

Method for stabilizing unstable periodic orbits in dynamic-mode atomic force microscopy

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We present a noninvasive feedback control scheme to access unstable periodic orbits in dynamic-mode atomic force microscopy. By utilizing this method we are able to explore the complete nonlinear frequency-response curves, including unstable branches between saddle-node bifurcations. The overall scheme is designed to be fast and derivative-free, which allows for simple experimental implementations. The control is closely related to phase-locked loop testing, a truncated Fourier discretization of periodic orbits, and an adaptive filter for online signal demodulation. We demonstrate the feedback control on various contact models for dynamic-mode atomic force microscopy and hope to motivate laboratory experiments by elucidating software and corresponding hardware implementations in detail.

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I. INTRODUCTION

In recent decades, efforts have been made to observe, understand, and manipulate objects at the nanoscale. Consequently, different imaging techniques for the topography of surfaces have been established. One option, the scanning tunneling microscope, was introduced by Binnig and Rohrer in 1983 [1] and uses the tunneling current between a sharp conducting tip and a conducting sample to sense the surface of the sample at the atomic scale. Only three years later in 1986, Binnig, Quate, and Gerber [2] generalized the idea and invented the atomic force microscope (AFM), also known as the scanning force microscope, which was no longer restricted to conductive materials. Instead of electron transport, its principle is based on tip-sample interaction forces. A commonly used operational mode of the AFM is the dynamic mode, due to its short interaction times with the sample and thus inherently less destructive behavior, as opposed to the contact mode, where the tip remains permanently in a repulsive interaction. In dynamic-mode atomic force microscopy a microcantilever is driven to oscillations above a sample. The dynamics of the tip, located at the end of the cantilever,

are monitored by a laser and reflected onto a segmented photodiode and can to a first approximation be described as a nonlinear driven damped harmonic oscillator. By demodulation of the displacement dynamics one can in general obtain surface properties.

New directions in dynamic-mode atomic force microscopy introduce multiharmonic excitation in order to reconstruct tip-sample interactions through Fourier mode mappings [3] or more recently by sparse identification of nonlinear dynamics (SINDy) [4,5]. We would like to highlight that the displacement dynamics of the tip under monoharmonic excitation is still not completely explored and might reveal features in order to gain further information on the interaction properties. This can be seen by varying the driving frequency adiabatically under constant forcing amplitude and tracking the solution, manifesting in multistable nonlinear frequency-response curves that experimentally only include stable periodic orbits [6,7]. As a result one observes jump phenomena at bifurcation points, located at the end of the stable branches in the frequency-response curves. Similar jump phenomena and transitions between stable orbits were reported by experimentally changing the separation distance [8]. From theoretical works [9–11] it is well established within the atomic force microscopy community that an unstable branch of solutions, consisting of unstable periodic orbits (UPOs) connects the saddle-node bifurcation points. Recently, successful stabilization of UPOs, with the control proposed here, have been reported in an actual AFM experiment [12]. Such new AFM methods could lead to

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novel spectroscopy and imaging methods due to the naturally unobtainable operating mode. Knowledge of the unstable branch can also be used to calibrate parameters of the system, as done, for example, in a nanoscopic Duffing oscillator [13] and in the context of atomic force microscopy for the estimation of the tip radius [14] or material parameters [15].

The aim of this work is to take recent developments in the field of experimental continuation and present a stabilization technique for UPOs in dynamic-mode atomic force microscopy that is suited not only for numerical continuation but also in particular for a laboratory scenario. Therefore, we focus on a fast, derivative-free, model-free and noninvasive feedback control scheme that allows for tracking of nonlinear frequency-response curves by changing the driving frequency. The paper is thus structured as follows. First, we will briefly introduce dynamic-mode atomic force microscopy. In Sec. II we present concepts and algorithms that will be necessary for the implementation of the feedback control law. In order to show that the scheme is able to stabilize periodic orbits on a vast variety of tip-sample interaction force models, in Sec. III we apply the control scheme numerically on a Duffing, Lennard-Jones and Derjaguin-Muller-Toporov model, respectively, and show that intrinsic limitations seem reasonable. This paper aims to provide a solid base for experimental implementations, while actual laboratory experiments will be covered in separate publications.

II. METHODS

Generally, in the field of control-based continuation, several methods have been developed that enable formerly unstable periodic solutions to be stabilized and therefore tracked in different experimental scenarios without changing the solution itself. The underlying idea is to actively manipulate the original dynamics of the system by a feedback control signal, which acts in such a way that we are able to reach the former unstable time-invariant set [16,17]. Once reached, the feedback control signal vanishes and only the original dynamics remain, in other words the control scheme is noninvasive [18–20]. One solely manipulates the linearization of the dynamical system and therefore stability around the time-invariant set. In this manner, unstable branches in many scenarios such as pedestrian flows [21], Zeeman catastrophe machines [22], gene synthesis networks [23], neuronal states [24], etc. were obtained. In fact, experimental nonlinear response curves with unstable branches were measured with such methods for multiple forced nonlinear oscillators [17,25–29]. An excellent introduction to experimental continuation can be found in the overview article [30], while more recent adaptations that include adaptive control can be found in [31]. The challenge to apply these methods in dynamic-mode atomic force microscopy can be boiled

down to the requirement to operate at the spatial nanoscale, implying inherent noise contributions as well as fast temporal dynamics. As shown for micro- and nanoelectromechanical systems, even stability of branches is often not sufficient to physically observe states on them, due to small basins of attraction [32]. Noninvasive feedback control can also be used to enlarge basins [33]. To illustrate these challenges we will briefly introduce dynamic-mode atomic force microscopy.

A. Nonlinear experiment—dynamic-mode atomic force microscopy

The overall setup consists of a microcantilever that is excited at the base by piezo actuators above a sample, in the near-resonance regime of the first mechanical mode of the cantilever. The motion of the tip of the cantilever is tracked by a laser and segmented photodiode [see Fig. 1(a)], and is strongly influenced by nonlinear interaction forces between tip and sample, which can be characterized by long-range attractive van der Waals forces and short-range repulsive interactions. The nonlinearity of the force can thus be adjusted by the separation s that measures the distance between the tip of the cantilever and the sample in the nondriven case without interaction forces [see Fig. 1(a)]. Under constant separation s and excitation amplitude F one can increase (forward sweep) or decrease (backward sweep) the driving frequency. By applying demodulation techniques on the time-dependent deflection voltage, which is proportional to the displacement x , and waiting until transients disappear, one can then observe frequency-response curves with jump phenomena at saddle-node bifurcation points [see Fig. 1(b)].

These frequency-response curves have to be tracked promptly in order to maintain constant internal parameters of the experiment. In general, thermal drift leads to changes in the separation s and therefore modifies the whole interaction, yielding different time-invariant sets (i.e., frequency-response curves). Consequently, the control algorithm to track the solutions should be designed to operate completely on the fly without the need for expensive computations that, for example, take place in common predictor-corrector pseudo-arc-length continuation schemes [17,25]. By applying the Euler-Bernoulli beam theory on the microcantilever one can obtain the tip dynamics described by coupling mechanical modes [34]. However, the first mechanical mode is dominant in most cases, therefore it is well established to model the dynamics of the tip in a rather simple damped driven harmonic oscillator with interaction forces given by

$$\frac{d}{dt}x = v, \quad (1)$$

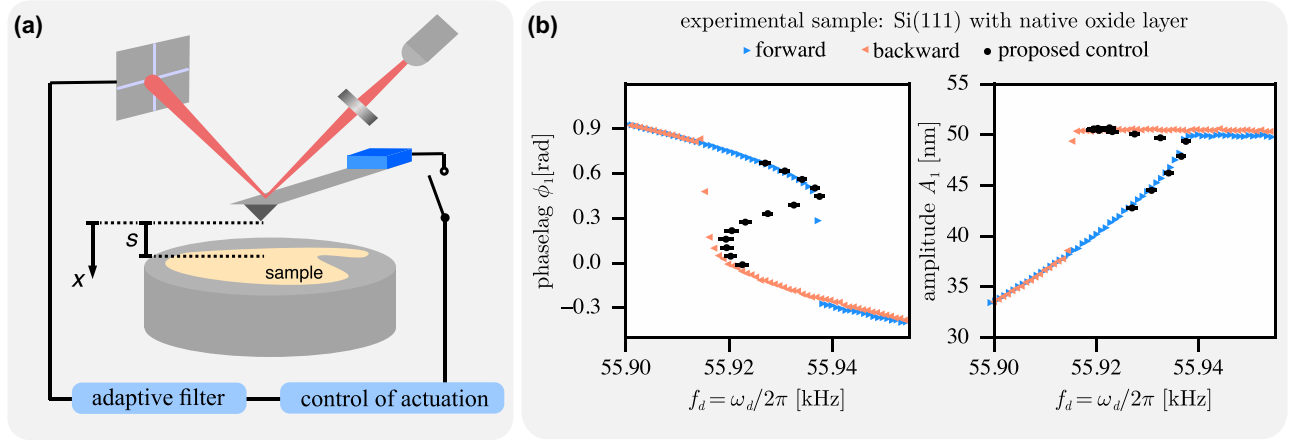


FIG. 1. (a) In dynamic-mode atomic force microscopy a microcantilever is monoharmonically vertically driven. The deflection of the tip $x(t)$ is tracked by a laser deflection scheme and a segmented photodiode (position-sensitive photodiode). The nonlinear interaction can be changed by the nominal separation s . Using adaptive filters, we can demodulate the deflection signal and can either feed information back onto the actuation via control or just manually change the driving frequency. (b) By varying the driving frequency f_d and waiting until the transients are eliminated, experimental frequency-response curves which display the fundamental phase lag ϕ_1 and amplitude A_1 can be obtained and clearly show bifurcation behavior. By use of control we are able to unveil the unstable branch experimentally on a Si(111) sample under ambient conditions, humidity levels between 17% and 36%, and a commercial NT-MDT NTEGRA Spectra295 Solar setup. For further experimental details see [12].

$$\frac{d}{dt}v = -\omega_0^2 x - \frac{\omega_0}{Q}v - \frac{\omega_0^2}{k}F_{\text{TS}}(x, v; s) \quad (2)$$

$$+ \frac{\omega_0^2}{k}F \cos(\psi), \quad (3)$$

$$\frac{d}{dt}\psi = \omega_d, \quad (4)$$

with cantilever angular eigenfrequency ω_0 , cantilever oscillation quality factor Q , spring constant k , external forcing F , driving angular frequency ω_d , a tip-sample interaction force F_{TS} , which is generally unknown, and an initial condition $(x(0), v(0), \psi(0))^T \in \mathbb{R}^2 \times \mathbb{S}_{[0, 2\pi)}$. For convenience of an autonomous system we introduced the instantaneous phase ψ in the excitation signal, which changes at the rate of the driving angular frequency. Note that infinitesimal changes in ψ lead to continuous changes in the excitation signal, whereas deviations in the driving angular frequency itself would result in discontinuous excitation signals due to the product $\omega_d t$, which will be a key observation to later introduce control. Even though we will not exploit the model for the continuation algorithm itself, we will use it for numerical validation.

B. Periodic orbits as steady states in a truncated Fourier space

The general issue within designing a control scheme that allows for tracking of UPOs is to formalize the problem in such a way that we can represent the targeted periodic orbit as a point. Feedback control towards a target point is then a well-defined root-finding or fixed-point problem that can

be solved by different techniques. From the analytical point of view, stroboscopic maps and therefore nonlinear control seem to be the most natural to use, since by design they capture periodic orbits as fixed points. Indeed such control algorithms have been designed and show promising results for Duffing and Toda oscillators [33, 35]. Closely related is time delay control, which uses a time-shifted output of a nonlinear system as a new actuation [36, 37]. A noise-robust alternative is to project the dynamics of the tip $x(t)$ onto basis functions. Periodic B-splines as a basis function set were recently proposed as an alternative to the typical Fourier approach [38]. Since we observe rather small deviations from elliptic orbits in experimental dynamic-mode atomic force microscopy, we use the more common and traditional ansatz

$$x(t) = \sum_{\omega_i \in \Omega} (X_{i,s} \sin \omega_i t + X_{i,c} \cos \omega_i t), \quad (5)$$

the validity of which is given by the theorem of Fourier. In practice, we focus on a finite set $\Omega = \{\omega_i\}$, that is, a truncated Fourier series, which approximates our signal $x(t)$ as $\tilde{x}(t)$. The general idea of truncation in Fourier space is spread across various disciplines, namely, harmonic balancing [39, 40], van der Pol transformations [41], and rotating-wave approximations [42]. However, it is not straightforward to choose a suitable set Ω due to nontrivial frequency conversions that take place in periodically forced nonlinear systems. As a result one should carefully investigate experimentally obtained time-series data and their respective frequency spectrum. In nonchaotic dynamic-mode atomic force microscopy we observe a

phase-locked behavior between the monoharmonic excitation signal $F \cos \omega_d t$ and cantilever deflection response $x(t)$ and additionally the presence of higher harmonics which motivates the ansatz for an approximation $\tilde{x}$ of the tip dynamics

$$\tilde{x}(T, t) = \frac{1}{2}X_0(T) + \sum_{\omega_i \in \Omega} (X_{i,s}(T) \sin \omega_i t + X_{i,c}(T) \cos \omega_i t) \quad (6)$$

with $\Omega = \{n\omega_d | n, N \in \mathbb{N} : 0 < n \leq N\}$, which essentially represents a truncated Fourier series approach. We will refer to

$$X(T) = (X_0, X_{1,s}, X_{1,c}, \dots, X_{N,s}, X_{N,c})^\top \in \mathbb{R}^{2N+1} \quad (7)$$

as the harmonic state, to $X_0, X_{i,s}, X_{i,c}$ as the harmonic variables, which change at a slow timescale $T \gg 2\pi / \min_i \omega_i$, and to N as the truncation order. Note that we are not inherently limited by a truncated Fourier series; Zhou *et al.* [43] also incorporated subharmonic resonances in their approximation [see Eq. (6)]. Since we are going to manipulate the driving frequency ω_d over time, but would like to obtain the harmonic state X based on the current actuation, we synchronize the clocks between actuation and Fourier discretization by introducing the current instantaneous phase ψ in Eq. (6),

$$\tilde{x}(T, \psi) = \frac{1}{2}X_0(T) + \sum_{\psi_i \in \Psi} (X_{i,s}(T) \sin \psi_i + X_{i,c}(T) \cos \psi_i), \quad (8)$$

$$\frac{d}{dt}\psi = \omega_d, \quad (9)$$

with $\Psi = \{n\psi \mid 0 < n \leq N \text{ with } n, N \in \mathbb{N}\}$ and $\psi(0) = 0$. One might think of this expansion as a projection onto a slow-fast dynamical system, in the rotating frame of the actuation, where we describe the fast oscillations by sines and cosines and the slow, transient behavior of the original system by the harmonic variables. If the finite set of frequencies Ω is sufficient and an equilibrium of the harmonic state X or equivalently a periodic orbit is reached, the harmonic variables are constant with respect to the slow timescale T and approximate the Fourier coefficients associated to the dynamics of the displacement of the tip. Therefore, we can formulate a root-finding problem

$$\frac{d}{dT}X^*(T; \mu) = 0 \quad (10)$$

to characterize the periodic orbit as an equilibrium point $X^* \in \mathbb{R}^{2N+1}$. By changing a bifurcation parameter μ , in our case ω_d , adiabatically and imposing Eq. (10), one can obtain a $(2N + 1)$ -dimensional μ -response curve.

C. Nonlinear frequency-response curves

Within both the harmonic balancing and control-based continuation communities one usually maps the truncated Fourier space to a collection of one-dimensional curves by harmonic amplitudes A_i and phase lags ϕ_i ,

$$A_i(T) = \sqrt{(X_{i,s}(T))^2 + (X_{i,c}(T))^2}, \quad (11)$$

$$\phi_i(T) = \arctan_2(X_{i,c}(T), X_{i,s}(T)), \quad (12)$$

for each frequency ω_i in the set Ω . The $\arctan_2$ expression is thus the inverse tangent function defined in all four quadrants. We would also like to emphasize that even though these quadrature interpretations [Eqs. (11) and (12)] are natural to choose to illustrate physically feasible quantities, there might exist alternative suitable maps

$$h: \mathbb{R}^{2N+1} \rightarrow \mathbb{R}, \quad X \mapsto h(X) \quad (13)$$

that are computationally less demanding for actual hardware such as microcontrollers or field programmable gate arrays and still manifest in S-shaped (or Z-shaped) frequency-response curves and allow for easy-to-implement experimental tracking. Continuation schemes for S-shaped curves C can be viewed as a special case of natural parameter continuation. By effectively swapping the meanings of the bifurcation parameter μ and observation $h(X)$, we can naturally parameterize the curve C by a grid of observations h . That is, we can reinterpret the bifurcation curve C as a single-valued function. As a result $\mu(h(X^*))$ is a single-valued function in at least the neighborhood of interest $\mu \in [\mu_a, \mu_b]$. It is assumed that such a help function h can be constructed that fulfills this property. This allows for avoidance of arc-length continuation. Using a grid of targets G_h that contain individual targets h^* , and assuming $h(X^*)$ follows an S-shape in the near-resonance regime, we can aim towards one target h^* by a simple proportional plus integral control law

$$\frac{d}{dt}\psi = \omega_s + K_P(h(X(T)) - h^*) + \lambda, \quad (14)$$

$$\psi(0) = \psi_0,$$

$$\frac{d}{dt}\lambda = K_I(h(X(T)) - h^*), \quad (15)$$

$$\lambda(0) = 0,$$

with a starting angular frequency ω_s , the current observation $h(X(T))$, the instantaneous phase ψ of the actuator, the integral part λ , and real control gains K_P, K_I . Note that such control laws are noninvasive by design. If we reach our target h^* by choosing proper gains K_P, K_I and

a steady-state of $h(X(T))$ is acquired with

$$\frac{d}{dt}\psi = \omega_s + \tilde{\lambda} = \omega_d, \quad (16)$$

$$\frac{d}{dt}\lambda = 0, \quad (17)$$

one again obtains a monoharmonic excitation signal, but now reaching the UPO characterized by h^* . Note that phase-locked loops (PLLs) are a special case of such control laws by using $h(X) = \phi_1(X)$. Indeed, PLLs have been successfully used to stabilize UPOs or extract backbone curves in experimental nonlinear dynamical systems [43–45]. Similar phase controls were established to achieve UPOs in the early 2010s [46,47], which utilize analog phase shifters. However, the latter are less versatile and more closely related to time-delay control. In our approach we can freely choose the map h [see (13)].

D. Online estimation of harmonic state

A drawback of the control scheme acting in a truncated Fourier space is the inherent time delay between obtaining the harmonic state $X(T)$ and the true dynamics of the displacement $x(t)$. One way of solving this problem is to design the controller *offline* by tracking time-series data $x(t)$ and applying a fast Fourier transform, between adaptations of the control signal, to gain information on the current observation $h(X(T))$. In fact, this would result in a time-splitting algorithm that enables high precision but lacks convergence speed. Within engineering or experimental sciences and digital signal processing one typically addresses this problem by estimating the harmonic variables online with a lock-in amplifier and hence multiorder low-pass filters. By choosing suitable cutoff frequencies at the low-pass filters one can achieve a balance between convergence speed towards the harmonic state X and precision. An alternative that is known to outperform low-pass filters in convergence speed are Lyapunov-based estimators, which are common in adaptive filter theory [48] and were first used in a truncated Fourier space for noise-canceling purposes by Widrow and Hoff [49]. Lately, they have also been introduced for demodulation in high-speed atomic force imaging [50]. The fundamental idea relies on the linear parametric form of our truncated Fourier series [see Eq. (8)]. By introducing the basis vector

$$c(\psi) = \left(\frac{1}{2}, \sin(\psi), \cos(\psi), \dots, \sin(N\psi), \cos(N\psi) \right)^T \in \mathbb{R}^{2N+1} \quad (18)$$

and substituting $c(\psi)$ into Eq. (8) we arrive at a short linear parametric form of our current approximation $\tilde{x}$ of the

displacement signal of the tip x :

$$\tilde{x}(T, \psi) = X^T(T)c(\psi), \quad \frac{d}{dt}\psi = \omega_d, \quad \psi(0) = 0. \quad (19)$$

An online estimator for the harmonic state can now be constructed by manufacturing a Lyapunovlike function based on the current error $e(t) = x(t) - \tilde{x}(T, \psi)$ between measurement and estimation. One arrives at update equations for the harmonic state X that minimize the error $e(t)$ exponentially

$$\frac{d}{dt}X(T) = \Gamma c(\psi) (x(t) - X^T(T)c(\psi)) \quad (20)$$

$$X(0) = 0$$

$$\frac{d}{dt}\psi = \omega_d, \quad \psi(0) = 0, \quad (21)$$

where the diagonal matrix $\Gamma = \text{diag}(\gamma_1, \gamma_2, \dots, \gamma_{2N+1})$ represents individual step sizes for each harmonic variable that have to be chosen carefully and determine individual bandwidths (for further details, see [51,52]). To ensure exponential convergence of the error $e(t)$ towards zero and therefore convergence of X , the basis vector c has to be persistently exciting, which is naturally given for a Fourier series approach if the frequency set Ω is chosen adequately [51]. Note that the Widrow-Hoff learning rule or least-mean-square (LMS) algorithm for online demodulation is a special case, where $\Gamma = \text{diag}(\gamma)$ and an Euler forward time discretization $\xi(n\Delta t_{\text{LMS}}) = \xi|_n$ is used:

$$X|_{n+1} = X|_n + \gamma \Delta t_{\text{LMS}} c(\psi|_n) (x|_n - X^T|_n c(\psi|_n)). \quad (22)$$

We thus arrive at a computationally efficient scheme to approximate the current harmonic state X . A different way to obtain Eq. (22) is to define a mean-square error cost function and apply stochastic gradient descent. In the context of experimental continuation the LMS algorithm was first applied by Abeloos *et al.* [53].

E. Online steady state detection—adapted Welford algorithm

In order to obtain the equilibrium of the harmonic state X^* and the associated bifurcation curve, we have to solve the zero problem [see Eq. (10)], and hence find fixed points of Eq. (22). This observation demonstrates the influence of the chosen adaptive filter on the total dynamics as well. The naive approach to determine X^* is to completely ignore the time derivative in the slow timescale T [see Eq. (10)] and just assume that we always settle on $X^*(T; \mu)$ after some constant time T_{wait} or constant number of iterations of the applied control law. Indeed, this solution is valid if we are able to approximate T_{wait} . However, such an approach tends to prolong sweeps of the bifurcation

parameter μ , since the transient times between different setpoints h^* vary. In the specific case of dynamic-mode atomic force microscopy this results in intolerable thermal drift and therefore different μ -response curves. Instead we use a different path and employ an adaptation of Welford's algorithm [54] for a circular buffer that computes the current variance Σ as well as the average of the circular buffer (moving window) on the fly. Pushing new elements of the current observation $h|_n = h(X|_n)$ with a sampling frequency of $1/\Delta t_C$ into the circular array of length L , we obtain

$$\langle h \rangle|_{n+1} = \langle h \rangle|_n + \frac{h|_n - H}{L}, \quad (23)$$

$$\Sigma|_{n+1} = \Sigma|_n + (h|_n + H - \langle h \rangle|_n - \langle h \rangle|_{n+1}) \times (h|_n - H), \quad (24)$$

time-explicit update equations for the average $\langle h \rangle$ and variance Σ of the circular buffer with head H which contains the last stored entry, namely $h|_{n-1}$. We assume that we have reached a steady-state of the harmonic state X and that therefore Eq. (10) is satisfied if the average of the observation is within some error bound Δh^* around the current target and additionally the standard deviation of the buffer is smaller than a given σ_{tol} :

$$\langle h \rangle|_{n+1} \in [h^* - \Delta h^*, h^* + \Delta h^*], \quad \sqrt{\frac{\Sigma|_{n+1}}{L-1}} \leq \sigma_{\text{tol}} \quad (25)$$

The length L of the buffer as well as the as sampling frequency $1/\Delta t_C$ should thus be chosen to account for the slow-time scale $T \gg 2\pi/\min_i \omega_i$, hence $L\Delta t_C \sim T$, where L should be at least 10. If conditions (25) are fulfilled, we effectively switch towards the next setpoint in the grid of targets G_h . For stability reasons it might be advantageous to choose finer grid distances at bifurcations points. Generally one should create such buffers for each individual harmonic variable in the harmonic state to ensure minimal invasiveness. Nevertheless we assume, for computational efficiency, that convergence of the observation $h(X)$ is sufficient to identify a periodic orbit, since we raise the same assumption for the control itself. Hence, we conclude that, in contrast to PLLs where $h(X) = \phi_1(X)$, taking into account help functions or, in other words, observations that consider further harmonic variables of the state X could be beneficial. The Welford algorithm not only allows for fast sweeps, due to individual transient times, but in principle also facilitates the calculation of error bars on the bifurcation set, by tracking the bifurcation parameter μ , here ω_d , over time in a circular buffer as well, which is especially desirable in experimental setups. However, the adapted *Welford* algorithm comes with the cost of memory and assumes that the frequency set $\Omega = \{\omega_i\}$ is chosen sufficiently large in order for Eq. (22) to converge.

F. Explicit update equations of the controller

The overall dynamics can be ordered at three different timescales: first, the position of the tip, and therefore the continuous-time equations of motion [see Eq. (1)]; second, the PI controller, which is limited by the information gain of the harmonic state X and therefore the LMS algorithm [see Eq. (22)]; and finally, the slowest timescale represented by filling the circular buffer with current observations and evaluating steady-state behavior [see Eqs. (23) and (24)]. In experimental implementations the continuous-time integral is replaced by the natural evolution of the physical system, whereas the control law and Welford algorithm have to be handled and accurately timed by processes implemented on the corresponding hardware (e.g., a field programmable gate array). In simulations we use an adaptive Runge-Kutta algorithm, namely `Tsit5()` of the open source Julia package *DifferentialEquations.jl* [55], to integrate the equations of motion. We use one periodic discrete callback with sampling time Δt_{LMS} to handle updates of the control law

$$\frac{d}{dt}\psi = \omega_s + u(t), \quad \psi(0) = \psi_0, \quad (26)$$

with starting angular frequency ω_s . Another periodic callback with sampling time Δt_C is employed to update Eqs. (23) and (24) of the circular buffer. The transfer function of our simple controller can be written in the continuous s -domain as

$$G(s) = K_P + K_I \frac{1}{s} + K_D \frac{s}{sN_{\text{low}} + 1}, \quad (27)$$

where we optionally introduced a filtered differential part with timescale N_{low} . Applying a Tustin transform [56] and introducing the error $e|_n = h(X|_n) - h^*$ at the timestep $n\Delta t_{\text{LMS}}$, the time-explicit PID control law $u|_{n+1} = p|_{n+1} + i|_{n+1} + d|_{n+1}$ can be evaluated by

$$p|_{n+1} = c_1 e|_n, \quad (28)$$

$$i|_{n+1} = i|_n + c_2 (e|_n + e|_{n-1}), \quad (29)$$

$$d|_{n+1} = c_3 (e|_n - e|_{n-1}) + c_4 d|_n, \quad (30)$$

with initial conditions $p|_0 = 0, i|_0 = 0, d|_0 = 0$, where we introduced the constants

$$c_1 = K_P, \quad (31)$$

$$c_2 = K_I \frac{\Delta t_{\text{LMS}}}{2}, \quad (32)$$

$$c_3 = \frac{2K_D}{2N_{\text{low}} + \Delta t_{\text{LMS}}}, \quad (33)$$

$$c_4 = \frac{2N_{\text{low}} - \Delta t_{\text{LMS}}}{2N_{\text{low}} + \Delta t_{\text{LMS}}}, \quad (34)$$

for abbreviation and $p|_{n+1}, i|_{n+1}, d|_{n+1}$ are the proportional, integral, and differential part, respectively. N_{low} defines a time constant in order to smooth out the derivative of the differential controller. Generally the PID control can be further optimized by antiwindup features and sigmoidal activation functions between different targets h^* . The positive gains $K = (K_P, K_I, K_D) \in \mathbb{R}_+^3$ are found by trial and error. From experience we advise testing proportional and integral gains around the natural frequency of the cantilever, which is in accordance with the stability analysis of a PLL-controlled Duffing oscillator [44]. For experimental implementations we suggest (depending on the actual hardware used) using fixed-point arithmetic and binary angular measurements of ψ for fast evaluation of the controller [see Eqs. (28)–(30)], and abusing overflow properties of the instantaneous phase over time, since numerical overflows can be used to naturally mimic the circular $\mathbb{S}_{[0,2\pi)}$ topology of the phase space. In order to comply with sinusoidal actuation, we should update the instantaneous phase at least 10 times per period ($\Delta t_{\text{LMS}} < 2\pi/10\omega_0$). An experimental alternative might be to further smooth out the actuation signal given by the control law using an appropriate low-pass filter.

G. Limitations by construction

By construction the overall setup, summarized in Fig. 2, has the following limitations.

- (1) By using a grid G_h of targets h^* , we assume that the driving frequency $\omega_d(h(X^*))$ is a single-valued function in the near-resonance regime. This is often expressed as an S-shaped bifurcation set.
- (2) We assume that we can stabilize the formerly UPOs using a simple PI control. Although this allows for simple experimental implementations, the control gains are for

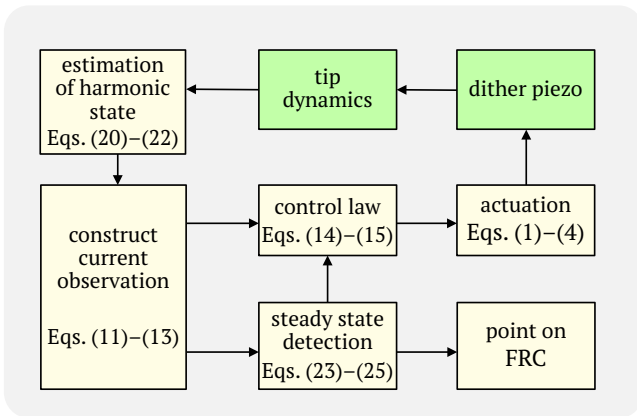


FIG. 2. High-level schematic of the proposed closed-loop control. The natural dynamics are highlighted in green boxes, whereas additional requirements for the feedback control and tracking of the bifurcation diagram are shown in yellow boxes.

now only found by coarse estimates and systematic trial and error. In experimental implementations we advise testing K_P in orders of magnitude of the natural frequency of the cantilever and increasing K_P, K_I if stability is not yet achieved, which is in accordance with [44]. Furthermore, it might be advantageous to restrict the output of the controller in such a way that solely driving frequencies in an interval around the natural frequency of the cantilever can be achieved, resulting in less rapid changes in the tip dynamics, related measurements, and overall less elongated transients.

(3) The effectiveness of the LMS algorithm to approximate the harmonic state $X(T)$ is strongly dependent on the sampling frequency of the deflection signal $x(t)$, as well as a sufficient frequency set $\Omega = \{\omega_i\}$ and step size γ . For experimental setups we advise investigating the frequency spectrum of stable periodic orbits near saddle-node bifurcations to choose a suitable set Ω . If the frequency set is not adequately chosen, the convergence of the LMS algorithm can no longer be guaranteed, since the basis vector is not persistently exciting. Nevertheless the results in the next section as well as experimental implementations [12] demonstrate that even a small set Ω is oftentimes sufficient in atomic force microscopy scenarios. To gain slow but precise harmonic state approximations we advise testing small LMS filter step sizes γ first. Increasing γ leads to fast coarse approximations of the harmonic state, but also overshooting and therefore prolonged transients.

III. RESULTS FOR VARIOUS INTERACTIONS

We will first demonstrate the feedback scheme on the well-known Duffing or Kerr nonlinearity and mention the connections between the constructed experimental continuation algorithm, the mathematical framework of averaging, and the stability of periodic orbits. Then we will show stabilization of unstable branches in more pertinent tip-sample interaction forces, namely a Lennard-Jones model with viscous damping and a Derjaguin-Muller-Toporov model.

A. Example I: Duffing/Kerr nonlinearity

In this subsection we consider the dynamical system

$$\begin{aligned} \frac{d}{dt}x &= v, & \frac{d}{dt}v &= -\omega_0^2 x - \varepsilon c v - \varepsilon \alpha x^3 + \varepsilon F \sin(\psi), \\ \frac{d}{dt}\psi &= \omega_d, \end{aligned} \quad (35)$$

which is the well-established forced Duffing oscillator with $\mathbb{R}^2 \times \mathbb{S}_{[0,2\pi)}$ phase space topology, soft excitation εF , and damping εc [57]. In addition to the traditional interpretation of a nonlinear spring, one might think of an extremely simplified interaction model (1), which solely contains a

repulsive, hardening $\alpha > 0$ or attractive, softening $\alpha < 0$ contribution. To analyze the forced system in Eq. (35) we apply Krylov-Bogoliubov averaging [41]. Alternatively, one can obtain the same results by the method of multiple scales, specifically the two-time method [57,58]. We begin by selecting the fast-time variable ψ , representing the instantaneous phase, and slow-time variable $T = \varepsilon t$, which will describe the envelope time evolution. We will solely cover the case of near-resonance driving $\omega_0^2 - \omega_d^2 = \varepsilon \Delta$, where $\varepsilon \Delta$ determines the detuning. By introducing the transformation

$$\begin{pmatrix} Y_{1,c}(T) \\ Y_{1,s}(T) \end{pmatrix} = A \begin{pmatrix} x \\ v \end{pmatrix}, \quad (36)$$

$$A = \begin{pmatrix} \cos(\omega_d t) & -\frac{1}{\omega_d} \sin(\omega_d t) \\ \sin(\omega_d t) & \frac{1}{\omega_d} \cos(\omega_d t) \end{pmatrix},$$

and substituting the inverse transformation A^{-1} into Eq. (35) one obtains a coupled first-order differential equation in the fast time scale t for the averaged sine and cosine quantities $Y_{1,s}, Y_{1,c}$. To obtain the slow-flow equations [see (37) and (38)] one can afterwards average the system by integrating over one period $\int_0^{2\pi/\omega_d} dt$ on both sides, as can be found in multiple textbooks (e.g., [41]), which yields

$$\frac{d}{dT} Y_{1,c} = \frac{\varepsilon}{2\omega_d} \left(-\omega_d c Y_{1,c} - \Delta Y_{1,s} - \frac{3\alpha}{4} Y_{1,s} (Y_{1,s}^2 + Y_{1,c}^2) \right), \quad (37)$$

$$\frac{d}{dT} Y_{1,s} = \frac{\varepsilon}{2\omega_d} \left(-\omega_d c Y_{1,s} + \Delta Y_{1,c} + \frac{3\alpha}{4} Y_{1,c} (Y_{1,s}^2 + Y_{1,c}^2) - F \right). \quad (38)$$

Frequency-response curves can now be obtained by finding roots of the right-hand side and varying ω_d . Note that this procedure closely resembles our feedback scheme by setting the frequency set solely to the driving frequency $\Omega = \{\omega_d\}$. However, care has to be taken in comparing both results, since in the feedback scheme the harmonic variables $X_{1,s}, X_{1,c}$ are, in contrast to the averaged quantities $Y_{1,s}, Y_{1,c}$, determined by a coupled fast-time ordinary

differential equation (ODE) themselves [see Eq. (20)], and therefore exist in a higher-dimensional dynamical system. Generally one can also obtain stability information on the steady states by linearization of the averaged ODE around the time-invariant sets. Promising results on the stability of the closed-loop system, which combines the adaptive filter, the original system dynamics, and a PLL, were found by Hippold *et al.* [45], where nevertheless full information on the nonlinearity is assumed, which is naturally not given in experimental AFM settings. Instead, we choose parameters of the controller by trial and error. As an example of averaging as well as the constructed continuation scheme we analyze the forced Duffing system [see Eq. (35)] with parameters listed in row 1 of Table I.

In Fig. 3(a) we showcase the ω_d -response curves, obtained by averaging and therefore essentially root-finding of Eqs. (37) and (38) and our proposed control. We notice small deviations between both results, since the first-order averaging approach only accounts for the fundamentals, whereas the feedback scheme relies on the more generous frequency set $\Omega = \{0, \omega_d, 3\omega_d, 5\omega_d\}$. The control strategy was to target linearly decreasing phase lags ϕ_1^* sequentially, which led to fast sweeps including the unstable branch. In fact, the control sweep was faster than open-loop sweeps due to close invariant sets along the sweep and shorter transients, since we actively manipulate the dynamics outside of invariant sets. In order to illustrate the multistability of the forced Duffing oscillator and grasp the difference between the time evolution of $(Y_{1,c}, Y_{1,s})^T$ and the harmonic state X , we consider the driving frequency $\omega_d/\omega_0 = 1.65$ marked as a dashed line in Fig. 3(a). The corresponding phase portrait of the averaged quantities is visualized in Fig. 3(b). We can observe that the slow-time vector field indeed has three time-invariant sets, which represent three solutions on the frequency-response curves. The unstable solution is thus topologically equivalent to a saddle-point and in a physical experiment not observable. To target the unstable solution, we effectively use polar coordinates to parameterize it by focusing on the angle. This can be considered as the fundamental phase-lag target $\phi_1^* = -2.15$ rad. To showcase how the feedback control manipulates the dynamics of the displacement x and actuation in order to reach the formerly unstable time-invariant set, we set up one initial condition $(x_0, v_0, \psi_0)^T = (0, 0, 0)^T$ with starting angular frequency $\omega_s = 1$ and target $\phi_1^* = -2.15$ rad. The transient

TABLE I. Parameters of the forced Duffing oscillator in the open-loop (system and adaptive filter) and additionally closed-loop system (system, adaptive filter and feedback). Parameters of the adaptive filter and feedback were found by trial and error.

	ω_0	$\varepsilon \alpha$	εF	εc	γ	Ω^a	Δt_{LMS}	Δt_C	K_P	K_I	σ_{tol}	L
1	1	0.05	2.5	0.2	0.1	{1, 3, 5}	0.01	10.2	0.4	0.004	1×10^{-4}	40
2	1	1	14	1	0.1	{1, 3, 5}	0.05	5.2	10	1	1×10^{-4}	40

^aIn terms of harmonics and additionally the direct current (dc) part.

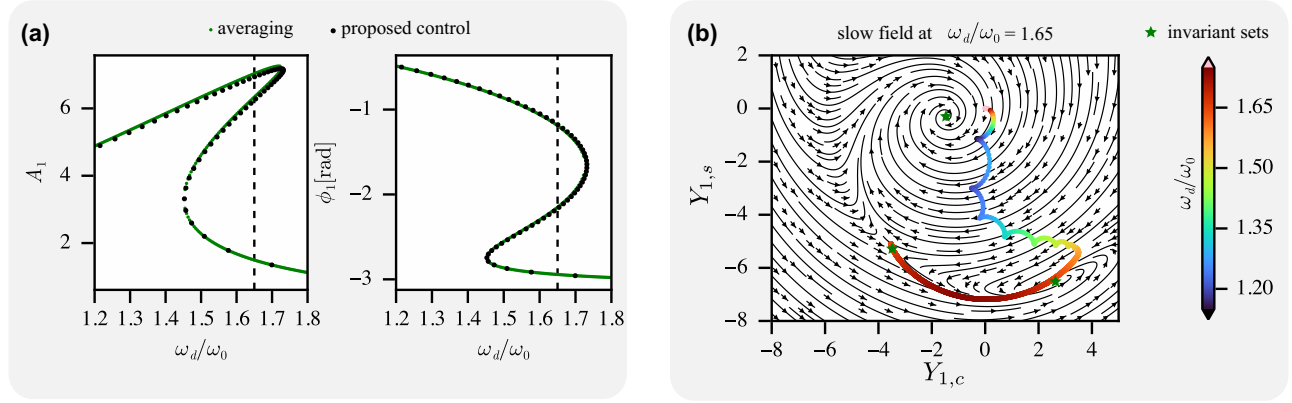


FIG. 3. (a) The fundamental amplitude A_1 and phase lag ϕ_1 for the averaged and controlled case of a repulsive Duffing oscillator for varying driving frequencies. Small deviations can be seen due to the multiharmonic approach for the control. (b) The slow-time vector field (37) and (38) at $\omega_d/\omega_0 = 1.65$. We projected the transient of the proposed control for a single target $\phi_1^* = -2.15$ [rad] onto the averaged phase space; the current driving frequency is used as color code.

of the harmonic state $X(t)$ of the displacement $x(t)$, estimated by the LMS algorithm (22), is projected onto the slow field, which approximates the open-loop behavior at $\omega_d/\omega_0 = 1.65$. The color code on the transient corresponds to the current driving angular frequency ω_d of the actuation. Interestingly, the control seems to be quite robust, despite being a simple PI controller, since at similar driving frequencies (red colors) we effectively trespass on another open-loop stable node-solution. We would like to highlight that the LMS algorithm in this scenario is cold started ($X = 0$). In continuation sweeps, as in Fig. 3(a), the distance between current and next harmonic states along the bifurcation curve $\|X^*(T; \mu) - X^*(T; \mu + \Delta\mu)\|$ is small if the targets h^* are spaced accordingly, resulting in less elongated transients in the phase space, since the LMS algorithm (22) has to adjust only slightly.

To showcase the versatility of the algorithm we apply the continuation via feedback control on different Duffing parameters [see row 2 of Table I], and track the bifurcation diagrams of the higher harmonics in the frequency set Ω as well. Figure 4 shows the complete bifurcation diagram for the fundamental and higher harmonic responses, achieved by manipulating the driving angular frequency ω_d by feedback control with observation $h(X(T)) = \phi_1(X(T))$ and linearly spaced targets. We observe that the continuation algorithm not only is able to track through stable periodic orbits, but also stabilizes formerly unstable time-invariant sets beyond the saddle-node bifurcation points, indicated by black squares, with just one set of closed-loop parameters. In Figs. 4(a) and 4(b) we see the fundamental amplitude and phase lag, respectively. The open-loop forward (blue) and backward (orange) sweeps as well as the control (gray) coincide for the stable branches of the system. In Fig. 4(a) we display the closed-loop harmonic variables $X_{1,s}$ and $X_{1,c}$, which themselves would require pseudo-arc-length schemes. Due to the range $[-\pi, \pi)$ of

$\arctan_2$ we color the top and bottom spines of the phase-lag coordinate systems with green lines, indicating the periodic boundary behavior. In Figs. 4(c)–4(f) we illustrate the harmonic variables and parametrizations of the third and fifth harmonics. Since bifurcations occur at the more fundamental level of the system state and we try to capture the system state by the harmonic state X , we see saddle-node bifurcations at exactly the same driving frequencies for each element in Ω . We would like to highlight that although we solely aim for a specific fundamental phase lag ϕ_1 , we inherently continued the whole harmonic state X , since the Lyapunov estimator or discrete LMS filter combines all elements within the frequency set Ω into one estimation of the displacement $\tilde{x}|_n = X^\top|_n c(\psi|_n)$, effectively coupling the dynamics of all harmonic variables over time [see Eq. (22)].

Interestingly, higher harmonic amplitudes, in contrast to A_1 , also exhibit S-curves and might be used as a set of targets to manipulate the driving frequency accordingly. By applying phase unwrapping, i.e. removing the 2π discontinuities by extending the range of the $\arctan_2$ function beyond $(-\pi, \pi)$, the higher-order phase lags can also serve as a suitable observation function $h(X)$. However, the harmonic variables corresponding to the higher harmonics are orders of magnitude smaller and could be more vulnerable to noise in real experimental scenarios. With these polynomial nonlinearities in mind, we now focus on more relevant force microscopy contact models.

B. Example II: Lennard-Jones model with viscous damping

One classical approach to model the interaction between tip and sample is by introducing a 12–6 potential, namely a Lennard-Jones interaction, and supplementing a viscous damping to account for nonlinear dissipation mechanisms

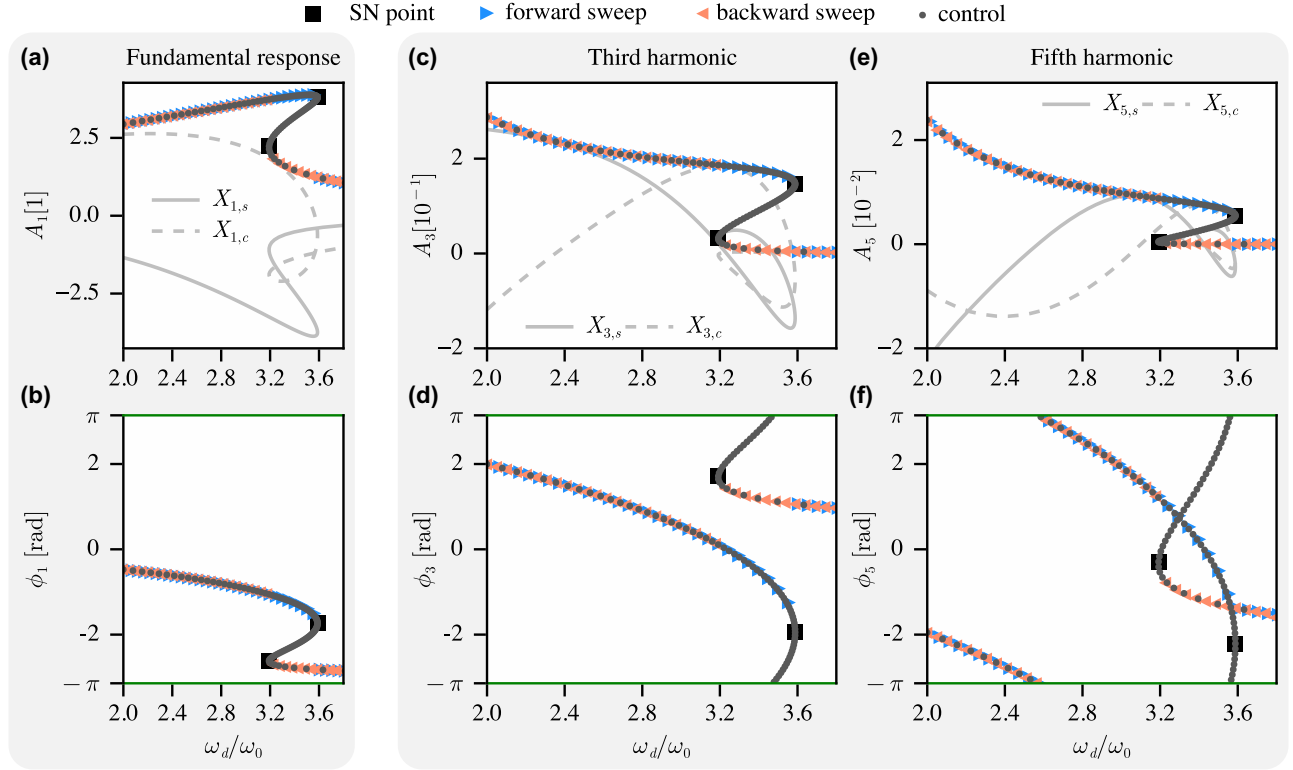


FIG. 4. Continuation of bifurcation diagram with feedback scheme on a Duffing oscillator with observation $h(X) = \phi_1(X)$ and parameters listed in row 2 of Table I. Additionally we used a differential controller with $K_D = 2.5$, $N_{\text{low}} = 2.5$. Panels (a),(b) showcase the fundamental responses with saddle-node bifurcation points, forward and backward open-loop sweeps, and applied control. The harmonic variables in (a) do not describe an S-curve, but the observation ϕ_1 in (b) shows and is utilized as a set of targets. Although we only target fundamental phase lags we intrinsically also achieve the stable and unstable periodic orbits on the higher harmonic responses [see (c)–(f)], due to the coupling of the frequencies in the Lyapunov estimator.

[59]. The Pauli part is active in case of pure hardening, and the van der Waals part in pure softening. In reality both parts participate because of the finite oscillation amplitudes, striking both regimes. Although for the attractive part a refined form was derived by Lifschitz, here we restrict ourselves to the Lennard-Jones model. We hence utilize dissipation introduced by introduced by [60], which translates in our coordinate system (1) and dynamical system to the tip-sample interaction

$$F_{\text{TS}}(x, v; s) = \frac{12V_0}{\sqrt{(x-s)^2}} \left(\left(\frac{\sigma^2}{(x-s)^2} \right)^6 - \left(\frac{\sigma^2}{(x-s)^2} \right)^3 \right) + \frac{cv}{(s-x)^3} \quad (39)$$

TABLE II. Parameters of the forced Lennard-Jones oscillator with viscous damping in the open-loop system.

$\frac{\omega_0}{2\pi}$ [kHz]	Q [1]	V_0 [aJ]	σ [nm]	k [N/m]	c [nN nm ² s]	s [nm]	F [nN]
55	400	4.2	2.8	0.7	$6 \cdot 10^{-4}$	60–120	0.3

with potential height determined by V_0 , potential minima distance proportional to σ , separation s , and nonlinear damping coefficient c . Different Lennard-Jones models [60] respect the geometry of the sample and cantilever tip. Here we simply use the interaction between two pseudo particles. In the Derjaguin-Muller-Toporov model [see Sec. III C] we will take care of geometry by modeling the tip as a ball and the sample as a flat surface. From the experimental point of view it is also interesting how the frequency-response curve changes with respect

TABLE III. Parameters of the forced Lennard-Jones oscillator with viscous damping in the open-loop (system and adaptive filter) and additionally closed-loop system (system, adaptive filter and feedback). Parameters of the adaptive filter and feedback were found by trial and error.

γ	Ω^a	$1/\Delta t_{\text{LMS}}$ [kHz]	$1/\Delta t_C$ [kHz]	K_P [kHz]	K_I [kHz/s]	σ_{tol} [rad]	L
0.05	{1, 2, 3, 4}	687.5	3.6	22	0.22	$5 \cdot 10^{-6}$	40

^aIn terms of harmonics and additionally the direct current (dc) part.

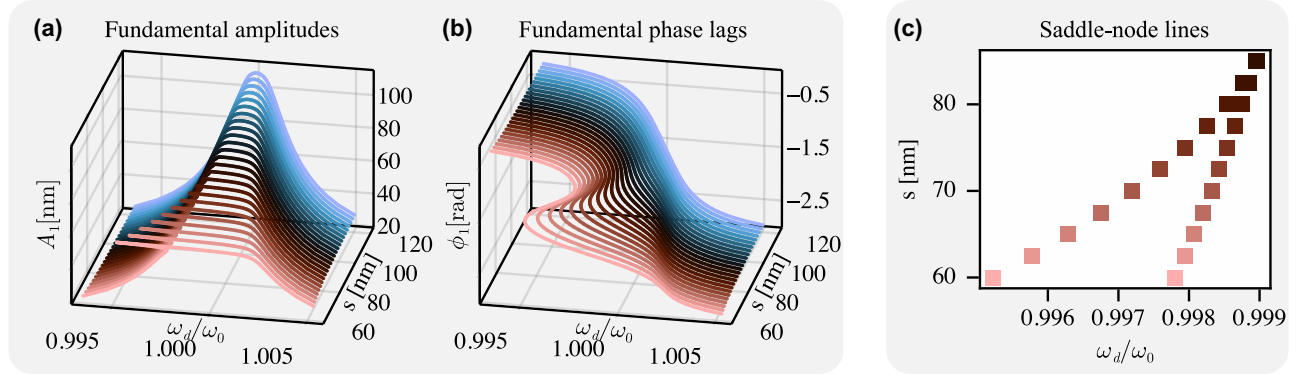


FIG. 5. Feedback control applied to Lennard-Jones model with parameters listed in Tables II and III. Illustrated in (a) and (b) are the fundamental amplitude A_1 and ϕ_1 for varying separations s , showing emergence of an unstable branch of periodic orbits for small s . In (c) we project the saddle-node bifurcation points to the (ω_d, s) -domain and therefore effectively track the saddle-node lines *a posteriori*, highlighting regions of multistability.

to the separation s , which will serve in the following as a second bifurcation parameter. We account for different separations by applying the feedback scheme for various values of s and thus construct a surface of all solutions in the (s, ω_d) domain, which include saddle-node and cusp-bifurcations [61].

Our control strategy is in this case to target 60 fundamental phase lags ϕ_1^* , for separations s between 60 nm and 120 nm. Generally one could achieve that in one single simulation, by changing the separation s after reaching all targets for a singular s . However, we are here opting for multiple simulations for each s that can easily be computed in parallel. In experimental scenarios the former case might be favorable. Surprisingly, we were able to find parameters for the control algorithm by trial and error that allowed us to stabilize UPOs for all the separations used here, listed in Table III. In Figs. 5(a) and 5(b) we see the various frequency-response curves of the fundamentals, leaning

towards driving frequencies, since the nonlinearity acts predominantly attractively with our parameters. Within the blue regime, and therefore big separations, we effectively observe Lorentzians associated to the linear theory of damped driven harmonic oscillators. Moving towards smaller separations, at the black curves (approx. 90 nm), we begin to see the existence of an UPO at a cusp point, related to $d\omega_d/d\phi_1 = 0$. At the most nonlinear red regime, we see in accordance with the experimental data a whole branch of UPOs lying extremely close to the stable periodic solutions in the amplitude. However, in the fundamental phase lag they are well separated. We can summarize the multistability by projecting the saddle-node bifurcation points *a posteriori* in the (ω_d, s) domain, as seen in Fig. 5(c), showcasing essentially a cusp catastrophe. Since our feedback scheme effectively continues the bifurcation curve for all frequencies in the set Ω , we now focus on one slice at constant separation $s = 65$ nm and analyze it more

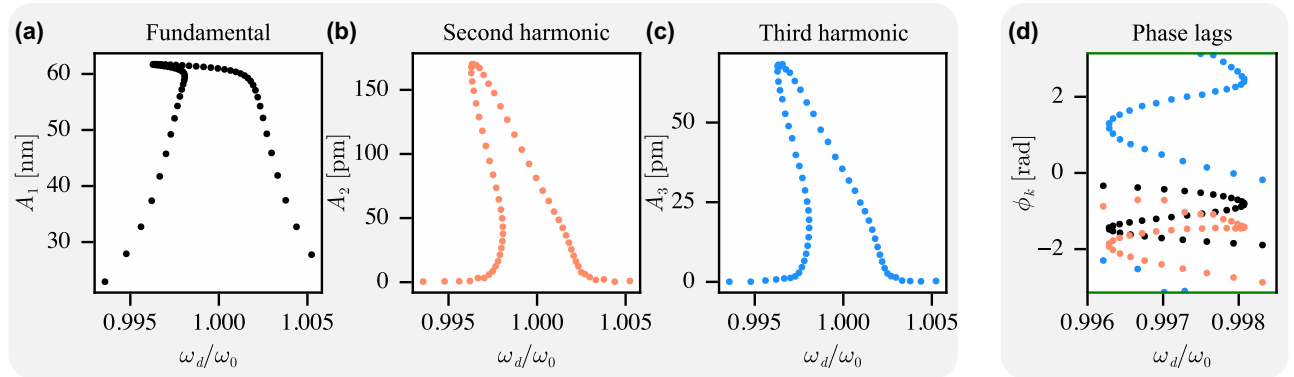


FIG. 6. Control algorithm applied to Lennard-Jones model listed in Tables II and III at constant separation $s = 65$ nm, indicating that we intrinsically track higher harmonic bifurcation curves. Panels (a)–(c) show the amplitudes of the respective harmonics. Using the same colors as in (a)–(c), we show the higher harmonic phase lags in (d). The top and bottom spines are thus colored green, indicating periodic boundaries, due to the range $[-\pi, \pi)$ of $\arctan_2$.

TABLE IV. Parameters of the forced DMT oscillator in the open-loop system. Parameters for the adaptive filter were found by trial and error.

$\omega_0/2\pi$ [kHz]	Q [1]	H [aJ]	k [N/m]	a_0 [nm]	R [nm]	F [nN]	γ	Ω^a
300	300	0.2	40	0.3	10	1.33	0.05	{1, 2, 3, 4}

^aIn terms of harmonics and additionally the direct current (dc) part.

closely. Similarly, as with the multiharmonic approach to the Duffing oscillator, the higher harmonic frequency-response curves for the Lennard-Jones interaction can also be conceptualized. As illustrated in Fig. 6(a), the amplitude of the unstable branch in the fundamental is nearly identical to that of the stable upper branch, further substantiating the assertion that pseudo-arc-length methods are not viable in the context of amplitude continuation. The same behavior is evident in the experimental data, as illustrated in Fig. 1. It is noteworthy that the unstable branches of the higher harmonics amplitudes are distinctly separated from the upper stable branch in magnitude, as illustrated in Figs. 6(b) and 6(c). It must be acknowledged, however, that amplitudes in the picometer regime may not be discernible in experimental frequency-response curves and, as a consequence, cannot be employed in arc-length schemes. Higher harmonic imaging is a prevalent technique within experimental dynamic-mode atomic force microscopy. These numerical results suggest that at least bistability for certain driving frequencies should be observable in this context. Figure 6(d) additionally plots the phase lags corresponding to the higher harmonics, which all show the S-curve property if unwrapped. Consequently, experimental higher harmonic phase contrast pictures of samples should indicate bimodal phase distributions for specific driving frequencies. We now focus on a different

dynamic-mode regime, often called the tapping mode, in which repulsive forces are also quite relevant.

C. Example III: Derjaguin-Muller-Toporov model

Another more commonly used tip-sample interaction force in dynamic-mode atomic force microscopy is the piecewise-defined Derjaguin-Muller-Toporov (DMT) model. The DMT model can be introduced in our dynamical system (1–4) by the tip-sample force F_{TS} , conditionally depending on the instantaneous distance

$$x < s - a_0 :$$

$$F_{TS}(x; s) = \frac{HR}{6(s-x)^2}, \quad (40)$$

$$x \geq s - a_0 :$$

$$F_{TS}(x; s) = \frac{HR}{6a_0^2} - \frac{4E}{3}\sqrt{R}(x - (s - a_0))^{3/2} \quad (41)$$

with the intermolecular distance a_0 , Hamaker constant H , tip-radius R , separation s , and effective elasticity module E . The Young modulus E is computed by individual elasticity modules $E_{t,s}$ of the tip and sample with respective Poisson ratios $\nu_{t,s}$ by

$$\frac{1}{E} = \frac{1 - \nu_t^2}{E_t} + \frac{1 - \nu_s^2}{E_s} \quad (42)$$

with $\nu_{t,s} = 0.3$, $E_t = 130$ GPa, and $E_s = 1$ GPa. The DMT model allows for modeling elasticity and penetration into the sample. For benchmark purposes we here choose the same parameters as Hoelscher *et al.* [11] in the tapping regime of AFM, listed in Table IV, and apply the noninvasive feedback control with parameters listed in Table V for 20 different linearly spaced separations s between 8.5 nm and 10.5 nm and 120 phase targets ϕ_1^* , which can be seen Figs. 7(a) and 7(b).

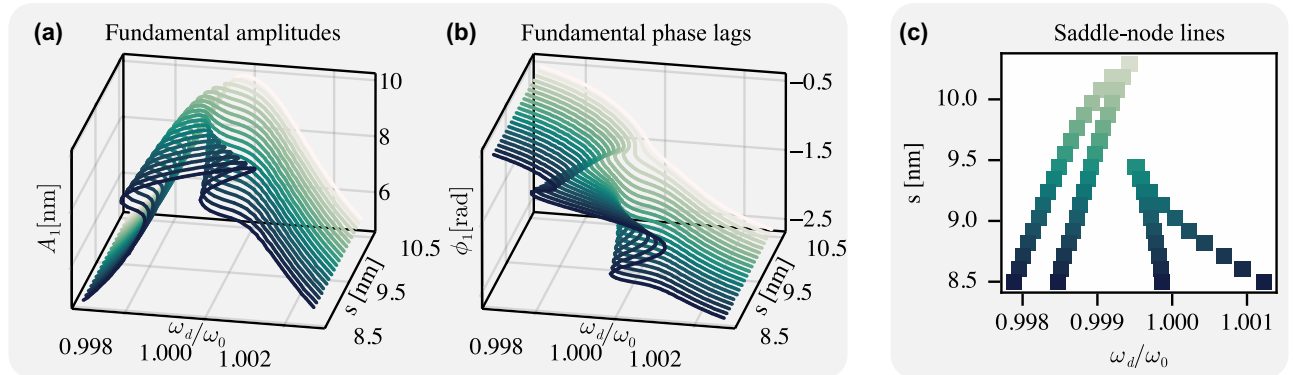


FIG. 7. Continuation algorithm applied to Derjaguin-Muller-Toporov model with parameters listed in Tables IV and V. By utilizing the same control hyperparameters for all separations s we are able to stabilize the whole manifold of solutions, including stable and unstable branches, as can be seen in (a) and (b). In (c) we project the saddle-node bifurcation points to the (ω_d, s) -domain and therefore effectively track the saddle-node lines *a posteriori*, highlighting regions of multistability.

TABLE V. Closed-loop parameters for the forced Derjaguin-Muller-Toporov system.

$1/\Delta t_{\text{LMS}}$ [MHz]	$1/\Delta t_C$ [kHz]	K_P [kHz]	K_I [kHz/s]	K_D [kHz · s]	N_{low} [μs]	σ_{tol} [rad]	L [1]
6	30	1.6	480	0.3	6.66	10^{-5}	50

From a theoretical standpoint, the DMT tip-sample interaction (40)–(41) presents a more difficult challenge due to the fact that it is no longer differentiable for all displacements x . Nevertheless, the continuation algorithm should remain operational as long as the harmonic state $X(T; \mu)$ undergoes continuous variation in response to alterations in the bifurcation parameter μ , specifically ω_d , and the observation $h(X(T; \mu))$ remains S-shaped. As illustrated in Figs. 7(a) and 7(b), the construction of a manifold encompassing all solutions and the effective tracking of stable and unstable periodic orbits with identical control parameters for all separations s are indeed feasible and in accordance with Hölscher *et al.* [11]. Unstable solutions can be characterized by $d\omega_d/d\phi_1 < 0$, whereas saddle-node bifurcation points correspond to $d\omega_d/d\phi_1 = 0$ and are projected in the (ω_d, s) -domain in Fig. 7(c), encapsulating regions of multistability. The saddle-node points thus merge at two distinguish cusp points. A critical factor of experimental implementations is the natural frequency f_0 of the cantilever. By choosing fast cantilevers, we intrinsically need, by the Nyquist limit, high sampling frequencies if we want to track higher harmonics. In this specific example $1/\Delta t_{\text{LMS}} = 6$ MHz might already be located at the upper bound of experimentally realistic sampling frequencies.

IV. CONCLUSION AND OUTLOOK

We have shown that stabilization of unstable periodic orbits in dynamic-mode atomic force microscopy is at least *numerically* possible by changing the driving frequency according to a noninvasive feedback control scheme. Experimental implementations show promising results and first unstable solutions were shown in Fig. 1, but are discussed more explicitly in a different publication [12]. In Sec. II we explained in detail the construction of the feedback control experimentally as well as in simulations, introduced an adaptive filter to gain the harmonic state online, and proposed a steady-state criterion to accelerate sweeps. Combining all three methods led to fast open-loop and closed-loop sweeps, which might inhibit problems arising by thermal drift in experimental settings. By applying these methods to numerical tip-sample interaction models in Sec. III, we concluded that inherent limitations of the feedback control seem manageable and even work for different separations, manifesting in surfaces with unstable branches and cusp bifurcations.

Generally force microscopy experiments might be an excellent framework to challenge and test even more sophisticated experimental continuation algorithms, due to the easily adjustable nonlinearities, by changing the sample itself (or the medium) or by using different separations s . The general framework with an observation function $h(X)$ is introduced in this context not only to justify approximations of $\arctan_2$ in experimental scenarios for acceleration purposes, but also to combine information of different harmonic modes into one observation in future theoretical works.

From the academic standpoint, such experiments can also be interesting due to still ongoing research in modeling tip-sample interactions, not only in the context of force microscopy, but also in tribology and electromechanical systems. Information on experimental (until now unreachable) unstable branches in dynamic-mode atomic force microscopy can effectively be used to benchmark competing theoretical models, where unstable solutions can be obtained by various numerical software (e.g., [62–65]). Another point we would like to emphasize is that in experimental settings numerous bifurcations can occur; here we only took into account saddle-node bifurcations. Future *theoretical* studies could revolve around control-based bifurcation analysis on liquid dynamic-mode AFM models or different continuation strategies, for example working on a constant driving frequency but changing the excitation amplitude.

V. DATA AND CODE AVAILABILITY

Data and code used for the numerical examples can be found on Zenodo [66]. The pipelines to create the figures in this paper with listed .csv files and *Makie.jl* [67] can also be found there.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [66].

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