ANALYTICAL CALCULATIONS FOR NANOSCALE ELECTROMECHANICAL SYSTEMS *

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A general model is presented for calculating of pull–in parameters of nano-electromechanical systems. Theory includes van der Waals forces and presents analytical expressions for pull–in voltage and gap. A role of atomistic corrections for the pull–in at the nanoscale is discussed at length.

I. INTRODUCTION

Nano-electromechanical systems (NEMS) become an essential part of modern science and technology [1]. A number of applications is already known: nanomanipulation, nanosensors, medical devices, nanofluidic devices, to name a few. Even more applications are anticipated to follow the technological progress in this field.

I address in this paper one of issues arising when we try to understand phenomena happened at the nanoscale with theoretical tools borrowed from an experience of macroscopic physics. The latter has to reach its limits and micromodels are required for a quantitative description of a nano–device. However, an essential part of the theory bases on very general assumptions. For example, a continuum modeling gives a perfect description of systems of atomic scale when using a microscopically derived parameterization for the theory.

The aim of this paper is to derive an atomistic correction for a micro–scale modeling and to discuss limits of applicability of simplest models. The object of study is a nano–electromechanical switch. Main changes in its operation at the nanoscale are related to an importance of van der Waals forces. These forces will change parameters, describing the equation of state of a NEMS. All derivation will be performed analytically, which allows one to apply this theory to a broad class of devices.

I will demonstrate how the van der Waals interaction changes two main parameters describing an instability point of a NEMS device, which are a pull–in voltage and a pull–in gap. The calculation is done within a continuum model. It allows to develop a common analytical approach for nanoscale switches of various geometry, various size and various material properties. I stress that the model includes a general form of the free energy.

The free energy of the system may be comprised of several terms. Corresponding gradients of the energy components are forces acting on the NEMS. In particular, I

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consider in details a role of dispersion forces, which are the van der Waals forces at the smallest distance, Casimir forces at intermediate distances, or thermal fluctuation forces at the largest separation. In order to be able to use the model for every force field, the power law dependence of the dispersion energy on the distance is used. It allows describing many–body corrections to the van der Waals energy, that have been discussed in Ref. [2]. These forces have a fractional power law dependence on the distance. The power law exponent enters the final analytical expression as a parameter and, thus, the model comprehends a wide class of phenomena in nanoscale systems. Of course, this purely analytical calculation can provide only an order of magnitude estimation without a detailed knowledge of the specific system.

II. ANALYTICAL MODEL

I start here with a calculation of the pull–in parameters of a general NEM system which is an elastic media (elastic manifold) subjected to external forces. The forces are changing during the NEMS operation and define a dynamic shape of the NEMS. The specific forces, considered below, are (i) the van der Waals force, (ii) the electrostatic force, and (iii) the elastic force, which is able to restore the initial equilibrium shape of the NEMS.

A further generalization to the case of non–zero dissipation is straightforward, as well as an addition of a media surrounding a NEMS is easy. As far as I consider static rather than dynamic effects, the friction is not important.

It is well known how to derive an equation of state for simple electromechanical devices at the micrometer scale [3]. This paper presents a theory giving a required generalization for nanodevices. In an earlier paper [4] an analytical derivation of the pull–in voltage for a specific device has been presented with account for the vdW correction. The second pull–in parameter, the gap, was treated as an independent quantity. Below I will extend the result of the paper [4] and give an accurate derivation for both pull–in parameters.

The equilibrium dynamic shape of the NEMS satisfies the force balance condition (A): the first derivative of the total NEMS energy is equal to zero. In general, one has to calculate the energy gradient at every point of the system and equate it to zero locally. This gives the equilibrium shape of the system at given external forces applied to the NEMS. Main approximation, which allowed me to yield an analytical solution of the problem, is to consider only one mechanical degree of freedom. This approximation gives a true answer for the pull–in up to a numerical factor which is geometry dependent. The numerical factor is not altered by changing force fields (e.g., by changing van der Waals to Casimir force) and has to be calculated only once for a given geometry.

Within this one parameter model, I write the first equation of state as:

$$\frac{\partial E}{\partial x} = 0 \tag{1}$$

where x is the single degree of freedom of a NEMS, for example, the gap, and E is the total energy given by

$$E(x, \varphi) = T(x, h; k) - V(x, \varphi; C) - W(x; \epsilon, \alpha). \tag{2}$$

Here, the energy depends on x and φ, the gap and the voltage, which are the parameters governing the instability point. Three energy components are the elastic strain energy, T, the electrostatic energy, V, and the dispersion (van der Waals) energy (vdWE), W. All three terms depend on the system design (geometry, shape etc.) as well as on the material parameters (elasticity, capacitance etc.). The first type of dependence is expressed in terms of the gap (or the NEMS degree of freedom), $0 \leq x \leq h$; in terms of the maximum (initial) gap, h; and the voltage, φ. The material properties are collected in four constants: an elastic stiffness with respect to the gap (degree of freedom), k, a general capacitance with respect to the voltage, C, and general vdW coefficients, α and ϵ, which have the meaning of a power law exponent and a specific vdWE for a given NEMS structure.

Let me define the stiffness, k, as a linear response to the strain induced by the gap variation:

$$k = \frac{\partial^2 T}{\partial x^2} + o(x^2) \tag{3}$$

and last terms of this expansion series will be omitted. Then, the elastic energy component reads as $T = k(h-x)^2/2$. One can easily recognize a mechanical linear oscillator model, which is widely used in MEMS analysis. Thus, numerical results given below will directly correspond to a continuum MEMS theory. In particular, beam equations may be useful to estimate k for a specific geometry. An advanced atomistic model (molecular mechanics and/or dynamics) may require to define the stiffness of a specific nanoscale device (for example, a parameterization for nanotubes is given in Ref. [5]). However, once parameterized for a concrete device, the model allows fast analysis of the device equation of state in various external fields.

I propose a similar definition for the specific capacitance:

$$C = \frac{\partial^2 V}{\partial \varphi^2} + o(\varphi^2). \tag{4}$$

The definition is consistent with the classic image charge energy, well known in MEMS physics, but not restricted to the classical electrostatics. One may use a micromodel to determine the energy, similarly to what has been done for calculating an atomistic capacitance of a single wall nanotube in Ref. [6]. The electrostatic energy term reads as $V = C\varphi^2/2$.

So far, the energy components are similar, at least formally, to what have been used in a standard MEMS theory [3]. Let me add an extra term which is the dispersion energy. The dispersion energy component is often approximated by a single attraction term [4,7], given by an attractive part of the vdWE, which depends on the distance between interacting surfaces. Integrating out all system geometry [7,8] will result in a simple dependence of the vdWE on the gap: $W \simeq \epsilon x^{-\alpha}$, where an exponent α defines the specific power law for the specific dispersion force. For example, for the pure van der Waals interaction between small objects (atoms) $\alpha = 6$, for the retarded Casimir force between atoms $\alpha = 7$, it can be fractional for the many–body terms in low dimensional systems [2,7]. To be consistent with this definition of a general dispersion (van der Waals) potential, I define the material coefficient ϵ and the exponent α as:

$$\epsilon = W(x)\ \exp\left[-x\log(x)\ \frac{\partial \log W}{\partial x}\right] + o(x). \tag{5}$$

$$\alpha = -x\frac{\partial \log W}{\partial x} + o(x) \tag{6}$$

With these definitions for the material constants I write the total energy of the NEMS as:

$$E(x,\varphi) = \frac{k(h-x)^2}{2} - \frac{C(x)\varphi^2}{2} - W(x;\epsilon,\alpha) \tag{7}$$

where the dependence of the capacitance on the gap, $C = C(x)$, has to be defined separately.

To find an instability point of the NEMS I write the second pull–in equation. It follows from the condition for disappearing of the stable solution of the Eq.(1). Since one defines a physical root of this equation, the merging of a stable root and an unstable root which is next to the physical solution, is a single possibility for device instability. It is equivalent to a condition (B): the second derivative of the expression (2) must equal zero:

$$\frac{\partial^2 E}{\partial x^2} = k - \frac{\varphi^2}{2}\frac{\partial^2 C}{\partial x^2} - \frac{\partial^2 W(x)}{\partial x^2} = 0. \tag{8}$$

III. GENERAL EQUATIONS FOR THE PULL–IN

Let me present a solution for the pull–in voltage, V_o, and the pull–in gap, x_o, for a standard electromechanical switch with planar electrodes. The capacitance of a planar capacitor is known to be $C = c_o/x$ in neglecting fringing fields, where $c_o = S/4\pi$ and S is a plate capacitor surface area. It results in simple relations for the capacitance derivatives: $\partial C/\partial x = -C/x$ and $\partial^2 C/\partial x^2 = 2C/x^2$. The equations of state (A) and (B) are written with use of these relations as follows:

$$\begin{cases} -k(h-x) + \frac{1}{2}\varphi^2\ \frac{C}{x} - \frac{\partial W}{\partial x} = 0 \\ \\ k - \frac{1}{2}\varphi^2\ \frac{2C}{x^2} - \frac{\partial^2 W}{\partial x^2} = 0. \end{cases} \tag{9}$$

In full neglecting the vdWE terms I obtain:

$$\begin{cases} -k(h-x) + \frac{1}{2}\varphi^2\ \frac{C}{x} = 0 \\ \\ k - \frac{1}{2}\varphi^2\ \frac{2C}{x^2} = 0, \end{cases} \tag{10}$$

which reproduces the classical MEMS result. The system of equations (10) is linear in variables x and φ^2 and always allows an analytical solution.

In what follows logarithmic derivatives of the energy components will be used. When the dependence of the energy components on the gap is given by a power law (the vdWE term and the electrostatic energy may be approximated by a power law at certain conditions), the logarithmic derivatives are simply constants depending on

the material properties and the geometry of the NEMS: $\beta_1 = -x\partial \log C/\partial x$, $\alpha_1 = -x\partial \log W/\partial x$, $\beta_2 = x^2 \left(\partial \log C/\partial x\right)^2 + x^2\partial^2 \log C/\partial x^2$ and $\alpha_2 = x^2 \left(\partial \log W/\partial x\right)^2 + x^2\partial^2 \log W/\partial x^2$.

In terms of α and β, which are just numbers, the general physical solution of Eq.(9) is as follows:

$$\begin{cases} x_o = h\dfrac{\beta_2}{\beta_1+\beta_2}\ \dfrac{1}{2}\left(1+\sqrt{1+4\dfrac{W(x_o)}{kh^2}\dfrac{\beta_1+\beta_2}{\beta_2}\dfrac{\alpha_2\beta_1-\alpha_1\beta_2}{\beta_2}}\right) \\ V_o = \dfrac{\sqrt{2k}h}{\sqrt{C(x_o)}}\dfrac{\sqrt{\beta_2}}{\beta_1+\beta_2}\times \\ \sqrt{\frac{1}{2}-\frac{W(x_o)}{kh^2}\frac{(\beta_1+\beta_2)(\alpha_1+\alpha_2)}{\beta_2}+\frac{1}{2}\sqrt{1+4\frac{W(x_o)}{kh^2}\frac{\beta_1+\beta_2}{\beta_2}\frac{\alpha_2\beta_1-\alpha_1\beta_2}{\beta_2}}}. \end{cases} \tag{11}$$

So far, this expression is still implicit because R.H.S. of the first equation depends on the amount of vdWE at the pull–in gap, $W(x_o)$. However, the vdWE component is normally small at large distances and I propose to substitute the bare value for the pull–in gap $x_o(0) = h\frac{\beta_2}{\beta_1+\beta_2}$ into the R.H.S. of the equations (11). This is allowed for large h because expanding the expression in series in W, one gets the difference of this approximation and an exact result only in the second order of $W/kh^2 \ll 1$. In the opposite, ultra–nanoscale, limit the solution of the first of Eqs.(11) must be substituted in the second one.

Several conclusions can be drawn from the general expression for the pull–in. It gives a required generalization of the MEMS result [3]. It describes how the electrode geometry, which is reflected in the specific capacitance, $C(x)$, influences the pull–in gap and voltage. It shows the role of the vdW interaction in the pull–in at the nanoscale. To the best of my knowledge this effect has not been studied with analytical theory to date, although numerical solution may indicate the discrepancy with standard MEMS expressions.

IV. NEGLECTING VDWE: MEMS LIMIT

The Eq.(11) gives a general solution for an electromechanical device operation. The solution includes the van der Waals correction which will be considered in the last section.

In full neglecting the van der Waals cohesion, the pull–in gap, x_o, is a fixed fraction of the initial gap, or the electrode separation, h.

$$x_o(0) \equiv x_o|_{W\to 0} = \frac{\beta_2}{\beta_1+\beta_2}h. \tag{12}$$

In the approximation of zero vdWE, the pull–in voltage is a product of the separation, h, and the inverse square root of the capacitance at the pull–in, $C^{-1/2}(x_o)$:

$$V_o(0) \equiv V_o|_{W\to 0} = \frac{\sqrt{\beta_2}}{\beta_1+\beta_2}\frac{\sqrt{2k}h}{\sqrt{C(x_o)}}. \tag{13}$$

If the NEMS electrode is an elastic plate (wide elastic rod), this expression simplifies to

$$V_o(0)|_{\beta\to 1} = \frac{2}{3}\frac{\sqrt{k}h}{\sqrt{C(x_o)}}, \tag{14}$$

and the pull–in gap

$$x_o(0)|_{\beta\to 1} = \frac{2}{3}h. \tag{15}$$

I receive $V_o(0) \propto h^{3/2}$, substituting $C^{-1}(x_o) \propto x_o \propto h$. Eqs.(14),(15) return the well–known MEMS result [3] that the pull–in voltage is a $3/2$ power law function of the separation. However, the actual dependence of the capacitance on the gap (the mechanical degree of freedom of the NEMS) has to be taken into account. A change of this dependence results in the change of the NEMS equation of state and, thus, of the pull–in gap and voltage. An example of an essential change of these parameters is a nanotube NEMS (to be presented elsewhere).

V. ROLE OF VAN DER WAALS ENERGY IN NEMS CHARACTERISTICS

I present here a limiting case for the general equation of state (9) when the electrostatic force can be described via a planar capacitor model: $C = c_o/x$ and the vdW contribution can be written as $W = \varepsilon/h^\alpha$. For completeness, I give here all logarithmic derivative coefficients: $\beta_1 = 1$, $\beta_2 = 2$, $\alpha_1 = \alpha$ and $\alpha_2 = \alpha(\alpha+1)$. Substituting these values into Eq.(11), I obtain:

$$\begin{cases} x_o = \dfrac{2}{3}h\left(\dfrac{1}{2} + \dfrac{1}{2}\sqrt{1 + 3\alpha(\alpha-1)\dfrac{W(x_o)}{kh^2}}\right) \\ V_o = \dfrac{2\sqrt{k}h}{3\sqrt{C(x_o)}}\sqrt{\dfrac{1}{2} - \dfrac{3}{2}\alpha(\alpha+2)\dfrac{W(x_o)}{kh^2} + \dfrac{1}{2}\sqrt{1 + 3\alpha(\alpha-1)\dfrac{W(x_o)}{kh^2}}}. \end{cases} \tag{16}$$

These equations may be further simplified for the small vdW forces: keeping only leading terms in W, I obtain:

$$\begin{cases} x_o \simeq h\dfrac{2}{3}\left(1 + \dfrac{3}{4}\alpha(\alpha-1)\dfrac{W(x_o)}{kh^2} + o(W/kh^2)\right) \\ V_o \simeq \dfrac{\sqrt{k}}{\sqrt{c_o}}\left(\dfrac{2}{3}h\right)^{3/2}\left(1 - \dfrac{9}{4}\alpha\dfrac{W(x_o)}{kh^2} + o(W/kh^2)\right). \end{cases} \tag{17}$$

The role of the vdW correction is to decrease the pull–in voltage via increasing the pull–in gap: at smaller distances the electrostatic term of the Eq.(2) becomes larger because the vdW force brings the electrode closer to the ground plane.

The numerical estimate for a selfconsistent solution of the equations (16) is presented in Fig.1 and Fig.2. The classical result (MEMS limit) is shown as a dash–dotted line, while solid lines represent selfconsistent solutions for the pull–in gap and

the pull–in voltage. The parameters taken for a numerical estimate are $k \simeq \varepsilon/nm^6$, $C \simeq (2/3)\sqrt{k}V/nm$. Typical value for the ε is about several eV Å^6.

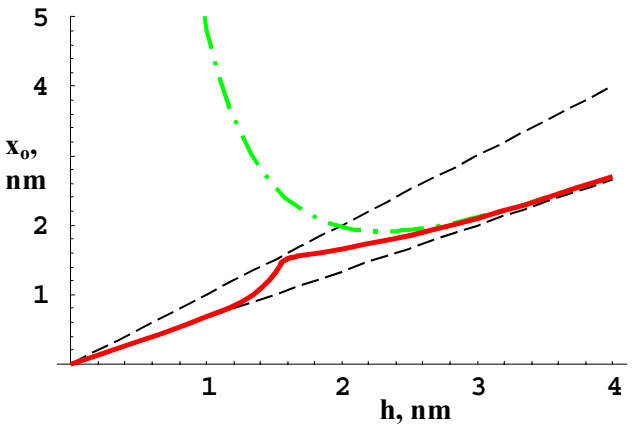

FIG. 1. The pull-in gap as a function of the initial device gap. Red (solid) curve represents the selfconsistent analytical result. Green (dash–dotted) curve shows the dependence in neglecting the van der Waals correction. Two dashed lines bound an operation region of a classical MEMS: $2h/3 \leq x_o < h$.

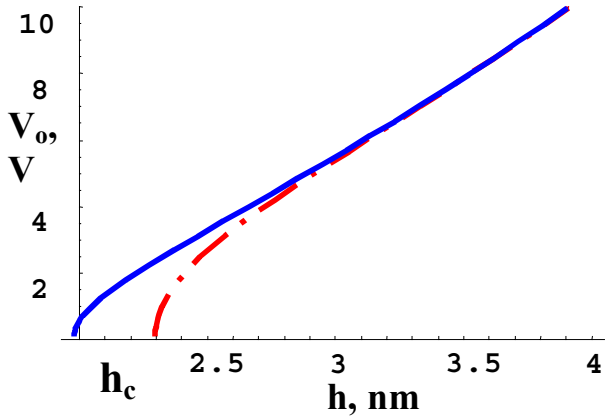

FIG. 2. The pull-in voltage as a function of the gap. Blue (solid) curve represents the analytical result explained in the text. Red (dash–dotted) curve shows the dependence in neglecting the van der Waals correction for the pull-in gap.

In contrast to a classical result, the pull–in voltage as a function of the initial separation, decreases to zero at $h = h_c$ (Fig.2). This is a critical size of a possible nano–electromechanical switch as discussed in the Ref. [4].

In summary, I present an analytical model for calculating pull–in parameters of an electromechanical system. Using continuum model with a single mechanical degree of freedom, I demonstrated the role of the van der Waals interaction for nanoscale devices. A general equation of state and a closed form of solution are derived for a planar capacitor NEMS. When operating NEMS at low gaps, the vdW corrections are written explicitly and it is discussed how the vdW interaction may restrict the

applicability of the classical MEMS theory at the distances close to a vdW limit. The theory presented in this paper allows one the calculating of the critical gap as a function of the material properties of the nanoswitch (to be discussed elsewhere).

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