Macroscopic quantum effects in nanomechanical systems

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Abstract. – We investigate quantum effects in the mechanical properties of elastic beams on the nanoscale. Transverse quantum and thermal fluctuations and the nonlinear excitation energies are calculated for beams compressed in longitudinal direction. Near the Euler instability, the system is described by a one dimensional Ginzburg-Landau model where the order parameter is the amplitude of the buckling mode. We show that in single wall carbon nanotubes with lengths of order or smaller than 100 nm zero point fluctuations are accessible and discuss the possibility of observing macroscopic quantum coherence in nanobeams near the critical strain.

Introduction. – The progress in miniaturization of electromechanical devices towards the nanometer scale (NEMS) is beginning to reach the limit, where quantum effects play an important role. For example, in nanoscale beams phonons may propagate ballistically, leading to a quantized thermal conductance. Moreover a sizeable contribution to the forces between plates and beams which are separated by less than one micron is the Casimir force between neutral objects due to the modification of the electromagnetic vacuum. The combination of electrical and mechanical properties may be studied via quantized transverse deflection due to charge quantization of charged, suspended beams in an electric field. Similarly the standard Coulomb-blockade in small metallic islands or in semiconducting quantum dots may be used to mechanically transfer single electrons with a nanomechanical oscillator. Regarding possible applications of nanomechanical sensors, Si-based resonators in the radio-frequency regime were recently fabricated and manipulated. In the present work we focus on quantum effects in mechanical resonators on the nanometer scale, in particular in single wall carbon nanotubes (SWNT). Due to their small masses and remarkable elastic properties down to nanometer scale, carbon nanotubes are ideally suited to study effects like phonon quantization, the generation of non-classical states of mechanical motion or macroscopic quantum tunnelling out of a metastable configuration. On the classical level, both the thermal Brownian motion of single nanotubes clamped on one side and the discrete eigenmodes of charged multiwall nanotubes excited by an ac-voltage have been detected experimentally. More recently, the thermal vibrations of doubly clamped SWNT’s
down to lengths of around 0.5μm have been observed with a scanning electron microscope \[16\]. In all of these cases it turns out that the measured transverse vibrations of nanotubes agree reasonably well with the predictions of an elastic continuum model. Its applicability even on the nm scale is also supported by molecular dynamics simulations which show that SWNT’s down to lengths of around 10nm are well described by an effective elastic continuum, responding in a reversible manner up to large deformations \[17\]. In the following, we will therefore use the standard theory of an elastic continuum \[18\] for carbon nanotubes which are clamped between two fixed end points. We calculate both thermal and quantum fluctuations of the nanotube under longitudinal compression, including properly the nonlinearity in the bending energy. It is shown that in SWNT’s with a length below 100nm the crossover from thermal to quantum zero point fluctuations is reached at accessible temperatures of around 30mK. We also discuss the possibility to realize coherent superpositions of macroscopically distinct states by observing the avoided level crossing near the degenerate situation above the critical force of the well known Euler-buckling instability.

**The Model.** – Our model system is a freely suspended SWNT of length \(L\) and diameter \(D\) which is fixed at both ends, allowing only transverse vibrations. In addition we consider a mechanical force \(F\) which acts on the beam in longitudinal direction \(\quad (F > 0 \text{ for compression})\). In a classical description the beam is then completely described by the transverse deflection \(\phi(s)\) parametrized by the arclength \(s \in [0, L]\). We assume the beam to be incompressible in longitudinal direction and only keep a single transverse degree of freedom for simplicity (see below). For arbitrary strong deflections \(\phi(s)\) the nonlinear Lagrangian of the system is then \[19\]

\[
L = \int_0^L ds \left[ \frac{\sigma}{2} \dot{\phi}^2 - \frac{\mu}{2} \left( \phi'' \right)^2 - \frac{\sigma}{2} \left( \phi' \right)^2 \right] - \frac{F}{2} \sqrt{1 - \left( \phi' \right)^2}.
\]

(1)

Here \(\sigma = m/L\) is the mass density, while the bending rigidity \(\mu = EI\) is the product of the elasticity modulus \(E\) and the moment of inertia \(I = \pi D^3 d/8\), with \(d\) an effective wall thickness. For small deformations \(|\phi'(s)| \ll 1\) the Lagrangian is quadratic, leading to the standard linear equation of motion

\[
\sigma \ddot{\phi} + \mu \phi''' + F \phi'' = 0
\]

(2)

for the transverse vibrations of an elastic beam under compression. The corresponding eigenmodes \(\phi_n\) and eigenfrequencies \(\omega_n\) depend on the boundary conditions. We assume that the experimental realization \[16\] is well described by clamped ends at both sides, \(\phi(0) = \phi(L) = 0\) and \(\phi'(0) = \phi'(L) = 0\). The exact \(\phi_n\)'s are then given by a superposition of trigonometric and hyperbolic functions, and the \(\omega_n\)'s by solving a transcendental equation \[18\]. In the following, for some of the analytic expressions, we will use boundary conditions without bending moments at the ends of the beam, \(\phi'(0) = \phi'(L) = 0\). This leaves the essential physics unchanged and permits one to write down simple expressions for the eigenfunctions in the normal mode expansion

\[
\phi(s) = \sum_n A_n \sin \frac{n \pi}{L} s
\]

(3)

and its eigenfrequencies

\[
\omega_n = \left( \frac{\mu (n \pi / L)^2 - F}{\sigma} \right)^{\frac{1}{2}} \frac{n \pi}{L}.
\]

(4)

Clearly the modes soften with increasing compression \(F\), up to a critical force \(F_c = \mu (\pi / L)^2\) where the fundamental frequency \(\omega_{n=1}(F)\) vanishes. Then the system reaches a bifurcation point, the well known Euler instability, beyond which \(\phi_1 \sim \sin (\pi s / L)\) becomes the new stable
solution of the static problem. For clamped boundary conditions with finite bending moments at \( s = 0, L \) the critical force is four times larger, and the shape of the stable solution in the static problem for \( F > F_c \) has the form \( \sin^2 \left( \frac{\pi s}{L} \right) \). Near criticality, the frequencies of higher modes \( n = 2, 3, \ldots \) remain finite. The dynamics at low frequencies is thus determined by the fundamental mode alone. The nonlinear field theory eq. (1) may be quantized in the standard manner by requiring canonical commutation relations 
\[
[\hat{\phi}(s, t), \hat{\Pi}(s', t)] = i\hbar \delta(s - s')
\]
between the field \( \phi \) and its canonically conjugate momentum \( \Pi = \sigma \dot{\phi} \) at equal times. In the linear regime, the problem is reduced to an infinite number of harmonic oscillators. Introducing oscillator lengths \( l_k^2 = \hbar / (m_k \omega_k) \) with \( k = n\pi/L \) and \( n = 1, 2, \ldots \), the amplitudes
\[
A_k = \frac{l_k}{\sqrt{2}} (a_k^\dagger + a_k)
\]
are expressed by the standard creation and annihilation operators \( a_k^\dagger \) and \( a_k \). The effective masses \( m_k \) arising in \( l_k \) turn out to be \( m_{\text{eff}} \simeq 3/8 \) of the beam mass for the fundamental mode but are generally mode dependent for clamped boundary conditions.

**Thermal vibrations.** – In the linearized theory, the mean square displacement of the beam is trivially calculated from the normal mode expansion eq. (3). Assuming a thermal occupation of the discrete phonon modes one obtains a maximum value at the center of the beam, which for unclamped boundary conditions reads
\[
\sigma^2 = \langle \phi^2(L/2) \rangle = \frac{l_0^2}{2} \sum_{n \text{ odd}} \frac{1}{n\sqrt{n^2 - 1 + \delta}} \coth \left( \frac{T_0}{2T} n\sqrt{n^2 - 1 + \delta} \right).
\]
Here the scale is set by the oscillator length \( l_0 = (\hbar/m_{\text{eff}} \omega_0)^{\frac{1}{2}} \) and the temperature \( T_0 = \hbar \omega_0/k_B \) is associated with the frequency scale of the fundamental mode \( \omega_0 = \omega_1(F \to F_c) \delta^{-\frac{1}{2}} \simeq 1.02 \omega_1(F = 0) \). The parameter \( \delta = (F_c - F)/F_c \) determines the dimensionless distance from the critical compression force. At temperatures larger than \( T_0 \) one obtains the usual equipartition theorem result, where \( \sigma^2 \sim T/\omega_0^2 \) increases linearly with \( T \) as observed on sufficiently long nanotubes [14, 16]. For low temperatures the mean square displacement remains finite due to zero point fluctuations. As shown in Fig. 1 the crossover to this regime occurs at \( T^* \simeq 0.4T_0 \) in the absence of an external force \( \delta = 1 \), giving accessible temperatures.

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**Fig. 1** – Mean square displacement at the center of a clamped beam in linearized theory for the free (\( \delta = 1 \)) and compressed (\( \delta = 1/4 \)) case. The dotted lines show the classical behaviour if one considers only the leading contribution of the first mode, the dashed-dotted line indicates the increasing zero point fluctuations versus decreasing crossover-temperature, \( \{\sigma^2(\delta, T \to 0), T^*(\delta)\} \), for compression approaching the critical force.
of around 30mK for typical SWNT's (see Table I). Unfortunately, the associated transverse deflection amplitude \( l_0 \) is only of order \( 10^{-2} \)nm and thus beyond accessibility of standard displacement detection techniques. There are a number of ways, however, to measure such tiny amplitudes, for instance by capacitively coupling the beam to the gate of a single electron transistor [20] or using its electrostatic interaction with a free-standing quantum dot [21]. Of course the fluctuations are strongly enhanced near the critical force \( F_c \), where only the fundamental mode \( n = 1 \) contributes and thus \( \sigma^2(T = 0) \) increases like \( l_0^2 / \sqrt{\delta} \). In this case, the problem of measuring the thermal to quantum crossover is somehow inverted, since now the decreasing crossover temperature \( T^*(\delta) \sim T_0 \sqrt{\delta} \) poses a limiting factor for an observation.

Moreover the divergence in eq.(6) for \( \delta \to 0 \) marks the breakdown of the linearized theory.

To explore the quantitative enhancement of the fluctuations and the change of the relevant length and energy scales near criticality, one has to include the nonlinear terms in the bending energy eq.(1).

**Buckling instability.**  
In order to describe the behaviour near the buckling instability, we insert the Fourier expansion eq.(3) into the corresponding nonlinear Hamiltonian. Keeping only the fundamental mode, since all higher modes have no influence near criticality due to their nonvanishing frequencies, the interacting field theory is reduced to a one particle problem in terms of the coordinate \( A_1 \), and its canonically conjugate momentum \( \mathcal{P} \equiv -\hbar \partial / \partial A_1 \).

The force term generates a negative contribution to the quartic term in \( A_1 \), driving the system unstable. The nonlinearity in the curvature term, however, over-compensates this and guarantees stability even for fixed length of the beam [19]. For clamped boundary conditions one can use the approximate shape \( \sin^2(\pi s/L) \) which becomes exact near \( \delta \to 0 \). One ends up with a quantum mechanical one particle Hamiltonian with an anharmonic oscillator potential

\[
H = \hbar^2 \left( -\frac{1}{2} \nabla^2 + \frac{1}{2} \frac{\delta}{\bar{\delta}} y^2 + \frac{1}{4} y^4 \right),
\]

and an anharmonic coefficient \( b_4 = (\pi/L)^4 F_c L \). A similar effective description of quantum effects near the buckling instability has been derived in [22]. The nonlinearity there, however, arises from longitudinal stretching while we keep the length of the nanotube fixed. It is now convenient to define a dimensionless coordinate \( y \) by \( A_1 = \bar{l} y \), where \( \bar{l} = \bar{l}_0 (2\pi)^{1/6} (L/l_0)^{1/3} \) is the characteristic magnitude of the deflection, where the quartic term due to the nonlinear bending energy is of the same order than the kinetic energy. The Hamiltonian is thus transformed to a dimensionless form

\[
\bar{H} = \hbar \bar{\omega} \left( -\frac{1}{2} \nabla^2 + \frac{1}{2} \frac{\delta}{\bar{\delta}} \bar{y}^2 + \frac{1}{4} \bar{y}^4 \right),
\]

with \( \bar{\omega} = \hbar / (m_{\text{eff}} \bar{l}^2) \) as the characteristic frequency scale near the critical compression force \( F_c \). It differs from the fundamental frequency \( \omega_0 \) of the classical transverse vibrations by a factor

\[
\frac{\bar{\omega}}{\omega_0} = (2\pi)^{1/3} \left( \frac{l_0}{L} \right)^{2/3} \sqrt{\bar{\delta}} \equiv \sqrt{\bar{\delta}}
\]

which also determines the size \( \bar{\delta} \) of the critical regime. For SWNTs with length \( L = 0.1\mu m \), \( \bar{\delta}^{1/2} \) is of order or smaller than \( 10^{-2} \) (see Table I). The potential energy in eq.(1) exhibits the standard Landau bifurcation from a single to a double well as the external force is increased through its critical value \( F_c \). Indeed our zero dimensional quantum problem is equivalent to a one dimensional classical Ginzburg Landau theory [23]. Let us consider first the mean square displacement at the center of the beam. In the harmonic approximation this diverges
as \( F \) approaches the critical value from below. For \( F \) much larger than \( F_c \) it is simply determined by the stable minimum of the effective Landau energy at \( y_{\text{min}} = \pm \left( \delta / \bar{\delta} \right)^{1/2} \) giving \( \sigma^2 = \bar{l}^2 |\delta| / \bar{\delta} \). As shown in Fig. 2, the exact result smoothly interpolates between those two limits giving a finite value \( \sigma(F_c) = 0 \) at \( F_c \), which is of order 0.1nm for typical SWNT’s (see Table I). A similar behaviour is found for the lowest excitation frequency of the beam. In the harmonic approximation it vanishes like \( \omega_1(F) = \bar{\omega} \cdot \left( \delta / \bar{\delta} \right)^{1/2} \). Above the critical force the lowest excitation is the small oscillation in one of the degenerate minima of the anharmonic oscillator. This is true, however, only in a classical description. Quantum mechanically, the lowest excitation is the exponentially small tunnelsplitting \( \Delta \) which lifts the degeneracy between the two states localized in the left or right well of the effective potential. Again, the exact numerical result for \( \omega = (E_1 - E_0) / \hbar \) starts to deviate from the harmonic expression at around \( \delta \approx 5 \bar{\delta} \) and approaches a finite excitation frequency \( \omega = 1.1 \bar{\omega} \) at \( F_c \) (see Fig. 3). For \( \delta < -3 \bar{\delta} \) it vanishes exponentially in good agreement with the WKB result eq. (10) for the tunnelsplitting \( \Delta \). It is remarkable that the excitation frequency precisely at \( F_c \), which is of order \( 2 \pi \cdot 0.01 \text{GHz} \) for the parameters of Table I is no longer related to the characteristic frequency \( \omega_0 \) of the classical problem but scales like \( \omega = \omega_0 (4 \hbar \omega_0 / F_c L)^{1/3} \), remaining finite only through a genuine quantum effect. Unfortunately, the smallness of the size \( \delta \approx 10^{-4} \) of the critical regime requires fine tuning the compression force \( F \) very close \( (\delta \approx \bar{\delta}) \) to its critical value in order to see deviations from classical behaviour near the buckling instability.

**Macroscopic Quantum Coherence (MQC).** In the regime beyond the critical buckling force, the state of lowest energy corresponds to a stationary finite deflection amplitude \( y_{\text{min}} = \pm \left( |\delta| / \bar{\delta} \right)^{1/2} \) which is lower in energy by \( \hbar \omega (\delta / \bar{\delta})^2 / 4 \) than the configuration with no deflection. The direction in which the buckling occurs is arbitrary, however, in a realistic setup like that in ref. [10] the boundary conditions in the buckled state are likely to break the perfect rotation symmetry assumed in [21]. In this situation, the transverse deflection is described by a single degree of freedom with only two degenerate states. Quantum mechanically, these states are split into a narrow doublet with energy separation \( \hbar \Delta \) due to tunnelling. Sufficiently far above
the critical force its magnitude may be determined from a WKB-calculation in the anharmonic oscillator potential, giving

\[
\Delta = \frac{\bar{\omega}}{2} \left( \frac{\delta}{\bar{\delta}} \right)^\frac{3}{2} \exp \left[ -B \left( \frac{\delta}{\bar{\delta}} \right)^\frac{2}{3} \right].
\]

(10)

with \( A = 3.8 \) and \( B = 0.94 \). Note that the validity of the WKB approximation is limited to \( \delta/\bar{\delta} < -2 \), above which the zero point energy of a harmonic approximation in one of the energy minima reaches the barrier height. In practice the perfectly degenerate situation is hardly achieved, introducing some bias energy \( \varepsilon \) which singles out a preferred ground state in which the beam is bent either to the left or right. We have thus an effective two state system with Hamiltonian

\[
\hat{H} = -\frac{\hbar}{2} \hat{\Delta} - \frac{\varepsilon}{2} \hat{\sigma}_z - \frac{\dot{\varepsilon}}{2} \hat{\dot{\sigma}}_z.
\]

(11)

and eigenenergies separated by \( \sqrt{(\hbar \Delta)^2 + \varepsilon^2} \). \( (\hat{\Delta}, \hat{\sigma}_x, \hat{\sigma}_y) \) are the Pauli spin matrices. In the absence of any asymmetry \( \varepsilon \) its eigenstates are coherent superpositions \( |L\rangle \pm |R\rangle \) of the \( \hat{\sigma}_z \) eigenstates \( |L\rangle \) and \( |R\rangle \), in which the nanotube is bent towards the left or right. The two states \( |L\rangle \) or \( |R\rangle \) are clearly macroscopically distinct [29]. Similar to experiments on flux qubits in SQUID rings [27, 28], the existence of linear superpositions of these states may indirectly be verified by observing the avoided level crossing at \( \varepsilon = 0 \). Such a macroscopic quantum coherence experiment with SWNT’s requires that the small level splitting \( \Delta \) can be detected against noise and damping in a mechanical resonance experiment and moreover, that the asymmetry \( \varepsilon \) can be tuned through zero from any accidental nonzero value by external means. As shown in [15], spectroscopy of the transverse vibrations of nanotubes is in principle possible by applying dc- plus ac-voltages on a charged nanotube. Moreover with a capacitive coupling the bias energy \( \varepsilon \) may be changed via an appropriate electrostatic gate potential. Due to the still large mass involved, the tunnel splitting is rather small (around \( \Delta = 2\pi \cdot 1 \text{MHz} \) for \( \delta/\bar{\delta} = -3 \)), and thus coherent superpositions with an accessible value of \( \Delta \) require nanotubes close to the buckling instability. Regarding the influence of damping effects, it is known [29] that the dynamics of a two-level system subject to an ohmic dissipation mechanism is determined by the size of the parameter \( \alpha = \eta q_0^2 / (2\pi \hbar) \). Here \( q_0 = 2y_{\text{min}} \) is the distance between the two minima and \( \eta \) the phenomenological damping parameter which appears in the equation of motion

\[
m_{\text{eff}} \ddot{A}_1 + \eta \dot{A}_1 + \frac{\partial}{\partial A_1} V(A_1) = 0.
\]

(12)

Coherence in the two level system is present only for \( \alpha < \frac{1}{2} \) at \( T = 0 \) and \( k_B T < \hbar \Delta / \alpha \) for finite temperature and very small \( \alpha \). This requires that the quality factor of the SWNT in the uncompressed case (which is related to \( \eta \) by \( Q = m_{\text{eff}} \omega_0 / \eta \)) obeys \( Q > 4|\delta| / (\pi \delta^{3/2}) \). For the above value of \( \delta \), this leads to \( Q > 220 \) in the relevant regime \( |\delta| \approx \bar{\delta} \). This condition does not seem too stringent for SWNTs, note that a quality factor of \( Q = 500 \) has been reached for Si-based resonators in the GHz regime [20].
Conclusions. – We have discussed quantum effects in the mechanical properties of single wall carbon nanotubes, in particular zero point fluctuations in the transverse vibrations and the possibility to see the analog of MQC in nanobeams below the Euler buckling instability. While thermal vibrations of clamped SWNT’s down to lengths $L = 0.5 \mu m$ have indeed been observed very recently \[16\], it remains a considerable challenge to measure the tiny zero point vibrations of order 0.1 nm predicted for SWNTs of length $L = 0.1 \mu m$ near the buckling instability. With the sensitivity attained very recently with Si-based resonators \[20\], however, reaching this goal in the near future seems to be quite realistic. As regards the possibility to see the analogue of MQC near or below the Euler buckling instability, this requires to tune these systems rather closely below the instability point and doing spectroscopy with both dc- and ac-driving. Provided the methods used for multivall nanotubes with lengths of several $\mu m$ \[15\] can be scaled down to clamped single wall nanotubes, quantum mechanics in its literal meaning would finally be of relevance in truly mechanical devices.

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REFERENCES

[1] Roukes M., *Physics World*, 14 (2001) 25.
[2] Craighead H. G., *Science*, 290 (2000) 1532.
[3] Cleland A. N., *Foundations of Nanomechanics* (Springer) 2003.
[4] Schwab K. *et al*, *Nature*, 404 (2000) 974.
[5] Chan H. B. *et al*, *Science*, 291 (2001) 1941.
[6] Buki E., Roukes M. L., *Phys. Rev. B*, 63 (2001) 033402.
[7] Sapmaz S. *et al*, *Phys. Rev. B*, 67 (2003) 235414.
[8] Erbe A. *et al*, *Phys. Rev. Lett.*, 87 (2001) 096106.
[9] Shekhter R. I. *et al*, *J. Phys. Cond. Matt.*, 15 (2003) 441.
[10] Pescini L., Lorenz H. and Blick R. H., *Appl. Phys. Lett.*, 82 (2003) 352.
[11] Roukes M., *Physica B*, 263-264 (1999) 1.
[12] Wilson-Rae I. Zoller P. and Imamoğlu A., *cond-mat*, 03066724 (2003) 1.
[13] Buki E., Roukes M. L., *Europhys. Lett.*, 54 (2001) 220.
[14] Treacy M. M. J., Ebbesen T. W. and Gibson J. M., *Nature*, 381 (1996) 678.
[15] Poncharal P. *et al*, *Science*, 283 (1999) 1513.
[16] Babić B. *et al*, *cond.mat*, 0307252 (2003) 1.
[17] Yakobson B. I., Braic B. J. and Bernholc J., *Phys. Rev. Lett.*, 76 (1996) 2511.
[18] Landau L. D. and Lifshitz E. M., *Theory of Elasticity* (Pergamon Press) 1959.
[19] Poston T. and Stewart I., *Catastrophe Theory and its Applications* (Pitman) 1978
[20] Knoebel R. G. and Cleland A. N., *Nature*, 424 (2003) 291.
[21] Kirschbaum J. *et al*, *Appl. Phys. Lett.*, 81 (2002) 280.
[22] Carr S. M., Lawrence W. E. and Wybourne M. N., *Phys. Rev. B*, 64 (2001) 220101.
[23] Scalapino D. J., Sears M. and Ferrell R. A., *Phys. Rev. B*, 6 (1972) 3409.
[24] Lawrence W.E., *Physica B*, 316 (2002) 448.
[25] Weiss U., *Quantum Dissipative Systems* (World Scientific) 1993.
[26] Leggett A. J., *J. Phys.: Cond. Mat.*, 14 (2002) R415.
[27] van der Wal C. H. *et al*, *Science*, 290 (2000) 773.
[28] Friedman J. R. *et al*, *Nature*, 406 (2000) 43.
[29] Leggett A. J. *et al*, *Rev. Mod. Phys*, 59 (1987) 1.