Sub-Poissonian phonon distributions in suspended carbon nanotubes

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Abstract. We study a quantum dot embedded into a vibrating suspended carbon nanotube. The out-of-equilibrium dynamics of the vibrational degrees of freedom is analyzed introducing the phonon Fano factor $F$ to characterize different phonon distributions. Sub-Poissonian distributions with $F < 1$ are found in selected transport regimes and are explained in terms of a selective population of phonon states due to a peculiar transport mechanism.

1. Introduction
Recent improvements in building nanoelectromechanical systems (NEMS) open a new scenario for studying the interaction between mechanical and electronic degrees of freedom at the nanoscale [1]. The electron-phonon coupling is responsible for such peculiar transport features as the Franck-Condon blockade [2]. A notable class of NEMS is represented by freely vibrating carbon nanotubes (CNTs), seamless cylinders of graphene [3] suspended between two metallic contacts at different voltages. Capacitive coupling to a gate electrode provides the possibility to modulate the effective charge in the system. The interest on such systems has increased considerably in the last years [4, 5, 6]. Signatures due to different vibrational modes, from the stretching ones [4, 5] to the radial breathing mode [6] have been detected in transport experiments and analyzed theoretically [7, 8, 9]. The properties of the out-of-equilibrium phonon populations of these systems have attracted however less attention [10]. In this paper we will theoretically study the vibron dynamics, which can exhibit a non-classical sub-Poissonian population of phonons, with fluctuations smaller than the average phonon number [11, 12].

2. Model
The CNT, of length $L$, is suspended between two metallic gates, see Fig. 1. Here, it is assumed that the CNT vibrates according to its fundamental stretching mode. Within the CNT, a quantum dot of length $L$ is formed due to structural defects at $x_1 = 0$ and $x_2 = L$, which act as tunnel barriers, while the CNT portions at $x < 0$ ($x > L$) act as source (drain) CNT contacts. A symmetric bias $V$, applied across the system forces electrons to flow from the source to the drain lead via the dot. Additionally, the dot is capacitively coupled to an external gate, at a voltage $V_g$, which tunes its excess charge.
Figure 1. Model setup: a suspended CNT (blue) connected to two metallic gates. Along the CNT two tunneling barriers create a quantum dot (red) between \( x_1 = 0 \) and \( x_2 = L \), capacitively coupled to a gate electrode.

The Hamiltonian of the CNT dot reads [13]

\[
H_d = \frac{E_c}{2} (N - N_g)^2 + \sum_{\eta, \sigma, j} \varepsilon_{\eta, \sigma, j} n_{\eta, \sigma, j},
\]

where \( E_c \) is the charging energy, \( n_{\eta, \sigma, j} = d_{\eta, \sigma, j}^\dagger d_{\eta, \sigma, j} \) is the occupation number of the \( j \)-th orbital electron state with spin \( \sigma = \pm 1 \) in the branch \( \eta = 1, 2 \). The spectrum is \( \varepsilon_{\eta, \sigma, j} = j\varepsilon_0 + (\eta - 1)\Delta \varepsilon \), with \( \varepsilon_0 \) the electronic level spacing and \( \Delta \varepsilon \) an energy mismatch between the two branches. Additionally, \( N = \sum_{\eta, \sigma, j} n_{\eta, \sigma, j} \) is the dot total charge while \( N_g \) is the charge induced by the gate voltage \( V_g \). The lowest quantized stretching mode (vibron) is modeled by (here and in the following, \( \hbar = 1 \))

\[
H_v = \Omega b^\dagger b,
\]

with \( \Omega \) the vibron frequency whose occupation is increased (decreased) by \( b^\dagger \) (\( b \)). In this work we consider a dot smaller than the vibron \((L < L_v)\). In such a situation, the Anderson-Holstein model provides an appropriate description of the coupling between electrons and the vibron. Deviations from this model, occurring for \( L \gtrsim L_v \), have been recently considered [9]. The vibron couples with the total dot charge via the Hamiltonian

\[
H_{d-v} = \Omega \lambda (b^\dagger + b)(N - N_g),
\]

with \( \lambda \) a coupling parameter. The dot is also connected with the external CNT leads via

\[
H_t = \sum_\alpha t_\alpha \sum_{\eta, \sigma, k, j} c_{\alpha, \eta, \sigma, k}^\dagger d_{\eta, \sigma, j} + \text{H.c.}
\]

with \( t_\alpha \) the tunneling amplitude on barrier \( \alpha = S, D \) and \( c_{\alpha, \eta, \sigma, k}^\dagger \) the creation operator for an electron with spin \( \sigma \) and longitudinal momentum \( k \) on the branch \( \eta \) of the lead \( \alpha \). The latter are treated as a noninteracting electron gas.

In order to diagonalize the linear coupling between the dot and the vibron we perform the Lang-Firsov canonical transformation [14] with generator \( \mathcal{U} = e^{\lambda (b^\dagger - b)(N - N_g)} \). The transformed total Hamiltonian \( \hat{H} = \mathcal{U}(H_d + H_v + H_{d-v})\mathcal{U}^\dagger \) and tunneling Hamiltonian \( \hat{H}_t = \mathcal{U}H_t\mathcal{U}^\dagger \) are expressed in terms of the original operators as

\[
\hat{H} = \frac{E_c}{2} (N - N_g)^2 + \sum_{\eta, \sigma, j} \varepsilon_{\eta, \sigma, j} n_{\eta, \sigma, j} + \Omega b^\dagger b
\]

\[
\hat{H}_t = \sum_{\alpha = S, D} t_\alpha e^{\lambda (b^\dagger - b)} \sum_{\eta, \sigma, k, j} c_{\alpha, \eta, \sigma, k}^\dagger d_{\eta, \sigma, j} + \text{h.c.}.
\]

In the following, we are interested in the low-energy dynamics of the vibrational degrees of freedom. Since \( \varepsilon_0 \gg \Omega \), as pointed out in recent experiments [5, 9], we can neglect the plasmonic excitations of the quantum dot. In this case, the dot states in branch \( \eta \) with spin \( \sigma \) are compactly
filled with \( N_{\eta,\sigma} \) electrons and the \( \tilde{H} \) can be labeled as \( \{|N_{\eta,\sigma}\}, l \) with \( l \) the occupation number of the vibron. Treating \( \tilde{H} \) to lowest order in \( t_\alpha \) and tracing out the leads degrees of freedom, one obtains a master equation for the occupation probability of the dot-vibron states \( P(\{N_{\eta,\sigma}\}, l) \)

\[
\dot{P}(\{N_{\eta,\sigma}\}, l) = \sum_{\alpha,\eta,\sigma} \Gamma^{(\alpha)}_{N_{\eta,\sigma}, l'\rightarrow N_{\eta,\sigma}, l} P(\{N'_{\eta,\sigma}\}, l') - \sum_{\alpha,\eta,\sigma} \Gamma^{(\alpha)}_{N_{\eta,\sigma}, l\rightarrow N_{\eta,\sigma}, l'} P(\{N_{\eta,\sigma}\}, l)
\]

where

\[
\Gamma^{(\alpha)}_{N_{\eta,\sigma}, l\rightarrow N'_{\eta,\sigma}, l'} = \Gamma_0 \left| \frac{t_{\alpha}}{|t_S|^2} \right|^2 X_{l'} \{ f_\alpha(\Delta E)\delta_{N',N+1} + [1 - f_\alpha(\Delta E)]\delta_{N',N-1} \}
\]

with \( \Gamma_0 = 2\pi \nu |t_S|^2 \), \( N = \sum_{\eta,\sigma} N_{\eta,\sigma} (N' = \sum_{\eta,\sigma} N'_{\eta,\sigma}) \), \( \nu \) the density of states of the leads (assumed constant and equal on both contacts), \( \Delta E \) the energy difference between the final and the initial states and \( f_{S/D}(E) = f(E \pm eV/2) \). Here, \( f(E) \) is the Fermi function at temperature \( T \) and \( e \) is the electron charge. In Eq. 7, we have introduced the Franck-Condon factors \( |\langle l | \exp \{\lambda (b - b') \}|l'\rangle|^2 = e^{-\lambda^2} \lambda^{2l'-l} (l_{\text{c}} < l') \lambda^{2l-l_{\text{c}}^2} \lambda^{2l-l_{\text{c}}^2} \) with \( l_{\text{c}} = \min\{l, l'\} \), \( l_{\text{c}} = \max\{l, l'\} \) and \( L_{\alpha}(x) \) the generalized Laguerre polynomials. It is also useful to introduce the asymmetry between the barriers with the source and the drain contacts \( A = |t_D|^2/|t_S|^2 \). In the following, we restrict the numerical solution of Eq. (6) in the steady state near the resonance between the two charge states of the dot \( N = 4N' \), with \( N_{\eta,\sigma} = N' \forall \eta, \sigma \), and \( N + 1 \) with one extra electron in the lowest unoccupied charge states, which occurs at \( N_g = 1/2 + 4N + \varepsilon_0/E_c \).

3. Results

In order to characterize the vibrational dynamics of the system, we introduce the vibron Fano factor \( \mathcal{F} = \text{var}(l)/\langle l \rangle [15] \), with \( \langle l \rangle \) the average vibron occupation number and \( \text{var}(l) = \langle l^2 \rangle - \langle l \rangle^2 \) its variance\(^1\). In analogy to the photon case, we can distinguish between sub-, super- and Poissonian distributions according to \( \mathcal{F} < 1 \), \( \mathcal{F} > 1 \) and \( \mathcal{F} = 1 \). For conventional boson distributions such as e.g. photons in a classical light field, a super-Poissonian Fano factor is typically expected [15].

**Figure 2.** (a) Density plot of \( \mathcal{F} \) as a function of \( V \) (units \( \Omega/|e| \)) and \( \bar{N}_g = N_g - 4N - \varepsilon_0/E_c \). White: \( \mathcal{F} = 1 \). (b,c) Phonon populations in different points of the \( (V, \bar{N}_g) \) plane: (b) \( |e|V = 2 \Omega \), \( \bar{N}_g = 0.54 \) (zone 1, with \( \mathcal{F} = 0.89 \)); (c) \( |e|V = 5.7 \Omega \), \( \bar{N}_g = 0.5 \), with \( \mathcal{F} = 1.7 \). In all plots, \( k_B T = 0.02 \Omega \), \( \lambda^2 = 0.6 \), \( A = 1/20 \), \( E_c = 20 \Omega \), \( \Delta \epsilon = 0.6\Omega \).

Figure 2a shows a density plot of \( \mathcal{F} \) in the plane \( (V, \bar{N}_g) \), where \( \bar{N}_g = N_g - 4N - \varepsilon_0/E_c \)

\(^1\) Both quantities contain contributions due to the dot charge state through the electron-vibron coupling [11].
obtained solving numerically the master equation (6) in the stationary regime. The solid thick lines denote transitions between states with $N$ and $N+1$ charges and the vibron in its ground state. These lines separate regions at low bias where transport is interdicted (Coulomb blockade) from areas where it is allowed. Thin solid (dashed) lines, with energy spacing $\Omega$, mark the onset of vibrational excitations triggered by tunneling events on dot states with $\eta = 1$ ($\eta = 2$).

For the non-equilibrated dynamics of the vibron in our system, a super-Poissonian Fano factor is typically obtained. However, in selected parameter regimes, $\mathcal{F} < 1$ can be achieved: this occurs in the regions of the $(V, N_\eta)$ plane denoted as “1” and “2” contoured in green in Fig. 2a. This phenomenon is linked with a peculiar selective population of the vibron states [11], in which $\mathcal{P}_0, \mathcal{P}_1 \gg \mathcal{P}_{l \geq 2}$, with $\mathcal{P}_l = \sum_{N_\eta, \sigma} P \{ \{N_\eta, \sigma\}, l\}$. This population is achieved, in selected regimes of bias and gate voltages, if $\lambda \lesssim 1$ and if $A \neq 1$ [11]. Figure 2b shows $\mathcal{P}_l$ calculated in the center of zone 1: here $\mathcal{P}_0 \approx 0.6$ and $\mathcal{P}_1 \approx 0.35$, with $\mathcal{P}_{l \geq 2} \ll 0.1$.

Let us analyze in more details the transport mechanisms leading to this kind of population. In zone 1, tunnel in events occur with $\Delta l = l_1 - l_1$ (with $l_1/l_1$ the vibron number of the final/initial state), while tunnel out transitions imply $\Delta l \leq 0$. Due to the above constraints, no direct population of the vibron states with $l_1 \geq 2$ from the vibrational ground state $l_1 = 0$ is allowed. Indeed the population of a state with given $l_1 \geq 2$ implies at least $l_1 - 1$ tunnel-out events starting from $l_1 = 0$. As a result, the population of vibron states with $l \geq 2$ scales as $\mathcal{P}_l \propto A^{-l}$. For $\lambda \lesssim 1$ and $A < 1$, this leads to a “filtering” of the probability distribution with $\mathcal{P}_0 \lesssim \mathcal{P}_1 \ll \mathcal{P}_{l \geq 2}$ and an ensuing $\mathcal{F} < 1$ [11]. In zone 2, tunnel out events from the state with $\eta = 2$ may occur with $\Delta l \leq 1$: this results in a stronger de-population of the $l = 1$ state and a weaker sub-Poissonian Fano factor.

For higher bias voltage, super-Poissonian distributions are generally achieved. Due to the large number of transport channels supporting vibron excitations, one finds broad phonon distributions with $\mathcal{F} > 1$. An example is shown in Fig. 2c.

4. Conclusions

In this work we have studied a quantum dot embedded into a freely-vibrating suspended CNT. We have analyzed the out-of-equilibrium occupation probability of vibron states, which in selected transport regimes exhibits a sub-Poissonian phonon distribution. We have explained this non-classical behavior as due to a selective population of vibron states.

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5. References

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