

# Surface dissipation in nanoelectromechanical systems: Unified description with the standard tunneling model and effects of metallic electrodes

C. Seoáñez and F. Guinea

*Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E28049 Madrid, Spain*

A. H. Castro Neto

*Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA*

(Received 5 December 2007; revised manuscript received 22 January 2008; published 7 March 2008)

By modifying and extending recent ideas [C. Seoáñez *et al.*, *Europhys. Lett.* **78**, 60002 (2007)], a theoretical framework to describe dissipation processes in the surfaces of vibrating micro- and nanoelectromechanical devices, thought to be the main source of friction at low temperatures, is presented. Quality factors as well as frequency shifts of flexural and torsional modes in doubly clamped beams and cantilevers are given, showing the scaling with dimensions, temperature, and other relevant parameters of these systems. Full agreement with experimental observations is not obtained, leading to a discussion of limitations and possible modifications of the scheme to reach a quantitative fitting to experiments. For nanoelectromechanical systems covered with metallic electrodes, the friction due to electrostatic interaction between the flowing electrons and static charges in the device and substrate is also studied.

DOI: [10.1103/PhysRevB.77.125107](https://doi.org/10.1103/PhysRevB.77.125107)

PACS number(s): 03.65.Yz, 62.40.+i, 85.85.+j

## I. INTRODUCTION

The successful race for miniaturization of semiconductor technologies<sup>2</sup> manifests itself spectacularly in the form of nanoelectromechanical systems (NEMS),<sup>3–6</sup> which are machines in the micron and submicron scales whose mechanical motion, integrated into electrical circuits, has a wealth of technological applications, including control of currents at the single-electron level,<sup>7</sup> single-spin detection,<sup>8</sup> subattoneutron force detection,<sup>9</sup> mass sensing of individual molecules,<sup>10</sup> high-precision thermometry,<sup>11</sup> or *in vitro* single-molecule biomolecular recognition.<sup>12</sup>

These mechanical elements (such as cantilevers or beams, see Fig. 1) are also the focus of attention and intensive research as experiments are approaching the quantum regime,<sup>13–15</sup> where manifestations of quantized mechanical motion of a macroscopic degree of freedom such as their center of mass should become apparent. Several schemes to prepare the mechanical oscillator in a nonclassical state and observe clear signatures of its quantum behavior have been recently suggested.<sup>16–21</sup>

A key figure of merit of the mechanical oscillation is its quality factor  $Q = \omega / \Delta\omega$ , where  $\Delta\omega$  is the measured linewidth of the corresponding vibrational eigenmode of frequency  $\omega$ . To reach the quantum regime, as well as for most practical applications, where the measured shifts of the resonant frequency  $\omega$  constitute the detectors principle, a very high  $Q$  is compulsory. Imperfections and the environment surrounding the oscillator result in both a finite linewidth  $\Delta\omega$  and a frequency shift  $\delta\omega$  with respect to the ideal case. Therefore, several works have been devoted to the analysis of the different sources of dissipation present in microelectromechanical systems and NEMS,<sup>22–32</sup> trying to determine the dominant damping mechanisms and the ways to minimize them. Among the different mechanisms affecting semiconductor-based NEMS, the most important and difficult to avoid are (i) clamping losses<sup>33,34</sup> through the transfer

of energy from the resonator mode to acoustic modes at the contacts and beyond, up to the substrate, (ii) thermoelastic damping,<sup>35–37</sup> and (iii) friction processes taking place at the surfaces.<sup>38–40</sup> At low temperatures and for decreasing sizes, the prevailing mechanism is the last one,<sup>6</sup> as indicated by the linear decrease of the quality factor of flexural modes with decreasing size (see Fig. 2) or the sharp increase of  $Q$  when the resonator is annealed.<sup>38,41</sup> Excitation of adsorbed molecules, movement of lattice defects, or configurational rearrangements irreversibly absorb energy from the excited eigenmode and redistribute it among the rest of the degrees of freedom of the system.

A theoretical quantitatively accurate description of surface dissipation proves therefore challenging, as many different dynamical processes and actors come into play, some of whom are not yet well characterized, so simplifications need to be done to provide a unified framework for all of them. In Ref. 1, such a scheme was given, based on the following considerations: (i) experimental observations indicate that surfaces of otherwise monocrystalline resonators acquire a

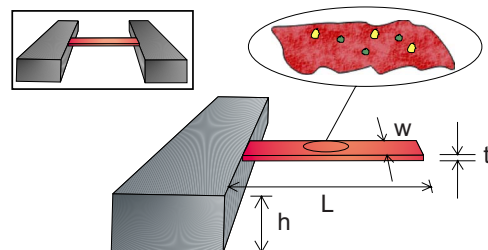


FIG. 1. (Color online) Sketch of the systems considered in the text. The inset shows a doubly clamped beam, while the main figure shows a cantilever characterized by its dimensions, width ( $w$ ), thickness ( $t$ ), and length, ( $L$ ), where  $w \sim t \ll L$ . The height above the substrate is  $h$ . A schematic view of the surface is given, highlighting imperfections such as roughness and adsorbates, which dominate dissipation at low temperatures.

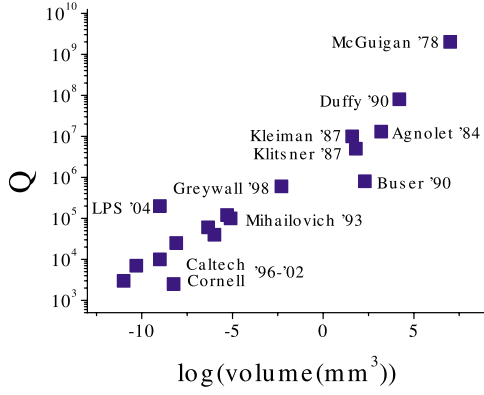


FIG. 2. (Color online) Evolution of reported quality factors in monocrystalline mechanical resonators with size, showing a decrease with linear dimension, i.e., with increasing surface-to-volume ratio, indicating a dominant role of surface-related losses (Ref. 6).

certain degree of roughness, impurities, and disorder, resembling an amorphous structure.<sup>42</sup> (ii) In amorphous solids, the damping of acoustic waves at low temperatures is successfully explained by the standard tunneling model,<sup>43–46</sup> which couples the acoustic phonons to a set of two-level systems (TLSs) representing the low-energy spectrum of all the degrees of freedom (DOFs) able to exchange energy with the strain field associated with the vibration. These DOFs correspond to impurities or clusters of atoms within the structure which have two energy minima separated by an energy barrier in their configurational space (similar to the dextro and/or levo configurations of the ammonia molecule), which are modeled as a DOF tunneling between two potential wells. At low temperatures, only the two lowest eigenstates have to be considered, characterized by the bias  $\Delta_0^z$  between the wells and the tunneling rate  $\Delta_0^x$  through the barrier. The standard tunneling model specifies the properties of the set of TLSs in terms of a probability distribution  $P(\Delta_0^x, \Delta_0^z)$  which can be inferred from general considerations<sup>43,44</sup> and is supported by experiments.<sup>46</sup> Note, however, that below a certain temperature the model breaks down due to the increasing role played by interactions among the TLSs (not shown).<sup>47,48</sup>

In Ref. 1, a description of the attenuation of vibrations in nanoresonators, due to their amorphouslike surfaces, in terms of an adequate adaptation of the standard tunneling model was intended to be given. An estimate for  $Q^{-1}(T)$  was provided, reproducing correctly the weak  $\sim T^{1/3}$  temperature dependence as well as the order of magnitude observed in recent experiments.<sup>30,32</sup> However, the way the standard tunneling model was adapted was not fully correct, and a revision of the results for  $Q^{-1}(T)$  obtained therein was mandatory.

In this work, we will (i) discuss in detail some important issues hardly mentioned in, Ref. 1 (ii) modify some points to obtain a theory fully consistent with the standard tunneling model and which includes all possible dissipative processes due to the presence of TLSs, (iii) extend the results and give expressions for the quality factor of cantilevers as well as damping of torsional modes and frequency shifts associated,

(iv) compare with available experimental data by discussing the validity of the model, range of applicability, and aspects to be modified and/or included to reach an accurate quantitative fit to experiments, and (v) study the dissipative effects associated with the presence of metallic electrodes frequently deposited on top of the resonators.

Section II starts with a brief summary of the model described in Ref. 1, discussing the approximations involved, while the different dissipative mechanisms due to the presence of TLSs are presented in Sec. III. Section IV analyzes and compares the two main mechanisms, namely, relaxational processes associated with asymmetric (biased) TLSs, and nonresonant damping of symmetric TLSs. The extension of the results to cantilevers and torsional modes is given in Sec. V. A brief account of the frequency shift expressions is found in Sec. VI. In Sec. VII, a comparison with experiments and a discussion of the applicability, validity, and further extensions of the model are made. Section VIII discusses dissipation effects due to the existence of metallic leads coupled to the resonator, which can be coupled to the electrostatic potential induced by trapped charges in the device. Under some circumstances, these effects cannot be neglected. Finally, the main conclusions of our work are given in Sec. IX. Details of some calculations are provided in the Appendixes.

We will not analyze here the dissipation due to clamping and thermoelastic losses, which may dominate dissipation in the case of very short beams and strong driving, respectively. We will also not consider direct momentum exchange processes between the carriers in the metallic circuit and the vibrating system.<sup>49</sup>

## II. SURFACE FRICTION MODELED BY TWO-LEVEL SYSTEMS

### A. Hamiltonian

We will consider a rod of length  $L$ , width  $w$ , and thickness  $t$  (see Fig. 1), and we use units such that  $\hbar=1=k_B$ . As described in Ref. 1, the vibrating resonator with imperfect surfaces is represented by its vibrational eigenmodes coupled to a collection of noninteracting TLSs, assuming that the main effect of the strain caused by the phonons is to modify the bias  $\Delta_0^z$  of the TLSs<sup>50</sup> as follows:

$$H = \sum_{k,j} \omega_{k,j} a_{k,j}^\dagger a_{k,j} + \sum_{\Delta_0^x, \Delta_0^z} \left\{ \Delta_0^x \sigma_x + \left[ \Delta_0^z + \sum_{k,j} \lambda_{k,j} (b_{k,j}^\dagger + b_{k,j}) \right] \sigma_z \right\}. \quad (1)$$

The index  $j$  represents the three kinds of modes present in a thin beam geometry:<sup>51</sup> flexural (bending), torsional, and compression modes. These modes will be present for wavelengths  $\lambda > t$ , while for shorter ones, the system is effectively three-dimensional (3D), with the corresponding 3D modes. The main effect of these high-energy 3D modes is to renormalize the tunneling amplitude, so we will take that renormalized value as our starting point  $\Delta_0^x$  and forget about the 3D modes in the following. The sum over TLSs is characterized by the probability distribution  $P(\Delta_0^x, \Delta_0^z) = P_0 / \Delta_0^x$ .<sup>43,44</sup>

This result follows, as explained in Refs. 44 and 45, due to (i) the exponential sensitivity of  $\Delta_0^x$  to the properties of the energy barrier of the two-well potential, giving rise to the TLS description of the system at low  $T$  [resulting in a  $1/\Delta_0^x$  dependence of  $P(\Delta_0^x, \Delta_0^z)$ ], and (ii) the characteristic energy scale of the distribution of asymmetries  $\Delta_0^z$ , much bigger than 1 K, which is the temperature at which experiments are performed and which, thus, fixes the scale of the bias of a TLS if it is to contribute significantly to dissipation,  $\Delta_0^z \leq 1$  K. [Therefore, the relevant TLSs have values of  $\Delta_0^z$  lying in a very narrow energy range around  $\Delta_0^z=0$  as compared to the variance of their probability distribution, allowing us to consider that  $P(\Delta_0^x, \Delta_0^z)$  to a first approximation does not depend on  $\Delta_0^z$ .] Unphysical divergencies do not appear, as  $\Delta_0^x > \Delta_{min}$ , with  $\Delta_{min}$  fixed by the typical time scale of the experiment, which is given by the time needed to obtain a spectrum around the resonance frequency of the excited vibrational eigenmode of the resonator, and  $\varepsilon = \sqrt{(\Delta_0^x)^2 + (\Delta_0^z)^2} < \varepsilon_{max}$ , which is estimated to be of the order of 5 K.<sup>46</sup> For typical amorphous insulators,  $P_0 \sim 10^{44} \text{ J}^{-1} \text{ m}^{-3}$ .

To see to which low-energy modes the TLSs are more coupled, inducing a more effective dissipation at low temperatures, the spectral function  $J(\omega, j) \equiv \sum_k |\lambda_{k,j}|^2 \delta(\omega - \omega_{k,j})$  characterizing the evolution of the strength of the coupling for each type of mode can be computed. Due to their non-linear dispersion relation  $\omega = \sqrt{EI/\rho t w k^2}$ , with  $I = t^3 w / 12$ ,  $E$  the Young modulus, and  $\rho$  the mass density, flexural modes show a sub-Ohmic behavior  $J_{flex}(\omega) = \alpha_b \sqrt{\omega_{co}} \sqrt{\omega}$ , with

$$\alpha_b \sqrt{\omega_{co}} = 0.3 \frac{\gamma^2}{t^{3/2} w} \frac{(1+\nu)(1-2\nu)}{E(3-5\nu)} \left( \frac{\rho}{E} \right)^{1/4}, \quad (2)$$

where  $\gamma \sim 5$  eV is a coupling constant appearing in  $\lambda_{k,j}$ ,  $\nu$  is Poisson's ratio, and  $\omega_{co} \approx \sqrt{EI/\rho t w} (2\pi/t)^2$  is the high-energy cutoff of the bending modes. A detailed derivation of  $J_{flex}(\omega)$  is given in Appendix A. Even though the length  $L$  of our system is finite, and thus the vibrational spectrum is discrete, a continuum approximation like this one will hold if  $kT \gg \hbar \omega_{fund}$ , with  $\omega_{fund}$  being the frequency of the fundamental mode.

The bending modes prevail over the other, Ohmic-like, modes as a dissipative channel at low energies, thanks to their weaker  $J_{flex}(\omega) \sim \omega^{1/2}$  dependence. One may ask at what frequency do the torsional and compression modes begin to play a significant role, and a rough way to estimate it is to see at what frequency do the corresponding spectral functions have the same value,  $J_{flex}(\omega^*) = J_{comp,tors}(\omega^*)$ . By using the expressions in Ref. 1, namely,  $J_{comp,tors}(\omega) = \alpha_c \omega$ , with  $\alpha_c = (\gamma \Delta_0^x / \Delta_0)^2 (2\pi^2 \rho t w)^{-1} (E/\rho)^{-3/2}$  and  $\alpha_t = C (\gamma \Delta_0^x / \Delta_0)^2 (8\pi^2 \mu t w \rho l)^{-1} (\rho l / C)^{3/2}$ , the results are  $\omega^* \sim 30(1+\nu)^2 (1-2\nu)^2 (E/\rho)^{1/2} / [t(3-5\nu)^2]$  for the case of compression modes and  $\omega^* \sim 300(1-2\nu)^2 (E/\rho)^{1/2} / [t(3-5\nu)^2(1+\nu)]$  for the torsional modes. By comparing these frequencies to that at the onset of 3D behavior,  $\omega_{co}$ , the frequencies are found to be similar, justifying a simplified model where only flexural modes are considered.

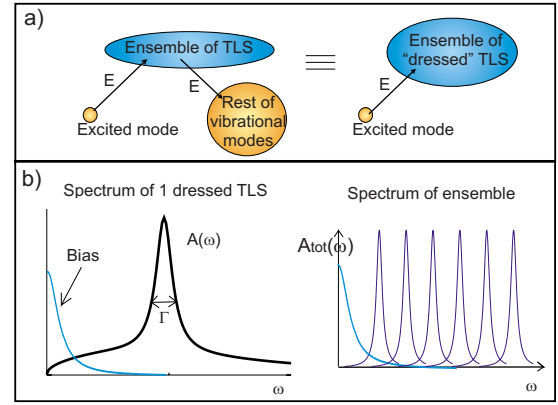


FIG. 3. (Color online) (a) Schematic representation of the irreversible flow of energy from the externally excited mode to the TLS ensemble, and from the ensemble to the rest of the vibrational modes. This process can be viewed as a flow of energy from the excited mode to an ensemble of dressed TLSs, with their dynamics modified by the presence of the vibrational modes. (b) Left: Spectral function  $A(\omega)$  of a single dressed TLS that is weakly damped ( $\Gamma < \Delta_0^x$ ). A peak around  $\omega=0$  arises if the system is biased, corresponding to the relaxational dissipation mechanism. Right: Total spectral function  $A_{tot}(\omega)$  of the ensemble of dressed TLSs.

## B. Two-level system dynamics

The interaction between the bending modes and the TLSs affects both of them. When a single mode is externally excited, as is done in experiments, the coupling to the TLSs will cause an irreversible energy flow from this mode to the rest of the modes through the TLSs, as depicted in Fig. 3(a). The dynamics of the TLSs in the presence of the vibrational bath determines the efficiency of the energy flow and thus the quality factor of the excited mode. By taking a given TLS plus the phonons, its dynamics is characterized by the Fourier transform of the correlator  $\langle \sigma_z(t) \sigma_z(0) \rangle$ , the spectral function  $A(\omega)$ , which at  $T=0$  reads

$$A(\omega) \equiv \sum_n |\langle 0 | \sigma_z | n \rangle|^2 \delta(\omega - \omega_n + \omega_0), \quad (3)$$

where  $|n\rangle$  is an excited state of the total system TLS plus vibrations. In Ref. 1, an analysis of  $A(\omega)$  was made for the case of a *symmetric* TLS ( $\Delta_0^z=0$ ), concluding that (i) if  $\Delta_0^x \ll \alpha_b^2 \omega_{co}$ , the tunneling amplitude is basically suppressed and the TLS does not participate in dissipative processes. For reasonable system dimensions, the coupling constant is very small,  $\alpha_b \ll 1$ , so this effect can be ignored. (ii) Around the resonance at  $\omega = \Delta_0^x$ , a broadening appears,  $\Gamma(\Delta_0^x)$ , which, for  $\Gamma(\Delta_0^x) \ll \Delta_0^x$ , is given by the Fermi golden rule result  $\Gamma(\Delta_0^x) = 16\alpha_b \sqrt{\omega_{co}} \sqrt{\Delta_0^x}$  [for  $T=0$  K; at  $T>0$ , Eq. (7) applies]. (iii) The coupling to phonons of all energies provides the "dressed" TLS with tails far from resonance,  $A(\omega) \propto \alpha_b \sqrt{\omega_{co}} \omega / (\Delta_0^x)^2$  for  $\omega \ll \Delta_0^x$  and  $A(\omega) \propto \alpha_b \sqrt{\omega_{co}} (\Delta_0^x)^2 \omega^{-7/2}$  for  $\omega \gg \Delta_0^x$  [see left side of Fig. 3(b)]. (iv) The main effect of the asymmetry  $\Delta_0^z$  is to suppress the TLSs dynamics, so the TLSs playing an active role in dissipation satisfy  $\Delta_0^x > |\Delta_0^z|$ .

Finally, for those low-energy overdamped TLSs such that  $\Gamma(\Delta_0^x) \gg \Delta_0^x$ , an incoherent decay  $\exp(-t/\tau)$  with time, with  $\tau(\Delta_0^x) = \Gamma(\Delta_0^x)^{-1}$ , was assumed.

Two points that Ref. 1 missed, and now will be considered, are the following: First, the effect of the asymmetry is not simply the one stated. An *underdamped biased* TLS develops an additional peak around  $\omega=0$ , as shown in Fig. 3(b), which corresponds to the relaxation mechanism that dominates the dissipation of acoustic waves in amorphous solids<sup>46</sup> [see Eq. (9)]. In Ref. 1, the relaxation mechanism associated with Eq. (9) was misinterpreted to correspond to friction due to overdamped TLSs, while in this work it will be linked to the presence of biased underdamped TLSs, consistent with the standard tunneling model. It will be described in more detail in the next section and taken into account in the computation of the total dissipation.

The second point missed by Ref. 1 is the following. One can estimate, using the probability distribution  $P(\Delta_0^x, \Delta_0^z)$ , the total number of overdamped TLSs in the volume fraction of the resonator having amorphous features,  $V_{amorph}$ . With  $V_{amorph} \sim V_{tot}/10$  and using  $\Gamma(E, T) = \Gamma(E, T=0) \coth[E/2T] \approx 2T\Gamma(E, T=0)/E$ , the number of overdamped TLSs,  $\Delta_0^x \leq \Gamma(\Delta_0^x, T) \rightarrow \Delta_0^x \leq [30\alpha_b \sqrt{\omega_{co} T}]^{2/3}$ , is  $N \approx P_0 t w L [30\alpha_b \sqrt{\omega_{co} T}]^{2/3}$ , which for typical resonator sizes  $L \sim 1 \mu\text{m}$  and  $t, w \sim 0.1 \mu\text{m}$  is less than 1 for  $T < 1$  K. Therefore, unless the resonator is bigger, and hence,  $P_0$  too, this contribution to dissipation can be safely neglected, as will be done in the following.

### III. DISSIPATIVE MECHANISMS

From the features of the spectral function  $A_{tot}(\omega) = \sum_{\Delta_0^x, \Delta_0^z} A(\Delta_0^x, \Delta_0^z, \omega)$  of the ensemble of dressed TLSs, one can classify into three kinds the dissipative mechanisms affecting an externally excited mode  $\omega_0$ .

#### A. Resonant dissipation

Those TLSs with their unperturbed excitation energies close to  $\omega_0$  will resonate with the mode, exchanging energy quanta, with a rate proportional to the mode's phonon population  $n_{\omega_0}$  to first order. For usual excitation amplitudes  $\sim 1 \text{ \AA}$ , the vibrational mode is so populated (as compared with the thermal population) that the resonant TLSs become saturated and their contribution to the transverse (flexural) wave attenuation becomes negligible, proportional to  $n_{\omega_0}^{-1/2}$ .<sup>52</sup>

#### B. Dissipation of symmetric nonresonant two-level systems

We show first that a correct description of the dissipation due to weakly damped TLSs is given by the approximate Hamiltonian used in Ref. 1, starting from Eq. (1), if one considers in some way that the presence of the relaxational peak at  $\omega=0$  is due to a finite bias  $\Delta_0^z \neq 0$ .

We focus the attention on a given TLS plus the vibrations (spin-boson model),  $H = \Delta_0^x \sigma_x + \Delta_0^z \sigma_z + H_{int} + H_{vibr}$ ,

$$H_{int} = \sigma_z \sum_k \lambda \frac{k^2}{\sqrt{\omega_k}} (a_k^\dagger + a_k), \quad (4)$$

with  $\lambda$  defined in Eq. (A4). In Ref. 1, a change of basis to the unperturbed eigenstates of the TLS was performed, obtaining  $H = \varepsilon \sigma_z + [(\Delta_0^x/\varepsilon) \sigma_x + (\Delta_0^z/\varepsilon) \sigma_z] \sum_k \lambda \frac{k^2}{\sqrt{\omega_k}} (a_k^\dagger + a_k) + H_{vibr}$ . Then the term  $(\Delta_0^z/\varepsilon) \sigma_z$  was ignored [remember  $\varepsilon = \sqrt{(\Delta_0^x)^2 + (\Delta_0^z)^2}$ ], arguing that the key role in dissipation is played by fairly symmetrical TLSs,  $|\Delta_0^z| \ll \varepsilon$ . This allowed us to simplify the spin-boson Hamiltonian to that of a symmetric TLS, which is much easier to analyze, with tunneling amplitude  $\varepsilon$  instead of  $\Delta_0^x$  and coupling  $\lambda(\Delta_0^x/\varepsilon)$  instead of  $\lambda$ . The consistency was kept by restricting the sums over the TLS ensemble to those such that  $|\Delta_0^z| \leq \Delta_0^x$ .

One can check this consistency by going back to the original basis, where the approximation of the Hamiltonian reads  $H \approx \Delta_0^x \sigma_x + \Delta_0^z \sigma_z + [(\Delta_0^x/\varepsilon)^2 \sigma_z - (\Delta_0^z \Delta_0^x/\varepsilon^2) \sigma_x] \sum_k \lambda \frac{k^2}{\sqrt{\omega_k}} (a_k^\dagger + a_k) + H_{vibr}$ . Restricting the application of this Hamiltonian to those TLSs such that  $|\Delta_0^z| \leq \Delta_0^x$  seems to be a fairly good approximation, but a price has been paid; namely, the spectral weight at  $\omega=0$  due to the bias has been lost in this effectively symmetric spin-boson approximation. This weight cannot be ignored, and it has to be added as a different mechanism (the relaxational mechanism), which will be done in the next section. Once this issue has been taken care of, all the dissipative processes due to the presence of TLSs are correctly included in this framework, and we can proceed describing nonrelaxational friction due to nonresonant, weakly damped, weakly biased TLSs.

As mentioned before, the coupled system TLSs + vibrations can be viewed, taking the coupling as a perturbation, from the point of view of the excited mode  $\omega_0$  as a set of TLSs with a modified absorption spectrum. The TLSs, dressed perturbatively by the modes, are entities capable of absorbing and emitting over a broad range of frequencies, transferring energy from the excited mode  $\omega_0$  to other modes. The contribution to the value of the inverse of the quality factor,  $Q^{-1}(\omega_0)$ , of all these nonresonant TLSs will be proportional to  $A_{\text{off-res}}^{\text{tot}}(\omega_0) = \sum_{\Delta_0^x=0}^{\omega_0 - \Gamma(\omega_0)} A(\Delta_0^x, \Delta_0^z, \omega_0) + \sum_{\omega_0 + \Gamma(\omega_0)}^{\varepsilon_{\text{max}}} A(\Delta_0^x, \Delta_0^z, \omega_0) \approx 2P\alpha_b \sqrt{\omega_{co}}/\omega_0$ , a quantity measuring the density of states which can be excited through  $H_{int}$  at frequency  $\omega_0$  (see Appendix B for details).

For an excited mode  $\omega_0$  populated with  $n_{\omega_0}$  phonons,  $Q^{-1}(\omega_0)$  is given by  $Q^{-1}(\omega_0) = \Delta E/2\pi E_0$ , where  $E_0$  is the energy stored in the mode per unit volume,  $E_0 \approx n_{\omega_0} \hbar \omega_0 / t w L$ , and  $\Delta E$  is the energy fluctuations per cycle and unit volume.  $\Delta E$  can be obtained from the Fermi golden rule as follows:

$$\Delta E_{\text{off-res}}^{\text{tot}} \approx \frac{2\pi}{\omega_0} \hbar \omega_0 \frac{2\pi}{\hbar} n_{\omega_0} \left( \lambda \frac{k_0^2}{\sqrt{\omega_0}} \right)^2 A_{\text{off-res}}^{\text{tot}}(\omega_0), \quad (5)$$

and the inverse quality factor of the vibration follows. For finite temperatures, the calculation of  $A_{\text{off-res}}^{\text{tot}}(\omega_0, T)$  is done in Appendix B. The result, valid for temperatures below the breakdown of the TLS approximate description of the two-well potential [ $T \sim 5$  K (Ref. 46)], is different from the one

given in Ref. 1, because there the value of  $Q^{-1}(\omega_0, T)$  was interpreted as corresponding to the net energy loss of the studied mode (subtracting emission processes from absorption ones), while in experiments the *observed linewidth* is due to the total amount of *fluctuations*, the addition of emission and absorption processes. So in this context, dissipation means fluctuations and not net loss of energy. The contribution of these kind of processes is thus

$$(Q^{-1})_{\text{off-res}}^{\text{tot}}(\omega_0, T) \approx 10P_0 t^{3/2} w \left(\frac{E}{\rho}\right)^{1/4} \frac{\alpha_b^2 \omega_{co}}{\omega_0} \text{cothanh}\left[\frac{\omega_0}{T}\right]. \quad (6)$$

### C. Contribution of biased two-level systems to the linewidth: Relaxation absorption

This very general friction mechanism arises due to the phase delay between stress and imposed strain rate. In our context, for a given TLS, the populations of its levels take a finite time to readjust when a perturbation changes the energy difference between its eigenstates.<sup>46,53</sup> This time  $\tau$  corresponds to the inverse linewidth and is given, for not too strong perturbations, by the Fermi golden rule result

$$\Gamma(\varepsilon, T) = 16\alpha_b \sqrt{\omega_{co}} \sqrt{\varepsilon} \text{coth}[\varepsilon/2T], \quad (7)$$

where  $\varepsilon = \sqrt{(\Delta_0^x)^2 + (\Delta^z)^2}$  is the energy difference between the levels. Notice that  $\Delta^z$  is not just the bare  $\Delta_0^z$  appearing in the Hamiltonian of the system, but the net bias including the modification due to the coupling to the vibrational modes,  $\Delta^z = \Delta_0^z + \xi_k \partial u_k$  ( $\xi_k$  is the corresponding coupling constant with the proper dimensions and  $\partial u_k$  is a component  $k$  of the deformation gradient matrix, defined recalling Eq. (4) as  $\partial u_k \sim \langle k, n_k | (k/\sqrt{\omega_k})(a_k^\dagger + a_k) | k, n_k \rangle$ , associated with a vibrational mode  $|k, n_k\rangle$ ). Equation (7) is valid in the range of applicability of the TLS description of the two-well potentials ( $T \leq 5$  K) and for values of  $\alpha_b$  such that  $\Gamma(\varepsilon, T) < \varepsilon$ . Therefore, the energy levels  $\varepsilon_{1,2} = \mp \frac{1}{2} \sqrt{(\Delta_0^x)^2 + (\Delta^z)^2} = \mp \frac{1}{2} \sqrt{(\Delta_0^x)^2 + (\Delta_0^z + \xi_k \partial u_k)^2}$  depend on  $\partial u_k$ , and to first order, the sensitivity of these energies to an applied strain is proportional to the bias

$$\frac{\partial \varepsilon_i}{\partial (\partial u_k)} = \frac{(\Delta_0^z + \xi_k \partial u_k)}{\varepsilon_i} \xi_k = \frac{\Delta_0^z}{\varepsilon_i} \xi_k, \quad (8)$$

with a response of the TLS  $\propto (\Delta^z/\varepsilon)^2$ . In Ref. 46, a detailed derivation is given, and the imaginary part of the response, corresponding to  $Q^{-1}$ , is also  $\propto \tau/(1 + \omega^2 \tau^2)$ , which, in terms of  $A(\omega)$ , is the Lorentzian peak at  $\omega=0$  of Fig. 3(b).

The mechanism is most effective when  $\tau \sim 1/\omega$ , where  $\omega$  is the frequency of the vibrational mode; then, along a cycle of vibration, the following happens (see Fig. 4): When the TLS is under no stress, the populations, due to the delay  $\tau$  in their response, are being still adjusted as if the levels corresponded to a situation with maximum strain [and therefore, of maximum energy separation between them; cf.  $\varepsilon_{1,2}(u_k)$ ], so that the lower level becomes overpopulated. As the strain is increased to its maximum value, the populations are still adjusting as if the levels corresponded to a situation with

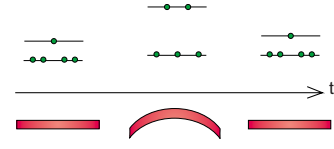


FIG. 4. (Color online) Schematic representation of the levels' population evolution of an ensemble of five identical TLSs with a response time  $\tau \sim 1/\omega$ , where  $\omega$  is the frequency of the excited bending mode, whose evolution is also depicted in the lower part of the figure. The delay  $\tau$  plus the bias  $\Delta_0^z$  give rise to the relaxational energy loss mechanism of the mode (see text).

minimum strain, thus overpopulating the upper energy level. Therefore, in each cycle, there is a net absorption of energy from the mechanical energy pumped into the vibrational mode.

If, on the other hand,  $\tau \gg 1/\omega$ , the TLS level populations are frozen with respect to that fast perturbation, while in the opposite limit,  $\tau \ll 1/\omega$ , the levels' populations are always in instantaneous equilibrium with the variations of  $\varepsilon_{1,2}$  and there is no net absorption of energy.

For an ensemble of TLSs, the contribution to  $Q^{-1}$  is<sup>46</sup>

$$Q_{\text{rel}}^{-1}(\omega, T) = \frac{P_0 \gamma^2}{ET} \int_0^{\varepsilon_{\text{max}}} d\varepsilon \int_{u_{\text{min}}}^1 du \frac{\sqrt{1-u^2}}{u} \frac{1}{\cosh^2(\varepsilon/2T)} \times \frac{\omega \tau}{1 + (\omega \tau)^2}. \quad (9)$$

The derivation of Eq. (9) only relies on the assumptions of the existence of well defined levels that need a finite time  $\tau$  to reach thermal equilibrium when a perturbation is applied and the existence of bias  $|\Delta_0^z| > 0$ . This implies that such a scheme is applicable also to our one-dimensional (1D) vibrations, but is valid only if the perturbation induced by the bath on the TLSs is weak, so that the energy levels are still well defined. Therefore, we will limit the ensemble to underdamped TLSs where  $\Gamma(\varepsilon, T) < \varepsilon$ . In Eq. (9), the factor  $\cosh^{-2}(\varepsilon/2T)$  imposes an effective cutoff  $\varepsilon < T$ , so that in Eq. (7), one can approximate  $\text{coth}[\varepsilon/2T] \sim 2T/\varepsilon$ , resulting in  $\Gamma(\varepsilon) \sim 1/\sqrt{\varepsilon}$  and thus the underdamped TLSs will satisfy  $\varepsilon \geq [30\alpha_b \sqrt{\omega_{co}} T]^{2/3}$ . For  $T \gg [32\alpha_b \sqrt{\omega_{co}}]^2$ , which is fulfilled for typical sizes and temperatures (see Appendix C for details),

$$Q_{\text{rel}}^{-1}(\omega_0, T) \approx \frac{20P_0 \gamma^4 (1+\nu)(1-2\nu)}{t^{3/2} w E^2 (3-5\nu)} \left(\frac{\rho}{E}\right)^{1/4} \frac{\sqrt{T}}{\omega_0}. \quad (10)$$

Here,  $V_{\text{amorph}} \sim V_{\text{tot}}/10$  was assumed.

## IV. COMPARISON BETWEEN CONTRIBUTIONS TO $Q^{-1}$ : RELAXATION PREVALENCE

It is useful to estimate the relative importance of the contributions to  $Q^{-1}$  coming from the last two mechanisms. For that sake, we particularize the comparison to the case of the fundamental flexural mode, which is the one usually excited and studied, of a doubly clamped beam, with frequency  $\omega_0 \approx 6.5(E/\rho)^{1/2} t/L^2$  (for a cantilever, these considerations

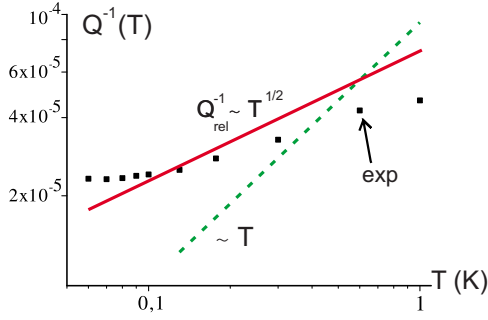


FIG. 5. (Color online) Example of fit of  $Q_{\text{rel}}^{-1}(\omega_0, T)$  [Eq. (10)] to experimental data. The data correspond to a Si resonator vibrating at  $\omega_0 = 12.028$  MHz (see Ref. 30). Although the predicted order of magnitude for the dissipation and the sublinear temperature dependence is observed, the experimental trend follows a weaker temperature dependence than the prediction  $T^{1/2}$ . For comparison, a linear temperature dependence is shown (dotted line). See the text for more details.

hold, with only a slight modification of the numerical prefactors; the conclusions are the same). The result is

$$\left[ \frac{Q_{\text{rel}}^{-1}(T)}{Q_{\text{off-res}}^{-1}(T)} \right]_{\text{fund}} \approx \frac{300t^{1/2}}{L} \frac{(3-5\nu)}{(1+\nu)(1-2\nu)} \frac{E}{\rho} \frac{1}{T^{1/2}}. \quad (11)$$

For a temperature  $T=1$  K, the result is as big as  $10^6$  even for a favorable case;  $t=1$  nm,  $L=1$   $\mu\text{m}$ ,  $E=50$  GPa,  $\nu=0.2$ , and  $\rho=3$  g/cm<sup>3</sup>. So for any reasonable temperature and dimensions, the dissipation is dominated by the relaxation mechanism, so that the prediction of the limit that surfaces set on the quality factor of nanoresonators is, within this model for the surface, Eq. (10) as follows:

$$Q_{\text{surface}}^{-1}(\omega_0, T) \approx Q_{\text{rel}}^{-1}(\omega_0, T) \sim \frac{T^{1/2}}{\omega_0}. \quad (12)$$

For typical values  $L \sim 1$   $\mu\text{m}$ ,  $t, w \sim 0.1$   $\mu\text{m}$ ,  $\gamma \sim 5$  eV,  $P_0 V_{\text{amorph}} / V_{\text{tot}} \sim 10^{44}$  J/m<sup>3</sup>, and  $T$  in the range 1 mK–0.5 K, the estimate for  $Q_{\text{surface}}^{-1} \sim 10^{-4}$  gives the observed order of magnitude in experiments such as Ref. 30 and also predicts correctly a sublinear dependence, but with a higher exponent, 1/2 versus the experimental fit 0.36 in Ref. 30 or 0.32 in Ref. 32 (see Fig. 5 for an example).

## V. EXTENSIONS TO OTHER DEVICES

### A. Cantilevers, nanopillars, and torsional oscillators

The extrapolation from doubly clamped beams to cantilevers<sup>54</sup> and nanopillars<sup>7</sup> is immediate, the only difference between them being the allowed  $(k, \omega(k))$  values due to the different boundary conditions at the free end [and even this difference disappears as one considers high frequency modes, where in both cases one has  $k_n \approx (2n+1)\pi/2L$ ]. All previous results apply, and one has just to take care in the expressions corresponding to the  $Q^{-1}$  of the fundamental mode, where there is more difference between the frequencies of both cases, the cantilever one being  $\omega_0^{\text{cant}} \approx (E/\rho)^{1/2} t/L^2$  as compared to the doubly clamped case,  $\omega_0^{\text{clamped}} \approx 6.5(E/\rho)^{1/2} t/L^2$ .

### B. Effect of the flexural modes on the dissipation of torsional modes

The contribution from the TLSs + sub-Ohmic bending mode environment to the dissipation of a torsional mode of a given oscillator can be also estimated. We will study the easiest (and experimentally relevant<sup>55</sup>) case of a cantilever. For paddle and double paddle oscillators, the geometry is more involved, modifying the moment of inertia and other quantities. When these changes are included, the analysis follows the same steps we will show.

#### 1. Relaxation absorption

We assume, based on the previous considerations on the predominant influence of the flexural modes on the TLSs dynamics, as compared with the influence of the other modes, that the lifetime  $\tau = \Gamma^{-1}$  of the TLSs is given by Eq. (7). The change in the derivation of the expression for  $Q^{-1}$  is shown in Eq. (8), where the coupling constant  $\xi_k^{\text{tors}}$  is different, which translates simply, in Eq. (9), into substituting  $\gamma^2 \leftrightarrow \gamma_{\text{tors}}^2$ , and the corresponding prediction for  $Q_{\text{rel}}^{-1}$  is as follows:

$$Q_{\text{rel}}^{-1}(\omega_0, T) \approx \frac{20P_0 \gamma_{\text{tors}}^2 \gamma^2 (1+\nu)(1-2\nu)}{t^{3/2} w} \frac{1}{E^2 (3-5\nu)} \left( \frac{\rho}{E} \right)^{1/4} \frac{\sqrt{T}}{\omega_0}, \quad (13)$$

where now  $\omega_0$  is the frequency of the corresponding flexural mode. The range of temperatures and sizes for which this result applies is the same as in the case of an excited bending mode.

#### 2. Dissipation of symmetric nonresonant two-level systems

The modified excitation spectrum of the TLS's ensemble,  $A_{\text{off-res}}^{\text{tot}}(\omega_0, T)$ , remains the same, and the change happens in the matrix element of the transition probability of a mode  $|k_0, n_0\rangle$  appearing in Eq. (5),  $(\lambda k_0^2 / \sqrt{\omega_0})^2$ . The operator yielding the coupling of the bath to the torsional mode which causes its attenuation is the interaction term of the Hamiltonian, which for twisting modes is [see Appendix D for the derivation of Eqs. (14) and (15)]

$$H_{\text{int}}^{\text{tors}} = \hbar \sigma_z \sum_k \gamma \sqrt{\frac{C}{8\mu t w}} \sqrt{\frac{1}{2\rho \hbar L}} \frac{k}{\sqrt{\omega_k}} (a_k^\dagger + a_k), \quad (14)$$

where  $\mu = E/[2(1+\nu)]$  is a Lande coefficient and  $C = \mu t^3 w/3$  is the torsional rigidity. Again,  $Q^{-1}(\omega_j) = \Delta E/2\pi E_0$ , where the energy  $E_0$  stored in a torsional mode  $\phi_j(z, t) = A \sin[(2j-1)\pi z/2L] \sin(\omega_j t)$  per unit volume is  $E_0 = A^2 \omega_j^2 \rho (t^2 + w^2)/48$  ( $z$  is the coordinate along the main axis of the rod). Expressing the amplitude  $A$  in terms of phonon number  $n_j$ , the energy stored in mode  $|k_j, n_j\rangle$  is

$$E_0(k_j, n) = \frac{1}{2} \frac{\hbar \omega_j}{(t^3 w + w^3 t) L} (t^2 + w^2) (2n_j + 1), \quad (15)$$

the energy fluctuations in a cycle of such a mode is

$$\Delta E = \frac{2\pi}{\omega_j} \hbar \omega_j \frac{2\pi}{\hbar} \frac{\gamma^2 \hbar \omega_j}{16Ltw\mu} n_j A_{\text{off-res}}^{\text{tot}}(\omega_j, T), \quad (16)$$

and the inverse quality factor

$$(Q^{-1})_{\text{off-res}}^{\text{tot}}(\omega_0, T) \approx 0.04 \frac{\gamma^4 P \rho^{1/4} (1+\nu)^2 (1-2\nu)}{t^{3/2} w E^{9/4} (3-5\nu)} \times \frac{1}{\sqrt{\omega_0}} \text{cothanh} \left[ \frac{\omega_0}{T} \right]. \quad (17)$$

For sizes and temperatures as the ones used for previous estimates, the relaxation contribution dominates dissipation.

## VI. FREQUENCY SHIFT

Once the quality factor is known, the relative frequency shift can be obtained via a Kramers–Kronig relation (valid in the linear regime), because both are related to the imaginary and real parts, respectively, of the acoustic susceptibility. First, we will demonstrate this, and afterwards, expressions for beam and cantilever will be derived and compared to experiments.

### A. Relation to the acoustic susceptibility

In the absence of sources of dissipation, the equation for the bending modes is given by  $-(12\rho/t^2)\partial^2 X/\partial t^2 = E\partial^4 X/\partial z^4$ . The generalization in the presence of friction is

$$-\frac{12\rho}{t^2} \frac{\partial^2 X}{\partial t^2} = (E + \chi) \frac{\partial^4 X}{\partial z^4}, \quad (18)$$

where  $\chi$  is a complex-valued susceptibility. Inserting a solution of the form  $X(z, t) = A e^{i(kx - \omega t)}$ , where  $k$  is now a complex number, one gets the dispersion relation  $\omega = \sqrt{t^2(E + \chi)/(12\rho)} k^2$ . Now, assuming that the relative shift and dissipation are small, implying  $\text{Re}(\chi) \ll E$  and  $\text{Im}(k) \ll \text{Re}(k)$ , the following expressions for the frequency shift and inverse quality factor are obtained in terms of  $\chi$ :

$$Q^{-1} = \Delta\omega/\omega = -\text{Im}(\chi)/E, \quad (19)$$

$$\delta\omega/\omega = \text{Re}(\chi)/2E.$$

Therefore, a Kramers–Kronig relation for the susceptibility can be used to obtain the relative frequency shift as follows:

$$\frac{\delta\omega}{\omega}(\omega, T) = -\frac{1}{2\pi} P \int_{-\infty}^{\infty} d\omega' \frac{Q^{-1}(\omega', T)}{\omega' - \omega}, \quad (20)$$

where  $P$  here means the principal value of the integral.

### B. Expressions for the frequency shift

Relaxation processes of biased, underdamped TLSs dominate the perturbations of the ideal response of the resonator, as we have already shown for the inverse quality factor. For most of the frequency range,  $\omega \gg [30\alpha_b \sqrt{\omega_{co} T}]^{2/3}$ ,  $Q^{-1}(\omega, T) \approx A\sqrt{T}/\omega$ , with  $A$  defined by Eq. (10). The associated predicted contribution to the frequency shift, using Eq. (20), is

$$\frac{\delta\omega}{\omega}(\omega, T) \approx -\frac{A}{2\pi} \frac{\sqrt{T}}{\omega} \log \left[ \left| 1 - \frac{\omega}{[30\alpha_b \sqrt{\omega_{co} T}]^{2/3}} \right| \right]. \quad (21)$$

For low temperatures,  $\omega \gg [30\alpha_b \sqrt{\omega_{co} T}]^{2/3}$ , the negative shift grows toward zero as  $\delta\omega/\omega(\omega, T) \sim \sqrt{T} \log[T^{2/3}/\omega]$ , reaching at some point a maximum value. For high temperatures,  $\omega < [30\alpha_b \sqrt{\omega_{co} T}]^{2/3}$ , the negative shift decreases as  $\delta\omega/\omega(\omega, T) \sim 1/T^{1/6}$ . Even though the prediction of a peak in  $\delta\omega/\omega(T)$  qualitatively matches the few experimental results currently available,<sup>30,32</sup> it does not fit them quantitatively.

## VII. APPLICABILITY AND FURTHER EXTENSIONS OF THE MODEL: DISCUSSION

As mentioned, the predictions obtained within this theoretical framework do qualitatively match the experimental results in terms of observed orders of magnitude for  $Q^{-1}(T)$ , weak sublinear temperature dependence, and the presence of a peak in the frequency shift temperature dependence. However, quantitative fitting is still to be reached. On the experimental side, more experiments need to be done at low temperatures to confirm the, until now, few results.<sup>30</sup>

The several simplifications involved in the model put certain constraints, some of which are susceptible to improvement. We enumerate them first and discuss some of them afterwards: (i) The probability distribution  $P(\Delta_0^x, \Delta_0^z)$ , borrowed from amorphous bulk systems, may be different for the case of the resonator's surface. (ii) The assumption of noninteracting TLSs, only coupled among them in an indirect way through their coupling to the vibrations, breaks down at low enough temperatures, where also the discreteness of the vibrational spectrum affects our predictions. (iii) When temperatures rise above a certain value, high-energy phonons with 3D character dominate dissipation, the two-state description of the degrees of freedom coupled to the vibrations is not a good approximation, and thermoelastic losses begin to play an important role. (iv) For strong driving, anharmonic coupling among modes has to be considered and some steps in the derivation of the different mechanisms, which assumed small perturbations, must be modified. This will be the case of resonators driven to the nonlinear regime, where bistability and other phenomena take place.

The solution to issue (i) is intimately related to a better knowledge of the surface and the different physical processes taking place there. Recent studies try to shed some light on this question,<sup>40</sup> and from their results, a more realistic  $P(\Delta_0^x, \Delta_0^z)$  could be derived, which is left for future work. Before that point, it is easier to wonder about the consequences of a dominant kind of dissipative process which corresponds to a set of TLSs with a well defined value of  $\Delta_0^x$  and a narrow distribution of  $\Delta_0^z$ 's of width  $\Delta_1$ , as was suggested for single-crystal silicon.<sup>56</sup> Following Ref. 56 a  $Q^{-1}(T) \sim \sqrt{T}$  behavior is obtained for low temperatures  $T < \Delta_1$  if  $\Gamma(\Delta_0^x, T) < \omega$ , and  $Q^{-1}(T) \sim 1/\sqrt{T}$  if  $\Gamma(\Delta_0^x, T) > \omega$ , while at high temperatures  $T > \Delta_1$ , a constant  $Q^{-1}(T) \sim Q_0$  is predicted for both cases. These predictions do not match bet-

ter with experiments than the results obtained with  $P(\Delta_0^x, \Delta_0^z) \sim P_0/\Delta_0^x$ , so issue (i) remains open. From the point of view of those who attribute the origin of the low-energy TLSs to the long range interaction between localized defects, a possible source of change for  $P(\Delta_0^x, \Delta_0^z)$  may be the decrease in size of the resonator below the correlation length of this interaction.

We try now to have a first estimate of the temperature for which interactions between TLSs cannot be ignored. Following the ideas presented in Ref. 46, we will estimate the temperature  $T^*$  at which the dephasing time  $\tau_{\text{int}}$  due to interactions is equal to the lifetime  $\tau(T) = \Gamma^{-1}(T)$  defined in Eq. (7), for the TLSs that contribute most to dissipation, which are those with  $\varepsilon = \sqrt{(\Delta_0^x)^2 + (\Delta_0^z)^2} \sim \Delta_0^x \sim T$ . For them,  $\tau^{-1}(T) = \Gamma(T) \approx 40\alpha_b \sqrt{\omega_{co}} \sqrt{T}$ . The interactions between the TLSs are dipolar, described by  $H_{\text{int}} = \sum_{i,j} U_{1,2} \sigma_1^z \sigma_2^z$ , with  $U_{1,2} = b_{12}/r_{12}^3$ ,  $b_{12}$  verifying  $\langle b_{12} \rangle \approx 0$ , and  $\langle |b_{12}| \rangle \equiv U_0 \approx \gamma^2/E$ .<sup>46,47</sup> From the point of view of a given TLS, the interaction affects its bias,  $\Delta_j^z = (\Delta_0^z)_j + \sum_i U_{ij} \sigma_i^z$ , causing the fluctuations of its phase  $\delta\varepsilon_j(t)$  (where  $t$  here means time and not thickness), which have an associated  $\tau_{\text{int}}$  defined by  $\delta\varepsilon_j(\tau_{\text{int}}) \tau_{\text{int}} \sim 1$ . These fluctuations are caused by those TLSs which, within the time  $\tau_{\text{int}}$ , have undergone a transition between their two eigenstates, affecting the value of the bias of our TLS through the interaction  $H_{\text{int}}$ . At a temperature  $T$ , the most fluctuating TLSs are those such that  $\varepsilon = \sqrt{(\Delta_0^x)^2 + (\Delta_0^z)^2} \sim \Delta_0^x \sim T$ , and their density can be estimated, using  $P(\Delta_0^x, \Delta_0^z)$ , as  $n_T \approx P_0 kT$ . They will fluctuate with a characteristic time  $\tau(T) \approx [40\alpha_b \sqrt{\omega_{co}} \sqrt{T}]^{-1}$ , so for a time  $t < \tau(T)$ , the amount of these TLSs that have made a transition is roughly  $n(t) \approx P_0 kT t / \tau(T)$ . For a dipolar interaction like the one described above, the average energy shift is related to  $n(t)$  by<sup>57</sup>  $\delta\varepsilon(t) \approx U_0 n(t)$ . Substituting it in the equation defining  $\tau_{\text{int}}$  and imposing  $\tau_{\text{int}}(T^*) = \tau(T^*)$  give the transition temperature  $T^* \approx [6\alpha_b \sqrt{\omega_{co}} / (U_0 P_0)]^2$ . For example, for a resonator such as the silicon ones studied in Ref. 30, with  $L = 6 \mu\text{m}$ ,  $t = 0.2 \mu\text{m}$ , and  $w = 0.3 \mu\text{m}$ , the estimated onset of interactions is at  $T^* \approx 10 \text{ mK}$ .

An upper limit  $T_{\text{high}}$  of applicability of the model due to high-energy 3D vibrational modes playing a significant role can be easily derived by imposing  $T_{\text{high}} = \omega_{\text{min}}^{\text{3D}}$ . The frequency  $\omega_{\text{min}}^{\text{3D}}$  corresponds to phonons with a wavelength comparable to the thickness  $t$  of the sample (do not confuse with time),  $\omega_{\text{min}}^{\text{3D}} = 2\pi\sqrt{E/\rho}/t$ . The condition is very weak, as the value, for example, for silicon resonators reads  $T_{\text{high}} \approx 400/t$ , with  $t$  given in nanometers and  $T_{\text{high}}$  in Kelvin. At much lower temperatures, the two-state description of the degrees of freedom coupled to the vibrations ceases to be realistic, with a high temperature cutoff in the case of the model applied to amorphous bulk systems of  $T \sim 5 \text{ K}$ .

## VIII. DISSIPATION IN A METALLIC CONDUCTOR

Many of the current realizations of nanomechanical devices monitor the system by means of currents applied through metallic conductors attached to the oscillators. The vibrations of the device couple to the electrons in the metallic part. This coupling is useful in order to drive and measure

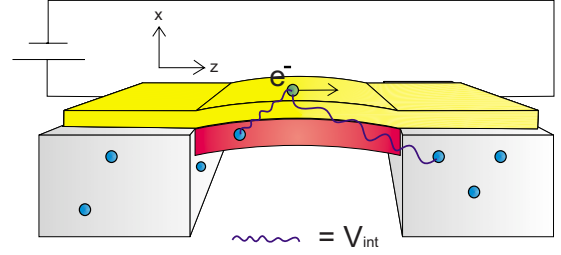


FIG. 6. (Color online) Sketch of the distribution of charges in the device. When the system oscillates, these charges induce time-dependent potentials which create electron-hole pairs in the metallic layer deposited on top of the beam, absorbing part of the mechanical energy of the flexural mode. See text for details.

the oscillations, but it can also be a source of dissipation. We will apply here the techniques described in Refs. 58 and 59 (see also Ref. 60) in order to analyze the energy loss processes due to the excitations in the conductor.

We assume that the leading perturbation acting on the electrons in the metal are offset charges randomly distributed throughout the device. A charge  $q$  at position  $\tilde{\mathbf{R}}$  interacts with an energy

$$V(\tilde{\mathbf{r}}, t) \equiv \frac{q^2}{\epsilon_0 |\tilde{\mathbf{R}}(t) - \tilde{\mathbf{r}}(t)|}, \quad (22)$$

with another charge  $q$  at a position  $\tilde{\mathbf{r}}$  inside the metal (see Fig. 6). As the bulk of the device is an insulator, this potential is only screened by a finite dielectric constant,  $\epsilon_0$ . The oscillations of the system at frequency  $\omega_0$  modulate the relative distance  $|\tilde{\mathbf{R}}(t) - \tilde{\mathbf{r}}(t)|$ , leading to a time-dependent potential acting on the electrons of the metal.

The probability per unit time of absorbing a quantum of energy  $\omega_0$  can be written, using second order perturbation theory, as<sup>58,59</sup>

$$\Gamma = \int d\tilde{\mathbf{r}} d\tilde{\mathbf{r}}' dt dt' V(\tilde{\mathbf{r}}, t) V(\tilde{\mathbf{r}}, t') \text{Im} \chi[\tilde{\mathbf{r}} - \tilde{\mathbf{r}}', t - t'] e^{i\omega_0(t-t')}, \quad (23)$$

where  $\text{Im} \chi[\tilde{\mathbf{r}} - \tilde{\mathbf{r}}', t - t']$  is the imaginary part of the response function of the metal.

### A. Charges in the oscillating part of the device

We write the relative distance as  $\tilde{\mathbf{R}}(t) - \tilde{\mathbf{r}}(t) = \tilde{\mathbf{R}}_0 - \tilde{\mathbf{r}}_0 + \delta\tilde{\mathbf{R}}(t) - \delta\tilde{\mathbf{r}}(t)$  and expand  $V(\tilde{\mathbf{r}}, t)$ , whose time-dependent part is approximately

$$V(\tilde{\mathbf{r}}, t) \approx \frac{q^2 [\tilde{\mathbf{R}}_0 - \tilde{\mathbf{r}}_0] \cdot [\delta\tilde{\mathbf{R}}(t) - \delta\tilde{\mathbf{r}}(t)]}{\epsilon_0 |\tilde{\mathbf{R}}_0 - \tilde{\mathbf{r}}_0|^3}. \quad (24)$$

For a flexural mode,  $[\tilde{\mathbf{R}}_0 - \tilde{\mathbf{r}}_0] \cdot [\delta\tilde{\mathbf{R}}(t) - \delta\tilde{\mathbf{r}}(t)]$  has turned into  $[X_0 - x_0][\delta X(t) - \delta x(t)] \sim tA \sin(\omega t)$ , where  $t = t_{\text{ins}} + t_{\text{metal}}$  is the thickness of the beam and  $A$  is the amplitude of vibration of the mode. Thus, the average estimate for this case for the correction of  $V(\tilde{\mathbf{r}}, t)$  is



$$\delta V(\tilde{\mathbf{r}}, t) \sim \frac{q^2 t A \sin(\omega t)}{\epsilon_0 L^3}, \quad (25)$$

$L$  being the resonator's length.

The integral over the region occupied by the metal in Eq. (23) can be written as an integral over  $\tilde{\mathbf{r}}_0$  and  $\tilde{\mathbf{r}}'_0$ . The dielectric constant of a dirty metal in the random phase approximation is<sup>61</sup>

$$\text{Im } \chi(\tilde{\mathbf{r}} - \tilde{\mathbf{r}}', t - t') = \int \frac{d\omega d\tilde{\mathbf{q}}}{(2\pi)^4} e^{i\tilde{\mathbf{q}}(\tilde{\mathbf{r}} - \tilde{\mathbf{r}}')} e^{i\omega(t-t')} \frac{|\omega|}{e^4 D \nu |\tilde{\mathbf{q}}|^2}, \quad (26)$$

where  $e$  is the electronic charge,  $D = \hbar v_F l$  is the diffusion constant,  $v_F$  is the Fermi velocity,  $l$  is the mean free path, and  $\nu \approx (k_F t_{\text{metal}})^2 / \hbar v_F$  is the one-dimensional density of states.

By combining Eqs. (23) and (26) and assuming that the position of the charge,  $\tilde{\mathbf{R}}_0$ , is in a generic point inside the beam and that the length scales are such that  $k_F^{-1}, t_{\text{metal}}, t \ll L$ , we can obtain the leading dependence of  $\Gamma$  in Eq. (23) on  $L$  as follows:

$$\Gamma \approx \frac{|\omega_0| A^2 \left(\frac{t}{L}\right)^2}{D \nu L} \approx \frac{|\omega_0| A^2 \left(\frac{t}{L}\right)^2}{l k_F^2 L^3 t_{\text{metal}}}, \quad (27)$$

where we also assume that  $|q| = e$ . The energy absorbed per cycle of oscillation and unit volume will be  $\Delta E = (2\pi / \omega_0) \hbar \omega_0 \Gamma_{\text{ph}} / t^2 L = 2\pi \hbar \Gamma_{\text{ph}} / t^2 L$  and the inverse quality factor  $Q_{\text{ph}}^{-1}(\omega_0)$  will correspond to

$$Q_{\text{ph}}^{-1}(\omega_0) = \frac{1}{2\pi} \frac{\Delta E}{E_0} = \frac{\hbar \Gamma_{\text{ph}}}{t \omega L} \frac{1}{\frac{1}{2} \rho \omega_0^2 A^2}, \quad (28)$$

where  $E_0$  is the elastic energy stored in the vibration and  $A$  is the amplitude of vibration. Substituting the result for  $\Gamma$ , one obtains

$$Q^{-1} \approx \frac{2\hbar}{l k_F^2 L^4 t^2 \rho \omega_0} \left(\frac{t}{t_{\text{metal}}}\right)^2. \quad (29)$$

In a narrow metallic wire of width  $t_{\text{metal}}$ , we expect that  $l \sim t_{\text{metal}}$ .

Typical values for the parameters in Eq. (29) are  $k_F^{-1} \approx 1 \text{ \AA}$ ,  $A \approx 1 \text{ \AA}$ ,  $l \sim t_{\text{metal}} \approx 10 \text{ nm} \sim 10^2 \text{ \AA}$ ,  $t \approx 100 \text{ nm} \approx 10^3 \text{ \AA}$ , and  $L \approx 1 \text{ } \mu\text{m} \approx 10^4 \text{ \AA}$ . Hence, each charge in the device gives a contribution to  $Q^{-1}$  of order  $10^{-20}$ . The effect of all charges is obtained by summing over all charges in the beam. If their density is  $n_q$ , we obtain

$$Q^{-1} \approx \frac{2\hbar n_q}{l k_F^2 L^3 \rho \omega_0} \left(\frac{t}{t_{\text{metal}}}\right)^2. \quad (30)$$

For reasonable values of the density of charges,  $n_q = l_q^{-3}$ ,  $l_q \gtrsim 10 \text{ nm}$ , this contribution is negligible,  $Q^{-1} \lesssim 10^{-16}$ .

### B. Charges in the substrate surrounding the device

Many resonators, however, are suspended at distances much smaller than  $L$  over an insulating substrate, which can also contain unscreened charges. As the Coulomb potential induced by these charges is long range, the analysis de-

scribed above can be applied to all charges within a distance of order  $L$  from the beam. Moreover, the motion of these charges is not correlated with the vibrations of the beam, so that now the value of  $|\delta \tilde{\mathbf{R}}(t) - \delta \tilde{\mathbf{r}}(t)|$  has to be replaced by

$$|\delta \tilde{\mathbf{R}}(t) - \delta \tilde{\mathbf{r}}(t)| \approx A e^{i\omega_0 t}, \quad (31)$$

and the value of  $|\tilde{\mathbf{R}}_0 - \tilde{\mathbf{r}}_0| \sim L$ . Assuming, as before, a density of charges  $n_q = l_q^{-3}$ , the effect of all charges in the substrate leads to

$$Q^{-1} \approx \frac{2\hbar L}{l(k_F t_{\text{metal}})^2 l_q^3 t^2 \rho \omega_0} \approx 0.3 \frac{\hbar L^3}{l(k_F t_{\text{metal}})^2 l_q^3 t^3 \sqrt{E\rho}}, \quad (32)$$

where the second result corresponds to the fundamental mode,  $\omega_0 \approx 6.5(t/L^2)\sqrt{E/\rho}$ . For values  $L \approx 1 \text{ } \mu\text{m}$ ,  $A \approx 1 \text{ \AA}$ ,  $k_F^{-1} \approx 1 \text{ \AA}$ ,  $l \sim t_{\text{metal}} \approx 10 \text{ nm}$ , and  $l_q \sim 10 \text{ nm}$ , we obtain  $Q^{-1} \sim 10^{-9}$ . Thus, given the values of  $Q^{-1}$  reached experimentally until now, this mechanism can be disregarded although it sets a limit to  $Q^{-1}$  at the lowest temperatures. Note also that this estimate neglects cancellation effects between charges of opposite signs.

## IX. CONCLUSIONS

Disorder and configurational rearrangements of atoms and adsorbed impurities at surfaces of nanoresonators dominate the dissipation of their vibrational eigenmodes at low temperatures. We have given a theoretical framework to describe in a unified way these processes, improving and extending previous ideas.<sup>1</sup> Based on the good description of low temperature properties of disordered bulk insulators provided by the standard tunneling model,<sup>43,44,46</sup> and in particular, of acoustic phonon attenuation in such systems, we adapt it to describe the damping of 1D flexural and torsional modes of NEMS associated with the amorphouslike nature of their surfaces.

Correcting some aspects of Ref. 1, we have calculated the damping of the modes by the presence of an ensemble of independent TLSs coupled to the local deformation gradient field  $\partial_i u_j$  created by vibrations. The different dissipation channels to which this ensemble gives rise to have been described, focusing the attention on the two most important: relaxation dynamics of biased TLSs and dissipation due to symmetric nonresonant TLSs. The first one is caused by the finite time it takes for the TLSs to readjust their equilibrium populations when their bias  $\Delta_0^z$  is modified by local strains, with biased TLSs playing the main role, as this effect is  $\propto [\Delta_0^z / \sqrt{(\Delta_0^z)^2 + (\Delta_0^x)^2}]^2$ . In terms of the excitation spectrum of the TLSs, it corresponds to a Lorentzian peak around  $\omega = 0$ . The second effect is due to the modified absorption spectrum of the TLSs caused by their coupling to all the vibrations, especially the flexural modes, whose high density of states at low energies leads to sub-Ohmic damping.<sup>62-64</sup> A broad incoherent spectral strength is generated, enabling the "dressed-by-the-modes" TLSs to absorb the energy of an excited mode and deliver it to the rest of the modes when they decay.

We have given analytical expressions for the contributions of these mechanisms to the linewidth of flexural [Eqs. (6) and (10)] or torsional modes [Eqs. (13) and (17)] in terms of the inverse quality factor  $Q^{-1}(\omega_0) = \Delta\omega_0/\omega_0$ , showing the dependencies on the dimensions, temperature, and other relevant parameters characterizing the device. We have compared the two mechanisms, concluding that relaxation dominates dissipation, with a predicted  $Q^{-1}(\omega_0, T) \sim T^{1/2}/\omega_0$ . Expressions have been provided for damping of flexural modes in cantilevers and doubly clamped beams as well as for damping of their torsional modes.

Analytical predictions for associated frequency shifts have also been calculated [Eq. (21)]. Some important findings have been achieved, such as the qualitative agreement with a sublinear temperature dependence of  $Q^{-1}(T)$ , the presence of a peak in the frequency shift temperature dependence  $\delta\omega/\omega(T)$ , or the observed order of magnitude of  $Q^{-1}(T)$  in the existing experiments studying flexural phonon attenuation at low temperatures.<sup>30,32</sup> Nevertheless, the lack of full quantitative agreement has led to a discussion on the assumptions of the model, its links with the physical processes occurring at the surfaces of NEMS, its range of applicability, and the improvements to reach the desired quantitative fit.

Finally, we have also considered the contributions to the dissipation due to the presence of metallic electrodes deposited on top of the resonators, which can couple to the electrostatic potential induced by random charges. We have shown that the coupling to charges within the vibrating parts does not contribute appreciably to the dissipation. Coupling to charges in the substrate, although more significant, still leads to small dissipation effects [Eq. (32)], imposing a limit at low temperatures of  $Q^{-1} \sim 10^{-9}$ , which is very small compared to the values reached in current experiments.<sup>30,32</sup>

#### ACKNOWLEDGMENTS

C.S. and F.G. acknowledge funding from MEC (Spain) through FPU grant (Grant No. FIS2005-05478-C02-01) and the Comunidad de Madrid through the program CITEC-NOMIK (No. CM2006-S-0505-ESP-0337). A.H.C.N. is supported through NSF Grant No. DMR-0343790.

#### APPENDIX A: CALCULATION OF THE SPECTRAL FUNCTION FOR THE BENDING MODES

The starting point is the Hamiltonian of Ref. 1,  $H = \Delta_0 \sigma_x + \gamma \sigma_z \partial_i u_j$ , where  $\partial_i u_j$  is a component of the deformation gradient matrix. In the case of the bending modes of a rod of dimensions  $L$ ,  $t$ , and  $w$ , and mass density  $\rho$ , there are two variables  $X(z)$ ,  $Y(z)$  (transversal displacements of the rod as a function of the position along its length,  $z$ ) obeying<sup>51</sup>

$$\begin{aligned} EI_y \frac{\partial^4 X}{\partial z^4} &= -\rho t w \frac{\partial^2 X}{\partial t^2}, \\ EI_x \frac{\partial^4 Y}{\partial z^4} &= -\rho t w \frac{\partial^2 Y}{\partial t^2} \end{aligned} \quad (\text{A1})$$

(where  $I_y = t^3 w / 12$  and  $I_x = w^3 t / 12$ ), so that there are plane waves  $X(z, t)$ ,  $Y(z, t) \sim e^{i(kz - \omega t)}$ , but with a quadratic disper-

sion relation,  $\omega_j(k) = \sqrt{\frac{EI_j}{\rho ab}} k^2$ . One can thus express  $X(z)$ ,  $Y(z)$  in terms of bosonic operators, for example,  $X(0) = \sum_k \sqrt{\frac{\hbar}{2\rho t w L \omega_k}} (a_k^\dagger + a_k)$ . We can relate this variables to the strain field  $\partial_i u_j$  through the free energy  $F$  as follows:

$$\begin{aligned} F_{rod} &= \frac{1}{2} \int dz EI_y \left( \frac{\partial^2 X}{\partial z^2} \right)^2 + EI_x \left( \frac{\partial^2 Y}{\partial z^2} \right)^2 \\ &= \frac{1}{2} \int dz \int dS \frac{1}{2} \lambda \sum_i u_{ii}^2 + \mu \sum_{i,k} u_{ik}^2 \\ &\approx \frac{1}{2} \int dz \int dS \left( \frac{3}{2} \lambda + 9\mu \right) u_{ij}^2, \end{aligned} \quad (\text{A2})$$

extracting an average equivalence for one component  $u_{ij}$ ,  $u_{ij} \approx 2\sqrt{EI_y/(3\lambda + 18\mu)tw} \partial^2 X/\partial z^2$ . The interaction term in the Hamiltonian is then

$$\begin{aligned} H_{int} &= \hbar \sigma_z \sum_k \lambda \frac{k^2}{\sqrt{\omega_k}} (a_k^\dagger + a_k) \\ &= \hbar \sigma_z \sum_{ij} \sum_k \left[ 2\gamma \frac{\Delta_0^x}{\Delta_0} \sqrt{\frac{EI_y}{(3\lambda + 18\mu)tw}} \sqrt{\frac{1}{2\rho t w \hbar L}} \right] \\ &\quad \times \frac{(k^{ij})^2}{\sqrt{\omega_k}} (a_k^{ij\dagger} + a_k^{ij}). \end{aligned} \quad (\text{A3})$$

So we have approximately nine times the same Hamiltonian, once for each  $u_{ij}$ , and the corresponding spectral function  $J(\omega)$  will be nine times the one calculated for

$$\begin{aligned} H_{int} &= \hbar \sigma_z \sum_k \lambda \frac{k^2}{\sqrt{\omega_k}} (a_k^\dagger + a_k) \\ &\approx \hbar \sigma_z \sum_k \left[ 2\gamma \frac{\Delta_0^x}{\Delta_0} \sqrt{\frac{EI_y}{(3\lambda + 18\mu)tw}} \sqrt{\frac{1}{2\rho t w \hbar L}} \right] \\ &\quad \times \frac{k^2}{\sqrt{\omega_k}} (a_k^\dagger + a_k). \end{aligned} \quad (\text{A4})$$

For a Hamiltonian of the class  $H = \Delta_0 \sigma_x + \hbar \sigma_z \sum_k \lambda_k (a_k^\dagger + a_k)$ , the spectral function  $J(\omega)$  is given by  $J(\omega) = \frac{1}{2\pi} \sum_k \lambda_k^2 \delta(\omega - \omega_k)$ , so that in our case the expression for it is

$$\begin{aligned} J(\omega) &= \frac{1}{2\pi} \sum_k \left[ 2\gamma \frac{\Delta_0^x}{\Delta_0} \sqrt{\frac{EI_y}{(3\lambda + 18\mu)tw}} \sqrt{\frac{1}{2\rho t w \hbar L}} \frac{k^2}{\sqrt{\omega_k}} \right]^2 \\ &\quad \times \delta(\omega - \omega_k). \end{aligned} \quad (\text{A5})$$

Taking the continuum limit ( $\frac{1}{L} \sum_k \rightarrow \frac{1}{\pi} \int dk$ ),

$$\begin{aligned} J(\omega) &= \frac{2L}{(2\pi)^2} \int_{k_{min}}^{k_{max}} dk \left[ 2\gamma \frac{\Delta_0^x}{\Delta_0} \sqrt{\frac{EI_y}{(3\lambda + 18\mu)tw}} \sqrt{\frac{1}{2\rho t w \hbar L}} \right]^2 \\ &\quad \times \frac{k^4}{\omega_k} \delta(\omega - \omega_k). \end{aligned} \quad (\text{A6})$$

Using the dispersion relation  $\omega_j(k) = \sqrt{\frac{EI_j}{\rho ab}} k^2 = ck^2$ , we express the integral in terms of the frequency as follows:

$$\begin{aligned}
J(\omega) &= \frac{L}{(2\pi)^2} \int_{\omega_{\min}}^{\omega_{co}} \frac{d\omega_k}{\sqrt{c\omega_k}} \left[ 2\gamma \frac{\Delta_0^x}{\Delta_0} \sqrt{\frac{EI_y}{(3\lambda + 18\mu)tw}} \right. \\
&\quad \times \left. \sqrt{\frac{1}{2\rho tw\hbar L}} \right]^2 \frac{k^4}{\omega_k} \delta(\omega - \omega_k) \\
&= \frac{L}{(2\pi)^2} \left[ 2\gamma \frac{\Delta_0^x}{\Delta_0} \sqrt{\frac{EI_y}{(3\lambda + 18\mu)tw}} \sqrt{\frac{1}{2\rho tw\hbar L}} \right]^2 \frac{\sqrt{\omega}}{c^{5/2}}.
\end{aligned} \tag{A7}$$

$J_{\text{flex}}(\omega)$  is just nine times this [Eq. (2)].

## APPENDIX B: DISSIPATION FROM OFF-RESONANCE DRESSED TWO-LEVEL SYSTEMS

We follow the method of Ref. 65. The form of  $A(\omega)$ , the spectral function of a single TLS, for frequencies  $\omega \ll \Delta$  and  $\omega \gg \Delta$  can be estimated using perturbation theory. Without the interaction, the ground state  $|s\rangle$  of the TLS is the symmetric combination of the ground states of the two wells and the excited state is the antisymmetric one,  $|a\rangle$ . We will use Fermi's golden rule applied to the sub-Ohmic spin-boson Hamiltonian,  $H = \Delta\sigma_x + \hbar\lambda\sigma_z\sum_k \left[ \frac{k^2}{\sqrt{\omega_k}} \right] (a_k^\dagger + a_k) + \sum_k \hbar\omega(k)a_k^\dagger a_k$ , where  $a_k$  is the annihilation operator of a bending mode  $k$ . Considering only the low-energy modes  $\omega(k) \ll \Delta$ , to first order the ground state and a state with energy  $\omega(k)$  are given by

$$\begin{aligned}
|g\rangle &\approx |s\rangle - \frac{\lambda k^2}{2\Delta} \frac{1}{\sqrt{\omega_k}} a_k^\dagger |a\rangle + \dots, \\
|k\rangle &\approx a_k^\dagger |s\rangle - \frac{\lambda k^2}{2\Delta} \frac{1}{\sqrt{\omega_k}} |a\rangle + \dots.
\end{aligned} \tag{B1}$$

We estimate the behavior of  $A(\omega)$  by taking the matrix element of  $\sigma_z$  between these two states, obtaining [remember that  $\omega(k) \propto k^2$ ]

$$A(\omega) \sim \frac{\hbar\alpha_b\sqrt{\omega_{co}}\sqrt{\omega}}{\Delta^2} + \dots, \quad \omega(k) \ll \Delta. \tag{B2}$$

The expression in the numerator is proportional to the spectral function of the coupling,  $J(\omega) = \alpha_b\sqrt{\omega_{co}}\sqrt{\omega}$ . Now we turn our attention to the case  $\omega(k) \gg \Delta$ , where the ground state  $|g\rangle$  and an excited state  $|k\rangle$  can be written as

$$\begin{aligned}
|g\rangle &\approx |s\rangle - \frac{\lambda k^2/\sqrt{\omega_k}}{\hbar\omega_k + 2\Delta} a_k^\dagger |a\rangle + \dots, \\
|k\rangle &\approx a_k^\dagger |s\rangle + \frac{\lambda k^2/\sqrt{\omega_k}}{\hbar\omega_k - 2\Delta} |a\rangle + \dots.
\end{aligned} \tag{B3}$$

The matrix element  $\langle 0|\sigma_z|k\rangle$  is  $\sim \frac{\lambda k^2}{\sqrt{\omega_k}} \frac{4\Delta}{(\hbar\omega_k)^2}$ , leading to

$$A(\omega) \sim \frac{\alpha_b\sqrt{\omega_{co}}\Delta^2}{\hbar^3\omega^{7/2}} + \dots, \quad \omega(k) \gg \Delta. \tag{B4}$$

## 1. Value of $A_{\text{off-res}}^{\text{tot}}(\omega_0)$

Now we will add the contributions of all the non-resonant TLSs using the probability distribution  $P(\Delta_0^x, \Delta_0^z) = P_0/\Delta_0^x$ .<sup>43,44</sup> For the case of weak coupling,  $\alpha_b < 1/2$  and  $\omega_0 \geq (2\alpha_b)^2\omega_{co}$ , which is the one found in experiments, one has

$$\begin{aligned}
A_{\text{off-res}}^{\text{tot}}(\omega_0) &\sim \int_{\hbar[\omega_0+\Gamma(\omega_0)]}^{\varepsilon_{\max}} d\Delta_0^x \int_{-\Delta_0^x}^{\Delta_0^x} d\Delta_z \frac{P}{\Delta_0^x} \frac{\hbar\alpha_b\sqrt{\omega_{co}}\sqrt{\omega_0}}{(\Delta_0^x)^2} \\
&\quad + \int_{\hbar(2\alpha_b)^2\omega_{co}}^{\hbar[\omega_0-\Gamma(\omega_0)]} d\Delta_0^x \int_{-\Delta_0^x}^{\Delta_0^x} d\Delta_z \frac{P}{\Delta_0^x} \frac{\alpha_b\sqrt{\omega_{co}}(\Delta_0^x)^2}{\hbar^3\omega_0^{7/2}},
\end{aligned}$$

obtaining the result  $A_{\text{off-res}}^{\text{tot}}(\omega_0) \approx 2P\alpha_b\sqrt{\omega_{co}/\omega_0}$ .

## 2. Off-resonance contribution for $T > 0$

Using the same scheme, the modifications due to the temperature will appear in the density of states of absorption and emission of energy corresponding to a dressed TLS,  $A(\Delta, \omega, T)$ . Now that there will be a probability for the TLS to be initially in the excited antisymmetric state,  $|a\rangle$ , proportional to  $\exp[-\Delta/kT]$ , and to emit energy  $\hbar\omega$ , giving it to our externally excited mode,  $|k, n\rangle$ , thus compensating the absorption of energy corresponding to the opposite case (transition from  $|s\rangle|k, n\rangle$  to  $|a\rangle|k, n-1\rangle$ ), but contributing in an additive manner to the total amount of fluctuations, which are the ones defining the linewidth of the vibrational mode observed in experiments, fixing the value of  $Q^{-1}(\omega, T)$ . The expression for  $A(\Delta, \omega, T)$  is given by

$$A(\omega, T) = \frac{1}{Z} \sum_i \sum_f \langle |i|\sigma_z|f\rangle^2 e^{-E_i/kT} \delta[\hbar\omega - (E_f - E_i)]. \tag{B5}$$

We consider a generic state  $|i_a\rangle = |a\rangle|k_1n_1, \dots, k_jn_j, \dots\rangle$  or  $|i_s\rangle = |s\rangle|k_1n_1, \dots, k_jn_j, \dots\rangle$ , and states that differ from it in  $\hbar\omega_j$ ,  $|f_{a\pm}\rangle = |a\rangle|k_1n_1, \dots, k_jn_j \pm 1, \dots\rangle$  and  $|f_{s\pm}\rangle = |s\rangle|k_1n_1, \dots, k_jn_j \pm 1, \dots\rangle$ . As for  $T=0$ , we will correct them to first order in the interaction Hamiltonian  $H_{\text{int}} = \hbar\lambda\sigma_z\sum_k \sqrt{\omega_k}(a_k^\dagger + a_k)$ , and then calculate the square of the matrix element of  $\sigma_z$ ,  $|\langle i|\sigma_z|f\rangle|^2$ .

Elements  $\langle i_{a,s}|\sigma_z|f_{a+,s+}\rangle^2$  correspond to absorption by the dressed TLS of an energy  $\hbar\omega_j$  from the mode  $k_j$ , while elements  $\langle i_{a,s}|\sigma_z|f_{a-,s-}\rangle^2$  correspond to emission and ‘‘feeding’’ of the mode with a phonon  $\hbar\omega_j$ . The expressions for the initial states are

$$\begin{aligned}
|i_s\rangle &= |s\rangle|k_1n_1, \dots, k_jn_j, \dots\rangle \rightarrow |s\rangle|k_1n_1, \dots, k_jn_j, \dots\rangle \\
&\quad + \sum_{k_i \ni n_i > 0} \frac{\hbar\lambda\sqrt{n_i}\omega_i}{\hbar\omega_i + 2\Delta} |a\rangle \dots k_in_i - 1 \dots \\
&\quad - \sum_{\forall k_i} \frac{\hbar\lambda\sqrt{(n_i+1)\omega_i}}{\hbar\omega_i - 2\Delta} |a\rangle \dots k_in_i + 1 \dots,
\end{aligned}$$

$$\begin{aligned}
 |i_a\rangle &= |a\rangle|k_1n_1, \dots, k_jn_j, \dots\rangle \rightarrow |a\rangle|k_1n_1, \dots, k_jn_j, \dots\rangle \\
 &+ \sum_{k_i \ni n_i > 0} \frac{\hbar\lambda\sqrt{n_i\omega_i}}{\hbar\omega_i - 2\Delta} |s\rangle \dots k_in_i - 1 \dots \rangle \\
 &- \sum_{\forall k_i} \frac{\hbar\lambda\sqrt{(n_i+1)\omega_i}}{\hbar\omega_i + 2\Delta} |s\rangle \dots k_in_i + 1 \dots \rangle, \quad (B6)
 \end{aligned}$$

and, for example, the state  $|f_{a+}\rangle$  is given by

$$\begin{aligned}
 |f_{a+}\rangle &= |a\rangle|k_1n_1, \dots, k_jn_j + 1, \dots\rangle \rightarrow |a\rangle|k_1n_1, \dots, k_jn_j \\
 &+ 1, \dots\rangle + \sum_{k_i \ni n_i > 0, i \neq j} \frac{\hbar\lambda\sqrt{n_i\omega_i}}{\hbar\omega_i - 2\Delta} |s\rangle \dots k_in_i - 1 \dots k_jn_j \\
 &+ 1 \dots \rangle + \frac{\hbar\lambda\sqrt{(n_j+1)\omega_j}}{\hbar\omega_j - 2\Delta} |s\rangle \dots k_jn_j \dots \rangle \\
 &- \sum_{\forall k_i, i \neq j} \frac{\hbar\lambda\sqrt{(n_i+1)\omega_i}}{\hbar\omega_i + 2\Delta} |s\rangle \dots k_in_i + 1 \dots k_jn_j + 1 \dots \rangle \\
 &- \frac{\hbar\lambda\sqrt{(n_j+2)\omega_j}}{\hbar\omega_j + 2\Delta} |s\rangle \dots k_jn_j + 2 \dots \rangle \quad (B7)
 \end{aligned}$$

with a similar expression for the rest of the states. The value of  $|\langle i_{a,s} | \sigma_z | f_{a+,s+} \rangle|$  (absorption) is  $|\langle i_{a,s} | \sigma_z | f_{a+,s+} \rangle| = \left| \frac{\lambda\sqrt{(n_j+1)\omega_j 4\Delta}}{(\hbar\omega_j)^2 - 4\Delta^2} \right|$ , with  $n_j=0, 1, \dots$ , while for emission, the result is  $|\langle i_{a,s} | \sigma_z | f_{a-,s-} \rangle| = \left| \frac{\lambda\sqrt{n_j\omega_j 4\Delta}}{(\hbar\omega_j)^2 - 4\Delta^2} \right|$ , with  $n_j=1, \dots$ . By taking the limits we considered at  $T=0$  ( $\hbar\omega_j \ll \Delta$  and  $\hbar\omega_j \gg \Delta$ ), the results are the same as for  $T=0$  for absorption, except for a factor  $(n_j+1)$ , and we also have now the possibility of emission, with the same matrix element but with the factor  $n_j$ :

$$\begin{aligned}
 \text{Absorption} &\begin{cases} \sim \frac{(n_j+1)\hbar\alpha_b\sqrt{\omega_{co}}\sqrt{\omega}}{\Delta^2}, & \hbar\omega_j \ll \Delta \\ \sim \frac{(n_j+1)\alpha_b\sqrt{\omega_{co}}\Delta^2}{\hbar^3\omega^{7/2}}, & \hbar\omega_j \gg \Delta, \end{cases} \\
 \text{Emission} &\begin{cases} \sim \frac{n_j\hbar\alpha_b\sqrt{\omega_{co}}\sqrt{\omega}}{\Delta^2}, & \hbar\omega_j \ll \Delta \\ \sim \frac{n_j\alpha_b\sqrt{\omega_{co}}\Delta^2}{\hbar^3\omega^{7/2}}, & \hbar\omega_j \gg \Delta. \end{cases} \quad (B8)
 \end{aligned}$$

Now we have to sum over all initial states, and by noting that the first order correction to the energy of any eigenstate is 0, the partition function  $Z$  is easy to calculate, everything factorizes, and the result is, for example, in the case  $\hbar\omega_j \ll \Delta$ , as follows:

$$\begin{aligned}
 A_{abs}(\Delta, \omega_j, T) &= \frac{1}{Z} \sum_{i \neq j, n_i=0}^{\infty} \sum_{n_j=0}^{\infty} \frac{\hbar\alpha_b\sqrt{\omega_{co}}\sqrt{\omega_j}}{\Delta^2} (n_j+1) \\
 &\times \exp\left(-\frac{\hbar\omega_j n_j}{kT}\right) \exp\left(-\frac{\hbar\sum_i n_i \omega_i}{kT}\right) \\
 &= \frac{\hbar\alpha_b\sqrt{\omega_{co}}}{\Delta^2} \frac{\sqrt{\omega_j}}{1 - e^{-\hbar\omega_j/kT}},
 \end{aligned}$$

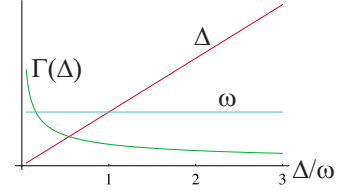


FIG. 7. (Color online) Evolution with  $\Delta_r$  of the different quantities determining the approximations to be taken in the integrand  $\omega_0\tau/[1+(\omega_0\tau)^2]$  of Eq. (9).

$$\begin{aligned}
 A_{em}(\Delta, -\omega_j, T) &= \frac{1}{Z} \sum_{i \neq j, n_i=0}^{\infty} \sum_{n_j=1}^{\infty} \frac{\hbar\alpha_b\sqrt{\omega_{co}}\sqrt{\omega_j}}{\Delta^2} n_j \\
 &\times \exp\left(-\frac{\hbar\omega_j n_j}{kT}\right) \exp\left(-\frac{\hbar\sum_i n_i \omega_i}{kT}\right) \\
 &= \frac{\hbar\alpha_b\sqrt{\omega_{co}}}{\Delta^2} \frac{\sqrt{\omega_j} e^{-\hbar\omega_j/kT}}{1 - e^{-\hbar\omega_j/kT}}. \quad (B9)
 \end{aligned}$$

In  $A_{abs}(\Delta, \omega_j, T)$ , we have added the contributions from the matrix elements  $|\langle i_s | \sigma_z | f_{s+} \rangle|^2 e^{\Delta/kT} + |\langle i_a | \sigma_z | f_{a+} \rangle|^2 e^{-\Delta/kT} = |\langle i_s | \sigma_z | f_{s+} \rangle|^2 [e^{\Delta/kT} + e^{-\Delta/kT}]$ . The sum of exponentials cancels with the partition function of the TLS (appearing as a factor in the total  $Z$ ), leading in this way to the expression above [the same applies for  $A_{em}(\Delta, -\omega_j, T)$ ]. The total fluctuations will be proportional to their sum, which thus turns out to be at this level of approximation  $\propto \coth[\hbar\omega_j/kT]$  as follows:

$$\begin{aligned}
 A_{diss}(\Delta, \omega_j, T) &= A_{abs}(\Delta, \omega_j, T) + A_{em}(\Delta, -\omega_j, T) = A_{diss}(\Delta, \omega_j, T \\
 &= 0) \coth\left[\frac{\hbar\omega_j}{kT}\right]. \quad (B10)
 \end{aligned}$$

In fact, this result applies for any other type of modes, independent of its dispersion relation, provided the coupling Hamiltonian is linear in  $\sigma_z$  and  $(a_{-k}^\dagger + a_k)$  and everything is treated at this level of perturbation theory. Moreover, it can be proven that if one has an externally excited mode with an average population  $\langle n_j \rangle$ , and fluctuations around that value are thermal-like, with a probability  $\propto \exp[-|n_j - \langle n_j \rangle|/kT]$ , one recovers again the same temperature dependence,  $\propto \coth[\hbar\omega_j/kT]$ .

### APPENDIX C: DERIVATION OF $Q_{rel}^{-1}(\omega_0, T)$ [EQUATION (10)]

As discussed after Eq. (9), we have to sum over underdamped TLSs,  $\varepsilon \geq [30\alpha_b\sqrt{\omega_{co}}T]^{2/3}$ , using the approximation for  $\Gamma$ ,  $\Gamma(\varepsilon, T) \sim 30\alpha_b\sqrt{\omega_{co}}T/\sqrt{\varepsilon}$ . Moreover, if  $\omega_0 \geq \Gamma(\varepsilon) = [30\alpha_b\sqrt{\omega_{co}}T]^{2/3}$ , then in the whole integration range  $\omega_0 \geq \Gamma(\varepsilon, T) \Leftrightarrow \omega_0\tau(\varepsilon, T) \geq 1$  (see Fig. 7), so that  $\omega_0\tau/[1+(\omega_0\tau)^2] \approx 1/(\omega_0\tau)$ .  $Q_{rel}^{-1}(\omega_0, T)$  follows

$$Q_{rel}^{-1}(\omega_0, T) \approx \frac{P_0\gamma^2}{ET} \int_{[30\alpha_b\sqrt{\omega_{co}}T]^{2/3}}^T d\varepsilon \int_{u_{min}}^1 \frac{du \sqrt{1-u^2} \Gamma(\varepsilon, T)}{u \omega_0}. \quad (C1)$$

For temperatures  $T \gg [30\alpha_b \sqrt{\omega_{co}} T]^{2/3}$ , which holds for reasonable  $T$  and sizes, the integral, which renders a result of the kind  $Q_{\text{rel}}^{-1}(\omega_0, T) \approx (1/\omega_0)(A\sqrt{T} - BT^{1/3})$ , can be approximated by just the first term, obtaining Eq. (10). In any case, for completeness, we give the expression for  $B$  as follows:

$$B \approx \frac{500P_0\gamma^{14/3}(1+\nu)^{4/3}(1-2\nu)^{4/3}}{t^2w^{4/3}} \frac{1}{E^{11/3}(3-5\nu)} \left(\frac{\rho}{E}\right)^{1/3}. \quad (\text{C2})$$

Also, for completeness, we give the result for higher temperatures, although for current sizes the condition  $\Gamma(\varepsilon=[30\alpha_b \sqrt{\omega_{co}} T]^{2/3}, T) > \omega_0$  implies values of  $T$  above the range of applicability of the standard tunneling model. Now for some range of energies,  $\Gamma(\varepsilon, T) > \omega_0$  and the range of integration is divided into two regions, one where  $\omega_0\tau \gg 1$  and one where the opposite holds:

$$Q_{\text{rel}}^{-1}(\omega_0, T) = \frac{P_0\gamma^2}{ET} \int_{u_{\min}}^1 du \frac{\sqrt{1-u^2}}{u} \left\{ \int_{[30\alpha_b \sqrt{\omega_{co}} T]^{2/3}}^{[16\alpha_b \sqrt{\omega_{co}} 2T/\sqrt{\omega_0}]^2} \times dE \omega_0 \pi(\varepsilon, T) + \int_{[16\alpha_b \sqrt{\omega_{co}} 2T/\sqrt{\omega_0}]^2}^T dE \frac{1}{\omega_0 \pi(\varepsilon, T)} \right\}. \quad (\text{C3})$$

The final result is  $Q_{\text{rel}}^{-1}(\omega_0, T) \approx -7P_0\gamma^2\omega_0/T + A\sqrt{T}/\omega_0 - CT/\omega_0^2$ , with  $A$  defined by Eq. (10) and  $C$  by

$$C \approx \frac{1500P_0\gamma^6(1+\nu)^2(1-2\nu)^2}{t^3w^2} \frac{1}{E^3(3-5\nu)^2} \left(\frac{\rho}{E}\right)^{1/2}. \quad (\text{C4})$$

All the results for  $Q_{\text{rel}}^{-1}(\omega_0, T)$  have to be multiplied by the fraction of volume of the resonator presenting amorphous features,  $V_{\text{amorph}}/tWL$ .

#### APPENDIX D: DERIVATION OF EQUATIONS (14) and (15)

To derive the interaction Hamiltonian [Eq. (14)], note that in terms of the deformation gradient matrix  $\partial_i u_j$ , it must be  $H_{\text{int}} = \gamma \sigma_z \partial_i u_j$ , where the deformations are caused in this case by the twisting of the resonator about its main axis. The twisting modes correspond<sup>51</sup> to the rotation angle around the longest main axis  $\phi$  obeying the wave equation

$$C \frac{\partial^2 \phi}{\partial z^2} = \rho I \frac{\partial^2 \phi}{\partial t^2} \quad (\text{D1})$$

so the variable  $\phi$  can be expressed in terms of boson operators

$$\phi(0) = \sum_k \sqrt{\frac{\hbar}{2\rho t w L \omega_k}} (a_k^\dagger + a_k),$$

$$\partial \phi|_{z=0} = \sqrt{\frac{\hbar}{2\rho t w L}} \sum_k \frac{k}{\sqrt{\omega_k}} (a_k^\dagger + a_k). \quad (\text{D2})$$

To obtain an approximate expression for  $\partial_i u_j$  in terms of the modes' operators  $a_k$ , we relate  $\partial u$  to  $\partial \phi$  through the expressions for the free energy of the rod in terms of both variables as follows:

$$F_{\text{rod}} = \frac{1}{2} \int dz C \left( \frac{\partial \phi}{\partial z} \right)^2 = \frac{1}{2} \int dz \int dS 4\mu \left[ \left( \frac{\partial u_x}{\partial z} \right)^2 + \left( \frac{\partial u_y}{\partial z} \right)^2 \right] \approx \frac{1}{2} \int dz \int dS 8\mu \left( \frac{\partial u_x}{\partial z} \right)^2 \quad (\text{D3})$$

and the approximate relation  $\partial u|_{z=0} = \partial u_x / \partial z = \sqrt{C/8\mu t w} \partial \phi|_{z=0}$  is found. This relation together with Eq. (D2) leads to the stated result [Eq. (14)].

#### 1. Calculation of $E_0$

To classically calculate the energy stored by a torsional mode  $\phi_j(z, t) = A \sin[(2j-1)\pi z/2L] \sin(\omega_j t)$ , we just calculate the kinetic energy in a moment where the elastic energy is zero, for example, at time  $t=0$ . If an element of mass is originally at position  $(x, y, z)$  ( $x, y$  transversal coordinates), with a torsion  $\phi(z, t)$  it moves to

$$\vec{r}(t) = \left( \sqrt{x^2 + y^2} \cos \left[ \arccos \frac{x}{\sqrt{x^2 + y^2}} + \phi \right], \sqrt{x^2 + y^2} \sin \left[ \arccos \frac{x}{\sqrt{x^2 + y^2}} + \phi \right], z \right). \quad (\text{D4})$$

The kinetic energy at time  $t=0$  is

$$E_0 = \int_0^L dz \int_{-t/2}^{t/2} dx \int_{-w/2}^{w/2} dy \cdot \frac{1}{2} \rho \left| \frac{d\vec{r}}{dt} \right|_{t=0}^2. \quad (\text{D5})$$

Substituting the expression for  $\vec{r}(t)$  in the integrand, one arrives at

$$E_0 = \int_0^L dz \int_{-t/2}^{t/2} dx \int_{-w/2}^{w/2} dy \frac{1}{2} \rho A^2 \omega_j^2 \sin^2 \left[ \frac{(2j-1)\pi}{2L} z \right] \times (x^2 + y^2) = \frac{1}{48} A^2 \omega_j^2 \rho L (t^3 w + w^3 t). \quad (\text{D6})$$

In terms of the creation and annihilation operators,  $\phi_j(z, t) = \frac{\hbar}{2L\rho I \omega_j} (a_j^\dagger + a_j) e^{i(k_j z - \omega t)}$ , so the mean square of its amplitude is  $\langle \phi_j^2 \rangle = A^2/2 = \hbar(2n+1)/2L\rho I \omega_j$ . Substituting this in Eq. (D6), Eq. (15) for  $E_0$  is obtained.

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