Interaction and size effects in open nanoelectromechanical systems

1. Introduction

Our system consists of a 2D quantum wire (QW) of length L_x and width L_y. A singly clamped nanoresonator of mass m_0 and frequency ω_0 is aligned to the y-axis such that its endpoint can vibrate above the QW. In the absence of a driving signal and of a time-dependent electrostatic coupling to the QW the NR is located at the equilibrium distance z_0. In this configuration the segment of length L_y belonging to the NR acts as an oscillating tip. Let us stress though that here we are looking for the quantum regime of the NR and therefore our calculations are not relevant for an AFM tip which is always is the classical regime. For that configuration one can rely on a classical description of the nanoresonator. The NR could be a simple beam or a carbon nanotube (CNT). Note that one can easily sweep the nanoresonator along the x axis and then record the changes in its dynamics or in the transport properties of the QW. We assume that the NR is cooled down such that the ratio $k_BT/\hbar\omega_0$ is not very large (typically we consider $k_BT \sim 10\hbar\omega_0$).

The electron-vibron electrostatic coupling depends essentially on the nanoresonator mass M and on its fundamental frequency ω_0 (through the oscillator length $\sqrt{\hbar/2M\omega_0}$) but also on the charge density of the mesoscopic system which reflects in turn the localization properties of its wavefunctions.

Our aim here is to investigate the effects of the electron-vibron coupling on the dynamics of the nanoresonator. In contrast to most of previous works we pay special attention to the description of the electrostatic QW-NR interaction (see below). The geometry of the nanowire and the Coulomb interaction effects are also taken into account. Also we provide calculations for both transient and steady-state regimes.

A brief discussion on the available frequency range is useful here. A transverse oscillation mode around 39 GHz has been reported for a suspended CNT [1] while stretching modes can go up to 200 GHZ [2]. Notably, short CNTs were also shown to display extremely high frequency strain-tunable bending modes (few hundred GHz!) [3]. Note however that first experiments involving both CNTs and semiconductor cantilevers coupled to single-electron transistors (SETS) have been performed at $\omega_0 \sim 150 - 450$ MHz. The main point here is that in order to record changes induced by the NR on the transport properties the vibrational level spacing must be discerned when the chemical potentials of the leads are varied (see the discussion below). On the other hand, we find that the tunneling processes in the QW always trigger a change in the average vibron occupation provided the electrostatic coupling leads to a mixture of states with different vibron numbers.

The theoretical studies on nano-electromechanical systems both in classical or quantum regimes rely on Master equation approaches [6, 7] or non-equilibrium Green's functions techniques. Starting from a single-level Anderson-Holstein Hamiltonian (SLAH) where the electron-vibron electrostatic coupling is parameterized by a simple constant λ, one performs the unitary polaronic (Lang-Firsov) transformation leading to vibronic sidebands. Notably, this polaron transformation involves a perturbative expansion w.r.t. the dimensionless ratio $\lambda/\hbar\omega_0$ and changes the lead-nanowire tunneling Hamiltonian H_T by adding the operator-valued exponential $e^{\lambda/\hbar\omega_0(a^\dagger+a)}$.

A different and much less explored route is to solve the Master equation in the basis of the fully coupled NR+SET system. To our best knowledge this route was first taken by Hubener and Brandes [8] for the simple case of a single-level quantum dot coupled to a classical oscillator. They ended up with a Franck-Condon Master equation which naturally embodies the overlap between different vibrational components of the interacting wavefunctions. The role of these position-dependent Franck-Condon terms on the mass sensing and transport properties of suspended CNTs has been later pointed out in the theoretical calculations of Remaggi *et al.* [4] and Donarini *et al.* [5]

Here we shall present some preliminary results on interaction and size effects in open nanoelectromechanical systems. As stated above we pay special attention to the description of the electron-vibron coupling. The transient and steady-state transport properties are discussed within the Master equation formalism.

2. Formalism

We introduce the main steps of the formalism. The Hamiltonian $H_{\rm QW}$ of the quantum wire embodies the geometrical details and the effect of the Coulomb interaction. The single-particle eigenenergies and eigenfunctions are denoted by ε_n and ψ_n. Then we introduce the Coulomb interaction and calculate numerically the low-energy interacting many-body configurations $|\nu\rangle$ and the associated eigenvalues E_ν, such that $H_{\rm QW}|\nu\rangle = E_\nu|\nu\rangle$. To be more specific, the Hamiltonian of the interacting quantum wire reads:

$$H_{\rm QW} = \sum_{i,\sigma} \varepsilon_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} + \frac{1}{2}\sum_{i,j}\sum_{\sigma,\sigma'} V_{ijji} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} c_{j\sigma} + \sum_{i,j}\sum_{\sigma,\sigma'} V_{ijij} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{j\sigma'} c_{i\sigma}, \qquad (1)$$

where V_{ijji} (V_{ijij}) stands for the exchange (direct) interaction terms and $c^\dagger_i(c_i)$ are the creation (annihilation) operators associate to a single particle state with energy ε_i. The QW-NR system is described by the Hamiltonian:

$$H_S = H_{\rm QW} + H_{\rm NR} + V_{\rm el-vb} := H_S^{(0)} + V_{\rm el-vb}, \qquad (2)$$

where $H_{\rm NR} = \hbar\omega_0 a^\dagger a$ and $V_{\rm el-vb}$ stands for the electron vibron coupling which can be written as:

$$V_{\rm el-vb} = \sum_{i\in QW} v_i c^\dagger_i c_i (a^\dagger + a). \qquad (3)$$

Here $a^\dagger/a$ are the raising/lowering operators associated to the vibrational mode. Note that $H_S^{(0)}|\nu, N\rangle = (E_\nu + N\hbar\omega_0)|\nu, N\rangle$ where we introduced the 'free' states of the system in the absence of the electron-vibron interaction $|\nu, N\rangle := |\nu\rangle \otimes |N\rangle$, being $|N\rangle$ the N-vibron state of the nanoresonator (i.e. $a^\dagger a|N\rangle = N|N\rangle$).

In Eq. (3) v_i denotes the electron-vibron coupling strength associated to the single-particle state ψ_i of the non-interacting QW. Its explicit form is obtained by expanding the QW-NR electrostatic interaction about the equilibrium position z_0 and by quantizing the displacement $u = z' - z_0$. The 1st order term associated to the i-th SPS reads:

$$\hat{\mathcal{V}}_i = \frac{eQ_{\rm tip}}{4\pi\varepsilon_0\varepsilon_r}\int_{NR} d\mathbf{r}' \int_{QW} d\mathbf{r}\mathcal{N}_i(\mathbf{r})\hat{u}\frac{\partial}{\partial z'}|\mathbf{r}-\mathbf{r}'|\Big|_{z'=z_0} = v_i(a^\dagger + a), \qquad (4)$$

where $\mathcal{N}_i(\mathbf{r}) = |\psi_i(\mathbf{r})|^2$ is the electronic density at site i and $Q_{\rm tip} = eN_{\rm tip}$ is the charge localized on the NR. In our discrete model the integrals will be simply replaced by sums over the sites describing the NR and the QW. Note that $v_i \sim \sqrt{\frac{\hbar}{2M\omega_0}}$ but it also depends on the geometry of the NR. For simplicity we omitted the 0-order term which only induces a global shift of the eigenstates of the nanoresonator.

The states of the coupled QW-NR system can be generally written as linear combinations of 'free' states:

$$|p\rangle = \sum_{\nu,N} C^{(p)}_{\nu N}|\nu, N\rangle, \qquad (5)$$

where the coefficients $C^{(p)}_{\nu N}$ are found by numerical diagonalization. It is however useful to introduce an alternative notation. Since the electron-vibron interaction conserves the electronic occupation of the quantum wire it follows that for any MB configuration ν one gets a subspace

of fully interacting states $\{\nu, s\}$ which only differ by the weights $A^{(\nu)}_{sN}$ of different vibron states $|N\rangle$:

$$|\nu, s\rangle = |\nu\rangle \otimes \left\{ \sum_N A^{(\nu)}_{sN} |N\rangle \right\} := |\nu\rangle \otimes |s_\nu\rangle, \tag{6}$$

where the notation s_ν recalls that the vibrational components depend on the many-body configuration. A similar notation was used in [8]. In practical calculations the number of vibronic states s must be limited to a cut-off value N_{eff} such that $s, N = 1, 2, ..., N_{\text{eff}}$. Note that for each many body configuration ν the coeficients $A^{(\nu)}_{sN}$ define a unitary transformation between $\{|N\rangle\}$ and $\{|s_\nu\rangle\}$. In other words the Hamiltonian of the QW-NR systems is block diagonal w.r.t $|\nu\rangle$. With this notation the eigenvalues of the coupled electron-vibron system are defined by $H_S|\nu, s\rangle = \mathcal{E}_{\nu s}|\nu, s\rangle$.

The transfer Hamiltonian describing the lead-QW coupling has a standard form:

$$H_T = \sum_\alpha \sum_{k,\sigma} \sum_{i \in \text{QW}} \left(V^\alpha_{i,k\sigma} c^\dagger_i c_{k\alpha\sigma} + h.c. \right), \tag{7}$$

where (k, σ) stand for the momentum and spin ofelectron in the reservoir α and $V^\alpha_{i,k\sigma}$ is the tunneling strength. We assume for simplicity that the tunneling processes conserve the spin such and does not depend on k.

The dynamics and the transport properties of the system are calculated from the Master equation of the reduced density operator $\rho(t) = \text{Tr}_{\text{leads}}\{W(t)\}$ where $W(t)$ is the density operator of the whole system, i.e solving $i\hbar\dot{W}(t) = [H_S + H_T + H_{\text{leads}}, W]$. The leads are suddenly coupled at some initial time t_0 and $\rho(t_0) = |\nu_0, N = 0\rangle\langle\nu_0, N = 0|$.

Within the Born-Markov approximation the Master equation reads:

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H_S, \rho(t)] - \mathcal{L}_{\text{leads}}[\rho(t)] - \mathcal{L}_\kappa[\rho(t)], \tag{8}$$

where $\mathcal{L}_{\text{leads}}$ takes into account the contribution of the particle reservoirs (i.e. the leads) and $\mathcal{L}_\kappa$ describes the damping of vibrons due to a thermal reservoir. By straightforward and standard calculations one finds that:

$$\mathcal{L}_{\text{leads}}[\rho(t)] = \frac{1}{\hbar^2} \int_0^\infty ds \text{Tr}_{\text{leads}} \left\{ \left[H_T, [\tilde{H}_T(-s), \rho(t)\rho_R] \right] \right\}, \tag{9}$$

where ρ_R is the equilibrium statistical operator of the reservoirs and the interaction picture w.r.t the Hamiltonian of the disconnected system reads $H_T(t) = e^{\frac{i}{\hbar}t(H_S + H_{\text{leads}})} H_T e^{-\frac{i}{\hbar}t(H_S + H_{\text{leads}})}$. To get to a more explicit form of $\mathcal{L}_{\text{leads}}$ one expresses H_T in the basis of fully interacting states $|\nu, s\rangle$. By doing so the Lindblad-like terms are expressed in a compact form (the sums run over the lead index $\alpha = L, R$ and the spin on leads $\sigma = \uparrow, \downarrow$):

$$\mathcal{L}_{\text{leads}}[\rho(t)] = \frac{\pi}{\hbar} \left(\sum_{\alpha,\sigma} [\mathcal{A}_{\alpha\sigma}, \mathcal{B}_{\alpha\sigma}\rho(t) - \rho(t)\mathcal{D}^\dagger_{\alpha\sigma}] + h.c \right). \tag{10}$$

The operators $\mathcal{A}, \mathcal{B}$ and $\mathcal{D}$ are given as follows:

$$\mathcal{A}_{\alpha\sigma} = \sum_{\nu s, \nu' s'} T^{\alpha\sigma}_{\nu s, \nu' s'} |\nu s\rangle\langle\nu' s'| \tag{11}$$

$$\mathcal{B}_{\alpha\sigma} = \sum_{\lambda r, \lambda' r'} (1 - f_\alpha(\mathcal{E}_{\lambda' r'} - \mathcal{E}_{\lambda r})) \overline{T}^{\alpha\sigma}_{\lambda r', \lambda r} |\lambda r\rangle\langle\lambda' r'| \tag{12}$$

$$\mathcal{D}_{\alpha\sigma} = \sum_{\lambda r, \lambda' r'} f_\alpha(\mathcal{E}_{\lambda r} - \mathcal{E}_{\lambda' r'}) T^{\alpha\sigma}_{\lambda r, \lambda' r'} |\lambda r\rangle\langle\lambda' r'|. \tag{13}$$

We introduced the Fermi functions $f_\alpha(E)$ and jump operators between pairs of fully interacting states ($D_{\alpha\sigma}$ is the density of states of the lead α):

$$T^{\alpha\sigma}_{\nu s,\nu' s'} = \sqrt{D_{\alpha\sigma}} \sum_{i\in \mathrm{QW}} V^{\alpha}_{i,\sigma} \langle \nu | c_i^\dagger | \nu' \rangle \cdot \langle s_\nu | s'_{\nu'} \rangle. \tag{14}$$

The thermal damping term reads simply as:

$$\mathcal{L}_\kappa = \frac{\kappa}{2} \left(a^\dagger a \rho + \rho a^\dagger a - 2 a \rho a^\dagger \right). \tag{15}$$

The Master equation will be solved w.r.t the fully interacting states $|\nu, s\rangle$ of the QW-NR system. Here 'fully interacting' means that both the Coulomb interaction within the QW and the electron-vibron coupling are taken into account. The main point here is that along the derivation of the Master equation the argument of the Fermi functions is given by the energy difference between two fully interacting states (e.g. $f_\alpha(\mathcal{E}_{\nu s} - \mathcal{E}_{\nu' s'})$). Essentially this means that the electron-vibron coupling renormalizes the tunneling energy $E_\nu - E_{\nu'}$ between two many-body configurations of the mesoscopic system. Note that the numbers of electrons for the pair ν, ν' obey the identity $|n(\nu) - n(\nu')| = 1$ (tunneling or tunneling out events) and that the scalar product between two vibrational components s_ν and $s_{\nu'}$ is nothing but the Franck-Condon factor.

As a particular case one can choose μ_L and μ_R such that $f_L = 1 - f_R = 1$. Then it is easy to see that:

$$\sum_{\nu s, \nu' s'} f_\alpha(\mathcal{E}_{\nu s} - \mathcal{E}_{\nu' s'}) T^{\alpha\sigma}_{\nu s,\nu' s'} |\nu s\rangle\langle \nu' s'| = \sum_{\nu,\nu'} T^{L\sigma}_{\nu\nu'} |\nu\rangle\langle\nu'| \otimes \mathbf{1}_{\mathrm{vb}}. \tag{16}$$

This means in particular that one could actually solve the Master equation w.r.t the 'free' states and that the dissipative term of the leads $\mathcal{L}_{\alpha,\sigma}$ does not depend explicitely on the electron-vibron coupling. In fact one check that $\mathcal{B}_{c\sigma} = \mathcal{A}^\dagger_{c\sigma}$ and that $\mathcal{D}_{v\sigma} = \mathcal{A}_{v\sigma}$. Consequently, the leads' dissipative term acquires the well known Lindblad form:

$$\mathcal{L}_{\alpha,\sigma}[\rho] = \mathcal{A}_{\alpha,\sigma}\mathcal{A}^\dagger_{\alpha,\sigma}\rho + \rho\mathcal{A}_{\alpha,\sigma}\mathcal{A}^\dagger_{\alpha,\sigma} - 2\mathcal{A}^\dagger_{\alpha,\sigma}\rho\mathcal{A}_{\alpha,\sigma}. \tag{17}$$

A different regime is in order if the different energy differences $\mathcal{E}_{\nu s} - \mathcal{E}_{\nu' s'}$ are found on both sides of the chemical potential of a given lead. Then the effect of the vibrons on the tunneling energies is not negligible and one has to solve the Master equation w.r.t full basis. Of course it is always possible to switch back to the 'free' state picture using the inverse transformation $|\nu, N\rangle = \sum_s \overline{A_{sN}} |s, N\rangle$ and look at the associated populations and coherences.

Now let us compute the observables in terms of the matrix elements of $\rho(t)$. We denote by $Q_S = eN_S = e\sum_i c_i^\dagger c_i$ the charge operator in the sample. The two time-dependent currents are identified and calculated from the continuity equation:

$$\frac{d}{dt}\mathcal{Q}_S(t) = e\mathrm{Tr}\{N_S \frac{d}{dt}\rho(t)\} = e\mathrm{Tr}\{N_S \mathcal{L}_{\mathrm{leads}}\} = J_L(t) - J_R(t). \tag{18}$$

By convention the current in the left contact J_L is positive if electrons flow from the contact into the QD, while the current in the right contact J_R is positive if electron leave the valence energy levels of the QD. Each current can be identified by noticing that $\mathcal{L}_{\mathrm{leads}} = \mathcal{L}_L + \mathcal{L}_R$.

The vibron number is calculated as $N_v = \mathrm{Tr}\{\rho(t) a^\dagger a\}$, while the electron number $\mathcal{N}_S = \mathrm{Tr}\{N_S \rho(t)\}$. Finally the displacement of the nanoresonator $d = \sqrt{\frac{\hbar}{2M_0\omega_0}}\mathrm{Tr}\{(a^\dagger + a)\rho(t)\}$.

As for the matrix elements of the reduced density operator we switch back to the 'free' basis as it is more convenient for discussions. As an example, the population of N-vibron states is defined as:

$$P_N = \sum_\nu \langle \nu, N | \rho(t) | \nu, N \rangle. \tag{19}$$

3. Results

The quantum wire is described by a two-dimensional discrete Laplacian with Dirichlet boundary conditions. The hopping energy is however related to the effective electron mass. L_x, L_y denote the size of the mesoscopic system in nm. A typical case is an InAs quantum wire for which $L_x = 75$nm and $L_y = 10$nm. Unless otherwise stated the temperature of the system is $T = 50$ mK; with the present cooling techniques such a regime was already achieved in experiments.

The nanoresonator geometry cannot be easily described and is beyond the scope of the present work. We adopt a minimal model which allows us to calculate the electrostatic coupling to the QW. More precisely we consider a collection of few sites ($N_{\rm tip}$) located above the QW at an equilibrium distance z_0 (on the z-axis). These sites simulate the endpoint of the cantilever. In order to calculate the QW-NR Coulomb potential we need the coordinates of the NR sites in the (x, y)-plane. To this end we use the same grid as for the QW and select the "mirror" sites $\{s_1, s_2, ..., s_{N_{\rm tip}}\}$ describing the tip. The QW-NR electrostatic coupling depends both on the position of the tip but also on the localization properties of the single-particle states in the QW. Suppose that the cantilever is one-dimensional and oriented along the y-axis. We also allow for some charge N_q on each site of the tip. This helps us to tune the QW-NR coupling besides varying ω_0, z_0 and M.

The semiinfinite leads attached to the NW are also described by discrete Laplacians. A two-dimensional lead is just a bunch of 1D "channels" coupled at consecutive sites of the sample edge. For the numerical calculations we considered four-channel leads. For simplicity we slected the chemical potentials of the leads such that no more than two electrons participate in transport. Then spin-up and spin-down electrons coming from the left lead occupy the lowest single-particle state of the dot which is mostly localized in the center of the QW but also extends towards its endpoints.

The Master equation is solved numerically by using a 4-point Runge-Kutta method.

We now present the main results obtained at this stage of the project.

• *Formal results.* The intertwined dynamics of the open NEMS is described within a generalized Master equation approach which is exact w.r.t. the electron-vibron coupling. More precisely, we implemented numerically a Franck-Condon Master equation by treating the intradot Coulomb interaction and the electron-vibron coupling on equal footing. This goes beyond most of the existing approaches which assume that a single electron contributes to the transport and to the interaction with the vibrons. The eigenfunctions of the nanoelectromechanical system are found using configuration-interaction methods. We analyze the effect of the electron-vibron coupling on the energy spectrum of the nanoelectromechanical system. This dependence can lead to the removal or the onset of the Coulomb blockade as the distance between the NR and the mesoscopic system is changed.

• *Improved model for the electron-vibron coupling.* Our approach captures the dependence of the electron-vibron coupling on the location of the nanoresonator and on the equilibrium distance to the open mesoscopic system. We calculated the populations associated to different vibron numbers and investigated their dynamics for various locations of the NR on the x-axis. The time-dependent (i.e. transient) filling of the vibronic states reflects the "climbing" of the harmonic oscillator states due to the electron-vibron coupling. The coupling of the nanoresonator to a thermal bath limits the number of vibronic states excited by the current passing through the wire and drives the system to a steady state. If the states participating to the transport are well within the bias window the nanowire cannot detect neither their dynamics nor a shift of the tip along the x-axis. The role of the open quantum wire remains however crucial as it sets the NR into motion and changes its equlibrium position.

• *Vibron dynamics in an unbiased (yet open) sytem.* We find that the electron-vibron coupling drives the nanoresonator out-of-equilibrium even in the absence of an applied bias. Fig. 1(a) shows the evolution of the average vibron number at equal chemical potentials of the

leads $\mu_L = \mu_R = \mu_0$ and for several values of the equilibrium distance z_0. We selected $\mu_{L,R}$ such that the QW accumulates at most one ($\mu_0 = 35$ meV) or two electrons ($\mu_0 = 80$ meV). The vibron number N_v displays periodic oscillations for all configurations in spite of the fact that the charge on the QW settles down rapidly (not shown) to $Q = 1$ or $Q = 2$. It is clear that the mechanism behind these oscillation is similar to the one leading to Rabi oscillation in quantum optics. Here the off-diagonal electron-vibron interaction $\langle \nu, N|V_{\rm el-vb}|\nu, N'\rangle$ couples 'neighbor' vibron states and therefore generates coherences w.r.t. the vibron number in the Master equation.

In the case of double-occupancy $Q = 2$ we show results for two values of the equilibrium distance z_0. As expected, when the NR approaches the system by just 10 nm the vibron number increases as the electrostatic coupling enhanced. For single-occupancy configuration ($Q = 1$) one has to reduce the initial position of the nanoresonator in order to capture the effect of electron-vibron coupling. In the long time limit the oscillations of N_v are damped by the coupling to a thermal bath (the corresponding rate κ was chosen such that $\hbar\kappa$ is 10 times smaller than the smallest matrix element of the el-vb interaction).

Further information could be extracted by looking at the populations of N-vibron states. Fig. 1(b) captures the out-of-phase oscillations of P_0 on one hand and $P_{1,2,3}$ on the other hand. We also see that the main contribution to the vibronic populations is due to the one and two vibron states while P_3 can be neglected.

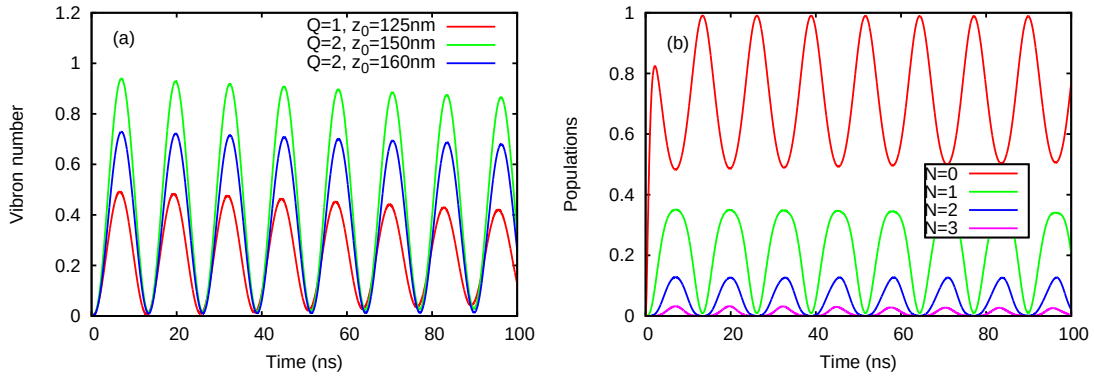

Figure 1: Left panel: The average vibron number for unbiased QW. The double occupancy $Q = 2$ is reached for $\mu_L = \mu_R = 80$ meV while single-electron configuration corresponds to $\mu_L = \mu_R = 35$ meV. Right panel: The populations of N-vibron states for the double-occupacy configuration at $z_0 = 160$ nm. Other parameters: $\omega_0 = 500$MHz, $M = 2.5 \cdot 10^{-15}$kg, $E_\uparrow = E_\downarrow = 31.85$ meV, $E_{\uparrow\downarrow} = 77.25$ meV.

The calculations discussed above were obtained starting from the initial state $|0, N = 0\rangle$ (that is there are no electrons or vibrons in the system before the coupling to the leads is switched on). Of course, the steady-state quantities do not depend on the choice of the initial state.

• *The dependence of the vibron number on the location of the NR on the x-axis.* For these simulations the system is also submitted to a bias and all states with at most one electron are available for tunneling IN and OUT processes. Similar results were obtained for a bias which activates as well the two-electron states. If the NR is placed above the center of the nanowire (i.e. for $L_{x,\rm tip} = 36.5$ nm) the charge density associated to the lowest energy single-particle state interacts strongly with the NR. Consequently the electron-vibron coupling reaches a maximum and states with up to 5 vibrons are populated (see Fig. 2(a)). By changing the position of the nanoresonator the minimal distance between the NR and the QW does not coincide to the maximum value of the charge density of the latter so the electrostatic potential decreases. This

has an effect on the average vibron number which drops from $N_v = 1.4$ to $N_v = 1.25$.

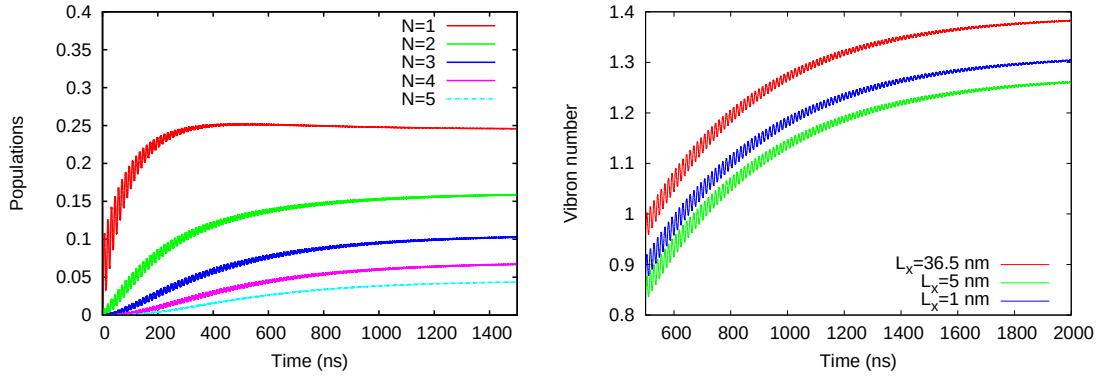

Figure 2: Left panel: Populations of N-vibron states for centered tip $L_x = 36.5$ nm. Right panel: Vibron number for different NR positions along the x-axis. Initial state: $|n = 0, N = 1\rangle$, $\omega_0 = 500$MHz, $M = 2.5 \cdot 10^{-15}$kg, $d_0 = 150$nm, $\mu_L = 35$ meV, $\mu_R = 25$ meV, $E_\uparrow = E_\downarrow = 31.85$ meV. $\kappa = 0.1V_0$, where V_0 is the smallest el-vb coupling associated to the pair of states $|1, N = 1\rangle$ and $|1, N = 0\rangle$.

Fig. 3(a) and (b) show the populations of the N-vibron states $P_N = \sum_\nu \langle \nu, N|\rho(t)|\nu, N\rangle$ as a function of time for several locations of the nanoresonator on the x-axis. As expected, if the NR is shifted towards the endpoints of the NW the electron-vibron coupling decreases. Consequently, the populations of excited vibron $P_{2,3,4,5}$ states presented in Fig. 3(b) settle down to smaller values while $P_{0,1}$ slightly increase. A similar effect is noticed on the average vibron number which drops from $N_v = 1.4$ to $N_v = 1.25$.

We also find that the displacement of the NR oscillates for a long time (μs) and settles down to a different value w.r.t to the initial equilibrium position (not shown). In contrast, if the chemical potentials of the leads are equal the NR returns to its equilibrium value z_0.

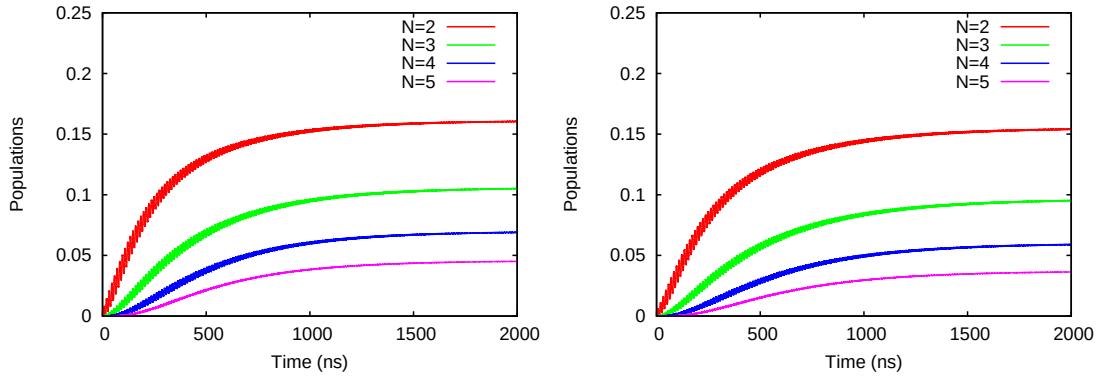

Figure 3: The population of N-vibron states for two locations of the NR on the x-axis. (a) $L_{x,\mathrm{tip}} = 36.5$ nm, (b) $L_{x,\mathrm{tip}} = 2$ nm. Other parameters: $\omega_0 = 500$MHz, $M_0 = 2.5 \cdot 10^{-15}$kg, $d_0 = 150$nm, $E_\uparrow = E_\downarrow = 31.85$ meV, $\mu_L = 35$ meV, $\mu_L = 25$ meV.

Remark: This 'senseless' regime of the QW corresponds to frequencies of hundreds MHz. Such frequencies were used in recent experiments [10] where a carbon nanotube is used *both* as a conducting system and as a nanoresonator driven by a microwave signal. Here setup is very different as the quantum wire and the NR are separate systems. In order to capture a

change in the transport properties due to the electron-vibron coupling one has to increase the level spacing of the vibronic states. This amounts to increase the NR frequency to tens or even hundreds of GHz such that the 'ladder' of harmonic oscillator levels $\mathcal{E}^{(0)}_{\nu N} = E_\nu + N\hbar\omega_0$ associated to a given many-body configuration ν of the QW can be individually scanned by varying the chemical potentials of the leads.

Some spectral analysis

Motivation: This analysis should help us understand the role of electron-vibron coupling in the transport properties.

The fully interacting eigenstates $|\nu, s\rangle$ and their corresponding eigenvalues $\mathcal{E}_{\nu s}$ are calculated by numerical diagonalization (there is no way to get analytical results). It is useful to look at the weights $|A^{(\nu)}_{sN}|^2$ of various vibron states $|N\rangle$ for different strenghts of the electron-vibron strenghts. We can easily guess their behavior and the degree of mxing between different states $|\nu, N\rangle$. On one hand, if the relevant electron-vibron interaction matrix elements are much smaller than $\hbar\omega_0$ one expects that for any interacting vibrational state $|s_\nu\rangle$ there exist a state $|\tilde{N}\rangle$ such that its weight $|A^{(\nu)}_{s\tilde{N}}|^2$ is much larger than any other weights appearing in $|s_\nu\rangle$. This situation corresponds to a weak mixing due to the el-vb interaction. On the other hand if the el-vb matrix elements increase, the relevant weights will be spread over many vibron numbers N. The stability of the diagonalization procedure is reached if by adding more vibron states in the calculation the weights remain unchanged. Remark that the diagonalization procedure provides a cutoff for an accurate calculation of the states and energies; the cutoff does not depend on the chemical potential of the leads so it is not clear yet how many vibron states must be included in the transport calculations.

It is clear that a strong mixing of the 'free' states prevents one to relate the fully interacting states to the so-called sidebands $E_\nu + N\hbar\omega_0$ which appear naturally if one performs the polaronic transformation. The weights of 'free' states are also crucial for the structure of the Franck-Condon terms appearing in the generalized tunneling coefficiens (see Eq. (14)) in which for any pair of many-body states $\{\nu, \nu'\}$ whose electronic occupations obey $|n(\nu) - n(\nu')| = 1$ one has:

$$\langle s'_{\nu'}|s_\nu\rangle = \sum_N \overline{A^{(\nu')}_{s'N}} A^{(\nu)}_{sN}. \tag{20}$$

It is not difficult to grasp that the largest FC factor is generated by states whose dominant vibronic numbers coincide (then both $A^{(\nu')}_{s'N}$ and $A^{(\nu)}_{sN}$ are of the same order for a given N). This can be checked easily on states for which $n(\nu) = 0$ and $n(\nu') = 1$ because the 'empty' states $|0, N\rangle$ cannot be mixed. The main idea is to look first at $T_{\nu s,0N}$ as a function of N and secondly to check the position of the energy differences $\mathcal{E}_{\nu s} - \mathcal{E}_{0N}$ w.r.t. the chemical potentials of the leads. This analysis should provide a hint on the changes in the transport when by varying the chemical potentials $f_\alpha(\mathcal{E}_{\nu s} - \mathcal{E}_{0N})$ is 0 or 1 for different pairs of states.

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