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Accessibility of quantum effects in mesomechanical systems

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We consider the quantum properties of an elastic bar subject to compression. If strain rather than stress is held fixed, the system remains stable beyond the buckling instability, supporting two potential minima. The classical equilibrium transverse displacement is analogous to a Ginsburg-Landau order parameter, with strain playing the role of temperature. We calculate the quantum and thermal fluctuations as a function of strain. Excitation energies and quantum fluctuation amplitudes are compared for silicon beams and carbon nanotubes.

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The drive towards semiconductor device miniaturization and integration has resulted in fabrication technologies that are capable of producing artificial structures with features approaching the ten nanometer length scale. To go beyond this scale, naturally occurring and chemically organized structures are receiving much attention. These top-down and bottom-up fabrication techniques have been used to make ultrasmall mechanical systems to probe new areas of mesomechanics.[1–5] Recently, two reports have appeared that describe two-state nanomechanical systems. In one,[6] crossed carbon nanotubes were suspended between supports and the suspended element was electrostatically flexed between two states. In the second,[7] it was proposed to use an electrostatically flexed cantilever to explore the possibility of tunneling in a nanomechanical system.

Here we discuss the accessibility of quantum effects in a two-state mechanical system that has a tunable, symmetric potential function. This mechanical system has analogies to the superconducting interference device in which the observation of a coherent superposition of macroscopically distinct states was recently reported.[8] Specifically, we consider an elastic bar under longitudinal compression. The compression is used to adjust the potential energy for transverse displacements, as illustrated in Fig. 1, with strain playing a role analogous to temperature in a Ginzburg-Landau system. As the compressional strain is increased toward the Euler buckling instability,[9] the frequency of the fundamental vibrational mode drops toward zero. By controlling the separation between the ends of the bar, i.e., fixing the strain, the system remains stable beyond the instability and develops a double-well potential for the transverse motion. Since both the well depth and asymmetry are tunable, a variety of quantum phenomena may be explored and controlled, including zero-point fluctuations, tunneling, and coherent superpositions of macroscopically distinct states. In the latter two cases, the system may provide a mechanical realization of models studied in Refs. 10 and 11, respectively. We have applied the model to silicon beams and carbon nanotubes, and show that in both cases the critical quantum fluctuations in position are about 0.1 Å, an order of magnitude greater than the relaxed values. We show that the crossover between the quantum and thermal fluctuation regimes is a function of strain as well as temperature. Finally, we comment on the fact that tunneling in this mechanical system will be difficult to observe because of the stringent requirements on the applied strain.

We start from the well-known[12] normal mode description of an elastic rectangular bar of length l, width w, and thickness d satisfying the conditions $l \gg w > d$. With d smaller than w, only transverse displacements $y(x,t)$ in the "d" direction are considered. The equation of motion for small displacements, when the bar is held fixed at both ends without strain, is

$$\mu \ddot{y} + \mathcal{F}\kappa^2 y^{(4)} = 0, \tag{1}$$

where $\mu = m/l$ is the mass per unit length and $\mathcal{F}$ is the linear modulus of the bar. $\mathcal{F}$ is related to the elastic modulus $\mathcal{Q}$ of the material by $\mathcal{F} = \mathcal{Q}wd$. The bending moment κ is given by $\kappa^2 = d^2/12$ for a bar of rectangular cross section.

The normal modes of the bar are described in general by a combination of trigonometric and hyperbolic functions, depending on the boundary conditions.[12] The boundary conditions appropriate to hinged end points, $y(\pm l/2) = 0 = y''(\pm l/2)$, lead to normal modes with (angular) frequencies

$$\omega_n = \sqrt{\frac{\mathcal{Q}}{\rho}}\,\kappa\left(\frac{n\pi}{l}\right)^2. \tag{2}$$

Clamped end points have boundary conditions $y(\pm l/2) = 0 = y'(\pm l/2)$, and their normal mode frequencies are given to good approximation by replacing n with $(n+\frac{1}{2})$ in Eq. (2). The following analysis applies equally well to both cases. In the few instances where it makes a numerical difference we shall refer to the hinged case because of its simplicity.

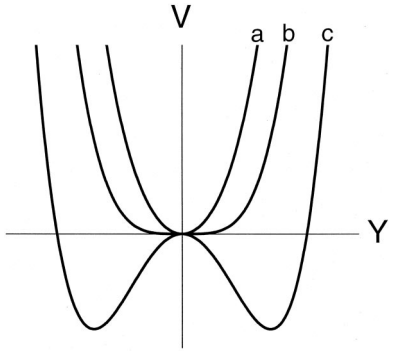

FIG. 1. Potential energy V as a function of the fundamental mode displacement Y. This function is harmonic above critical strain $\varepsilon > \varepsilon_c$ (a), quartic at critical strain $\varepsilon = \varepsilon_c$ (b), and a double-well below, $\varepsilon < \varepsilon_c < 0$ (c).

The mean square displacement of the bar, which includes both quantum and thermal contributions, is an incoherent superposition of contributions from each normal mode. At the center, only even-parity modes contribute, so that

$$\langle [y(0)]^2 \rangle = \sum_{\text{odd } n} \frac{\hbar}{2m^* \omega_n} [1 + 2\, f(\hbar \omega_n / kT)], \tag{3}$$

where $f(x) = 1/(e^x - 1)$ is the thermal excitation number of the nth mode. For hinged boundary conditions, $m^* = m/2$ exactly, whereas in the clamped case m^* is slightly smaller and weakly mode dependent. In either case the fundamental mode is responsible for more than half the total mean square displacement.

Longitudinal compression of the bar lowers the frequencies, with a corresponding increase in the zero-point motion. Compressive or tensile strain contributes the ''elastic'' potential energy $V_e = (\mathcal{F}/2l_0)(l_t - l_0)^2$, where $l_t = \int dx \sqrt{1 + (y')^2} \approx l + \frac{1}{2}\int dx (y')^2$ is the total (dynamic) length of the bar, l is the end-point separation, and l_0 is the unstressed equilibrium length. We subtract the static contribution $(\mathcal{F}/2l_0)(l - l_0)^2$ since it contributes nothing to the dynamics, and add the ''bending'' contribution $V_b \sim \int dx (y'')^2$ to get

$$V[y(x)] = \frac{1}{2} \int dx [\mathcal{F}\kappa^2 (y'')^2 + \mathcal{F}\varepsilon (y')^2] + \frac{\mathcal{F}}{8 l_0} \left(\int dx (y')^2 \right)^2, \tag{4}$$

where $\varepsilon \equiv (l - l_0)/l_0$ is the strain, positive if tensile and negative if compressive. From the Lagrangian, $L[y(x,t)] = (\mu/2)\int dx (\dot{y})^2 - V[y(x)]$, we find the equation of motion,

$$\mu \ddot{y} + \mathcal{F}\kappa^2 y^{(4)} - \mathcal{F}\varepsilon y'' - \frac{1}{2}\mathcal{F}\left(\int dx' [y'(x')]^2 \right) y'' = 0, \tag{5}$$

which generalizes Eq. (1). The third term represents the tension induced by externally-imposed stretching, and the anharmonic fourth term is the enhancement of tension due to the dynamic stretching effect of transverse motion; this term arises from the geometry of the system.

In the harmonic regime where the fourth term can be neglected, the normal mode frequencies under hinged boundary conditions are given by

$$\tilde{\omega}_n^2 = \omega_n^2 \left[1 + \varepsilon \left(\frac{l}{n\pi\kappa} \right)^2 \right], \tag{6}$$

where ω_n are the relaxed ($l = l_0$) frequencies of Eq. (2). The quantum and thermal fluctuations are given by Eq. (3) with ω_n replaced by $\bar{\omega}_n$. Of course, the harmonic approximation breaks down for the fundamental mode as we approach its critical strain,

$$\varepsilon_c \equiv \frac{l_c - l_0}{l_0} = -\left(\frac{\pi\kappa}{l} \right)^2. \tag{7}$$

At critical strain, the effective potential for the fundamental mode is purely quartic whereas the higher modes remain harmonic in leading order, with the first harmonic frequency being reduced by about 13% from its relaxed (uncompressed) value.

To address the quantum properties when the fundamental mode becomes anharmonic, we consider the Hamiltonian

$$H = \frac{1}{2\mu} \int dx \Pi^2 + V[y(x)], \tag{8}$$

where $\Pi(x,t) = \delta L/\delta \dot{y}(x,t) = \mu \dot{y}(x,t)$ is the canonical momentum. In the subcritical compression regime, a normal mode expansion of H leads to a phonon description of the transverse motion with interactions arising from the anharmonic term. These interactions occur physically because transverse phonons stretch the bar. Even the zero-point motion has a stretching effect, but this can be absorbed in the length parameter l. Thus, at temperatures below the first harmonic threshold, $kT < \hbar\tilde{\omega}_2$, the anharmonic effect on the fundamental is its own self-interaction. So the effective Hamiltonian for the fundamental mode, obtained by taking the ground-state expectation value in all higher modes, is a quartic function of the ''fundamental displacement'' Y, the Fourier component of the fundamental mode.[13] The energy eigenvalues E and eigenfunctions $\Psi(Y)$ describing the fundamental vibrational states are then given by the Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial Y^2} + \frac{\alpha}{2} Y^2 + \frac{\beta}{4} Y^4 \right) \Psi(Y) = E\Psi(Y), \tag{9}$$

where $-i\hbar\partial/\partial Y = P$ is the momentum operator canonically conjugate to Y. This simple description is possible because the intrinsic nonlinearity is restricted to a single mode. Since this fundamental transverse mode has a very small wave number (π/l), the continuum elastic theory is valid and determines both the form and parameter values of Eq. (9).

The potential energy has the form of a Ginzburg-Landau free energy,[14] with strain playing the role of temperature:

$$\alpha = m^* \tilde{\omega}_1^2 = m^* \omega_1^2 \left(\frac{\varepsilon_c - \varepsilon}{\varepsilon_c} \right). \tag{10}$$

The displacement Y is analogous to the order parameter, in that its classical equilibrium value vanishes above critical strain but takes a nonzero value $Y \to \pm Y_{\min} = \pm\sqrt{|\alpha|/\beta}$ below it ($\varepsilon < \varepsilon_c < 0$, Fig. 1), breaking the reflection symmetry of the Hamiltonian. Of course the quantum mechanical ground state has $\langle Y \rangle = 0$, but sufficiently far into the double-well regime, this ground state is a superposition of macroscopically distinct states. Thus, monitoring the position of the bar on a time scale less than the tunneling time would yield results clustered about just one of the potential minima, $Y_{\min}$ or $-Y_{\min}$, not both. The usual definition of quantum fluctuations, $\Delta Y^2 = \langle Y^2 \rangle - \langle Y \rangle^2$, becomes inappropriate as the system moves into the double-well regime. A more appropriate measure of the observable quantum fluctuations is $\Delta Y^2 = \langle \min(Y \pm Y_{\min})^2 \rangle$, the rms departure from the nearest potential minimum. We plot the ground- and first-excited-state energies in Fig. 2(a), and in Fig. 2(b) the ground-state quantum fluctuations ΔY, as functions of the strain near its

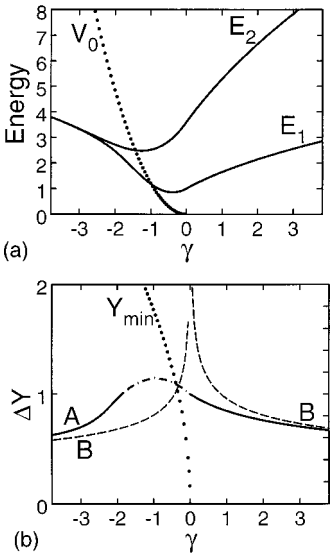

FIG. 2. (a) Ground- and first-excited-state energies, E_1 and E_2, respectively, of the fundamental vibrational mode as functions of the departure from critical strain γ. The dotted curve shows the barrier height dependence on γ. (b) Curve A is the ground-state fluctuation ΔY, calculated using the full quartic potential. The solid portions of the curve are obtained from the calculations; the dot-dashed region is a guide to the eye. For comparison, curve *B* shows ΔY obtained in the harmonic approximation. The dotted curve shows the position $Y_{\min}$ of the potential minimum.

critical value. These are plotted in dimensionless energy and length units, E/E_c and $\Delta Y/\Delta Y_c$, where E_c and ΔY_c are the ground-state values at critical strain,

$$E_c = 0.42\left(\frac{\hbar^2}{m^*}\right)^{2/3}\beta^{1/3} \quad \text{and} \quad \Delta Y_c = 0.68\left(\frac{\hbar^2}{m^*\beta}\right)^{1/6}, \tag{11}$$

and the departure from critical strain, $\gamma=(1.6\kappa/\Delta Y_c)^2(\varepsilon_c-\varepsilon)/\varepsilon_c$, is scaled so that $\gamma=-1$ when the barrier height $V_0=\alpha^2/4\beta$ is equal to E_1. Figure 2(b) shows that ΔY as defined above is much less than the well separation for fairly modest negative values of γ. In the region $\gamma\sim-1$, where this is no longer the case, this definition loses its physical meaning and larger fluctuations may be expected, as suggested by the dot-dash line in Fig. 2(b). The dashed curves B show ΔY similarly defined but calculated in the harmonic approximation, with the result $\Delta Y\sim|\varepsilon-\varepsilon_c|^{-1/4}$. The harmonic approximation is accurate outside a small region near the critical point (roughly $-6<\gamma<3$), where the divergence is prevented by the quartic term in the potential energy.

To address the magnitude of quantum fluctuations in real systems, Table I lists the first excitation energies $\Delta E=E_2-E_1$ and ground-state (quantum) fluctuations ΔY (Ref. 13) for rectangular silicon bars and cylindrical multiwalled carbon nanotubes. Numbers are given for two cases—the critical and the relaxed states. Schrödinger equation parameters are calculated using hinged boundary conditions, with the results $m^*=m/2$ and $\beta=m^*(\omega_1/2\kappa)^2$. Nanotube frequencies were found using Eq. (2) with $\kappa^2=(d_2^2+d_1^2)/16$, where d_1 and d_2 are inner and outer diameters. The dimensions of

TABLE I. Table of excitation energies $\Delta E=E_2-E_1$ and rms midpoint fluctuations ΔY for Si bars (linear dimensions *l, d, w*), and C nanotubes of length *l* and outer (inner) diameters $d_2(d_1)$. The Young's modulus and density of Si are $Q=130$ GPa and $\rho=2330$ kg/m^3. The values taken for C nanotubes are (Ref. 15) $Q=1.8$ TPa and $\rho=2150$ kg/m^3. Energies ΔE are given in temperature units (note that 1 GHz=48 mK).

	Si bar	Si bar		C nanotube	C nanotube
l (nm)	500	50	l (nm)	500	50
d (nm)	10	5	d_2 (nm)	10	5
w (nm)	20	10	d_1 (nm)	5	1
		Relaxed			
ΔE_0 (mK)	6.5	330		24	1100
ΔY_0 (Å)	0.0081	0.0072		0.0080	0.0066
		Critical			
ΔE_c (mK)	0.023	1.7		0.086	5.9
ΔY_c (Å)	0.12	0.092		0.12	0.083

the larger tubes listed are typical of the multiwalled tubes studied by Treacy *et al.*,[15] whose vibrational properties are consistent with continuum elastic theory. The smaller dimensions listed represent the smallest multiwalled tube observed to buckle without losing its elastic integrity.[16] In the critical and double-well regimes, because of cylindrical symmetry, the nanotube states will be described by a Mexican hat potential rather than the one-dimensional double well appropriate for the rectangular silicon bars. Figures 2(a) and 2(b) refer specifically to the one-dimensional case. For nanotubes, Eq. (9) still applies with Y replaced by a two-component vector. To compare nanotubes and silicon bars, the entries in Table I refer to a single Cartesian component of Y.

Remarkably, quantum fluctuations may be enhanced by an order of magnitude by applying critical strain. At the same time, the excitation energies are reduced by about two orders of magnitude, so that thermal fluctuations can exceed the quantum contributions. Thus, these mesomechanical systems offer the possibility for parametrically controlled quantum fluctuations, and a means to explore the region between quantum and thermal fluctuations.

The large differences between the relaxed and compressed energy scales suggests that these systems could be supercooled by compression toward their critical points. For example, the smaller carbon nanotube could be prepared initially very close to its ground state by cooling to 500 mK. Critical compression without heat transfer would then cool the tube to a few mK, at the same time enhancing its zero-point motion by a factor of about 10 (see Table I). Subsequent equilibration[17] to 500 mK would then bring the tube to a "classical" equilibrium state with thermal fluctuation $\Delta Y_t \approx 0.25$ Å,[18] a further factor of 3 enhancement.

Finally, we comment on the possibility of observing tunneling in mesomechanical systems such as those considered here. The barrier height V_0 divided by the level spacing $\hbar\tilde{\omega}_1$ provides a rough estimate for the number N of bound states with energy below the top of the barrier:

$$N \sim \left(\frac{\kappa}{\Delta Y_0}\right)^2 \left(\frac{\varepsilon_c - \varepsilon}{\varepsilon_c}\right)^{3/2}. \quad (12)$$

Taking the smaller bar, if we go to twice the critical compression, $\varepsilon = 2\varepsilon_c$, then $N \sim 3 \times 10^6$. In order to tune the potential to hold about 10 bound states in each well, one would have to apply strain with extreme delicacy, $\varepsilon - \varepsilon_c \sim 10^{-4}\varepsilon_c$. Controlling the strain to this precision for sufficient time to identify tunneling, as distinct from thermal or other noise, will be difficult. Thus, while the observation of tunneling will be challenging, the prospect of exploring tunable quantum fluctuations in this system, and the connection to Ginzburg-Landau theory, are intriguing.

[1] M. L. Roukes, Phys. World **14**, 25 (2001).
[2] H. G. Craighead, Science **290**, 1532 (2000).
[3] H. Park, J. Park, A. K. L. Lim, E. H. Anderson, A. P. Alivisatos, and P. L. McEuen, Nature (London) **407**, 57 (2000).
[4] A. Erbe, R. H. Blick, A. Tilke, A. Kriele, and J. P. Kotthaus, Appl. Phys. Lett. **73**, 3751 (1998).
[5] A. N. Cleland and M. L. Roukes, Appl. Phys. Lett. **69**, 2653 (1996).
[6] T. Rueckes *et al.*, Science **289**, 94 (2000).
[7] A. N. Cleland and M. L. Roukes, in *Proceedings ICPS-24*, edited by D. Gershoni (World Scientific, Singapore, 1999).
[8] J. R. Friedman, V. Patel, W. Chen, S. K. Tolpygo, and J. E. Lukens, Nature (London) **406**, 43 (2000).
[9] L. Euler, in *Elastic Curves*, translated and annotated by W. A. Oldfather, C. A. Ellis, and D. M. Brown, reprinted from ISIS, No. 58 XX(1), 1774 (Saint Catherine Press, Bruges, Belgium).
[10] A. O. Caldeira and A. J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1983).
[11] A. J. Leggett *et al.*, Rev. Mod. Phys. **59**, 1 (1987).
[12] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon, Oxford, 1986), pp. 64–86.
[13] We scale Y to be equal to the central displacement in the fundamental mode, so that $y(x) = Y y_1(x)/y_1(0)$. The rms fluctuations are then $(\Delta Y)^2 = \langle [y(0)]^2 \rangle$.
[14] This is not a close analogy: The potential applies to the single degree of freedom Y, not to the field $y(x)$, so that the usual "stiffness" term $\sim(\partial/\partial x)^2$ of Ginzburg-Landau theory is absent. The present $(\partial/\partial Y)^2$ term is a quantum mechanical operator usually absent in Ginzburg-Landau theory.
[15] M. M. J. Treacy, T. W. Ebbesen, and J. M. Gibson, Nature (London) **381**, 678 (1996).
[16] O. Lourie, D. M. Cox, and H. D. Wagner, Phys. Rev. Lett. **81**, 1638 (1998).
[17] Equilibration in this case consists of populating the fundamental with many phonons, while higher modes remain frozen. The precise mechanism and relaxation time for this are interesting open questions.
[18] Calculated using the generalized equipartition result that degrees of freedom appearing quartically in the Hamiltonian contribute $kT/4$ to the internal energy.