Quantum Effects in the Mechanical Properties of Suspended Nanomechanical Systems

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We explore the quantum aspects of an elastic bar supported at both ends and 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 Ginzburg-Landau order parameter, with strain playing the role of temperature. We calculate the quantum fluctuations about the classical value as a function of strain. Excitation energies and quantum fluctuation amplitudes are compared for silicon beams and carbon nanotubes.

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The continuing drive towards semiconductor device miniaturization and integration has resulted in fabrication and micromachining 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. The availability of these top-down and bottom-up nanofabrication capabilities has initiated the new area of nanomechanics [1, 2, 3, 4, 5] in which ultra small mechanical systems are used to explore both fundamental and applied phenomena. Recently, two reports have appeared on 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.

In this Letter we discuss 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 first observation of a coherent superposition of macroscopically distinct states was recently reported [8]. Specifically, we consider a suspended elastic bar under longitudinal compression. The compression is used to adjust the potential energy for transverse displacements from the harmonic to the double-well regime, as shown in Fig. 1, with strain playing a role analogous to temperature in a Ginzburg-Landau system. As the compressional strain is increased to the buckling instability [9], the frequency of the fundamental vibrational mode drops continuously to 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, including zero-point fluctuations, tunneling, and coherent superpositions of macroscopically distinct states. In the latter two cases, the system may provide a mechanical realization (at least in theory) of models studied in Refs. [10] and [11], respectively. We have applied the model to suspended silicon beams and carbon nanotubes, and show that in both cases the quantum fluctuations in position approach 0.1 Å; an order of magnitude greater than the relaxed values. We argue that compressing a carbon nanotube at low temperature may cause a crossover between the quantum and thermal fluctuation regimes. Further, we suggest that

![FIG. 1: Potential energy \( V \) as a function of the fundamental mode displacement \( Y \). The shape of the potential energy is harmonic for \( \varepsilon > \varepsilon_c \), quartic for \( \varepsilon = \varepsilon_c \equiv \text{critical strain} \) \((\varepsilon_c < 0)\), and a double-well for \( \varepsilon < \varepsilon_c \).](image-url)
tunneling in this mechanical system may be difficult to achieve because it will require precise regulation of the applied strain.

As a starting point, we consider the normal modes and associated quantum properties of an elastic rectangular bar of length \( l \), width \( w \) and thickness \( d \) satisfying \( l \gg w > d \), supported at both ends without strain. We suppose that \( d \) is smaller than \( w \) so that transverse displacements \( y(x, t) \) only occur in the “d” direction. The equation of motion for small displacements is [12]

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

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

The normal modes of the bar, \( y(x, t) = y_n(x) \exp(\pm i\omega_n t) \), have the general spatial dependences

\[
y_n(x) = a_n \cos k_n x + b_n \cosh k_n x, \quad n = 1, 3, 5, \ldots \tag{2}
y_n(x) = a_n \sin k_n x + b_n \sinh k_n x, \quad n = 2, 4, 6, \ldots \tag{3}
\]

with \( a_n/b_n \) and wavenumbers \( k_n \) fixed by the boundary conditions. The boundary conditions for hinged endpoints, \( y(\pm l/2) = 0 = y'(\pm l/2) \), lead to normal modes with \( b_n = 0 \), \( k_n = n\pi/l \), and (angular) frequencies

\[
\omega_n = \sqrt{Q/\rho} \kappa k_n^2 = \sqrt{Q/\rho} \kappa \left( \frac{n\pi}{l} \right)^2, \quad \text{(hinged b.c.)} \tag{4}
\]

Clamped endpoints have boundary conditions \( y(\pm l/2) = 0 = y'(\pm l/2) \); both \( a_n \) and \( b_n \) are nonzero, and the normal mode frequencies are given to good approximation by replacing \( n \) with \((n + \frac{1}{2})\) in Eq. (4). Because of their simplicity, we shall refer to hinged boundary conditions when specific results are quoted.

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

\[
\langle (y(0))^2 \rangle = \sum_{\text{odd } n} \frac{\hbar}{2m^* \omega_n} \left[ 1 + 2f(h\omega_n/kT) \right], \tag{5}
\]

where \( f(x) = 1/(e^x - 1) \) is the thermal excitation number of the \( n \)-th 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 moves the frequencies downward, with a corresponding increase in the zero-point motion. Compressive or tensile strain contributes the “elastic” potential energy \( V_c = (\mathcal{F}/2l_o)(l - l_o)^2 \), where \( l_c = \int dx \sqrt{1 + (y')^2} \approx l + \frac{1}{2} \int dx (y')^2 \) is the total (dynamic) length of the bar, \( l \) is the endpoint separation, and \( l_o \) is the unstressed equilibrium length. We subtract the static contribution \( (\mathcal{F}/2l_o)(l - l_o)^2 \) since it contributes nothing to the dynamics, and add the “bending” contribution \( V_b \sim \int dx (y')^2 \) to get

\[
V[y(x)] = \frac{1}{2} \int dx \left( \mathcal{F} \kappa^2 (y'')^2 + \mathcal{F} \varepsilon (y'')^2 \right) + \frac{\mathcal{F}}{8l_o} \left( \int dx (y')^2 \right)^2, \tag{6}
\]

where \( \varepsilon \equiv (l - l_o)/l_o \) is the strain, positive if tensile and negative if compressive. From the Lagrangian, \( L[y(x), t] = (\mu/2) \int dx (y'')^2 - V[y(x)] \), we find the equation of motion,

\[
\mu \ddot{y} + \mathcal{F} \kappa^2 y^{(4)} - \mathcal{F} \varepsilon y'' - \frac{1}{2} \mathcal{F} \left( \int dx (y')^2 \right) y'' = 0, \tag{7}
\]

which generalizes Eq. (4). The third term represents the tension induced by externally-imposed stretching, and the anharmonic fourth term is the enhancement of tension due to dynamic stretching; this term arises from the geometry of the system.

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

\[
\tilde{\omega}_n^2 = \omega_n^2 \left( 1 + \varepsilon \left( \frac{l - l_o}{l_o} \right)^2 \right), \tag{8}
\]

where \( \omega_n \) are the relaxed \((l = l_o)\) frequencies of Eq. (4). The zero-point fluctuations are given by Eq. (8) with \( \omega_n \) replaced by \( \tilde{\omega}_n \). Of course, the harmonic approximation breaks down for the fundamental mode as we approach its critical strain,

\[
\varepsilon_c \equiv \frac{l_c - l_o}{l_o} = - \left( \frac{\pi \kappa}{T} \right)^2. \tag{9}
\]

At critical strain, the effective potential for the fundamental mode is purely quartic (see Fig. 1) whereas the higher modes remain harmonic in leading order, with the first harmonic frequency being reduced by about 13% from its uncompressed value.

To go beyond the harmonic approximation and calculate the excitation energies and quantum fluctuations of the fundamental mode, we consider the Hamiltonian

\[
H = \frac{1}{2\mu} \int dx \Pi^2 + V[y(x)], \tag{10}
\]

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 with interactions arising from the anharmonic term. These interactions occur physically because 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 [3]. The quantum states and associated energy spectrum of fundamental vibrational states are then given by the Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial Y^2} + \frac{\alpha}{2} Y^2 + \frac{\beta}{4} Y^4\right) \Psi(Y) = E \Psi(Y)$$ \hspace{1cm} (11)

where $E_m$ and $\Psi_m(Y)$ are the energy eigenvalues and eigenfunctions, and $-i\hbar\partial/\partial Y = P$ is the momentum operator canonically conjugate to $Y$.

The potential energy has the form of a Ginzburg-Landau free energy [4], with strain playing the role of temperature:

$$\alpha = m^* \omega_1^2 = m^* \omega_1^2 \left(\frac{\varepsilon_c - \varepsilon}{\varepsilon_c}\right).$$ \hspace{1cm} (12)

The displacement $Y$ is analogous to the order parameter, in that its classical equilibrium value vanishes below critical strain but takes a nonzero value $Y \to \pm Y_{\text{min}} = \pm \sqrt{|\alpha|/\beta}$ above it, 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, $Y_{\text{min}}$ or $-Y_{\text{min}}$, not both. With this in mind, we plot the ground and first excited state energies in Fig. 2 and in Fig. 3 the ground state quantum fluctuations $\Delta Y$, as functions of the strain near its critical value. These are plotted in dimensionless energy and length units, $E/E_c$ and $\Delta Y/\Delta Y_c$, where $E_c$ and $\Delta Y_c$ are the ground state values at critical strain,

$$E_c = 0.42 \left(\frac{\hbar^2}{m^*}\right)^{2/3} \beta^{1/3} \quad \text{and} \quad \Delta Y_c = 0.68 \left(\frac{\hbar^2}{m^*\beta}\right)^{1/6},$$ \hspace{1cm} (13)

and $\gamma$ is the departure from critical strain,

$$\gamma = \frac{\varepsilon_c - \varepsilon}{\varepsilon_c} \left(1.68 \Delta Y_c\right)^2,$$ \hspace{1cm} (14)

scaled so that $\gamma = -1$ when the barrier height $V_0 = \alpha^2/4\beta$ is equal to $E_1$. In defining $\Delta Y$, care should be taken to account for the onset of a nonzero mean displacement as one moves into the double well regime. In the subcritical and near-critical regimes, the usual definition $\Delta Y^2 = \langle Y^2 \rangle - \langle Y \rangle^2$ surely applies, where brackets indicate ground state expectation values and $\langle Y \rangle = 0$. However, the comments above suggest that deeper in the double well regime, a more sensible practical definition is $\Delta Y^2 = \langle \text{min}(Y \pm Y_{\text{min}})^2 \rangle$, the $rms$ departure from the nearest potential minimum. Fig. 3 shows that quantum fluctuations defined in this way become much less than the well separation at fairly modest (negative) values of $\gamma$. In the region $\gamma \sim -1$, the latter definition of $\Delta Y^2$ loses its physical meaning and larger fluctuations may

FIG. 2: Ground and first excited state energies, $E_1$ and $E_2$, of the fundamental vibrational mode as functions of the departure from critical strain $\gamma$. The dotted curve shows the barrier height dependence on $\gamma$. 

FIG. 3: Curve A is the ground state fluctuation $\Delta Y$, calculated using the full quartic potential. The solid portions of the curve are obtained from the calculations; the dot-dash region is a guide to the eye. For comparison, curve B shows $\Delta Y$ obtained in the harmonic approximation. The dotted curve shows the position of the potential minimum, $Y_{\text{min}}$. 
be expected, as suggested by the dot-dash line on Fig. 3 which is only a guide to the eye.

A useful perspective is provided by comparing the exact quantum fluctuations with those given by the harmonic approximation. Indeed, making this approximation in the double well regime requires that one of the wells is ignored while fluctuations are defined about the minimum of the other, which clearly will become invalid as $\Delta Y$ approaches $Y_{\text{min}}$ in the near-critical regime. As shown in Fig. 3, this approximation predicts that the fluctuation $\Delta Y$ diverges as $|\varepsilon - \varepsilon_c|^{-1/4}$. It is nonetheless a very good approximation outside a small region around 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 $\Delta Y$ for rectangular silicon bars and cylindrical multiwalled carbon nanotubes. Numbers are given for two cases - the critical and the relaxed (uncompressed) states. The remaining Schrödinger equation parameters are calculated using hinged boundary conditions, with the results

$$m^* = m/2 \quad \text{and} \quad \beta = m^* (\omega_1/2\kappa)^2.$$  \hspace{1cm} (15)

The larger tubes have dimensions typical of the multiwalled tubes whose vibrational properties were studied by Treacy et al. \footnote{13}. The smaller tube is probably the smallest that would support buckling and retain its elastic integrity \footnote{16}. Nanotube frequencies were found using Eq. (4) with $\kappa = (d_2^2 + d_1^2)/16$, where $d_1$ and $d_2$ are inner and outer diameters. In the critical and double well regimes, because of cylindrical symmetry, the nanotube states will be described by a Mexican hat potential rather than a double well. In this case, Eq. (11) still applies, with $Y$ replaced by a two-component vector. In order to make a comparison to silicon bars, the nanotube entries in Table I refer to a single Cartesian component of $Y$. Fig. 3 refers specifically to one-dimensional transverse motion; the Mexican hat potential would have its main effect in the negative $\gamma$ regime where the first excitation energy $E_2 - E_1$ would fall less rapidly because the excitations are rotational rather than tunneling in nature.

For all systems shown, the zero-point fluctuations predicted in the relaxed states are enhanced by nearly an order of magnitude by applying critical compression. On the other hand, the excitation energies are all reduced by about two orders of magnitude, so that thermal fluctuations can swamp the quantum contributions. On the other hand, the large differences between the relaxed and compressed energy scales suggests that the relaxed 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 6 (see Table I). Subsequent equilibration to 500 mK would then bring the tube to a “classical” equilibrium state with thermal fluctuation $\Delta Y_t \approx 0.25 \AA$ \footnote{17}, a further factor of 5 enhancement.

Finally, we comment on the possibility of observing tunneling in nanomechanical systems such as those considered here. We can roughly estimate the number of bound states with energy below the top of the barrier; it is of the order of the barrier height $V_o$ divided by the level spacing $h\omega_1$. From Eqs. (4) \footnote{12} and (3) we find

$$N \sim \left( \frac{\kappa}{\Delta Y_o} \right)^2 \left( \frac{\varepsilon_c - \varepsilon}{\varepsilon_c} \right)^{3/2}.$$  \hspace{1cm} (16)

Taking the smaller bar, if we go to twice the critical com-
pression, $\varepsilon = 2\varepsilon_c$, 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 likely be very challenging, the prospect of exploring tunable quantum fluctuations in this system, and the connection to Ginzburg-Landau theory, are intriguing.

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