixed parameter in order to better fit the interaction force behaviour shown in Figure 1b. In addition, we assume that the first order harmonic is measurable. Under these hypotheses, upper and lower bounds on high order harmonics are provided. The paper is organized as follows. In Section II the problem of finding bounds on high order harmonics at the output of a class of nonlinear filter is defined and formalized as an optimization problem; in Section III an approach to compute harmonic bounds for an AFM model in a Lur'e form is described; Section IV shows some simulations results and summarizes the main points while in Section V all proofs are illustrated in detail.

II. Harmonic bounding as an optimization problem

We consider an AFM model defined by a feedback connection of a linear dynamic filter $L(s)$ and a nonlinear static filter $n(\cdot)$ excited by a sinusoidal signal $\gamma(t) = \Gamma\cos(\omega t + \phi_1)$ as depicted in Figure 2. In a symbolic form the system equation is

$$y = L\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)[\gamma(t) - n(y)] \tag{1}$$

where $y(t)$ is the cantilever position at the instant t. The output z of the nonlinear filter is such that $\exists\ l > 0 : y > -l \Rightarrow z = n(y) = 0$. We suppose that there exists a periodic solution $y(t)$ of the same period of the forcing. We define Y_k and Z_k as the k-th harmonic components of $y(t)$ and $z(t)$ respectively (scaled by a multiplicative factor for sake of notation)

$$Y_k := \int_{-\pi/\omega}^{\pi/\omega} y(t)\mathrm{e}^{ik\omega t}\mathrm{d}t \qquad Z_k := \int_{-\pi/\omega}^{\pi/\omega} z(t)\mathrm{e}^{ik\omega t}\mathrm{d}t.$$

We suppose that Y_1, the first harmonic component of $y(t)$ is measured and therefore it can be assumed known. Without loss of generality, we can scale and shift the time axis to obtain $\omega = 1$ and $arg(Y_1) = 0$. In addition, we assume that the interaction time $t_{\max}$ between the tip and the sample cannot be more than half period. These assumptions are not restrictive considering most operating conditions. In typical tapping mode operation the first order harmonic can be measured with good accuracy and the time of the tip-sample interaction is small when compared to the period time and the tip softly touches the sample [8]. We wish to obtain upper and lower bounds to the harmonics of $y(t)$. In other words we would like to evaluate, $\forall k \in \mathrm{N}$, $\underline{Y}_k$ and $\overline{Y}_k$ such that

$$\underline{Y}_k \leq \left|\int_{\pi}^{\pi} y(t)\mathrm{e}^{it}\mathrm{d}t\right| \leq \overline{Y}_k.$$

Towards this aim, let us consider the signal $z(t)$. Note that $|Z_1| = \left|\frac{Y_1}{L(i1)} - \Gamma\mathrm{e}^{i\phi_1}\right|$. Suppose there exist H such that $0 \leq z(t) \leq H$ and $t_{\max} < \pi$: $|t| \leq \frac{t_{\max}}{2}$ implies that $z(t) = 0$. For every harmonic of $z(t)$, an upperbound $\overline{Z}_k$ can be obtained by solving the following optimization problem:

$$\begin{array}{l} \overline{Z}_k = \max_{z(\cdot)} \left|\int_{-t_{\max}/2}^{t_{\max}/2} z(t)\mathrm{e}^{ikt}\mathrm{d}t\right| \\ 0 \leq z(t) \leq H \\ \left|\int_{-t_{\max}/2}^{t_{\max}/2} z(t)\mathrm{e}^{it}\mathrm{d}t\right| = |Z_1|. \end{array} \tag{2}$$

Consider the following lemma

Lemma II.1. *If $z(t)$ is a 2π-periodic signal then*

$$\forall k \in \mathrm{N} \qquad |Z_k| = \max_{\phi_k \in [-\pi,\pi]} \int_{-\pi}^{\pi} z(t)\cos(kt + \phi_k)\mathrm{d}t.$$

***Proof*.** See Appendix □

With the above lemma, (2) is equivalent to

$$\begin{array}{l} \overline{Z}_k = \max_{\phi_k \in [-\pi,\pi]} \int_{-\pi}^{\pi} z(t)\cos(kt + \phi_k)\mathrm{d}t. \\ 0 \leq z(t) \leq H \\ \left|\int_{-t_{\max}/2}^{t_{\max}/2} z(t)\mathrm{e}^{it}\mathrm{d}t\right| = |Z_1|. \end{array} \tag{3}$$

Moreover, the two following lemmas allow us to relax the problem (2) substituting the constraint on the first order harmonic with conditions much easier to handle.

Lemma II.2. *Let $z(t)$ be a 2π-periodic signal such that $0 \leq z(t) \leq H$. Let $0 \leq \tau_m \leq \pi$ such that*

$$H\int_{-\tau_m/2}^{\tau_m/2} \cos(t)\mathrm{d}t = |Z_1|$$

Then

$$H\tau_m \leq Z_0.$$

***Proof*.** See Appendix □

Lemma II.3. *Let $z(t)$ be a 2π-periodic signal with $0 \leq z(t) \leq H$. Let $0 < t_{\max} < \pi$ be such that if $t_{\max}/2 < |t| < \pi$ then $z(t) = 0$. Let $0 \leq \tau_M \leq t_{\max}/2$ be such that*

$$H\left\{\int_{-t_{\max}/2}^{-\frac{t_{\max}-\tau_M}{2}} + \int_{\frac{t_{\max}-\tau_M}{2}}^{t_{\max}/2}\right\}\cos(t)\mathrm{d}t = |Z_1|$$

Then

$$|Z_0| \leq H\tau_M.$$

***Proof*.** See Appendix □

With the above two lemmas problem (2) assumes the following relaxed form:

$$\begin{array}{l} \overline{Z}_k = \max_{z(\cdot)} \max_{\phi_k} \int_{t_{\max}/2}^{t_{\max}/2} z(t)\cos(kt + \phi_k)\mathrm{d}t \\ -\pi \leq \phi_k \leq \pi \\ 0 \leq z(t) \leq H \\ H\tau_m \leq \int_{t_{\max}/2}^{t_{\max}/2} z(t)\mathrm{d}t \leq H\tau_M. \end{array} \tag{4}$$

Defining $\overline{t}_{\max}(k) := \lceil k\frac{t_{\max}}{2\pi}\rceil\frac{2\pi}{k}$, we can further relax the problem extending the integration extrems and introducing an invariant property to ϕ_k-shifts as stated in the following result.

Lemma II.4. *Consider an optimization problem of the form (4). Let $t_{\max}$ be a multiple of $\frac{2\pi}{k}$. Then the optimization in (4) on the variable ϕ_k can be neglected and without loss of generality ϕ_k can be assumed 0.*

***Proof*.** See Appendix □

Letting $\phi_k = 0$, we can write a final relaxed form of the problem (2) given by:

$$\begin{array}{l} \overline{Z}_k = \max_{z(\cdot)} \int_{-\overline{t}_{\max}(k)/2}^{\overline{t}_{\max}(k)/2} z(t)\cos(kt)\mathrm{d}t \\ 0 \leq z(t) \leq H \\ H\tau_m \leq \int_{-\overline{t}_{\max}(k)/2}^{\overline{t}_{\max}(k)/2} z(t)\mathrm{d}t \leq H\tau_M \end{array} \tag{5}$$

Similarly, but with no need of any relaxing on the interval extremes, we can formulate an analogous optimization problem for lower bounds

$$\begin{array}{l} \overline{Z}_k = \min_{z(\cdot)} \max_{\phi} \int_{t_{\max}/2}^{t_{\max}/2} z(t)\cos(kt + \phi_k)\mathrm{d}t \\ -\pi \leq \phi_k \leq \pi \\ 0 \leq z(t) \leq H \\ H\tau_m \leq \int_{-t_{\max}/2}^{t_{\max}/2} z(t)\mathrm{d}t \leq H\tau_M \end{array} \tag{6}$$

A. Solution to the upper bound problem

The problem (5) can be solved by the direct application of Lemma (II.5) with $w(t) = \cos(kt)$.

Lemma II.5. *Consider the optimization problem*

$$\begin{array}{l} M := \max_{z(\cdot)} \int_D wz \\ 0 \leq z(t) \leq H \\ H\tau_m \leq \int_D z \leq H\tau_M \end{array}$$

where $z(\cdot)$ and $w(\cdot)$ are functions defined on a compact set D. Let $w(\cdot)$ also be continuous on D. Let $E_0 := \{x : w(x) \geq 0\}$ and let E be a set satisfying the property that $\xi_1 \in E$ and $\xi_2 \in D \setminus E$ implies that $w(\xi_1) \geq w(\xi_2)$. Let E also be a *union of closed intervals. If one of the following conditions is met*

$$\begin{aligned} \mu(E_0) > \tau_M \quad &\text{and} \quad \mu(E) = \tau_M && \text{(7a)}\\ \tau_m \le \mu(E_0) \le \tau_M \quad &\text{and} \quad \mu(E) = \mu(E_0) && \text{(7b)}\\ \mu(E_0) < \tau_m \quad &\text{and} \quad \mu(E) = \tau_m && \text{(7c)} \end{aligned}$$

Then it follows that $M = H \int_E w(t)\mathrm{d}t$.

Let us define $m(k) := \lceil \frac{k}{2\pi} t_{\max} \rceil$. It represents the number of periods of a $2k\pi$-periodic sinusoid in the time interval $\bar{t}_{\max}$. It is trivial to show that $\mu(E_0(k)) = m(k)\frac{\pi}{k}$. Let us define

$$\tau_{opt}(k) = \begin{cases} \tau_M & \text{if} \tau_M < \mu(E_0(k)) \\ \mu(E_0(k)) & \text{if} \tau_m \le \mu(E_0(k)) \le \tau_M \\ \tau_m & \text{if} \mu(E_0(k)) < \tau_m \end{cases}$$

Defining $E(k) := \{t : |t| < \bar{t}_{\max}(k)/2$ and there exists n in Z such that $|2n\pi - t| < \tau_{opt}/(2m(k))\}$ we find that it satisfies conditions of the Lemma (II.5). Thus, denoting with $\chi_A(t)$ the characteristic function of a set A, we find that $z(k,t) := H\chi_{E(k)}(t)$ is an optimal solution for (5) with

$$\overline{Z}_k = m(k)H \int_{\chi_E(k)} \cos(kt)\mathrm{d}t = \frac{m(k)}{k} H \int_{-\frac{k\tau_{opt}}{2m(k)}}^{\frac{k\tau_{opt}}{2m(k)}} \cos(t)\mathrm{d}t.$$

By inspection, when $m(k) = 1$, that is equivalent to $t_{\max} < \frac{2\pi}{k}$ the solution $z(t)$ is null if $|t| < t_{\max}/2$ so that it reveals optimal also for the problem (4).

B. Solution to the lowerbound problem

We can exploit the following result to solve the problem (6).

Lemma II.6. *Let us consider the problem*

$$\begin{aligned} &M = \min_{z(\cdot)} \max_{\phi_k} \int_{-t_{\max}/2}^{t_{\max}/2} z(t)\cos(kt + \phi_k)\mathrm{d}t \\ &-\pi \le \phi_k \le \pi \\ &0 \le z(t) \le H \\ &H\tau_m \le \int_{-t_{\max}}^{t_{\max}} z(t)\mathrm{d}t \le H\tau_M \end{aligned}$$

Then
If $t_{\max} \le \pi/k + \tau_m/2$ *then* $\phi_k = 0$ *and*

$$z(t) = \begin{cases} H & \text{if} \frac{t_{\max} - \tau_m}{2} \le |t| \le \frac{t_{\max}}{2} \\ 0 & \text{otherwise} \end{cases}$$

is a solution of the problem and

$$M = H \left\{ \int_{-t_{\max}/2}^{-t_{\max}/2 + \tau_m/2} + \int_{t_{\max}/2 - \tau_m/2}^{t_{\max}/2} \right\} \cos(kt)\mathrm{d}t$$

Proof. See Appendix □

Lemma (II.6) solves the problem (6) when $t_{\max} \le \pi/k + \tau_m/2$ giving as solution

$$M = H \left\{ \int_{-t_{\max}/2}^{-t_{\max}/2 + \tau_m/2} + \int_{t_{\max}/2 - \tau_m/2}^{t_{\max}/2} \right\} \cos(kt)\mathrm{d}t$$

When $t_{\max} > \pi/k + \tau_m/2$ we will assume 0 as a trivial bound.

III. Bounds on harmonics in the Lur'e system

In the previous section we have obtained bounds for a signal $z(t)$ provided that it is nonnegative, bounded by a constant H and has a support contained in a set $[-t_{\max}/2, t_{\max}/2]$ with $t_{\max} < \pi$. Let us assume that there exists Y_h such that

$$|y(t) - Y_1 \cos(t)| < Y_h.$$

With this assumption we can evaluate

$$\begin{aligned} &t_{\max} := \begin{cases} 0 & \text{if} \quad Y_1 + Y_h < l \\ \min\{2\arccos \frac{l}{Y_1 + Y_h}, \pi\} & \text{otherwise} \end{cases} \\ &H = \max_{|y| < Y_1 + Y_h} n(y) \end{aligned}$$

In this scenario it is possible to apply the results of the previous section to bound every $|Z_k|$

$$\begin{aligned} &\overline{Z}_k = \overline{Z}_k(Y_h) = H \int_{-k\tau_{opt}(k)/(2m(k))}^{k\tau_{opt}(k)/(2m(k))} \cos(t)\mathrm{d}t \\ &\underline{Z}_k = \underline{Z}_k(Y_h) = \begin{cases} H \left\{ \int_{-t_{\max}/2}^{-t_{\max}/2 + \tau_m} + \int_{t_{\max}/2 - \tau_m/2}^{t_{\max}/2} \right\} \cos(kt)\mathrm{d}t \\ \quad \text{if } t_{\max} < \pi/k + \tau_M \\ 0 \quad \text{otherwise.} \end{cases} \end{aligned} \tag{8}$$

Finally, we can evaluate bounds for $|Y_k|$ using the relation $Y_k = L(ik)Z_k$.

$$\begin{aligned} \overline{Y}_k &= |L(ik)|\overline{Z}_k(Y_h) \\ \underline{Y}_k &= |L(ik)|\underline{Z}_k(Y_h). \end{aligned}$$

It must be observed that obtained bounds are dependent on the value of Y_h that is unknown, but an estimate on Y_h can even be used (for example results in ([6]) can used as initial bound).
Using the closed loop equation (1), if Y_h is a valid bound so is $\sum_k \overline{Y}_k$. Let us define the map $T : \Re^+ \to \Re^+$ in following manner

$$Y_h(j+1) = T(Y_h(j)) = \sum_k \overline{Y}_k(Y_h(j)) \tag{9}$$

It is possible starting from a conservative bound to use results of previous section to obtain bounds on high order harmonics assuming that the first one is known. In addition, the closed loop equation allows to improve the bounds by iterating the map (9). In particular, we note that if the map T has a unique attracting fixed point $\hat{Y}_h$ in $[0, Y_h]$ then $\overline{Y}_k(\hat{Y}_h)$ is the best bound that can be obtained with this approach.
Conditions under which T is a contraction, has a single fixed point or admits more fixed points are still subject of investigation, but the fact that obtained bounds have a closed analytical form and are not evaluated numerically can allow to obtain analytical results. However, in all performed simulations, T has always exhibited a unique attracting fixed point with good converging properties.

A. Extension to the repulsive-attractive case

The described approach can be extended to obtain bounds even when the function $z(t)$ does not have a defined sign. In fact it can be split as a sum of two sign-defined functions: $z(t) = z^+(t) + z^-(t)$ where $z^+(t) \ge 0$ and $z^-(t) \le 0$. Applying separately the proposed technique to z^+ and z^- bounds on Z_k can be, for example, obtained in the following manner

$$\begin{aligned} \overline{Z}_k &:= |\overline{Z}_k^+| + |\overline{Z}_k^-| \\ \underline{Z}_k &:= \left| |\overline{Z}_k^+| - |\overline{Z}_k^-| \right|. \end{aligned}$$

IV. SIMULATIONS AND CONCLUSIONS

The model identified by experimental data described in [2] has been simulated. In the considered model the nonlinearity is a simple piecewise function. Upper bounds and lower bounds have been evaluated exploiting the proposed method using a starting $Y_h(0)$ equal to $10nm$. The numerically computed map T reveals to be a contraction on the whole interval $[0, Y_h(0)]$, showing a unique attractive fixed point. In Figure 3 the estimated upper and lower bounds are compared to magnitudes of harmonics computed from simulated data showing a very good agreement. A technique to obtain upper

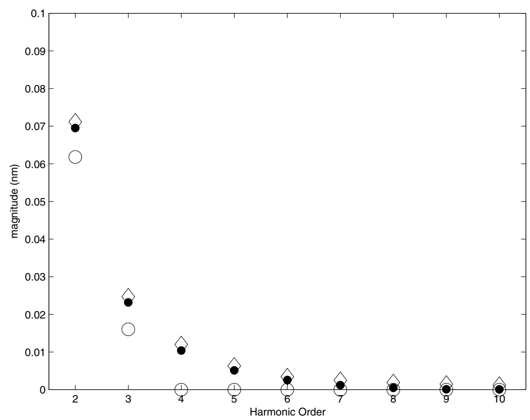

Fig. 3. Upperbounds (diamonds) and lowerbounds (circles) obtained for an AFM model identified by experimental data. Dots represent the computed harmonics obtained by a simulation of the model. The free tip oscillation amplitude is $25nm$ while the separation l is $20nm$

and lower bounds on the high order harmonics of the periodic solution in a tapping AFM has been presented. The proposed method considers a class of nonlinearity capable to well fit the tip-sample interaction and the problem of evaluating bounds is casted in the form of an optimization problem. An analytical solution for a relaxation of the problem has been provided allowing a fast computation. Finally a good agreement between simulation data and theoretical results seems to validate the approach.

V. APPENDIX

Lemma V.1 (*Generalized Mean Value Theorem*). *Let $f(\cdot)$ be a continuous function on an interval $I = [a, b]$ and let $g(\cdot)$ a function Riemann-integrable on the same interval I: $\int_a^b g(x)\mathrm{d}x \neq 0$. Then*

$$\exists\ \xi \in (a, b) : \int_a^b f(x)g(x)\mathrm{d}x = f(\xi)\int_a^b g(x)\mathrm{d}x.$$

Proof. We define $F(x) = \int_a^x f(t)g(t)\mathrm{d}t$ and $G(x) = \int_a^x g(t)\mathrm{d}t$. From the Cauchy's theorem there exists $\xi \in (a, b)$ such that

$$\frac{F(b) - F(a)}{G(b) - G(a)} = \frac{F'(\xi)}{G'(\xi)}.$$

Thus,

$$\frac{\int_a^b f(x)g(x)\mathrm{d}x}{\int_a^b g(x)\mathrm{d}x} = \frac{f(\xi)g(\xi)}{g(\xi)} = f(\xi)$$

□

Lemma V.2 (*Mean Value Theorem on union of intervals*). *Let D be the union of disjoint closed intervals I_j and f_1, f_2 two functions on D. Let $f_1(\cdot)$ be continuous in D and let $f_2(\cdot)$ be nonnegative. Then there exists K such that $\inf_D f_1(x) \leq K \leq \sup_D f_1(x)$ and $\int_D f_1(t)f_2(t)\mathrm{d}t = K\int_D f_2(t)\mathrm{d}t$*

Proof. By the lemma (V.1)

$$\int_D f_1(t)f_2(t)\mathrm{d}t = \sum_j f_1(\xi_j)\int_{I_j} f_2(x)\mathrm{d}t$$

If $\int_D f_2(t)\mathrm{d}t = 0$ then the theorem is obvious. Otherwise we define $S := \int_D f_2(t)\mathrm{d}t > 0$

$$\int_D f_1(t)f_2(t)\mathrm{d}t = S\sum_j f_1(\xi_j)\frac{\int_{I_j} f_2(t)\mathrm{d}t}{S}$$

We observe that

$$0 \leq \frac{\int_{I_j} f_2(t)\mathrm{d}t}{S}$$

and

$$\sum_j^N \frac{\int_{I_j} f_2(t)\mathrm{d}t}{S} = 1.$$

Thus,

$$\inf_D f_1 \leq K := \sum_j^N f_1(\xi_j)\frac{\int_{I_j} f_2(t)\mathrm{d}t}{S} \leq \sup_D f_1.$$

□

Proof of Lemma II.1

If $Z_k = 0$ then we have that

$$0 = |Z_k| = |\mathrm{e}^{i\phi_k}|\left|\int_{-\pi}^{\pi} z(t)\mathrm{e}^{ikt}\mathrm{d}t\right|.$$

This means that for every ϕ_k we obtain

$$|Z_k| = \int_{-\pi}^{\pi} z(t)\cos(kt + \phi_k)\mathrm{d}t.$$

Otherwise, if $Z_k \neq 0$, consider

$$q = \frac{\mathrm{conj}(Z_k)}{|Z_k|} = \mathrm{e}^{i\phi_k}$$

and ϕ_k can always be chosen in $[-\pi, \pi]$. We can evaluate

$$|Z_k| = qZ_k = \mathrm{Re}(qZ_k) = \int_{\pi}^{\pi} z(t)\cos(kt + \phi_k)\mathrm{d}t$$

Considering that $\mathrm{Re}(qZ_k) \leq |qZ_k| = |Z_k|$, we have the thesis.

Proof of Lemma II.2

By lemma (II.1)

$$\exists\phi : \int_{-\pi}^{\pi} z(t)\cos(t + \phi)\mathrm{d}t = |Z_1| =$$
$$= H\int_{-(\tau_m/2)-\phi}^{(\tau_m/2)-\phi} \cos(t + \phi)\mathrm{d}t$$

This implies that

$$\left\{\int_{-\pi}^{-(\tau_m/2)-\phi}+\int_{(\tau_m/2)-\phi}^{\pi}\right\} z(t)\cos(t+\phi)\mathrm{d}t =$$
$$= \int_{-(\tau_m/2)-\phi}^{(\tau_m/2)-\phi}(H-z(t))\cos(t+\phi)\mathrm{d}t$$

For the mean value theorem there exist $\xi_1 \in \left(-\frac{\tau_m}{2}-\phi, \frac{\tau_m}{2}-\phi\right)$, $\xi_2 \in \left(\pi, -\frac{\tau_m}{2}-\phi\right)$ and $\xi_3 \in \left(\frac{\tau_m}{2}-\phi, \pi\right)$:

$$\cos(\xi_2)\int_{-\pi}^{-\tau_m/2-\phi} z(t)\mathrm{d}t + \cos(\xi_3)\int_{\tau_m/2-\phi}^{\pi} z(t)\mathrm{d}t =$$
$$= \cos(\xi_1)\int_{-\tau_m/2-\phi}^{\tau_m/2-\phi}(H-z(t))\mathrm{d}t.$$

Thus,

$$H\tau_m = \int_{-(\tau_m/2)-\phi}^{(\tau_m/2)-\phi} z(t)\mathrm{d}t + \frac{\cos(\xi_2)}{\cos(\xi_1)}\int_{-\pi}^{-(\tau_m/2)-\phi} z(t)\mathrm{d}t +$$
$$+ \frac{\cos(\xi_3)}{\cos(\xi_1)}\int_{(\tau_m/2)-\phi}^{\pi} z(t)\mathrm{d}t$$

It can be noted that $\cos(\xi_1) \geq \cos(\xi_2)$ and $\cos(\xi_1) \geq \cos(\xi_3)$. In addition, since $\tau_m < \pi$, we have that both $\cos(\xi_2)/\cos(\xi_1)$ and $\cos(\xi_3)/\cos(\xi_1)$ are lesser than 1. Finally, observing that the last two integrals in the right hand side are non negative we have

$$H\tau_m \leq \int_{-\pi}^{\pi} z(t)\mathrm{d}t = Z_0.$$

Proof of Lemma II.3
First we observe, by Lemma II.1, that

$$\int_{-\frac{t_{\max}}{2}}^{\frac{t_{\max}}{2}} z(t)\cos(t)\mathrm{d}t \leq |Z_1| = H\left\{\int_{-\frac{t_{\max}}{2}}^{-\frac{t_{\max}-\tau_M}{2}} + \right.$$
$$\left. + \int_{\frac{t_{\max}-\tau_M}{2}}^{\frac{t_{\max}}{2}}\right\}\cos(t)\mathrm{d}t.$$

Steps similar to the ones in the previous lemma yield

$$\int_{\frac{-t_{\max}+\tau_M}{2}}^{\frac{t_{\max}-\tau_M}{2}} z(t)\cos(t)\mathrm{d}t \leq$$
$$\leq \left\{\int_{-t_{\max}/2}^{-\frac{t_{\max}-\tau_M}{2}} + \int_{\frac{t_{\max}-\tau_M}{2}}^{t_{\max}/2}\right\}(H-z(t))\cos(t)\mathrm{d}t;$$

thus

$$\int_{\frac{-t_{\max}+\tau_M}{2}}^{\frac{t_{\max}-\tau_M}{2}} z(t)\cos(t)\mathrm{d}t \leq$$
$$\leq \int_{-t_{\max}/2}^{-\frac{t_{\max}-\tau_M}{2}} [2H - z(t) - z(-t)]\cos(t)\mathrm{d}t.$$

This implies that $\exists \xi_1 \in [-t_{\max}/2 + \tau_M/2, t_{\max}/2 - \tau_M/2]$ and $\xi_2 \in [-t_{\max}/2, -t_{\max}/2 + \tau_M/2]$ such that

$$\cos(\xi_1)\int_{\frac{-t_{\max}+\tau_M}{2}}^{\frac{t_{\max}-\tau_M}{2}} z(t)\mathrm{d}t \leq$$
$$\cos(\xi_2)\int_{-t_{\max}/2}^{-\frac{t_{\max}-\tau_M}{2}} [2H - z(t) - z(-t)]\mathrm{d}t.$$

This implies that

$$\cos(\xi_1)\int_{\frac{-t_{\max}+\tau_M}{2}}^{\frac{t_{\max}-\tau_M}{2}} z(t)\mathrm{d}t + \cos(\xi_2)\left\{\int_{-t_{\max}/2}^{-\frac{t_{\max}-\tau_M}{2}} + \right.$$
$$\left. \int_{\frac{t_{\max}-\tau_M}{2}}^{t_{\max}/2}\right\} z(t)\mathrm{d}t \leq \cos(\xi_2)H\tau_M$$

Since $|\xi_2| < t_{\max}/2 < \pi/2$ we can write

$$\frac{\cos(\xi_1)}{\cos(\xi_2)}\int_{\frac{-t_{\max}+\tau_M}{2}}^{\frac{t_{\max}-\tau_M}{2}} z(t)\mathrm{d}t + \left\{\int_{-t_{\max}}^{-\frac{t_{\max}-\tau_M}{2}} + \right.$$
$$\left. + \int_{\frac{t_{\max}-\tau_M}{2}}^{t_{\max}}\right\} z(t)\mathrm{d}t \leq H\tau_M$$

and finally obtain, observing that $\cos(\xi_1)/\cos(\xi_2) \geq 1$ and $z(t) \geq 0$,

$$Z_0 = \int_{-t_{\max}/2}^{t_{\max}/2} z(t) \leq H\tau_M$$

Proof of Lemma II.4
Let us suppose that the solution of the problem is $\{z(\cdot), \phi_k\}$ with $\phi_k \neq 0$. Without any loss of generality we assume $\phi_k > 0$ otherwise $(z(-t), -\phi_k)$ is a solution with $-\phi_k > 0$. We consider the couple $\{z'(\cdot), 0\}$ where

$$z'(t) = \begin{cases} z(t-\phi_k/k) & \text{if } -\frac{t_{\max}}{2}+\frac{\phi_k}{k} \leq t \leq \frac{t_{\max}}{2} \\ z(t+t_{\max}-\phi_k/k) & \text{if } t < -t_{\max}+\phi_k/k \end{cases}$$

Note that

$$\overline{Z}_k = \int_{-t_{\max}/2}^{t_{\max}/2} z(t)\cos(kt+\phi_k)\mathrm{d}t =$$
$$= \left\{\int_{-\frac{t_{\max}}{2}}^{-\frac{t_{\max}-\phi_k/k}{2}} + \int_{\frac{t_{\max}-\phi_k/k}{2}}^{\frac{t_{\max}}{2}}\right\} z(t)\cos(kt+\phi_k)\mathrm{d}t$$

Using the substitution $s = t + \phi/k$

$$\overline{Z}_k = \left\{\int_{\frac{-t_{\max}}{2}+\phi/k}^{\frac{t_{\max}}{2}} + \int_{\frac{t_{\max}}{2}}^{\frac{t_{\max}}{2}+\phi/k}\right\} z(s-\phi/k)\cos(ks)\mathrm{d}s$$

Using the substitution $\sigma = s - t_{\max}$ in the second integral

$$\overline{Z}_k = \int_{-\frac{t_{\max}}{2}+\phi/k}^{\frac{t_{\max}}{2}} z(s-\phi/k)\cos(ks)\mathrm{d}s +$$
$$+ \int_{-\frac{t_{\max}}{2}}^{-\frac{t_{\max}}{2}+\phi/k} z(\sigma+t_{\max}-\phi/k)\cos(k\sigma)\mathrm{d}\sigma$$
$$= \int_{-\frac{t_{\max}}{2}}^{\frac{t_{\max}}{2}} z'(t)\cos(kt)\mathrm{d}t$$

Following the same arguments

$$\int_{-t_{\max}/2}^{t_{\max}/2} z(t)\mathrm{d}t = \int_{-t_{\max}/2}^{t_{\max}/2} z'(t)\mathrm{d}t.$$

Other constraints are trivially satisfied.

Proof of Lemma II.5
Note that if $z'(t)$ is a feasible element such that $H\int_E w < \int_D z'w$, then there exist, by lemma V.1, K_1 and K_2: $K_1 \leq \sup_{D\setminus E} w(\cdot) \leq \inf_E w(\cdot) \leq K_2$ and $K_2\int_E (H-z') < K_1 \int_{D-E} z'$.

- If (7a) holds, then

$$K_2 H\tau_M < K_2 \int_E z' + K_1 \int_{D-E} z' \leq$$
$$\leq K_2 \int_E z' \leq K_2 H\tau_M.$$

- Let us suppose that (7b) holds. First we want to show that $\mu(E) \geq \mu(E_0)$ implies $K_1 \int_{D-E} z' \leq 0$.
If $K_1 \leq 0$ the statement is true. So let us consider $K_1 > 0$. We have that $\sup_{D\setminus E} w(\cdot) > 0$ and this implies that $\exists \hat{x} \in D\setminus E : w(\hat{x}) > 0$. We can write the following relations

$$E \subseteq \{x \in D : w(x) \geq w(\hat{x}) > 0\} \subseteq E_0.$$

It follows that E and E_0 differ only by a zero measure set. Thus also $D \setminus E$ and $D \setminus E_0$ differ only by a zero measure set and we can write

$$K_1 \int_{D\setminus E} z' = \int_{D\setminus E} wz' = \int_{D\setminus E_0} wz' = K'_1 \int_{D\setminus E_0} z' \leq 0$$

where the inequality comes from the fact that $K'_1 \leq \sup_{D\setminus E_0} \leq 0$.
Analogously, we can show that $\mu(E) \leq \mu(E_0)$ implies $K_2 \int_{D-E} (H - z') \geq 0$.
If $K_2 \geq 0$ the statement is true. So let us consider $K_2 < 0$. We have that $\inf_E w(\cdot) < 0$ and this implies that $\exists \hat{x} \in E : w(\hat{x}) < 0$. We can write the following relations

$$D \setminus E \subseteq \{x \in D : w(x) \leq w(\hat{x}) < 0\} \subseteq D \setminus E_0.$$

It follows that $D \setminus E$ and $D \setminus E_0$ differ only by a zero measure set. Thus also E and E_0 differ only by a zero measure set and we can write

$$K_2 \int_E (H - z') = \int_E w(H - z') =$$
$$= \int_{E_0} w(H - z') = K'_2 \int_{E_0} (H - z') \geq 0$$

where the last inequality comes from the fact that $K'_2 \geq \inf_{E_0} \geq 0$.
So we obtain the following contradiction

$$0 \leq K_2 \int_E (H - z') < K_1 \int_{D-E} z' \leq 0$$

- If (7c) holds, then

$$K_2 H\tau_m < K_2 \int_E z' + K_1 \int_{D-E} z' \leq K_2 \int_E z' \leq K_2 H\tau_m.$$

Proof of Lemma II.6

We will show that the solution candidate is a saddle point for the problem. The proposed function $z(t)$ is a even function so $\phi = 0$ maximize the value of

$$\left| \int_{-t_{\max}/2}^{t_{\max}/2} z(t)\cos(kt + \phi_k)\mathrm{d}t \right|$$

But the integral is nonnegative so, fixed $z(t)$, $\phi = 0$ is maximal point also for the target function.

We observe that the function $z(t)$ can be always considered even. In fact, the considered problem is equivalent to the following one

$$M = \min_{z(\cdot)} \left| \int_{-t_{\max}/2}^{t_{\max}/2} z(t)\cos(kt) \right|$$
$$0 \leq z(t) \leq H$$
$$H\tau_m \leq \int_{-t_{\max}}^{t_{\max}} \leq H\tau_M$$

If z is a non even solution then $z^{(e)} := (z(t) + z(-t))/2$ satisfies all constraints and has a lesser or equal cost. In fact $|Z_k^{(e)}| = 1/2(Z_k + conj(Z_k)) \leq |Z_k|$. So, by contradiction, we can assume that there exists an optimal even function $z'(t)$:

$$\int_{-\frac{t_{\max}}{2}}^{\frac{t_{\max}}{2}} z'(t)\cos(kt)\mathrm{d}t < H \left\{ \int_{-\frac{t_{\max}}{2}}^{-\frac{t_{\max}-\tau_m}{2}} + \int_{\frac{t_{\max}-\tau_m}{2}}^{t_{\max}/2} \right\} \cos(kt)\mathrm{d}t$$
$$0 \leq \left\{ \int_{-\frac{t_{\max}}{2}}^{-\frac{t_{\max}-\tau_m}{2}} + \int_{\frac{t_{\max}-\tau_m}{2}}^{\frac{t_{\max}}{2}} \right\} (H - z'(t))\cos(kt)\mathrm{d}t +$$
$$- \int_{-t_{\max}/2+\tau_m/2}^{t_{\max}/2-\tau_m/2} z'(t)\cos(kt)\mathrm{d}t$$
$$0 \leq K_1 \left\{ \int_{-t_{\max}/2}^{-t_{\max}/2+\tau_m/2} + \int_{t_{\max}/2-\tau_m/2}^{-t_{\max}/2} \right\} (H - z'(t))\mathrm{d}t +$$
$$- K2 \int_{-t_{\max}/2+\tau_m/2}^{t_{\max}/2-\tau_m/2} z'(t)\mathrm{d}t$$

where $K_1 \leq K_2$ and $0 < K_2$ by the hypotheses on $t_{\max}$. So we obtain

$$\int_{-t_{\max}/2}^{t_{\max}/2} z'(t)\mathrm{d}t < \frac{K_1}{K_2} \left\{ \int_{-t_{\max}/2}^{-t_{\max}/2+\tau_m/2} + \right.$$
$$\left. + \int_{t_{\max}/2-\tau_m/2}^{t_{\max}/2} \right\} H\mathrm{d}t < H\tau_m$$

and it is a contradiction since $z'(t)$ should satisfy the constraints of the problem. The couple $\{0, z(t)\}$ is a saddle point and so it is optimal.

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