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Accuracy of Theoretical Solutions of a Single Degree of Freedom Model for Micro-Probe Vibration Amplitude in Atomic Force Microscope

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Abstract— In this study, we focus on investigating the amplitude characteristics of micro-probe vibration for atomic force microscope for the theoretically-derived solutions. To achieve this, we assume a higher quality factor than in our previous works and compare the theoretical solutions with the associated numerical results. Our findings indicate that using a large approximation order for the nonlinear interaction force is crucial for obtaining an accurate theoretical solution.

1. Introduction

Atomic Force Microscope (AFM) is a type of scanning probe microscope (SPM) that utilizes a small cantilever probe as a sensor to investigate the surface of a sample. AFM enables observation and manipulation of the shape of micro/nano-scale samples and is used for observing various samples [1, 2]. In D-AFM, a harmonic external force that oscillates in the vicinity of the natural frequency of the micro-scale cantilever probe is applied. At each scanning point of the probe, the oscillation modulated by the van der Waals force (atomic force) between the probe tip and the sample surface is detected and is feedback-controlled to obtain information on the surface shape. The atomic force shows a large nonlinearity when the probe and the sample surface are in close proximity. This causes a nonlinear problem in cases where the vibration amplitude of the probe is large or the probe intermittently contacts the sample surface in tapping mode [3–10].

The cantilever probes used in conventional AFMs are characterized by their sharp and pointed tips, which result in the atomic force acting on the probe tip becoming dominant [1]. Moreover, when the probe tip is bent towards the opposite side, the external force dominates the system. Therefore, to derive an approximated theoretical solution, we assume a nonlinear system as a perturbation to the harmonic oscillation when a small external force is applied, and the distance between the probe and the sample surface is kept relatively constant [10].

In this study, we investigate the approximated theoretical solution for micro-cantilevers for D-AFM by assuming the Morse potential for atomic force and approximating it with a single degree of freedom mass-spring model [11]. By comparing the theoretical solutions with the associated numerical results, we investigate the relationship between the accuracy of the approximated theoretical solutions and the approximation order. When the quality factor Q with no interaction force increases, the scanning speed becomes slower when investigating the amplitude modulation in scanning probe microscopy (SPM). In such a case, the theoretical solution plays a crucial role in understanding the oscillation state of the probe tip in SPM. To address this subject, we investigate the results for higher values of Q than those assumed in our previous works [10, 11].

2. Cantilever Model and its Approximated Theorical Solution

In this study, we consider a mass-spring model with a single degree of freedom to model the lateral oscillation of a probe tip, as shown in Fig. 1. The normalized equation of motion in the lateral direction (z) is written by the follwing [11]:

$$\frac{d^2z}{d\tau^2} + \frac{1}{Q}\frac{dz}{d\tau} + (z - \varepsilon) = a_e \cos(\omega\tau) + F(z), \tag{1}$$

where the normalized time is represented by the variable τ. The parameters a_e and ω correspond to the amplitude and the angular frequency of the external force, respectively. Note that $\omega = 1$ means that the natural frequency of the probe is same with the frequency of the external force. The parameters ε and Q correspond to the tip-sample distance and quality factor, respectively. The force $F(z)$ represents the atomic force as a function of z where we assume that the force obtained from the Morse potential [12]:

$$F(z) = -\beta e^{-(\alpha z+\gamma)}(1 - e^{-(\alpha z+\gamma)}), \tag{2}$$

where α, β, and γ are parameters that determine the shape of the characteristic curve of the atomic force. In the

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subsequent results, we set the parameters $\alpha = 3.29315$, $\beta = 70.1232$, and $\gamma = -2.6$ referring to our previous study [9] where we assume that both the probe and sample are made of silicon material, and the sample surface is sufficiently large compared to the probe.

In this study, we adopt the concept of the harmonic balance method [10] to derive an approximated theorical solution of Eq. (1). First, we assume the lateral oscillation in the steady state as follows:

$$z(\tau) = \varepsilon + a(\tau)\cos\omega\tau + b(\tau)\sin\omega\tau, \qquad (3)$$
$$(u(\tau) \equiv a(\tau)\cos\omega\tau + b(\tau)\sin\omega\tau),$$

Here, we consider amplitude variables $a(\tau)$ and $b(\tau)$ as slowly time-varying variables. Moreover, we substitute Eq. (3) into Eq. (1) and ignore the following small terms based on the above assumption and the condition $Q \gg 1$:

$$\frac{d^2a(\tau)}{d\tau^2} \ll 1, \quad \frac{d^2b(\tau)}{d\tau^2} \ll 1,$$
$$\frac{1}{Q}\frac{da(\tau)}{d\tau} \ll 1, \quad \frac{1}{Q}\frac{db(\tau)}{d\tau} \ll 1. \qquad (4)$$

In this study, we consider the exponential term in the following equation and perform a Taylor expansion around the tip-sample distance ε:

$$e^{-(\alpha z(\tau)+\gamma)} \simeq e^{-\gamma}\left\{\sum_{n=0}^{N}\frac{f^{(n)}(\varepsilon)}{n!}(-\varepsilon + z(\tau))^n\right\}, \qquad (5)$$
$$\left(f(z) = e^{-\alpha z(\tau)}\right),$$

Here, $f^n(z)$ represents the nth order derivative of $f(z)$ with respect to τ. Moreover, N is the approximation order in the Taylor expansion. In addition, by ignoring the higher-order components of ω in the power series of $z(\tau)$, we can derive the differential equations for the amplitude $A(\tau)(= a(\tau)^2 + b(\tau)^2)$ and initial phase $\phi(\tau)(= -\tan^{-1}\{b(\tau)/a(\tau)\})$:

$$\frac{dA(\tau)}{d\tau} = g_1(N, \boldsymbol{\lambda}), \quad \frac{d\phi(\tau)}{d\tau} = g_2(N, \boldsymbol{\lambda}). \qquad (6)$$

Here, $\boldsymbol{\lambda}$ represents a set of parameters $\boldsymbol{\lambda} = (\alpha, \beta, \gamma, \varepsilon, a_e, \omega) \in \mathbb{R}^6$ that include normalized parameters from the fundamental Eq. (1) and the interaction force in Eq. (2). Furthermore, $g_1(\eta, \boldsymbol{\lambda})$ and $g_2(\eta, \boldsymbol{\lambda})$ are expressed as functions that depend on the Taylor approximation order N in Eq. (5). Therefore, it is possible to derive approximated theoretical solutions for the amplitude $A(\tau)$ and initial phase $\phi(\tau)$, and obtain frequency response characteristics with respect to the amplitude and the phase difference between the amplitude of the probe tip and external force at steady-state(the explicit form of the approximated theoretical solution is omitted due to space constraints). In addition, the influence of the approximation order N and the parameters can be discussed.

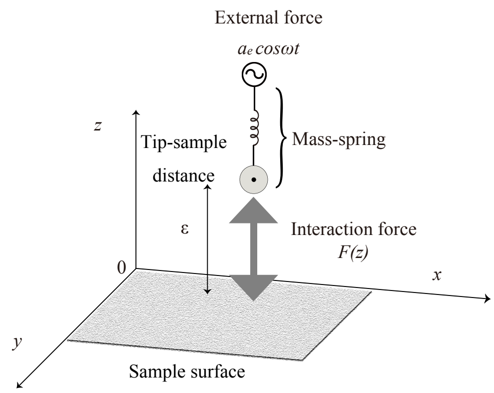


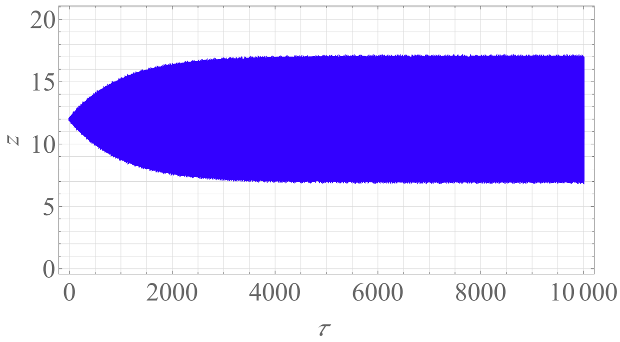
Figure 1: Mass-spring model for the lateral oscillation of a forced probe tip.

3. Accuracy of the approximated theoretical solutions

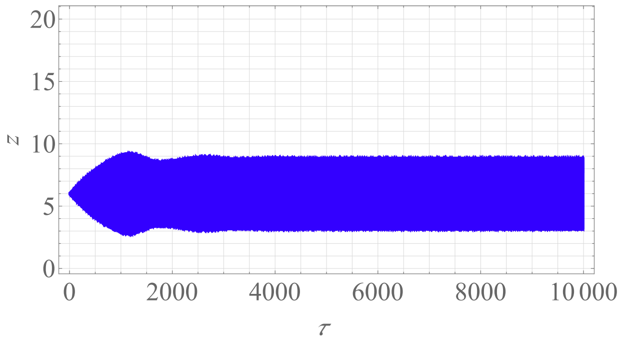
In this study, we aim to investigate the relationship between the accuracy of approximated theoretical solutions and the approximation order N. To achieve this, we compare the theoretical solutions with the associated numerical results. When the quality factor Q in Eq. (1) with no interaction force is increased n times, the transient time is also multiplied by n. This phenomenon indicates that the scanning speed becomes slower for larger Q when investigating the amplitude modulation in SPM. In such cases, a theoretical solution is crucial to understand the oscillation state of the probe tip in SPM. To obtain results, we set the quality factor Q=500, which is five times higher than that in our previous works [10, 11]. In the following results, we fix the amplitude of the etxternal force $a_e = 0.01$.

Figures 2 (a) and (b) show the numerically-obtained timeseries of the probe tip for $\omega = 1$ with the initial condition $(z(0), \dot{z}(0)) = (\varepsilon, 0)$ when we set the tip-sample distance $\varepsilon = 12$ and $\varepsilon = 6$, respectively. The amplitude of free oscillation is determined to be a_eQ. In Fig. 2 (a), we observe that the oscillation-amplitude of the probe tip at steady-state is close to that of a free oscillation when $\varepsilon = 12$, indicating that the interaction force is negligible and has little effect on the oscillation amplitude. Whereas the amplitude of oscillation for $\varepsilon = 6$ in Fig. 2 (b) decreases due to the interaction force. As shown in the results, the steady-state amplitude of the tip ($= A_p$) decreases as a function of the tip-sample distance ε because the attractive force dominates [8].

To assess the accuracy of the approximated theoretical solutions, we plot the frequency response curves for the amplitude obtained from Eq. (6) when we set $\varepsilon = 6$ for three values of the approximation order $N = 3, 5,$ and 7 in Figs. 3(a)–(c). Although the same value of ε is used, the larger N has stronger effect on the characteristic curve.



(a) $\varepsilon = 12$.



(b) $\varepsilon = 6$.

Figure 2: Numerically-obtained timeseries of the probe tip for $\omega = 1$.

When $\omega = 1$, the theoretically-obtained result for $N = 7$ shows the best fit with the numerical result in Fig. 2 (b). To further investigate the influence of ε, we calculate the theoretically-obtained amplitude when we set $\omega = 1$ for three values of the approximation order as shown in Figures 4(a)–(c), where the numerically-obtained amplitude A_p is superimposed. From the figures, we can see that the theoretically-obtained results are not consistent with the numerically-obtained results when the amplitude begins to decrease from that of a free oscillation. However, the amplitude curve for larger N shows better fit with the numerically-obtained result. The results indicate that we can obtain the accurate approximated theoretical solution by using the large N when we investigate the oscillation amplitude for large value of Q.

4. Conclusions

The results of this study suggested that the use of a large N was effective in obtaining an accurate approximated theoretical solution when investigating the oscillation amplitude for large values of Q. As demonstrated in Fig. 3 and Fig. 4, the theoretical results with larger N exhibited a better fit with the numerically-obtained results, particularly when the amplitude began to decrease from that of a free oscillation.

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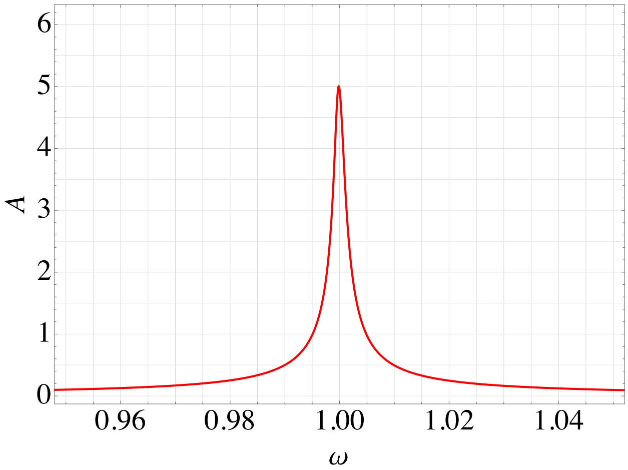
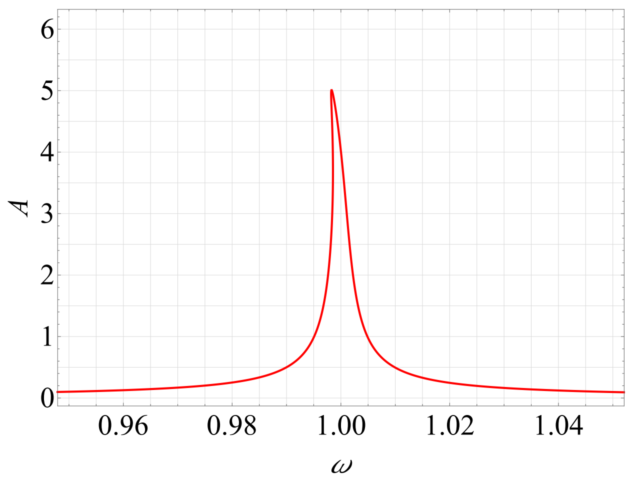
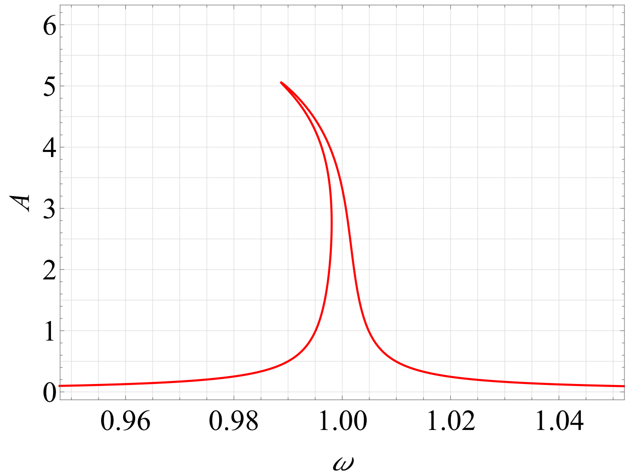


(a) $N = 3$.

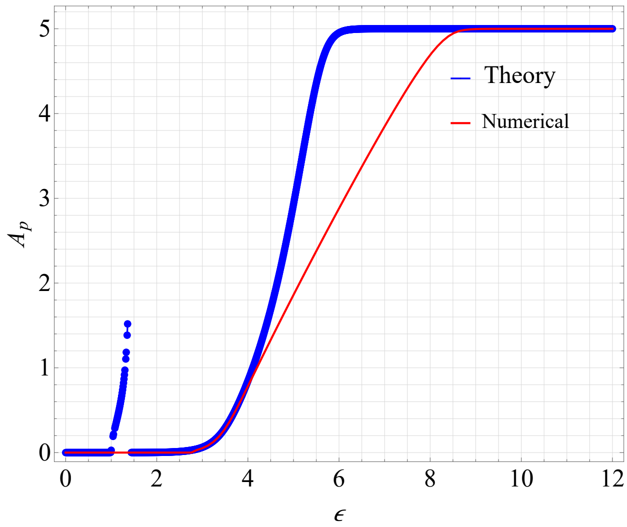


(b) $N = 5$.

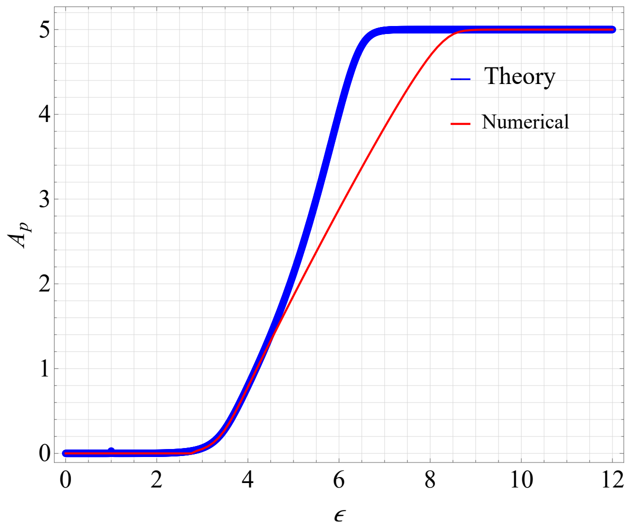


(c) $N = 7$.

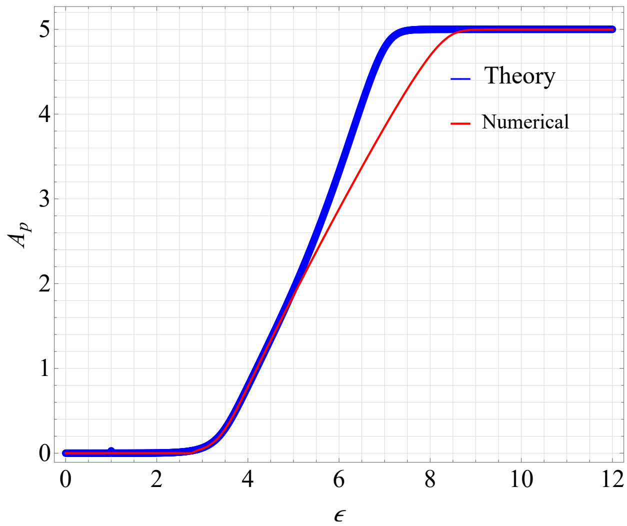
Figure 3: Frequency response curves for the amplitude obtained from Eq. (6) when we set $\varepsilon = 6$ for three values of the approximation order $N = 3, 5$, and 7.



(a) $N = 3$.



(b) $N = 5$.



(c) $N = 7$.

Figure 4: Theoretically-and numerically-obtained amplitude decaying characteristics when we set $\omega = 1$ for three values of the approximation order.