Quantum Friction of Micromechanical Resonators at Low Temperatures

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Dissipation of micro- and nanoscale mechanical structures is dominated by quantum-mechanical tunneling of two-level defects intrinsically present in the system. We find that at high frequencies — usually, for smaller, micron-scale structures — a novel mechanism of phonon pumping of two-level defects gives rise to weakly temperature-dependent internal friction, Q^{-1}, concomitant to the effects observed in recent experiments. Because of their size, comparable to or shorter than the emitted phonon wavelength, these structures suffer from superradiance-enhanced dissipation by the collective relaxation of a large number of two-level defects contained within the wavelength.

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Physical properties of physically and chemically engineered micromechanical systems are of immense fundamental and technical interest [1]. Some of the recent spectacular examples of micromechanical structures include the measurement of vortex motion in high-T_c superconductors [2], biomolecular recognition [3], actuation of sensors via Casimir force [4], and shuttling of an electron charge in a quantum dot [5]. Important to all these experiments is the oscillation of a particular set of micron-sized resonators at a resonance frequency determined by the geometry and material properties. Changes in the "resonant" oscillation frequency or the oscillation amplitude mostly determine the magnitude of the force of interest, to which the micromechanical structure is coupled. Detrimental to the detection of force is the damping of the resonant structure, quantified by quality factor Q or dissipation Q^{-1}.

The essential problem inherent to the types of force measurement mentioned above is the low quality factor Q, observed in small resonators. In many experiments, intrinsic two-level defects [6,7] are found to be the dominant cause of internal friction Q^{-1} in crystalline resonators [8–10]. The observed linear temperature dependence of $Q^{-1} \propto T$ [8] could be explained assuming reasonable density of defects within a linear response theory of two-level systems (TLS) [11,12]. Despite the success of the TLS mechanism, dissipation at low temperatures continues to hold many challenges, notably the observation of a weak temperature dependence [10] and the nonmonotonic dependence of $Q^{-1}(T)$ in silicon resonators [13]. Most recent experiments merely add to the list of problems yet to be understood.

Previous theoretical works on the acoustic response of TLS use the linear response approximation or adiabatic approximation for nonlinear response [14,15]. The question we would like to explore is whether the anomaly can be explained in terms of TLS if both assumptions are abandoned. For dissipation in micromechanical resonators, such issues become terribly important, as a new parameter space emerges with decreasing size. For example, emitted phonon wavelength becomes much longer ($\gg 1\ \mu$m) compared to the system size at low temperatures, bringing novel correlation effects [16], extremely relevant to mesoscopic structures.

In this work, we evaluate internal friction Q^{-1} when the two-level defects operate nonlinearly and nonadiabatically. We show that the nonlinear response of Q^{-1} results in a large contribution at low temperatures at high driving frequencies due to the process of *phonon pumping*. We propose and demonstrate a mechanism of how Q^{-1} can be significantly enhanced by the phonon pumping process through *cooperative emission* of phonons. Cooperative emission becomes possible because of the long wavelength of the emitted phonons, which allows the correlated decay of two-level systems contained within the wavelength. Our theory provides a mechanism for enhanced dissipation in micromechanical resonators within the context of two-level systems.

The Hamiltonian of a TLS is fully characterized by the asymmetry energy Δ and the tunneling matrix element Δ_0. The asymmetry energy of a TLS is the energy splitting due to the static strain $\pm\frac{1}{2}\Delta_s$ and the applied time-dependent strain field $\epsilon_0 \cos\omega t : \Delta(t) = \Delta_s + 2\gamma\epsilon_0 \times \cos\omega t$, where γ is the constant of coupling between the acoustic wave and the asymmetry energy. Friction due to thermal phonons is described by the Hamiltonian for the single TLS coupled to phonon fields [7]:

$$H = \frac{\Delta_s + 2\gamma\epsilon_0 \cos\omega t}{2}\sigma_z + \frac{\Delta_0}{2}\sigma_x + \sum_{\mathbf{q},\alpha} \hbar\omega_\alpha(\mathbf{q}) a^\dagger_{\mathbf{q},\alpha} a_{\mathbf{q},\alpha} + \sum_{\mathbf{q},\alpha} \gamma_\alpha \sqrt{\frac{q\hbar}{2\rho \mathcal{V} v_\alpha}} \sigma_z (a_{\mathbf{q},\alpha} + a^\dagger_{-\mathbf{q},\alpha}), \quad (1)$$

where $\mathcal{V}$ and ρ are the volume and the mass density of the resonator, v_α is the sound velocity for polarization α, $a_{\mathbf{q},\alpha}(a^\dagger_{\mathbf{q},\alpha})$ is the phonon annihilation (creation) operator. γ_α is the coupling constant which relates the change in the asymmetry energy to the local elastic strain.

In crystalline materials with many TLSs, it is known that the static asymmetry energy Δ_s has a wide distribution due to the randomness of the local strain, while tunneling splitting energy Δ_0 has a well-defined value [11]. For simplicity, we consider a rectangular distribution [12] of Δ_s with n number of TLS per unit volume in $0 < \Delta_s < \Delta_s^{\max}$. The underlying assumption, $\hbar\omega \ll \gamma\epsilon_0 \ll \Delta_s^{\max}$, holds in most experiments.

The internal friction Q^{-1} is related to the energy loss per unit volume δE in a cycle of the acoustic wave; $Q^{-1} = [(\delta E)/(2\pi E_0)]$, where $E_0 = 2\rho\epsilon_0^2 v^2$ is the acoustic wave energy stored per unit volume [7]. The time-averaged phonon emission power $\bar{P}(\Delta_s, T)$ of a TLS is related to Q^{-1}: $Q^{-1}(T) = (n/2\rho v^2) \times (1/\epsilon_0^2\omega) \int_0^{\Delta_s^{\max}} \bar{P}(\Delta_s, T) d\Delta_s$. Furthermore, we divide the two-level systems into two kinds based on their asymmetry energy Δ_s: (i) $\Delta_s < 2\gamma\epsilon_0$, and (ii) $\Delta_s > 2\gamma\epsilon_0$, which contribute to the total dissipation according to $Q^{-1}(T) = Q_1^{-1} + Q_2^{-1}$:

$$Q_1^{-1}(T) = \frac{n}{2\rho v^2} \frac{1}{\epsilon_0^2 \omega} \int_0^{2\gamma\epsilon_0} \bar{P}(\Delta_s, T) d\Delta_s, \qquad (2)$$

$$Q_2^{-1}(T) = \frac{n}{2\rho v^2} \frac{1}{\epsilon_0^2 \omega} \int_{2\gamma\epsilon_0}^{\Delta_s^{\max}} \bar{P}(\Delta_s, T) d\Delta_s. \qquad (3)$$

In linear response theory where ϵ_0 is infinitesimally small, all the TLS belong to category (ii), and $Q_1^{-1} = 0$. However, even a small experimental value of $\epsilon_0 = 10^{-6}$ will give rise to nonlinear behavior [8], which implies that TLS with $\Delta_s < 2\gamma\epsilon_0$ may also play an important role [12].

Usually a time-dependent unitary transformation U is used for solving the time-dependent Hamiltonian in the nonlinear regime, so that the TLS has time-dependent energy levels given as $\pm\frac{1}{2}E(t)$, $[E(t) = \sqrt{\Delta(t)^2 + \Delta_0^2}]$. In the standard adiabatic limit [14,15] used to explain the low-frequency experiments, the acoustic field frequency is assumed to be very low so that the additional term due to the unitary transformation $-i\hbar U^\dagger[(\partial U)/(\partial t)] = \sigma_y[(\Delta_0\gamma\epsilon_0)/(E(t)^2)]\hbar\omega \sin\omega t$ can be safely neglected. In contrast, here we consider the high-frequency regime where the matrix element of this additional term cannot be neglected in comparison to the diagonal term $\frac{1}{2}E(t)\sigma_z$ even at the level-crossing point $E(t) = \Delta_0$:

$$\frac{\gamma\epsilon_0\hbar\omega}{\Delta_0} \gg \Delta_0. \qquad (4)$$

Under this condition, as the tunneling motion between the two sites is not fast compared to the rapid time evolution of the acoustic wave, it is not useful to take the TLS bonding states of the two sites as the basis states. Instead, it is more natural to consider the localized basis states in each local potential minimum and consider the tunneling term $\frac{1}{2}\Delta_0\sigma_x$ as a perturbation.

We treat the coupling to the acoustic wave adiabatically and treat the tunneling term and the coupling to the thermal phonon perturbatively. The approximation is guaranteed by the fact that TLS-phonon interaction can be treated perturbatively whenever the two-level approximation is valid [17]. Let $|l\rangle$ and $|r\rangle$ be the left and the right localized states, respectively. The leading term for the transition from one state to the other is the second order process involving the tunneling and emission (absorption) of a phonon; at low temperatures the single phonon process dominates. The thermal averaged relaxation rate is written as $[1/\tau(\Delta)] = A\Delta_0^2\Delta \coth[\Delta/(2k_BT)]$, where $A = \sum_\alpha[\gamma_\alpha^2/(2\pi\hbar^4 v_\alpha^5\rho)]$. Here we assume the Debye density of states of phonon with a linear dispersion: $\omega_\alpha = v_\alpha q$.

Time evolution of the occupation number $n_r(= 1 - n_l)$ follows the rate equation [14] for the time-dependent asymmetry energy $\Delta(t) = 2\gamma\epsilon_0 \cos\omega t + \Delta_s$:

$$\frac{dn_r}{dt} = -\frac{n_r - n_r^{(0)}}{\tau[\Delta(t)]}; \qquad n_r^{(0)}(t) = 1/(e^{\beta\Delta(t)} + 1), \qquad (5)$$

where $\beta = 1/k_BT$. The typical process is depicted in Fig. 1. In the regime $\Delta_s < 2\gamma\epsilon_0$, the two energy levels cross, and at this point population inversion arises. Note that the population inversion process ($A \to B \to C$) is followed by the spontaneous emission of phonon ($C \to D$). The high-frequency assumption of Eq. (4) is crucial for the pumping process near the level-crossing point. In the conventional adiabatic limit ($\gamma\epsilon_0\hbar\omega/\Delta_0 \ll \Delta_0$) with TLS energies of $\pm\frac{1}{2}E(t)$, level crossing is avoided and the TLS in the low (high) energy state remains mostly in the low (high) energy state.

The time-averaged phonon emission power [14] can be obtained by solving Eq. (5) for $n_r(t)$:

$$\bar{P}(\Delta_s, T) = -\frac{\omega}{2\pi} \int_0^{\frac{2\pi}{\omega}} dt \Delta(t) \frac{dn_r(t)}{dt}. \qquad (6)$$

For the general case of asymmetric TLS, numerical

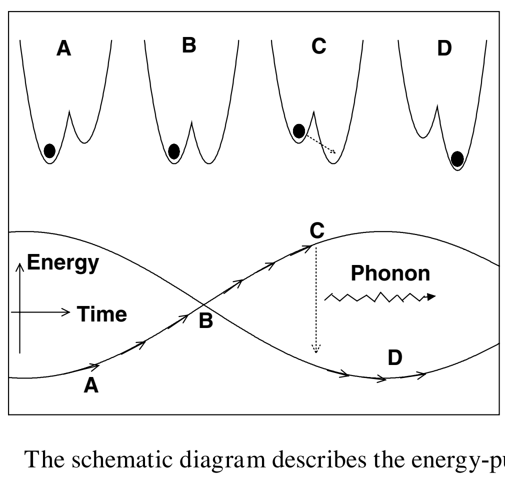

FIG. 1. The schematic diagram describes the energy-pumping process of the two-level atom from the acoustic wave to phonons. The crossing curves represent the time evolution of the two energy levels with the energy gap of $\Delta(t) = 2\gamma\epsilon_0 \cos\omega t + \Delta_s$. The energy diagrams of the two-level atom as a function of the configuration coordinates are depicted in the upper panel.

integration of Eq. (5) gives $\bar{P}$ as a function of the static asymmetry energy Δ_s and temperature T, and Eq. (2) subsequently gives Q_1^{-1}. For the particular case of symmetric TLS ($\Delta_s = 0$), Eq. (6) can be rewritten using an analytic solution of $n_r(t)$ at $T = 0$:

$$\bar{P} = \frac{2\gamma^2 \epsilon_0^2 A \Delta_0^2}{\pi\omega} \int_{-\frac{\pi}{2\omega}}^{\frac{\pi}{2\omega}} \cos^2\omega t \frac{\exp(\frac{\sin\omega t}{\omega\tau_\epsilon})}{\cosh(1/\omega\tau_\epsilon)} dt, \quad (7)$$

where τ_ϵ is a typical relaxation time scale of symmetric TLS at zero temperature when $\omega\tau_\epsilon > 1$:

$$\frac{1}{\tau_\epsilon} = 2A\Delta_0^2\gamma\epsilon_0. \quad (8)$$

When $\Delta_s > 2\gamma\epsilon_0$, the TLS always stays in the lower energy state at zero temperature, hence the TLS does not emit a phonon in its steady state, $\bar{P}(\Delta_s > 2\gamma\epsilon_0, T = 0) = 0$. Since $\bar{P}(\Delta_s, T = 0)$ is a smoothly decaying function of Δ_s, an analytic formula for $Q_1^{-1}(T = 0)$ can be obtained using the approximation $\int_0^{2\gamma\epsilon_0} \bar{P}(\Delta_s, T = 0) d\Delta_s \approx \gamma\epsilon_0[\bar{P}(0,0) + \bar{P}(\gamma\epsilon_0, 0)] = \gamma\epsilon_0 \bar{P}(0,0)$. From Eq. (7), the zero temperature internal friction Q_1^{-1} is found to be

$$Q_1^{-1}(T = 0) \approx \frac{n\gamma^2}{\rho v^2} \mathrm{sech}\left(\frac{1}{\omega\tau_\epsilon}\right) I_1\left(\frac{1}{\omega\tau_\epsilon}\right), \quad (9)$$

where $I_1(x)$ is the first kind modified Bessel function of order 1.

Now let us turn to Q_2^{-1}. For weak strain $2\gamma\epsilon_0 < \Delta_s$, where the energy levels do not cross, the phonon pumping process does not take place. This is the regime where the usual linear response theory is a good approximation for describing internal friction. In the linear response theory [6,11], $Q_2^{-1}(T)$ in Eq. (3) for $k_B T \gg \hbar\omega > \hbar/\tau(\Delta_0)$ can be written as [6] $Q_2^{-1}(T) = [(n\gamma^2)/(\rho v^2 k_B T)] (1/\omega) \int_{2\gamma\epsilon_0}^{\Delta_s^{\max}} (\Delta^2/E^2) \mathrm{sech}^2[E/(2k_B T)] \tau^{-1}(E) d\Delta$, where $E = \sqrt{\Delta^2 + \Delta_0^2}$. For $\Delta_0 \ll \gamma\epsilon_0 \ll \Delta_s^{\max}$, an expression for Q_2^{-1} is easily found:

$$Q_2^{-1}(T) = \frac{n\gamma^2}{\rho v^2} \frac{2}{\omega\tau_\epsilon} f\left(\frac{k_B T}{2\gamma\epsilon_0}\right), \quad (10)$$

where $f(x)$ is an almost linear function, defined by $f(x) = x \int_{1/x}^{\infty} dt (t/\sinh t)$.

Figure 2 shows the temperature dependence of $Q^{-1} = Q_1^{-1} + Q_2^{-1}$ for $\omega\tau_\epsilon = 1$, calculated from Eqs. (2), (3), (5), (6), and (10). Q^{-1} shows a weak temperature dependence with decreasing temperature, as Q_1^{-1} becomes more important than Q_2^{-1} at low temperatures. The low-temperature saturation value of Q^{-1} for $\omega\tau_\epsilon \gtrsim 1$ is well approximated by $\sim 0.3(1/\omega\tau_\epsilon)(n\gamma^2/\rho v^2)$. Now, let us estimate τ_ϵ from experimental data [8]. Since $n\gamma^2/\rho v^2$ is roughly the high-temperature saturation [6] value of Q^{-1}, for the single-crystalline silicon data in Ref. [8], we estimate $n\gamma^2/\rho v^2 \sim 10^{-6}$–$10^{-5}$ from the experiments at $\omega \sim 10^3$–10^4 Hz. Since the low-temperature saturation value of Q^{-1} was found to be $\sim 10^{-7}$–10^{-6} for these

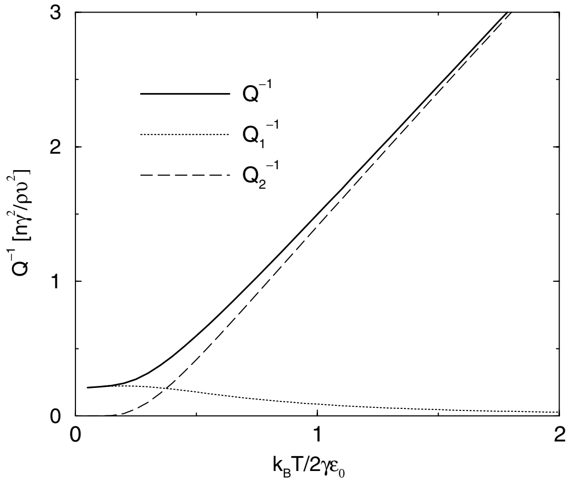

FIG. 2. The internal friction $Q^{-1} = Q_1^{-1} + Q_2^{-1}$ as a function of temperature for $\omega\tau_\epsilon = 1$.

frequencies, we estimate $\omega\tau_\epsilon \sim 1$, which means $\tau_\epsilon \sim 10^{-3}$–$10^{-4}$ sec. However, these values of τ_ϵ are anomalously small compared to the direct estimate using Eq. (8) with reasonable values of parameters [6,7,11]. By using $\gamma \sim 1$ eV, $\epsilon_0 \sim 10^{-6}$, $A \sim 10^8$ s^{-1} k_B^{-3} into Eq. (8), we get $\tau_\epsilon \sim 1$ sec. In other words, the low-temperature dissipation in experiments [8] is anomalously larger than our direct theoretical estimation.

Here we propose and discuss the origin of the anomalously small relaxation time τ_ϵ. We believe that the *cooperative emission* [18] of phonons provides a natural mechanism for the short relaxation time. In Dicke superradiance [18], N number of two-level atoms within a distance shorter than the emitted photon wavelength emits photons cooperatively, therefore the lifetime of the atom in the excited state is effectively reduced by a factor of N. In the usual treatment of phonon emission of TLS, as we have done so far, the emission of the phonon is calculated by assuming that the TLSs are totally independent. However, this assumption is not valid when a number of TLS are contained within a distance shorter than the wavelength of the emitted phonon. This phonon wavelength, $\lambda_{\text{ph}} \sim [(\hbar v_s)/(\gamma\epsilon_0)]$ (v_s is the sound velocity), can be considerably larger ($\gtrsim \mu$m), leading to the cooperative emission from a large number of two-level systems.

Now let us consider N two-level systems within a volume λ_{ph}^3. In the context of phonon emission, pumping of the two-level system is done by the acoustic wave applied to the resonator. The many-TLS Hamiltonian in Eq. (1) can be generalized to $H = H_0 + H_{\text{tun}} + H_{\text{TLS-ph}}$ where $H_0 = H_{\text{TLS}} + H_{\text{ph}} = \frac{1}{2}\Delta(t)\sum_{i=1}^N \sigma_{i,z} + \sum_{\mathbf{q},\alpha} \times \hbar\omega_\alpha(\mathbf{q}) a_{\mathbf{q},\alpha}^\dagger a_{\mathbf{q},\alpha}$, $H_{\text{tun}} = (\Delta_0/2)\sum_{i=1}^N \sigma_{i,x}$, and $H_{\text{TLS-ph}} = \sum_{i=1}^N \sum_{\mathbf{q},\alpha} \gamma_\alpha \sqrt{[(q\hbar)/(2\rho \mathcal{V} v_\alpha)]} \sigma_{i,z}(a_{\mathbf{q},\alpha} + a_{-\mathbf{q},\alpha}^\dagger)$.

The many-TLS state $|l, l, l, \ldots l\rangle$, where all the TLS are in the l state, is the maximally excited state or the ground state. We consider the set of many-TLS states generated from $H_{\rm TLS\text{-}ph} + H_{\rm tun}$, which are $|M\rangle = \sqrt{[(N/2 - M)!/N!(N/2 + M)!]}(\sum_{i=1}^{N} \sigma_i^{+})^{N/2+M}|l, l, l, \ldots l\rangle$, where $M = -N/2, \ -N/2 + 1, \ -N/2 + 2, \ldots, N/2$. These states satisfy $H_{\rm TLS}(t)|M\rangle = M\Delta(t)|M\rangle$. As in the case of a single TLS, a perturbation analysis finds the transition rate $w_{M\pm1,M}$ from $|M\rangle$ to $|M \pm 1\rangle$ to be $w_{M\pm1,M}(t) = w[\mp\Delta(t)](\frac{N}{2} \mp M)(\frac{N}{2} \pm M + 1)$, where $w(\Delta) = A\Delta_0^2[\Delta/1 - \exp(-\Delta/k_B T)]$. Here, we have used the relation $\langle M \pm 1|\sum_{i=1}^{N} \sigma_i^{\pm}|M\rangle = \sqrt{(N/2 \mp M)(N/2 \pm M + 1)}$. Now the rate equation for the many-TLS remains to be solved numerically: $[(dn_M)/(dt)] = w_{M,M+1}(t)n_{M+1} - w_{M-1,M}(t)n_M + w_{M,M-1}(t)n_{M-1} - w_{M+1,M}(t)n_M$. The time-averaged power $\bar{P}_N$ emitted by N number of TLS can be obtained as $\bar{P}_N = -(\omega/2\pi)\int_0^{2\pi/\omega} dt \sum_{M=-N/2}^{N/2} M\Delta(t) \times \{[dn_M(t)/(dt)]\}$.

Note that for phonons independently emitted by the TLSs, $\bar{P}_N$ is simply proportional to the number N; $\bar{P}_N = N\bar{P}$. However, in cooperative emission, the lifetime of the excited state of a single TLS is N times shorter, hence the phonon emission power of a single TLS should be N times larger when $\omega\tau_\epsilon > 1$ [19]. This means that $\bar{P}_N$ should be proportional to N^2 for $\omega\tau_\epsilon > 1$. Our numerical results indeed show that the $\bar{P}_N$ has a quadratic dependence of N (see Fig. 3).

When N number of TLS are within $\lambda_{\rm ph}$, one obtains Q_1^{-1} by replacing $\bar{P}$ with its effective value $\bar{P}^* = \bar{P}_N/N$. The enhanced phonon emission power due to superradiance $\bar{P}^* \sim N\bar{P}$ then provides a natural explanation of the anomalously large internal friction at low temperatures. Including the phonon superradiance effect, Eq. (9) for $\omega\tau_\epsilon > 1$ can be rewritten as

$$Q^{-1}(T = 0) = Q_1^{-1}(T = 0) \sim \frac{1}{\omega\tau_\epsilon^*}\frac{n\gamma^2}{\rho v^2}, \qquad (11)$$

where $\tau_\epsilon^* \approx \tau_\epsilon/N$ is the renormalized relaxation time and N is the number of cooperating TLSs. Thus, the enhancement of Q^{-1} at low temperature by a factor of 10^3–10^4 compared to our initial estimate in the independent TLS model [Eq. (9)] indicates that a large number of $\sim 10^3$–10^4 TLS emit phonons cooperatively. By taking $\lambda_{\rm ph} \sim 10\ \mu$m from $\lambda_{\rm ph} = [(\hbar v_s)/(\gamma\epsilon_0)]$, the total number of TLSs in the volume $\lambda_{\rm ph}^3$ is $\sim 10^5$ according to Ref. [11] or $\sim 10^3$ according to Ref. [12], which is a reasonably large enough number for the cooperative emission by 10^3 TLSs.

In conclusion, we formulate a theory of internal friction of micro- and nanomechanical resonators, which invokes intrinsic two-level defects in the nonlinear regime at high frequencies. As temperature decreases, the mechanical friction crosses over from the linear regime to the nonlinear regime, resulting in the saturation behavior as T goes to zero. Because of the phonon superradiance, the low-temperature saturation value of Q^{-1} is strongly enhanced by a factor given by the number of two-level systems contained within the emitted phonon wavelength.

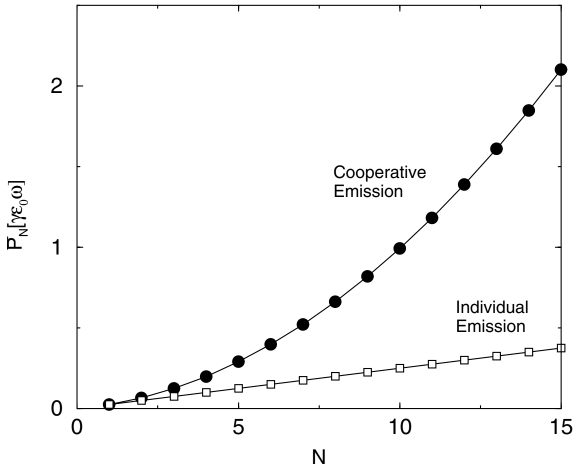

FIG. 3. The time-averaged phonon emission power $\bar{P}_N$ of N symmetric TLSs ($\Delta_s = 0$) at $T = 0.1\gamma\epsilon_0/k_B$ and $\omega\tau_\epsilon = 20$, which was numerically calculated (see the text).

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