

Diffusion-Induced Bistability of Driven Nanomechanical Resonators

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We study nanomechanical resonators with frequency fluctuations due to diffusion of absorbed particles. The diffusion depends on the vibration amplitude through inertial effect. We find that, if the diffusion coefficient D is sufficiently large, the resonator response to periodic driving displays bistability. The lifetime of the coexisting vibrational states exponentially increases with increasing D and displays a scaling dependence on the parameters close to bifurcation points.

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Micro- and nanomechanical resonators are studied in various contexts, from macroscopic quantum physics [1–4] to charge and mass sensing [5–9] to atomic and magnetic force microscopy [10]. They often have extremely narrow spectral lines at the fundamental mode frequency ω_0 , with linewidth $\lesssim 10^{-5}\omega_0$. An important factor in determining the line shape can be decoherence due to random frequency modulation. In turn, the modulation can itself depend on the vibration amplitude. An example is provided by the decoherence due to diffusion of massive particles along the resonator [11,12]. It occurs because the change of the resonator frequency depends on the particle positions [8]. However, because of inertia the particles themselves are driven toward the antinode of the mode [9], as beads on a vibrating string.

The dynamics of a resonator with diffusing particles becomes particularly interesting in the presence of a comparatively strong periodic driving at frequency ω_F close to ω_0 . Here one can think of the occurrence of two vibrational states. In one of them the vibration amplitude is large, and the diffusing particles concentrate close to the mode antinode and tune the vibration frequency of the resonator close to ω_F , leading self-consistently to a large amplitude. In the second state the vibration amplitude is small, and diffusion leads to an almost uniform distribution of particles over the resonator, tuning the vibration frequency further away from ω_F , which results, self-consistently, in a small vibration amplitude; see Fig. 1.

In this Letter, we show that driven nanoresonators can display diffusion-induced bistability (DIB), and the DIB may arise even where there are only a few or even one diffusing particle. Besides the physics of nanoresonators, the phenomenon is interesting from a broader perspective. Indeed, particle diffusion causes fluctuations of the nanoresonator frequency, and if the system is bistable, they lead to fluctuational switching between the coexisting states $i = 1, 2$. The notion of bistability is meaningful where the switching rates W_{ij} are much smaller than the vibration relaxation rate Γ , so that switching events are short and rare. The strong inequality $W_{ij} \ll \Gamma$ requires that the

fluctuation intensity \mathcal{D} be small; for example, for Gaussian fluctuations W_{ij} displays an activation dependence on \mathcal{D} [13]. One might think that, since frequency fluctuations are due to diffusion, \mathcal{D} is proportional to the diffusion coefficient D , and thus the DIB requires small D . In fact, the DIB occurs for large D , where diffusion largely averages out frequency fluctuations, and, as we show, W_{ij}/Γ is exponentially small, with $|\ln W_{ij}| \propto D$.

The DIB bears on noise-induced transitions [14], where the stationary probability distribution of a system changes from single- to double-peaked with increasing noise intensity. The occurrence of such a change does not indicate bistability, unless the peaks are well separated; moreover, in a bistable system the heights of the distribution peaks are strongly different (exponentially different, for the DIB for large D), with ratio $\propto W_{12}/W_{21}$, and become close only in a narrow parameter region where $W_{12} \approx W_{21}$. The DIB is somewhat closer to the noise-induced bistability seen in numerical simulations of a biomolecular system [15]; however, the conditions for the onset of the bistability and the parameter range where it occurs were not discussed in Ref. [15].

The suppression of fluctuations that leads to the DIB for one or a few diffusing particles can be understood for diffusion along a doubly clamped nanobeam; see Fig. 1.

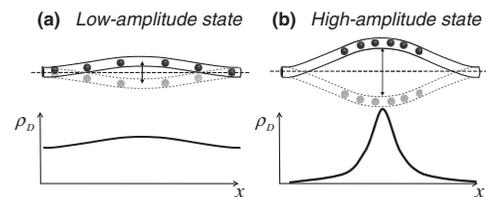


FIG. 1. Nanobeam resonator with diffusing particles. (a) In the low-amplitude vibrational state, the particle density $\rho_D(x)$ is almost uniform. (b) In the high-amplitude state, the particles are driven toward the antinode, and the distribution has a pronounced maximum there. Because of the different mass distribution, the resonator eigenfrequencies in (a) and (b) are different, which can lead to bistability of the resonant response.

Such diffusion was seen in a recent experiment [12], and its effect on the spectrum of linear response was analyzed earlier [11]. If the beam length is L , for a fixed vibration amplitude the particle distribution is formed over the diffusion time $t_D = L^2/D$ or faster. The distribution depends on the amplitude. In turn, it determines the nanobeam eigenfrequency. Then, if t_D is small compared to the vibration decay time $t_r = 1/\Gamma$, one can think of the eigenfrequency as being a function of the instantaneous amplitude. This is a familiar cause of bistability of forced vibrations [16]. Fluctuations are determined by small non-adiabatic corrections, are generally non-Gaussian, and as we show have intensity $\propto t_D/t_r \ll 1$.

We will consider a nanobeam with N diffusing particles of mass m and assume that $Nm \ll M$, where M is the nanobeam mass. In the fundamental mode, the transverse nanobeam displacement as a function of the longitudinal coordinate x (see Fig. 1) has the form $q(t)\phi(x)$, where $\phi(x)$ describes the spatial profile of the mode and $q(t)$ gives the vibration amplitude; we set $\int \phi^2 dx = L$. The vibrational kinetic energy is

$$\mathcal{T}_{\text{kin}} = \frac{1}{2} \int dx \mu(x) \dot{\phi}^2(x) \dot{q}^2. \quad (1)$$

Here, $\mu(x) = M/L + m \sum_n \delta(x - x_n)$, where x_n is the n th particle position along the beam. From Eq. (1), the particles change the nanobeam eigenfrequency from its value without them, ω_0 , to $\omega_e \approx \omega_0 - (m\omega_0/2M) \sum_n \phi^2(x_n)$. At the same time, the vibrations create an effective potential $-m\dot{q}^2 \phi^2(x)/2$ for the diffusing particles.

In the presence of friction and a force $F \cos \omega_F t$, the vibrations are described by the equation $\ddot{q} + 2\Gamma\dot{q} + \omega_e^2 q = (F/M) \cos \omega_F t$. We will assume that $\Gamma, t_D^{-1}, |\omega_F - \omega_0| \ll \omega_F$ and separate fast oscillations at frequency ω_F from their slowly varying amplitude and phase. To this end, we change from q and \dot{q} to dimensionless slow complex variables u and u^* :

$$u(t) = (2M\Gamma/F)(\omega_F q - i\dot{q}) \exp(-i\omega_F t), \quad (2)$$

dimensionless slow time $\tau = \Gamma t$, and dimensionless particle coordinates $z_n = x_n/L$. In the neglect of fast-oscillating terms, from Eq. (2)

$$\begin{aligned} \frac{du}{d\tau} &= K_r + K_D, & K_r &= -(1 + i\Omega)u - i, \\ K_D &= -iu \sum_n \nu(z_n), & \Omega &= (\omega_F - \omega_0)/\Gamma, \end{aligned} \quad (3)$$

where K_r and K_D describe the resonator dynamics without diffusing particles and the effect of these particles, respectively; $\nu(z) = (m\omega_0/2\Gamma M)\phi^2(Lz)$ is the scaled frequency shift of the resonator due to a particle at point $x = Lz$. We disregarded thermal noise in Eq. (3); it is usually weak for nanoresonators and does not change the qualitative results below.

The diffusing particles are usually overdamped. Their equation of motion in the neglect of fast-oscillating terms, inertia, and particle-particle interaction is

$$\frac{dz_n}{d\tau} = -|u|^2 \partial_{z_n} \Phi(z_n) + \theta^{1/2} \xi(\tau), \quad \theta = l_D^2/L^2. \quad (4)$$

Here, $\Phi(z) = -(F/4M\Gamma L)^2 (\Gamma\kappa)^{-1} \phi^2(Lz)$, with κ being the particle friction coefficient. The scaled potential $|u|^2 \Phi(z)$ is due to beam vibrations. Function $\xi(\tau)$ is white Gaussian noise that leads to diffusion, $\langle \xi(\tau) \xi(\tau') \rangle = 2\delta(\tau - \tau')$.

Parameter θ in Eq. (4) is determined by the diffusion length during the resonator relaxation time $l_D = (D/\Gamma)^{1/2}$; $\theta^{-1} \ll 1$ is the small parameter of the theory. The noise term in Eq. (4) is thus not small.

The probability density of the system $\rho = \rho(u, u^*; \{z_n\})$ is given by the Fokker-Planck equation

$$\partial_\tau \rho = -\{\partial_u [(K_r + K_D)\rho] + \text{c.c.}\} + \sum_n \Lambda_{z_n} \rho, \quad (5)$$

$$\Lambda_z \rho = \partial_z [|u|^2 \partial_z \Phi(z) + \theta \partial_z] \rho$$

with boundary conditions $\rho \rightarrow 0$ for $|u| \rightarrow \infty$ and the particle current equal to zero at the nanobeam boundaries $z = \pm 1/2$.

We will study first the most interesting case where there is just one particle on the nanobeam. Here, for $\theta \gg 1$ one can use the adiabatic approximation, in which the particle *distribution* adjusts to the slowly varying amplitude $|u|$ and phase $\varphi = -(i/2) \ln(u/u^*)$ of nanobeam vibrations. We consider an auxiliary eigenvalue problem

$$\Lambda_z \psi_\alpha = -\lambda_\alpha \psi_\alpha \quad (6)$$

with boundary conditions $[|u|^2 \partial_z \Phi + \theta \partial_z] \psi_\alpha = 0$ for $z = \pm 1/2$, where both λ_α and ψ_α depend parametrically on $|u|^2$. This is a standard Sturm-Liouville problem. It has an eigenstate with zero eigenvalue:

$$\lambda_0 = 0, \quad \psi_0(z; |u|^2) = Z^{-1} \exp[-|u|^2 \Phi(z)/\theta], \quad (7)$$

whereas the eigenvalues with $\alpha \geq 1$ are positive and large, $\lambda_{\alpha > 0} \gtrsim \theta$; in Eq. (7), $Z = \int dz \exp[-|u|^2 \Phi(z)/\theta]$. From Eqs. (5) and (6), in short time $\tau \sim \theta^{-1}$ the distribution with respect to z approaches a quasistationary, or adiabatic, value ψ_0 .

We seek the overall distribution as $\rho = \sum_\alpha P_\alpha(u, u^*, \tau) \psi_\alpha(z; |u|^2)$. Substituting this expression into Eq. (5), multiplying by the left eigenvectors $\bar{\psi}_\alpha$ of operator Λ_z , and integrating over z , we obtain

$$\begin{aligned} \partial_\tau P_\alpha &= -\lambda_\alpha P_\alpha - [\partial_u (K_r P_\alpha) + \text{c.c.}] - \sum_\beta k_{\alpha\beta} P_\beta \\ &+ \sum_\beta \nu_{\alpha\beta} \partial_\varphi P_\beta, \end{aligned} \quad (8)$$

$$\nu_{\alpha\beta} = \int dz \bar{\psi}_\alpha(z) \nu(z) \psi_\beta(z).$$

Here, $k_{\alpha\beta} = \int dz \bar{\psi}_\alpha (K_r \partial_u + \text{c.c.}) \psi_\beta$; we note that, since $\bar{\psi}_0 = 1$, $k_{0\alpha} = 0$.

From Eq. (8), function p_0 evolves on dimensionless time ~ 1 . The relaxation time of functions p_α with $\alpha > 0$ is $\lambda_\alpha^{-1} \lesssim \theta^{-1} \ll 1$. In this time they reach quasistationary values, which can be found from Eq. (8) by setting $\partial_\tau p_{\alpha>0} = 0$. Close to a maximum of p_0 , where $|\partial_\varphi p_0| \lesssim p_0$, we have $p_\alpha \approx -(k_{\alpha 0} p_0 - \nu_{\alpha 0} \partial_\varphi p_0) / \lambda_\alpha \sim p_0 / \theta$. To zeroth order in θ^{-1} , in Eq. (8) for p_0 the terms with $p_{\alpha>0}$ can be disregarded. This leads to the mean-field approximation: $p_0 \approx p_{\text{MF}}$,

$$\partial_\tau p_{\text{MF}} = -\partial_u(\tilde{K}_r p_{\text{MF}}) + \text{c.c.}, \quad \tilde{K}_r = K_r - iu\nu_{00}. \quad (9)$$

Parameter $\nu_{00} \equiv \nu_{00}(|u|^2)$ gives the shift of the nanoresonator frequency, $\omega_0 \rightarrow \omega_0 - \Gamma\nu_{00}$, which is determined by the vibration amplitude and the diffusion coefficient through Eq. (7).

Equation (9) corresponds to fluctuation-free motion in the rotating frame: $du/d\tau = \tilde{K}_r$. The stationary states $u = \text{const}$ determine periodic vibrational states of the resonator. Their scaled squared amplitude can be found from the equation

$$|u_{\text{st}}|^2 = \{1 + [\Omega + \nu_{00}(|u_{\text{st}}|^2)]^2\}^{-1}. \quad (10)$$

Equation (10) can have 1 or 3 solutions. The case of 3 solutions corresponds to the diffusion-induced bistability qualitatively explained in Fig. 1; only the solutions with the largest and smallest $|u_{\text{st}}|^2$ are stable.

The nonlinear response of the resonator displays the dependence on the field amplitude F and frequency ω_F , which is similar to the familiar response of an oscillator with cubic nonlinearity [16]. The parameter range where the bistability occurs is limited by the bifurcation lines where two solutions of Eq. (10) merge. This range has a characteristic wedgelike shape shown in Fig. 2.

A major effect of fluctuations caused by diffusion and disregarded in Eq. (9) is switching between the coexisting vibrational states. Such switching can be seen in the inset in Fig. 2 that illustrates the time dependence of $|u|^2$ obtained by numerical simulations. The resonator mostly performs small-amplitude fluctuations about the stable states determined by Eq. (10). However, occasionally there occurs a large fluctuation that drives it sufficiently far away to cause switching.

The switching rates are determined by the tail of the probability distribution for u far from its stable values. This tail is steep, with $|\partial_u p_\alpha| \propto \theta p_\alpha$ in Eq. (8). The approximation that led to Eq. (9) does not apply on the tail.

The analysis simplifies if the system is close, but not too close, to a saddle-node bifurcation point where a stable state merges with an unstable state and disappears. Here the rate of switching from the stable state W becomes larger, which facilitates observing switching; the bifurcation range is also interesting, because W often displays scaling behavior [17–19].

For Ω (or F) close to a bifurcational value, Ω_B (or F_B), the mean-field equation $du/d\tau = \tilde{K}_r$ is simplified. If we write $u = u_B + u' + iu''$, where u_B is the stationary value

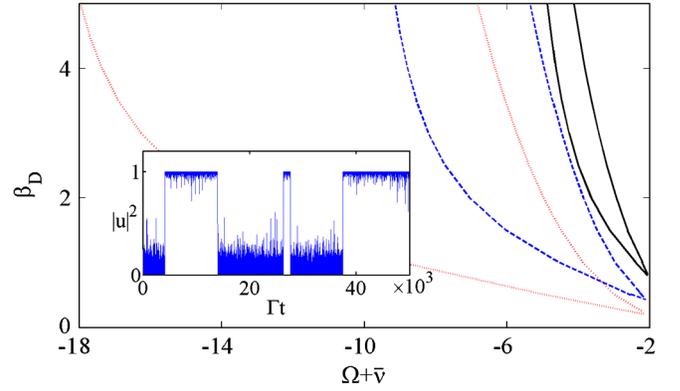


FIG. 2 (color online). Regions of bistability of a nanoresonator on the plane of the scaled intensity $\beta_D = (F/4M\Gamma)^2/\kappa D$ and frequency detuning Ω of the modulating field. The solid, dashed, and dotted lines show the pairs of bifurcation lines for $\bar{\nu} = Nm\omega_0/2M\Gamma = 5, 10, \text{ and } 20$, respectively, and for $\phi(x) = 2^{1/2} \cos(\pi x/L)$; the bistability occurs inside the corresponding wedges. The inset shows a simulated scaled squared amplitude of forced vibrations $|u|^2$ as a function of the scaled time Γt for $\theta = 1.01$, $\bar{\nu} = 10$, $\Omega = -18.95$, and $\beta_D = 5$.

of u at the bifurcation point, we find that the relaxation time of u' is $1/2$, whereas u'' varies much slower than u' for small $|u - u_B|$. By adiabatically eliminating u' , we obtain $du''/d\tau \approx \eta - bu''^2$, where $\eta \propto (\Omega - \Omega_B)$ is the distance to the bifurcation point, $|\eta| \ll 1$, whereas $|b| \sim 1$. The bistability exists for $\eta/b > 0$.

Since $|\tilde{K}_r| \ll 1$ for small $|\eta|$ and $|u - u_B|$, one can assume, and check afterwards, that in Eq. (8) $\partial_u p_\alpha / \theta p_\alpha$ is also small even where $|\partial_u p_\alpha / p_\alpha| \gg 1$. Then the quasistationary solution of Eq. (8) is $p_\alpha \approx \nu_{\alpha 0} \partial_\varphi p_0 / \lambda_\alpha$ for $\alpha > 0$. Substituting this into Eq. (8) for p_0 , we obtain

$$\partial_\tau p_0 = -[\partial_u(\tilde{K}_r p_0) + \text{c.c.}] + \mathcal{D} \partial_\varphi^2 p_0, \quad (11)$$

$$\mathcal{D} = \sum_{\alpha \geq 1} \frac{|\nu_{0\alpha}|^2}{\lambda_\alpha} = \int_0^\infty d\tau \langle \{ \nu[z(\tau)] - \nu_{00} \} \nu[z(0)] \rangle_u.$$

Here, $z(\tau)$ is given by Eq. (4) with $|u|^2 = \text{const}$, and $\langle \dots \rangle_u$ means averaging with $|u|^2 = \text{const}$. Since we are close to the bifurcation point, $\mathcal{D} \equiv \mathcal{D}(|u|^2) = \mathcal{D}(|u_B|^2)$.

Equation (11) is a Fokker-Planck equation in the resonator variables only. It corresponds to $\nu(z)$ in Eq. (3) being white Gaussian noise with mean ν_{00} and intensity $\mathcal{D} \propto 1/D$. Interestingly, \mathcal{D} becomes small for large D . This is because $1/D$ gives the correlation time of $\nu(z)$. For slowly varying in time p_0 , we have $\mathcal{D} |\partial_u p_0| \sim |\tilde{K}_r| p_0 \ll p_0$, justifying the earlier assumption.

The analysis of the switching rate near a bifurcation point can be done by using the method of Ref. [17]. It gives

$$W = (\Gamma |\eta b|^{1/2} / \pi) \exp(-4 |\eta|^{3/2} / 3 \mathcal{D} u_B^2 |b|^{1/2}). \quad (12)$$

From Eq. (12), the rate W displays activation dependence on $\mathcal{D} \propto 1/D$. Also, $\ln W$ scales with the distance to the bifurcation point η as $\eta^{3/2}$.

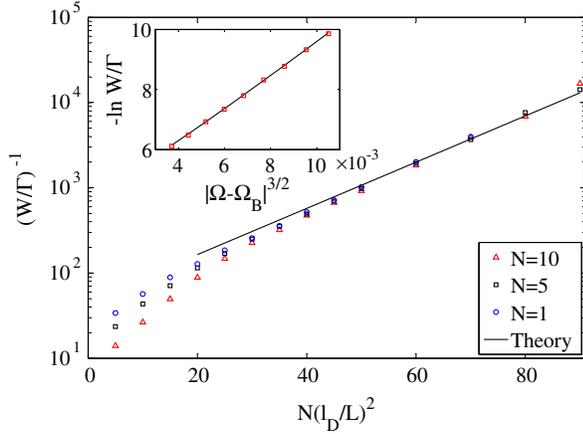


FIG. 3 (color online). The switching rate W near a bifurcation point as a function of the product of the diffusion coefficient D and the number of particles N for $\beta_D = 5$, $\bar{\nu} = 10$, and $\Omega - \Omega_B = 0.03$ ($\Omega_B = -19.145$). Inset: Scaling of $\ln W/\Gamma$ with the distance to the bifurcation point $\Omega - \Omega_B$ for the same β_D and $\bar{\nu}$; $\theta = 5.1$ and $N = 1$. The data are the results of simulations; the solid lines show the analytical predictions.

We now consider the case of many diffusing particles: $N \gg 1$; still we assume that their total mass is small: $Nm \ll M$. To the leading order in $1/N$, fluctuations from the particle diffusion are averaged out in the equation of motion for the resonator (3). The mean-field resonator dynamics is described by Eq. (9) with $\tilde{K}_r = K_r - iuN\nu_{00}$; i.e., m for the single particle case is replaced by Nm .

To describe fluctuations for $N \gg 1$ and given Nm , one can think of the term $\zeta(\tau) = N^{-1} \sum_n \nu[z_n(\tau)]$ in Eq. (3) as Gaussian noise with intensity $\propto 1/N$. Generally, $\zeta(\tau)$ is not δ -correlated. However, if the relaxation time t_D of diffusing particles is small, $\theta^{-1} \ll 1$, or if the system is close to a bifurcation point, so that its relaxation time is long ($\propto |\eta|^{-1/2}$) and largely exceeds t_D , the noise becomes effectively δ -correlated. Its intensity is \mathcal{D}/N , and the distribution of the resonator is described, respectively, by the Fokker-Planck equation (11) with \mathcal{D} replaced by \mathcal{D}/N . For large N and $\theta^{-1} \ll 1$, this equation is not limited to the vicinity of the bifurcation point.

The above analysis shows that the switching rate should display activation dependence on $\mathcal{D}/N \propto 1/ND$. This was indeed found in numerical simulations, as seen in Fig. 3, where $|\ln W| \propto ND$ for large ND and does not depend on N otherwise, for fixed Nm . The simulations also demonstrate the $3/2$ scaling of $|\ln W|$ with the distance to the bifurcation point.

The DIB should arise in nanoresonators and should display the described characteristic behavior provided the time of diffusion of attached particles over the resonator length exceeds the oscillation period but is smaller than the vibration decay time. For frequency $\omega_0/2\pi = 300$ MHz, decay rate $\Gamma = 10^5$ s $^{-1}$, and length $L = 1$ μ m, the appropriate range of the diffusion coefficient D is

$10^{-3} - 1$ cm 2 /s. In addition, the particle mass should not be too small, so that, for a large vibration amplitude, the energy gain from localizing a particle near the antinode, which is determined by Eq. (1), exceeds the temperature. Conceivable candidate systems are doubly clamped nanobeams or cantilevers based, for example, on carbon nanotubes, with $M \gtrsim 10^{-18}$ g, that have small metallic clusters, with $m \lesssim 10^{-20}$ g, diffusing along them. The intrinsic (Duffing-type) nonlinearity of such resonators can be small [5,6] and should not mask the effect.

In conclusion, we have demonstrated that diffusion of particles in a nanomechanical resonator can cause bistability of forced vibrations. The bistability can arise even for a single particle, given that the diffusion coefficient D is sufficiently large. In this case, the rate of switching scales as $-\ln W \propto D$ and is much smaller than the relaxation rate of the resonator. We also find the scaling behavior of W near bifurcation points. The analytical results are in excellent agreement with simulations, including the scaling of W with the number of particles.

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