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Electromechanical stiffening of rods and tubes

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Electrostatic interactions are shown to exert a significant effect on the buckling instability of a rod. In particular, the threshold value of the compressional force needed to induce buckling is found to be independent of rod length for long charged rods. In the case of rods of intermediate length, the critical buckling force crosses over from the classic inverse-square length dependence to asymptotic length-independent form with increasing rod length. It is suggested that this effect leads to the possibility of electromechanical stiffening of nanotubes, which would allow relatively long segments of them to be used as atomic force probes. © 2004 American Institute of Physics. [DOI: 10.1063/1.1757018]

When slender objects are subjected to external compressional elastic forces, they are susceptible to bending deformations. The onset of such a deformation is known generically as the buckling instability.^{1,2} An elastic rod of a given material and length can resist compressional forces up to a so-called *critical buckling force* F_c that increases with the (effective) bending stiffness of the rod, and decreases with an inverse-square law with its length L ($F_c \sim 1/L^2$). Because of this length dependence, longer filaments possess much lower critical buckling forces.¹

The limitation on rod length imposed by the buckling instability is a major structural issue in nano-scale mechanics [atomic force microscopy (AFM)-tips, nanotubes³ and nanorods,⁴ etc.] as well as the micro- and macro-scale. However, this limitation results from the local nature of elasticity, and may in principle be overcome if long-ranged interactions also exert a stiffening influence. Here we study the mechanical response of an elastic charged rod to external compressional forces, and in particular the onset of Euler buckling instability, taking into account the nonlocal nature of electrostatic self-interactions.⁵ For a cylindrical charged rod of radius r and surface number charge density σ , we find that long-ranged electrostatics leads, in the limit of a long rod, to a nonvanishing critical buckling force

$$F_c(L \rightarrow \infty) = \Delta \frac{\pi}{\epsilon_0} e^2 \sigma^2 r^2, \quad (1)$$

in which ϵ_0 is the permittivity of free space, e is the electron charge, and $\Delta = \gamma + \psi(1/2) + 3/2 \cong 0.1137056$ is a universal numerical prefactor.⁶ In the case of rods with a finite length L , we find that the above-mentioned result smoothly crosses over to a local $1/L^2$ dependence as L decreases. Crossover to

this dependence occurs when L is small enough that the accumulated electrostatic self-interaction has not yet overwhelmed local elasticity. As will be shown, we are also able to determine the shape of the rod at the onset of buckling, and show that the buckling rod becomes considerably flatter in the interior as a result of electrostatic self-repulsion.

The elastic charged rod is considered to be inextensible, and its energy consists of two contributions. The first part results from the elastic bending energy $E_b = (K/2) \int_0^L ds H(s)^2$. This energy is controlled by the intrinsic bending modulus K of the elastic rod and contains no electrostatic contributions. The curvature $H(s)$ is assumed to be a function of the arclength parameter s . For a homogeneous elastic rod of circular cross section that is made of a material with a Young's modulus E , we have $K = (\pi/4)r^4 E$.² The second contribution to the energy arises from electrostatic interactions, which can be written as

$$E_{\text{el}} = \frac{Y}{2} \int_0^L ds \int_0^L ds' \frac{1}{|\mathbf{r}(s) - \mathbf{r}(s')|},$$

for a rod whose conformation is represented by a space curve $\mathbf{r}(s)$. The electrostatic coupling constant is defined as $Y = e^2/(4\pi\epsilon_0 a^2)$, a being the average separation between neighboring charges along the line (see Fig. 1). Considering the cylindrical geometry of the rod, one can express the linear number charge density $1/a$ in terms of the surface num-

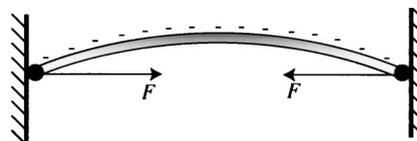


FIG. 1. The elastic charged rod is hinged at two ends and is subject to a compressional force F .

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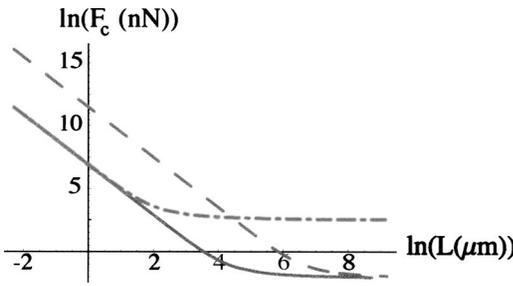


FIG. 2. The critical buckling force for a charged rod as a function of its length (log-log plot). (a) The solid line corresponds to $K=1 \times 10^{-19} \text{ N m}^2$ and $Y=1 \text{ nN}$. (b) The dashed line corresponds to $K=100 \times 10^{-19} \text{ N m}^2$ and $Y=1 \text{ nN}$. (c) The dash-dotted line corresponds to $K=1 \times 10^{-19} \text{ N m}^2$ and $Y=100 \text{ nN}$.

ber charge density σ through $a=(2\pi r\sigma)^{-1}$, which yields $Y=(\pi/\epsilon_0)e^2\sigma^2r^2$. Finally, to study the onset of buckling upon applying a compressive force F , we add a term $E_{\text{ex}}=F\int_0^L ds \cos\theta(s)$ to the total energy, where $\theta(s)$ is the angle that the rod's local unit tangent vector makes with its unperturbed orientation, and is related to the curvature via $H(s)=d\theta(s)/ds$.

One can estimate the critical buckling force for a neutral rod using a simple force balance argument. Imagine that the rod is bent into an arc of a circle of radius R with a corresponding arc angle θ , so that $L=R\theta$. Then we can calculate the bending energy $E_b(\theta)=KL/2R^2=K\theta^2/2L$, and the end-to-end distance $x(\theta)=2R\sin(\theta/2)=L\sin(\theta/2)/(\theta/2)$ as a function of the bending angle θ . The elastic force that resist bending at the onset of such arc formation can be found as $F_b=-\partial E_b(\theta)/\partial x(\theta)|_{\theta=0}=12K/L^2$, which slightly overestimates the exact critical buckling force $F_{c0}=\pi^2K/L^2$ (Ref. 2) due to the artificial assumption of constant curvature. A similar argument can be used to qualitatively account for Eq. (1) in the case of a charged rod with negligible intrinsic rigidity. Imagine that charges of unit magnitude are placed along the rod in a regular pattern at a distance a from each other. The electrostatic repulsive force that the first charge experiences can then be calculated as the sum of the contributions from all the neighbors, namely, $F_{\text{el}}(1)=Y(1+1/2^2+1/3^2+\dots)=\pi^2Y/6$. If the charged rod is to undergo compressional failure, the external force has to be greater than this Coulomb repulsion, thus yielding the scaling form for the critical buckling force as reported in Eq. (1). To obtain the correct numerical prefactor, however, one should look for collective failure corresponding to the lowest threshold critical force.⁷

We study the spectrum of the total energy operator numerically,⁸ and use it to find the critical buckling force and the shape of a charged rod of arbitrary length at the onset of compressive failure. In Fig. 2, the critical buckling force is plotted as a function of the length of the rod, for various values of K and Y . As shown in the plot, when L is small, the critical force is proportional to $1/L^2$. As L passes through a crossover length scale $\ell_x \propto \sqrt{K/Y}$, the force saturates at an L -independent value.

The critical buckling forces corresponding to different values of the parameters K , Y , and L can be collapsed onto a universal curve as shown in Fig. 3, if normalized with the critical buckling force of the neutral chain F_{c0} and plotted as a function of the dimensionless charging parameter Q

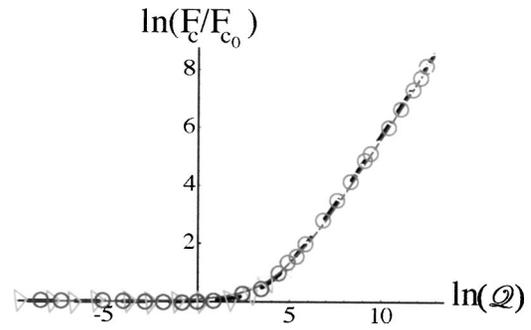


FIG. 3. The rescaled critical buckling force for a charged rod as a function of the charging parameter $Q=YL^2/K$. Note that three distinct series of data (open circles, triangles, and dashed line), corresponding to the different curves in Fig. 2, have been collapsed on top of a universal curve. The solid line represents the interpolation formula of Eq. (2) for comparison.

$=YL^2/K$. An interpolation formula of the form

$$\frac{F_c}{F_{c0}} = 1 + \frac{1}{\pi^2} \sqrt{\frac{Q}{2}} + \frac{\Delta}{\pi^2} Q, \tag{2}$$

is found to satisfactorily represent the universal curve as revealed by the comparison in Fig. 3.

The shape of the charged rod at the onset of buckling is also calculated, and shown in Fig. 4 for various values of the charging parameter Q . It appears that charging leads to deviations in the shape of the buckling rod from the sinus-profile² in that there is enhanced flattening in the interior. This is to be expected because the interior of the charged rod is subject to stronger electrostatic self-repulsion than the end-segments where ‘‘half’’ of the repelling charges are absent. A similar effect has also been observed in the bending response of charged elastic rods.⁹

The familiar image of a long-haired girl touching the van de Graaff machine suggests that a practical way of imposing the required charging is by applying a voltage. For a conducting cylinder of length L and radius r that is kept at a potential V relative to ‘‘infinity,’’¹⁰ one can calculate the induced surface charge density, and deduce from it the corresponding asymptotic critical buckling force as

$$F_c(L \rightarrow \infty, V) = \frac{\Delta \pi \epsilon_0 V^2}{[\ln(L/r)]^2}. \tag{3}$$

For a thread of human hair we have $r \approx 0.1 \text{ mm}$ and $K_{\text{hair}} \sim 10^{-11} \text{ N m}^2$, which yields for $L=1 \text{ cm}$ a critical force of $F_c \approx 10^{-6} \text{ N}$. Applying a voltage of $V=50 \text{ kV}$ (typical of van de Graaff generators) then results in a critical force of $F_c \approx 10^{-4} \text{ N}$ for a 1-m-long piece of hair!

Perhaps the most interesting venue in which these results find application will be in hardening of atomic force probes. Carbon nanotubes have been found to be structurally quite

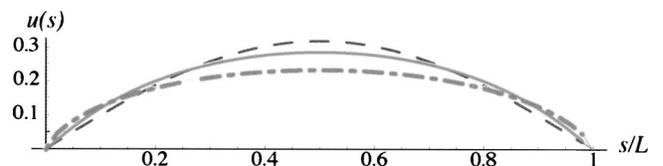


FIG. 4. The shape of a charged rod at the onset of Euler buckling instability. The dashed line corresponds to $Q=0$, the solid line corresponds to $Q=10^3$, and the dash-dotted line corresponds to $Q=10^6$. The buckling charged rod flattens in the interior as the charging is increased.

robust and have exceptionally high Young's modulus (in the TPa range).¹¹ However, the fact that they can grow to microns in length while having nanometric diameters renders them quite susceptible to buckling. The buckling of multiwalled carbon nanotubes has been recently investigated experimentally by Dong *et al.*¹² In their experiment, a 6.9- μm -long nanotube is subjected to compression, and its critical buckling force (typically in the nN range for micron-sized nanotubes) is determined. From this measurement the bending rigidity of the nanotube is found to be $K_{\text{nanotube}} = 8.641 \times 10^{-20} \text{ N m}^2$.¹² Using Eq. (3), we can now estimate that a carbon nanotube 30 nm in diameter can resist forces up to ~ 1 nN even when it is 1 mm long, provided it is kept at a voltage of 200 V. This implies a remarkable "electromechanical stiffness," in contrast with the intrinsic mechanical resistance to buckling which is diminished by a factor of 10^6 when the length of the nanotube is increased from a micron to a millimeter.^{13,14} Stiffening due to charging may also be useful in the nanometer-scale electromechanical actuator based on a multiwalled carbon nanotube that has been recently reported.¹⁵

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⁸Details of the numerical method are explained in Ref. 8.

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¹⁰If a conducting rod is held at a constant electrostatic potential, the charge distribution along the rod is known to be nearly uniform. The slight logarithmic buildup of charge at the ends of the rod leads to no significant change in the electrostatic energetics of the buckled rod; the conclusions reported in the body [Eq. (3) and the related discussions] are not materially affected.

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¹³The stability of carbon nanotubes under an applied voltage against charge leakage has been studied in Ref. 15 using density functional theory. It has been shown that beyond a critical voltage V_c the charged carbon atoms at the end of the tubes are ejected. The critical voltage is shown to depend on the length and end-conditions, with closed tubes being considerably more stable than the open ones. The critical voltage appears typically very high, with values of the order of 60 V for $L = 1$ nm and 120 V for $L = 10$ nm, for closed tubes (Ref. 15). Extrapolating the approximately logarithmic dependence yields a critical voltage $V_c \approx 420$ V for $L = 1$ mm, which is a factor of 2 larger than the suggested applied voltage to ensure the length-independence of the critical buckling force.

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