

Supplemental material to the paper : “Signatures of the current blockade instability in suspended carbon nanotubes”

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We provide details about the analytical derivations of the displacement spectral density $S_{xx}(\omega)$ and dephasing time γ_φ^{-1} of the carbon nanotube mechanical oscillator.

I. EVALUATION OF THE DISPLACEMENT SPECTRAL DENSITY $S_{xx}(\omega)$

In this section, we discuss how to obtain analytically the displacement spectral density $S_{xx}(\omega)$ of the carbon nanotube mechanical resonator. The effective potential $U(x)$ for the mechanical oscillator at low voltage can be expanded in Taylor series, and only the two first orders, the quadratic and quartic in x are relevant for effective temperatures $T_{\text{eff}} \ll \Gamma$ (in the following, we set both the Planck constant \hbar and the Boltzmann constant k_B to 1). We thus derive in the following analytical expressions for $S_{xx}(\omega)$ for the two limiting cases (i) where the quartic term is a small perturbation to the quadratic one, and (ii) when the quadratic term vanishes (for $\varepsilon_P = \varepsilon_c$) and the potential is purely quartic in x .

Following Dykman *et al.* in Ref. [1], in the regime of very small damping rate $A/m \ll \Delta\omega$, with $\Delta\omega$ the width of the main peak in the spectral density induced by the non-linearity, the autocorrelation function for the oscillator position can be well approximated by:

$$S_{xx}(t) = \int dx_0 dy_0 P_{\text{st}}(x_0, p_0) \tilde{x}_{x_0 p_0}(t) \tilde{x}_{x_0 p_0}(0) \quad (1)$$

where $x(t)$ is the periodic function that satisfies the equation of motion $m\ddot{x} = F(x)$ with initial conditions $x(0) = x_0$, and $\dot{x}(0) = p_0/m$ and $\tilde{x}_{x_0 p_0}(t) = x_{x_0 p_0}(t) - \langle x_{x_0 p_0}(t) \rangle$. The integration is taken over the whole phase space for the classical oscillator and $P_{\text{st}}(x, p)$ is the stationary distribution that, as discussed in the main text, for $eV \ll \Gamma$ has the Gibbs form $P_{\text{st}}(x, p) = \mathcal{N} e^{-E(x, p)/T_{\text{eff}}}$, with $E(x, p) = p^2/2m + U(x)$, and \mathcal{N} is such that the distribution is normalized $\int dx dp P_{\text{st}}(x, p) = 1$. The effective temperature $T_{\text{eff}} = eV/4$ is induced by the charge fluctuations on the dot due to the finite voltage across the leads. The damping A/m and the fluctuation D enter this expression in defining the form of P_{st} , but not in the dynamics of $x(t)$.

The expression (1) can be rewritten as follows:

$$\int_0^{+\infty} dE \int_0^{T(E)} d\tau P_{\text{st}}(E) \tilde{x}_E(t + \tau) \tilde{x}_E(\tau), \quad (2)$$

where $T(E)$ is the period of the closed trajectory $x_E(t)$ of fixed energy E and $P_{\text{st}}(E) = \mathcal{N} e^{-E/T_{\text{eff}}}$. Since $x(t)$ is periodic with a period $T(E) = 2\pi/\omega(E)$, we can introduce

its Fourier series:

$$\tilde{x}_E(t) = \sum_n e^{in\omega(E)t} x_n(E). \quad (3)$$

The spectrum then takes the form:

$$S_{xx}(\omega) = \int_0^{+\infty} dE \mathcal{P}(E) \sum_n 2\pi \delta(\omega - n\omega(E)) x_n^2(E), \quad (4)$$

with $\mathcal{P}(E) = P_{\text{st}}(E)T(E)$. Finally, introducing the energies E_n which satisfy the equation $\omega = n\omega(E_n)$, we obtain the expression for the spectral function (with $\omega > 0$) as:

$$S_{xx}(\omega) = \mathcal{N} \frac{(2\pi)^2}{\omega} \sum_{n=0}^{+\infty} \frac{e^{-E_n/T_{\text{eff}}}}{|\omega'(E_n)|} x_n^2(E), \quad (5)$$

with $\omega'(E_n) = (d\omega/dE)|_{E_n}$. The computation of S_{xx} is now reduced to the computation of $\omega(E)$ and $x_n^2(E)$.

A. Computation of $\omega(E)$

The expression for the effective force F is given in the main text for the case $\varepsilon_0 = (\mu_L + \mu_R + \varepsilon_P)/2$:

$$F(y) = -ky + (F_0/2\pi) \sum_{a=\pm 1} \arctan[(F_0 y + a eV/2)/\Gamma], \quad (6)$$

where $y = x - F_0/2k$. For $\varepsilon_P < \varepsilon_c$ there is only a single stable equilibrium position for $y = 0$. Expanding $F(y)$ around this point for $V = 0$ we obtain for the potential $U(y) = -\int_0^y dy' F(y')$:

$$U(y) = \frac{m\omega_0^2}{2} \left(1 - \frac{\varepsilon_P}{\varepsilon_c}\right) y^2 + \frac{\Gamma}{12\pi} \left(\frac{yF_0}{\Gamma}\right)^4, \quad (7)$$

where $\varepsilon_c = \pi\Gamma$. The period in terms of U reads:

$$T(E) = (m/2)^{1/2} \oint [E - U(y)]^{-1/2} dy. \quad (8)$$

that can be evaluated in terms of elliptic integrals:

$$\frac{\omega(E)}{\omega_0} = \frac{\pi}{2K[-m(E)]} \left(1 - \frac{\varepsilon_P}{\varepsilon_c}\right)^{1/2} \left(\frac{1 + C(E)}{2}\right)^{1/2}, \quad (9)$$

with

$$C(E) = \left(1 + \frac{4\pi^2}{3} \frac{\varepsilon_P^2 E}{\varepsilon_c^3 (1 - \varepsilon_P/\varepsilon_c)^2} \right)^{1/2}, \quad (10)$$

and $m(E) = \frac{C(E)-1}{C(E)+1}$. $K[-m(E)]$ is the complete elliptic integral of the first kind with parameter $-m(E)$ [see Ref. [2]]. We will need in the following the derivative of $\omega(E)$ for vanishing energy:

$$\omega'(0) \equiv \left. \frac{d\omega}{dE} \right|_{E=0} = \frac{\pi^2 \omega_0}{4} \left(\frac{\varepsilon_P}{\varepsilon_c} \right)^2 \left(1 - \frac{\varepsilon_P}{\varepsilon_c} \right)^{-3/2}. \quad (11)$$

B. Case (i) weakly non linear oscillator

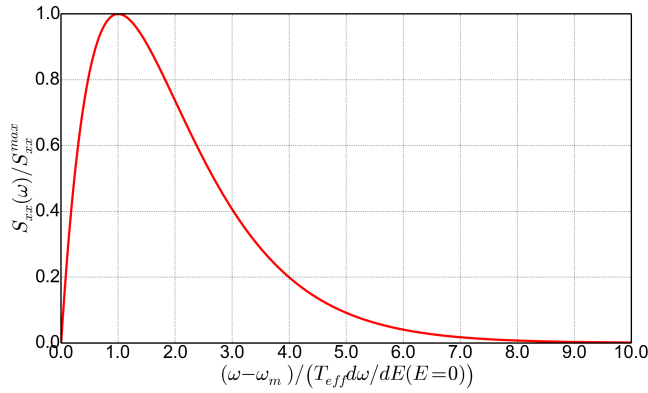


FIG. 1. Normalized displacement spectral density $S_{xx}(\omega)/S_{xx}^{max}$ as a function of the rescaled frequency $(\omega - \omega_m)/T_{\text{eff}}\omega'(0)$, in the case of weak electro-mechanical coupling ($\varepsilon_P \ll \varepsilon_c$).

Sufficiently far from the transition ($\varepsilon_P \ll \varepsilon_c$), the oscillator is weakly non-linear and we can treat the quartic part of the potential as a small perturbation. We can thus calculate S_{xx} by expanding the expression (5) to leading order in the non-linearity. The main contribution comes from the first harmonic whose amplitude can be approximated with the harmonic expression $x_1^2(E) \approx E/2m\omega_0^2$. The energy dependent resonating frequency is approximated by the expression:

$$\omega(E) = \omega_m + \omega'(0)E + \dots \quad (12)$$

where $\omega_m/\omega_0 = (1 - \varepsilon_P/\varepsilon_c)^{1/2}$. We obtain then:

$$S_{xx}(\omega) = \frac{\pi\omega_m\varepsilon_c}{m\omega_0^2(\varepsilon_c - \varepsilon_P)\omega|\omega'(0)|} \frac{\omega - \omega_m}{\omega'(0)T_{\text{eff}}} e^{-\frac{\omega - \omega_m}{\omega'(0)T_{\text{eff}}}}. \quad (13)$$

From Eq. (13) and Fig. 1 we see that the spectral density is defined for $\omega > \omega_m$ (there is actually an upper bound of the order of ω_0 , but the effective temperature being very low this limit is not visible) and has a maximum at

$\omega = \omega_m + \omega'(0)T_{\text{eff}}$. The full width at half maximum (FWHM) of the spectral line $\Delta\omega$ reads

$$\Delta\omega = \Delta_2\omega'(0)T_{\text{eff}}, \quad (14)$$

where $\Delta_2 \approx 2.446$ is a numerical coefficient corresponding to the FWHM in Fig. 1.

We thus find that the effect of the non-linearity on the width of the resonance is linear with the bias voltage eV and controlled by $\omega'(0)$, at least as far as the quartic terms does not become dominant. We will estimate at the end of the next subsection the limit of validity of this approach by comparing with the result of the purely quartic term.

C. Case (ii) purely quartic oscillator

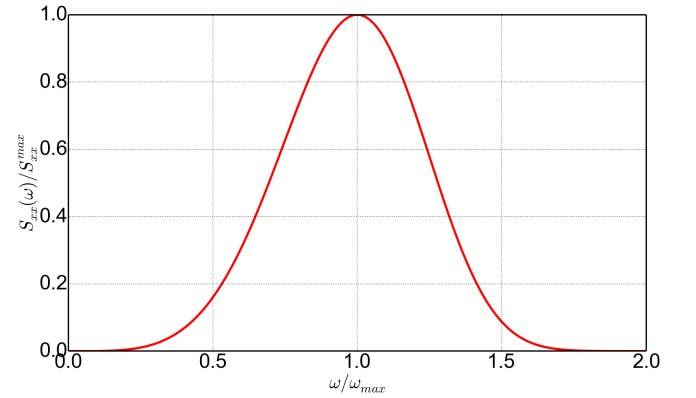


FIG. 2. Normalized displacement spectral density $S_{xx}(\omega)/S_{xx}^{max}$ as a function of the rescaled frequency ω/ω_{max} , at the critical point ($\varepsilon_P = \varepsilon_c$). The spectral line maximum is located at frequency $\omega_{max} = B\omega_0 (eV/4\Gamma)^{1/4}$.

At the critical point ($\varepsilon_P = \varepsilon_c$), the quadratic part of the potential vanishes and the mechanical oscillator becomes purely quartic. In this regime, we obtain for the oscillator frequency:

$$\frac{\omega(E)}{\omega_0} = B \left(\frac{E}{\Gamma} \right)^{1/4}, \quad (15)$$

with $B = \frac{1}{2} \left(\frac{\pi^3}{3} \right)^{1/4} \frac{\Gamma[3/4]}{\Gamma[5/4]} \approx 1.212$ a numerical constant and $\Gamma[x]$ the Euler gamma function [2]. The oscillator frequency has thus a scaling in energy $\propto (E/\Gamma)^{1/4}$.

Remarkably, the displacement spectral density of the quartic oscillator also has a simple analytical expression:

$$S_{xx}(\omega) = \tilde{B} \frac{\Gamma^2}{\omega_0 F_0^2} \left(\frac{\Gamma}{T_{\text{eff}}} \right)^{3/4} \sum_{n=1}^{+\infty} e^{-E_n/T_{\text{eff}}} \frac{\alpha_n^2 E_n}{n\Gamma}, \quad (16)$$

where $\tilde{B} = 16 \cdot 3^{3/4} \pi^{1/4} f(1) / \Gamma[3/4]$ is a numerical constant. $\alpha_n = \int_{-1}^1 du \frac{u}{f(1)\sqrt{1-u^4}} \cos\left(n\pi \frac{f(u)}{f(1)}\right)$ is a parameter depending on the harmonic index n and involving the integral function $f(u) = \int_{-1}^u dv / \sqrt{1-v^4}$. The energy $E_n = (3^{1/4} f(1) \omega / \pi^{5/4} n \omega_0)^4 \Gamma$ satisfies the equation $\omega = n\omega(E_n)$. We evaluate numerically the values of α_n for the first harmonics: $\alpha_1 \approx -0.477$, $\alpha_3 \approx -0.021$ and $\alpha_5 \approx -9.3 \cdot 10^{-4}$. In Eq. (16), the main contribution to $S_{xx}(\omega)$ is given by the first harmonic $n = 1$, the other harmonics $n \geq 3$ having a smaller weight. The normalized line shape of the displacement spectral density can be further approximated, retaining only the contribution of the first harmonic by:

$$\frac{S_{xx}(\omega)}{S_{xx}(\omega_{max})} \approx \left(\frac{\omega}{\omega_{max}}\right)^4 e^{-[(\frac{\omega}{\omega_{max}})^4 - 1]}, \quad (17)$$

where $\omega_{max} = B\omega_0 (T_{eff}/\Gamma)^{1/4}$ is the position of the maximum of the spectral density. From Eq. (17) and Fig. 2, we see that the spectral density has a different line shape compared to the weak non linear oscillator in Fig. 1. Its FWHM is given by:

$$\Delta\omega = \Delta_4 \omega_{max}. \quad (18)$$

where $\Delta_4 \approx 0.585$ is a numerical coefficient corresponding to the FWHM in Fig. 2. Finally, we get $\Delta\omega \approx 0.709\omega_0 (T_{eff}/\Gamma)^{1/4}$.

In contrast to the quasi-harmonic oscillator [see Eq. (14)], the resonance width of the quartic oscillator at the critical point does not scale linearly with the effective temperature, but with a scaling law $\propto (T_{eff}/\Gamma)^{1/4}$. Let's finally find the range of validity of the approximation used in Sec. IB. We first remark that $\Delta\omega$ in Eq. (14) diverges close to the transition, signaling the breakdown of the quasi-harmonic approximation. At the transition, $\Delta\omega$ expressed in Eq. (18) is finite. We estimate the crossover between both regions to happen when both estimations of the resonance width $\Delta\omega$ in Eq. (14) and in Eq. (18) are equal. We find that the crossover between the two regimes takes place for $1 - \varepsilon_P/\varepsilon_c \approx 1.71(eV/\varepsilon_c)^{1/2}$.

II. EVALUATION OF THE OSCILLATOR DEPHASING TIME γ_φ^{-1}

A. Linear response of the oscillator under weak driving

We now consider that the mechanical oscillator is under the influence of a weak driving force of frequency ω_D and amplitude F_D , so that the total force applied on the oscillator is $F(x) + F_D \cos(\omega_D t)$. The evolution equation for the probability distribution is then given by:

$$\partial_t P = \{\mathcal{L}_0 + 2\mathcal{L}_D \cos(\omega_D t)\} P, \quad (19)$$

where $\mathcal{L}_D = -F_D \partial_p / 2$. One can show that for weak driving, an approximate solution of Eq. (19) has the form $P(x_0, p_0, t) = P_{st}(x_0 - x_i(t), p_0 - p_i(t))$, where $x_i(t)$ and $p_i(t)$ are solutions of the equations of motion $\dot{x}_i(t) = p_i(t)/m$ and $\dot{p}_i(t) = F(x_i) + F_D \cos(\omega_D t) - A(x_i)p_i(t)/m$. Namely, the probability distribution for the oscillator in presence of driving is obtained by moving rigidly the centre of the stationary Gibbs distribution along the deterministic trajectory of the damped oscillator. If the driving is weak compared to the effective temperature, one can expand $P(x_0, p_0, t)$ to linear order in the driving strength:

$$P(x_0, p_0, t) \approx P_{st}(x_0, p_0) \left\{ 1 - \frac{x_i(t)F(x_0) - p_i(t)p_0/m}{T_{eff}} \right\}. \quad (20)$$

B. Ring-down response of the oscillator

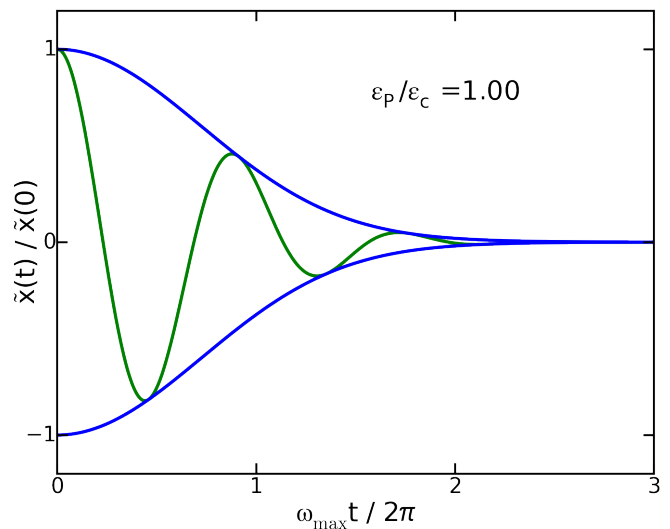


FIG. 3. Normalized ring-down displacement of the oscillator $\tilde{x}(t)/\tilde{x}(0)$ (green curve) and its envelope (blue curve) at the critical point $\varepsilon_p = \varepsilon_c$.

In the following, we suppose that the driving has been imposed far in the past. The linear response to this driving generates at time $t = 0$ an initial condition that we choose for simplicity to be $x_i(0) = x_i$ and $p_i(0) = 0$. At this same time $t = 0$, the driving is suddenly switched off and the system is let relaxing toward equilibrium. The ring-down dynamics at time $t > 0$ is encoded into the average response of the oscillator displacement $x(t) = \int \int dx_0 dp_0 P(x_0, p_0, 0) x_{x_0, p_0}(t)$.

Introducing $\tilde{x}_{x_0 p_0}(t) = x_{x_0 p_0}(t) - \langle x_{x_0 p_0}(t) \rangle$, we obtain from Eq. (20):

$$\tilde{x}(t) \approx -\frac{x_i}{T_{eff}} \int \int dx_0 dp_0 P_{st}(x_0, p_0) F(\tilde{x}_0) \tilde{x}_{x_0, p_0}(t), \quad (21)$$

which can be rewritten as:

$$\tilde{x}(t) \approx -\frac{x_i}{T_{\text{eff}}} \int_0^{+\infty} dE \int_0^{T(E)} dt P_{st}(E) F[\tilde{x}_E(0)] \tilde{x}_E(t). \quad (22)$$

Similarly to Sec.I, we perform the Fourier expansion of the periodic trajectories $\tilde{x}_E(t) = \sum_n e^{in\omega(E)t} x_n(E)$. In the case where $\varepsilon_P < \varepsilon_c$, the electronic force acting upon the oscillator is given by Eq. (7). We can further perform the average over energy and phase of the orbit in Eq. (22):

$$\tilde{x}(t) \approx \frac{x_i}{T_{\text{eff}}} \int_0^{+\infty} dE \mathcal{P}(E) \left\{ m\omega_m^2 \sum_n x_n^2(E) e^{in\omega(E)t} + \sum_{\{n_i\}} \frac{F_0^4 x_{n_1}(E) x_{n_2}(E) x_{n_3}(E) x_{n_4}(E)}{3\pi m \Gamma^3} e^{in_4\omega(E)t} \delta_{n_4, \sum_{j=1}^3 n_j} \right\}. \quad (23)$$

Eq. (23) enables to compute the ring-down dynamics of the oscillator displacement $\tilde{x}(t)$ as well as to extract a characteristic dephasing time γ_φ^{-1} of the mechanical oscillator.

In the following, we derive analytical expressions for $\tilde{x}(t)$ for the two limiting cases (i) where the quartic term is a small perturbation to the quadratic one, and (ii) when the quadratic term vanishes (for $\varepsilon_P = \varepsilon_c$) and the potential is purely quartic in x .

1. Case (i) weakly non linear oscillator

Far from the transition ($\varepsilon_P < \varepsilon_c$), the oscillator is weakly non-linear, and we can use the same approximations as in Sec.IB to derive from Eq. (23) an analytical expression for the oscillator displacement:

$$\tilde{x}(t) \approx x_i \frac{\left(1 - (\gamma_\varphi t)^2\right) \cos(\omega_m t) - 2\gamma_\varphi t \sin(\omega_m t)}{\left(1 + (\gamma_\varphi t)^2\right)^2}, \quad (24)$$

where the dephasing time γ_φ^{-1} of the oscillator is given by:

$$\gamma_\varphi^{-1} = \frac{1}{\omega'(0)T_{\text{eff}}}. \quad (25)$$

Eq. (25) shows that after the driving has been switched off, the oscillator follows an oscillating behaviour given by the natural frequency of the vibration $\omega_m = \omega(0)$. This fast oscillation decays as a power law.

As expected, we find that the typical decay or dephasing time γ_φ^{-1} of the oscillator is inversely proportional to the broadening of the displacement spectral density $\Delta\omega$ [see Eq. (14)], namely:

$$\Delta\omega = \Delta_2 \gamma_\varphi. \quad (26)$$

C. Case (ii) purely quartic oscillator

At the critical point ($\varepsilon_P = \varepsilon_c$), the quadratic part of the potential vanishes and the mechanical oscillator becomes purely quartic. We adopt the same approximations as in Sec.IC to derive from Eq. (23) an analytical expression for the oscillator displacement:

$$\frac{\tilde{x}(t)}{\tilde{x}(0)} \approx \frac{1}{\Gamma[7/4]} \int_0^{+\infty} dy y^{3/4} e^{-y} \cos(\omega_{max} y^{1/4} t), \quad (27)$$

where the frequency $\omega_{max} = B\omega_0 (T_{\text{eff}}/\Gamma)^{1/4}$ is the same as in Sec.IC. The oscillator displacement in Eq. (27) is plotted in Fig. 3.

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- [1] M. Dykman, S. Soskin, and M. Krivoglaz, *Physica A: Statistical Mechanics and its Applications* **133**, 53 (1985).
 [2] M. Abramowitz and I. A. Stegun, *Handbook of mathematical functions: with formulas, graphs, and mathematical tables*, 55 (Courier Corporation, 1964).