I. INTRODUCTION

Nanoelectromechanical systems (NEMS) convert electrical current into mechanical motion on a nanoscale and vice versa. These systems can be viewed as the successors of microelectromechanical devices (MEMS), which operate at a micron scale and are found in commercial applications. An improved performance is expected from NEM devices due to their small sizes, and higher eigenfrequencies. M(N)EMS have already been used for high-precision measurements of force, electric charge, the thermal conductance quantum, and the Casimir force. From a fundamental point of view, nanotubes have been previously fabricated, and their properties have been measured. We consider a single-wall nanotube, we obtain

II. DISPLACEMENT, STRESS, AND ENERGY

A. Equilibrium position

We consider a SWNT (modeled as a rod of length $L$ along the $x$ axis), freely suspended between source and drain electrodes, in the vicinity of a gate (see Fig. 1). The nanotube is attached to the electrodes via tunneling contacts. An electrostatic force (gate voltage) bends the tube; the deviation from a straight line is denoted by $\zeta(x)$ with $0 < x < L$. The elastic energy of the bent tube is

$$W_\sigma[\zeta(x)] = \int_0^L dx \left\{ \frac{EI}{2} \zeta'^2 + \frac{T_0}{2} \zeta'^2 + ES \int_0^L \zeta'^2 dx \right\},$$

where $E$, $I = \pi r^4/4$, and $S = \pi r^2$ are the elastic modulus, the inertia moment, and the cross section, respectively. Here, $r$ is the (external) radius of the tube. The first term in Eq. (1) is the energy of an unstressed bent rod; other two terms describe the effect of the stress force $T = T_0 + T$. Here, $T_0$ is the residual stress which may result, e.g., from the fabrication, and the induced stress $T$ is due to the elongation of the tube caused by the gate voltage,

$$T = \frac{ES}{2L} \int_0^L \zeta'^2 dx.$$

To write down the electrostatic energy, we denote the capacitances of the barriers connecting the nanotube with the source and drain as $C_L$ and $C_R$, respectively (see Fig. 1). The capacitance to the gate per unit length is $c(z)$. Approximating the gate by an infinite plane at a distance $R$ from the nanotube, we obtain
where the Taylor expansion restricts validity to $z \ll R$. In this limit, van der Waals forces between the nanotube and the substrate can be neglected. The electrostatic energy of the system reads

$$W_{es}[z(x)] = \frac{(ne)^2 - 2ne(C_LV + C_GV_G)}{2(C_L+C_R+C_G)} - \frac{C_L(C_R+C_G)V^2}{2(C_L+C_R+C_G)} - 2C_LC_GV^2,$$

Substituting this into Eq. (2), a relation between the stress $T$ and the external force $K_0$ is obtained. In the limiting cases, it reads

$$T = \begin{cases} K_0^2L^6S/(60480E^2), & T \ll EI/L^2 \\ (ES/24)^{1/3}(K_0L)^{2/3}, & T \gg EI/L^2 \end{cases},$$

The first line corresponds to weak bending of the tube. The energy associated with the bending exceeds the energy of the stress. Generally, it is realized for $z \ll r$. The second line describes strong bending, when the tube displacement is large ($r < z \ll R, L$).

For the displacement of the tube center $z_n^{max} = z_n(L/2)$, we find

$$z_n^{max} = 0.003 \frac{(ne)^2L^2}{Er^4R}, \quad T \ll E^3/L^2 \quad \left(n \ll \frac{Er^5R}{e^2L^2}\right)$$

$$z_n^{max} = 0.24 \frac{(ne)^{2/3}L^{2/3}}{E^{1/3}r^{2/3}R^{1/3}}, \quad T \gg E^3/L^2 \quad \left(n \gg \frac{Er^5R}{e^2L^2}\right).$$

For a SWNT with $r = 0.65$ nm, $E = 1.25$ TPa, $L = 500$ nm, and $R = 100$ nm (to be referred to as the $E$ nanotube), the crossover from weak to strong bending, $T \sim E^3/L^2$, occurs already at $n \sim 5 - 10$. In the strong-bending regime, the displacement of the $E$ nanotube is (in nanometers) $z_n^{max} = 0.24n^{2/3}$. Note that this regime is not accessible with state-of-the-art silicon submicron devices, which are always in the weak-bending limit.

### B. Charge and energy

For comparison with experiments, we have to relate the charge $ne$ to the gate voltage by minimizing the energy. The expression for the energy (elastic plus electrostatic) of the tube at equilibrium in the limiting cases reads

$$W_n[z(x)] = W_{el}[z(x)] + W_{es}[z(x)],$$

with respect to $z$, one finds the equation determining the tube position,

$$IEz'' - Tz'' = K_0 = \frac{(ne)^2}{L^2R^2},$$

where $K_0$ is the electrostatic force per unit length, which we approximate by a constant. Higher-order terms are small for $z \ll R$. To solve Eq. (6), we have to assume that the stress force $T$ is constant, and find it later from the self-consistent condition [Eq. (2)].
The first two terms represent the electrostatic energy of a straight tube, and the third one is due to the elastic degrees of freedom of the nanotube. The negative sign of the nanomechanical contribution is easily understood. As the gate voltage changes, the movable tube adjusts not only its charge but also its position, which leads to a lower energy as compared to the fixed-position system.

The value of \( n \) which minimizes the energy is

\[
W_n = W_{\text{eq}} - \delta W = \frac{(ne)^2}{2} \ln \left( \frac{r}{r_0} \right) - neV_G - \left\{ \begin{aligned}
0.0009 & (ne)^4 L / (E r^4 R^2), \quad T \ll E/L^2 \\
0.08 & (ne)^{1/3} / (E r^2 R L)^{1/3}, \quad T \gg E/L^2.
\end{aligned} \right.
\]

The two limiting cases represent the electrostatic energy of a straight tube, and the third one is due to the elastic degrees of freedom, stress, bending, and change of \( C_G \) due to displacement. This nonlinear, nanomechanical term is typically a small correction. For the \( E \) nanotube, it becomes of the same order as \( W_{\text{el}} \) if \( n \sim 3000 \) in which case Eq. (3) is not valid anymore.

The variance of the position of the tube center at a given gate voltage is

\[
\var Z_n = \left\{ \begin{aligned}
e^{\frac{2}{3} \left( -W_n + (2 \ln 2 - 1) V_G \right)} & , \quad n \neq 0 \\
e^{-1} & , \quad n = 0
\end{aligned} \right.
\]

where \( \Theta \) is the temperature. Except for \( n = 0 \), the functional integral in Eq. (11) is no Gaussian and has to be linearized around the equilibrium solution \( z_n(x) \), Eq. (7). The remaining Gaussian integral can be calculated, and we arrive at

\[
\var Z_n = k_B \Theta z_n(x) / 2 L
\]

In the two limiting cases of weak and strong bendings, the solution of Eq. (13) yields

\[
\var Z_n = \left\{ \begin{aligned}
k_B \Theta ^{1/2} / (2 L) & , \quad n \neq 0 \\
& , \quad n = 0
\end{aligned} \right.
\]

where the stress \( T \) is still given by the lower line of Eq. (8). Thus, the fluctuations in the tube position are expected to grow linearly with temperature. However, their magnitude is small. For the \( E \) nanotube, at 100 K the fluctuations in the \( n = 0 \) state are of the order of 0.1 nm, and at least an order of magnitude less in the strong-bending regime.

In the calculations, we have assumed that the charge \( ne \) is a fixed quantity. Close to the degeneracy points \( W_n^{eq} = W_n^{eq-1} \), thermal fluctuations may induce switching between the states with charges \( ne \) and \( (n + 1)e \), in this case Eq. (14) is no longer valid. However, the range of voltages, where switching is important, is narrow.

III. COULOMB EFFECTS AND BISTABILITY

A. Coulomb blockade

Since the nanotube is attached to the electrodes by tunneling contacts, it is in the Coulomb-blockade regime. We define the energy to add the \( n \)th electron to the tube as \( S_n = W_n - W_{n-1} \). Then, if the nanotube contains \( n > 0 \) electrons, the conditions that current cannot flow is Coulomb blocked are \( S_n < 0, \quad eV < S_{n+1} \). In quantum dots, \( S_n \) depends linearly on the bias \( V \) and gate \( V_G \) voltages. Thus, in the \( V_G - V \) plane, regions with zero current are confined within Coulomb diamonds, that are identical diamond-shape structures repeating along the \( V_G \) axis.

In a suspended carbon nanotube, in addition to the purely Coulomb energy, we also have the nanomechanical corrections. Generally, these corrections make the relations between \( V \) and \( V_G \), which describe the boundaries of Coulomb-blockade regions, nonlinear. Consequently, the Coulomb “diamonds” in suspended nanotubes are not diamonds any more, but instead have a curvilinear shape (with
the exception of the case $C_L = C_R = 0$). Their size is also not the same and decreases with $|V_G|$. Thus, the mechanical degrees of freedom affect the Coulomb-blockade diamonds. However, since these effects originate from the nanomechanical term, which is typically a small correction, its influence on Coulomb diamonds is small as well. For the $E$ nanotube, these effects do not exceed several percent for typical gate voltages.

B. Two-gate setup and bistability

To demonstrate that the nanomechanical effects cannot generally be omitted, we consider a suspended tube symmetrically placed in between two gates and show below that bistability in the tube position occurs.\textsuperscript{26}

Figure 1 again presents the schematic setup, but the suspended tube is placed between two gates, labeled up ($U$) and down ($D$). Since up and down capacitances are connected in parallel, their sum $C_G = C_U + C_D$ matters. Assuming that the distance of the straight tube to both gates is the same, we write

$$C_{U,D} = \int_0^L \frac{dx}{2 \ln \frac{2(\alpha + z)}{r}}.$$

Expanding this for $z \ll R$ and calculating the electrostatic force, we arrive at an equation similar to Eq. (6), with a constant force $K_0$ that is replaced by $\gamma z$, where

$$\gamma = \left(\frac{ne^2}{2L^2R^2}\right)(\ln 2 R/r + 2).$$

We now solve this equation in the strong-bending regime. For this purpose\textsuperscript{25} we disregard the term $IE\gamma''$, and use the boundary conditions $z(0) = z(L) = 0$. Multiple solutions emerge; the ones with the lowest energy are

$$z = \pm \frac{2L^2}{\pi^2} \sqrt{\frac{\gamma}{ES}} \sin \frac{\pi x}{L}.$$

Thus, the tube in the strong-bending regime can oscillate between the two symmetric positions. This creates a basis for observation of quantum effects, as discussed in Ref. 26. We emphasize once again that within this model, the multistability is due to the charging of the tube in combination with the nonlinearity.

IV. EIGENMODES

The eigenfrequency of a particular eigenmode is an important, directly measurable\textsuperscript{22} property. In future experiments on suspended tubes, we expect that the eigenmodes influence tunneling ("phonon-assisted tunneling") in a similar way as observed for a single $C_{60}$ molecule.\textsuperscript{10} Below, we demonstrate that the effect of the electrostatic interactions on the elastic properties (specifically, eigenfrequencies) is strong and changes the behavior qualitatively.

To find the eigenmodes, we apply a gate voltage with a large dc (single gate) and a small ac component. The displacement $z(x,t)$ is time dependent, which provides an external force $-\rho S\dddot{z}$ to Eq. (6), where $\rho$ equals $1.35$ g/cm$^3$. Equation (6) must be solved first with a constant stress, and then the stress is found self-consistently. The tube displacement has a small ac component $\dddot{z}$ on top of a large static one. The self-consistency procedure is essentially the same and again leads to Eq. (8). Thus, the dc component of the gate voltage determines the stress $T$ and it therefore controls the eigenmodes.

The frequencies of the (transverse) eigenmodes are found from the requirement that the equation

$$IE \dddot{z} - T \dddot{z} - \rho S \omega^2 \ddot{z} = 0$$

with the boundary condition $\dddot{z}(0) = \dddot{z}(L) = \dddot{z}'(0) = \dddot{z}'(L) = 0$ has a nonzero solution. This yields the following equation for the frequency $\omega$,

$$\cosh \gamma_1 \cos \gamma_2 - \frac{1}{2} \gamma_1^2 \gamma_2^2 \sinh \gamma_1 \sin \gamma_2 = 1$$

$$\gamma_{1,2} = \frac{L}{\sqrt{2}} \left(\frac{\sqrt{\gamma^2 + 4 \lambda^2 \pm \sqrt{\gamma^2 + 4 \lambda^2}}}{\gamma^2 + 4 \lambda^2}\right)^{1/2}, \quad \lambda = \sqrt{\frac{\rho S}{EI} \omega}.$$

In the following, we restrict ourselves to the fundamental (lowest frequency) eigenmode $\omega_0$. In the limiting cases, the solutions of Eq. (18) are

$$\omega_0 = \sqrt{\frac{EI}{\rho S}} \left(22.38 L^{-2} + 0.28 \xi^2, \quad 0 \ll 1, \quad \xi L \ll 1, \quad \xi L \gg 1,$$

The second terms on the right-hand side represent small corrections to the first ones.

The frequency dependence $\omega_0 \propto L^{-2}$ is associated with a loose string, while $\omega_0 \propto L^{-1}$ means that the string is tied like in a guitar. Our results show that the behavior of the tube crosses over from “loose” to “tied” as $V_G$ increases. For the fundamental mode, the crossover occurs at $\xi L \sim 1$, corresponding to the crossover from weak to strong bending. The middle curve in Fig. 3 shows the frequency of the fundamen-
tal mode as a function of gate voltage (zero residual stress). The arrow denotes the cross over from weak to strong bending.

The gate voltage dependence of the frequency is a stepwise function, as shown in the inset of Fig. 3. Steps occur whenever an additional electron tunnels onto the tube. For the E nanotube, their height is \( \sim 5 \text{ MHz} \), which is measurable. Note that the present submicron silicon devices are always in the weak-bending regime so that corrections due to the second term in Eq. (19) are too small to be measured. Furthermore, one should realize that frequency quantization is only observable if the frequency itself is greater than the inverse tunneling time for electrons.

We now consider the effect of a residual stress \( (T_0 \neq 0) \). First, we obtain the stress by solving Eqs. (2) and (6) in the latter, \( T \) is replaced by \( T + T_0 \). In particular, for a negative stress \( T + T_0 < 0 \), \( T_0 - E \pi /L^2 \), Eq. (2) acquires several solutions. This signals Euler instability: the tube bends in the absence of an external force.

If the residual stress is large, \( T_0 \approx E \pi /L^2 \), the tube always acts like a tied string (upper curve in Fig. 3). The frequency depends weakly on \( V_G \) for low voltages, and above \( T \sim T_0 \) (denoted with the arrow) grows with an envelope \( \propto V_G^{2/3} \). For negative \( T_0 \), the picture is qualitatively different (lower curve in Fig. 3). Whereas for large gate voltages the envelope is still proportional to \( V_G^{2/3} \), the frequency dives below the value for an unstressed tube \( [22.38/(E \pi /5)]^{1/2} L^{-2} \), represented by the thin solid line in Fig. 3), when the overall stress becomes negative. It further drops to zero at the Euler instability threshold.

The qualitative difference between the various regimes means that by measuring the gate voltage dependence of \( \omega_0 \), one can determine the sign of \( T_0 \) and get a quantitative estimate. On the other side, the gate effect can be used to tune the eigenfrequencies. We also mention that in the absence of charging effects, the steps vanish but the overall shape of the curves in Fig. 3 remains the same.

V. RELAXING THE APPROXIMATIONS

While considering equilibrium displacement and eigenmodes of the nanotube, we made a number of simplifying approximations. In this section, we consider two of them—disregarding the capacitances \( C_{L,R} \) and uniform distribution of the charge—and show that relaxing these approximations affects the above results quantitatively, but not qualitatively.

In this section, we consider the case of zero residual stress \( T_0 = 0 \).

A. Finite capacitances to the leads

We now relax the limitation \( C_L, C_R = 0 \). For the general case, Eq. (6) still holds, however, the force \( K_0 \) must be adjusted.

\[
K_0 = \frac{1}{L^2 R} \left( \frac{C_0^2}{(C_0 + C_R + C_L)^2} \right) \left[ n e + (C_L + C_R) V_G - C_L V \right]^2.
\]

\[ \tag{20} \]

\[ \text{FIG. 4. Above: Displacement as a function of gate voltage for the E nanotube with finite capacitances to the leads. The four curves correspond to different values of the parameter } \phi, \text{ defined as } C_L = \phi C_G. \text{ The inset is an enlargement of the main figure. Below: The frequency of the fundamental mode normalized to the fundamental frequency of an unstressed tube } \Omega = 22.38 L^{-2} (E \pi /5)^{1/2} = 141 \text{ MHz for the same parameters as above.} \]

where \( C_0 = L/(2 \ln 2 R/\pi) \) is the capacitance of the straight nanotube to the gate. The results of the numerical solutions for the displacement and the frequency of the fundamental mode are plotted in Fig. 4. For simplicity, we have taken \( C_L = C_R = \phi C_G \); the four curves correspond to different values of the parameter \( \phi \). The curves with \( \phi = 0 \) are the same as the ones in Figs. 2 and 3.

The plots demonstrate that the qualitative picture remains the same if we include finite capacitances to the leads. The steps observed for \( \phi = 0 \) become skewed with the increase of \( C_L \) and \( C_R \) (see inset of Fig. 4). At a certain \( \phi \) these disappear. For \( \phi > 10 \) the plots are, on the scale presented, the same.

B. Nonuniform charge distribution

Above, we have assumed a uniform charge distribution along the nanotube. Rather than trying to analyze the effect in general, we consider the opposite situation when the excess charge is concentrated at one point (to be more precise, in a concise region of the tube radius \( r \)), which may represent, for instance, a pinning center. This center is placed in the middle of the nanotube. Though we believe that the charge distribution in suspended nanotubes is closer to uniform, this situation applies to a suspended quantum dot as realized recently.\[27\]

The gate-charge capacitance \( C_G \) in this geometry is

\[ C = \frac{1}{\frac{1}{r} - \frac{1}{2R}}. \]

\[ \tag{21} \]
and we proceed to obtain the equations of motion

$$IE z'' - T z'' = F \delta \left( x - \frac{L}{2}, x \right), \quad F = \frac{(ne)^2}{4R^2}, \quad (22)$$

where we again set $C_L = C_R = 0$.

The solution with the same boundary conditions as previously, $z(0) = z(L) = z'(0) = z'(L) = 0$, and with $z$, $z'$, and $z''$ all continuous at $x = L/2$, is

$$z(x) = \frac{F}{2EI\xi^3} \left\{ \tanh \frac{\xi L}{2} \left[ \cosh \xi x - 1 \right] - \sinh \xi x + \xi x \right\}$$

(23)

for $0 < x < L/2$. For $L/2 < x < L$, the coordinate $x$ should be replaced by $(L - x)$ because $z(x) = z(L - x)$. As before, $\xi = (T/EI)^{1/2}$ and Eq. (2) is used to obtain the stress consistently,

$$T = \begin{cases} F^2L^4S/(3072EI^2), & T \ll EI/L^2, \\ (1/2)(ESF^2)^{1/3}, & T \gg EI/L^2. \end{cases}$$

(24)

Consider now the strong-bending regime and compare the results for the stress $T_u$ for the uniform [lower line of Eq. (8)] and $T_n$ for the concentrated [lower line of Eq. (24)] charge distributions,

$$T_n = T_u \left( \frac{\sqrt{3}L}{4R} \right)^{2/3}. \quad (25)$$

For $L \gg R$, we formally have $T_n \gg T_u$. This means that for the same gate voltage, more stress is induced at the nanotube if the charge is concentrated at one point. Also, the displacement of the tube is greater in the concentrated case,

$$z^n_{\text{max}} = 0.87 \left( \frac{L}{R} \right)^{1/3} z^u_{\text{max}}.$$

Thus, if the charge distribution is concentrated, NEMS are “more effective” than for the uniform charge. For the $E$ nanotube, the ratio of nonuniform to uniform maximal displacement is 1.49. The difference between uniform and nonuniform charge distributions is illustrated in Fig. 5.

**VI. DISCUSSION**

The presented model is simplified in many respects. Mechanical degrees of freedom are introduced via classical theory of elasticity: The nanotube (modeled by a rod) is considered as incompressible and without internal structure. This is justified, since so far the theory of elasticity has described all existing experiments on carbon nanotubes well. For SWNT’s it has also been supported by simulations (Ref. 15). Creation of defects in SWNT starts at deformations of the order of 10%. For larger deformations (see, e.g., Ref. 28), we expect strong deviations from the behavior we describe, but this typically lies outside our applicability range $z \ll R$. We have neglected damping, which is also expected to originate from the creation of the defects and to be irrelevant in this range. We also disregarded quantum effects (cotunneling and finite spacing of quantum levels of electrons in the tube). These issues need to be clarified for a detailed comparison with the experimental data, and will be a subject of future research.

Our main result is that the nanotube can be manipulated by the gate voltage, which determines its deformation and stress, and modifies the eigenmodes. Though the eigenmodes of nanotube ropes have been measured in Ref. 22 three years ago, the strain dependence of the eigenmodes was only recently reported in Ref. 29, which was published after this manuscript had been submitted for publication. Reference 29 demonstrates this effect for singly-clamped multiwall carbon nanotubes. We expect that our predictions will soon be tested in experiments on doubly clamped SWNTs.

We also mention one more paper published after the submission of our manuscript, Ref. 27, which shows measurements on a suspended quantum dot. Though the focus of our study was on carbon nanotubes, all the calculations can be immediately applied to this case as well.

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26 S.M. Carr, W.E. Lawrence, and M.N. Wybourne, Phys. Rev. B 64, 220101 (2001) discuss a bistability as a result of externally applied negative residual tension. We emphasize that in our case it appears for an arbitrary residual tension, in the regime when the charging effects drive the tube into the strong-bending regime.