Spectrum and Franck-Condon factors of interacting SWCNT

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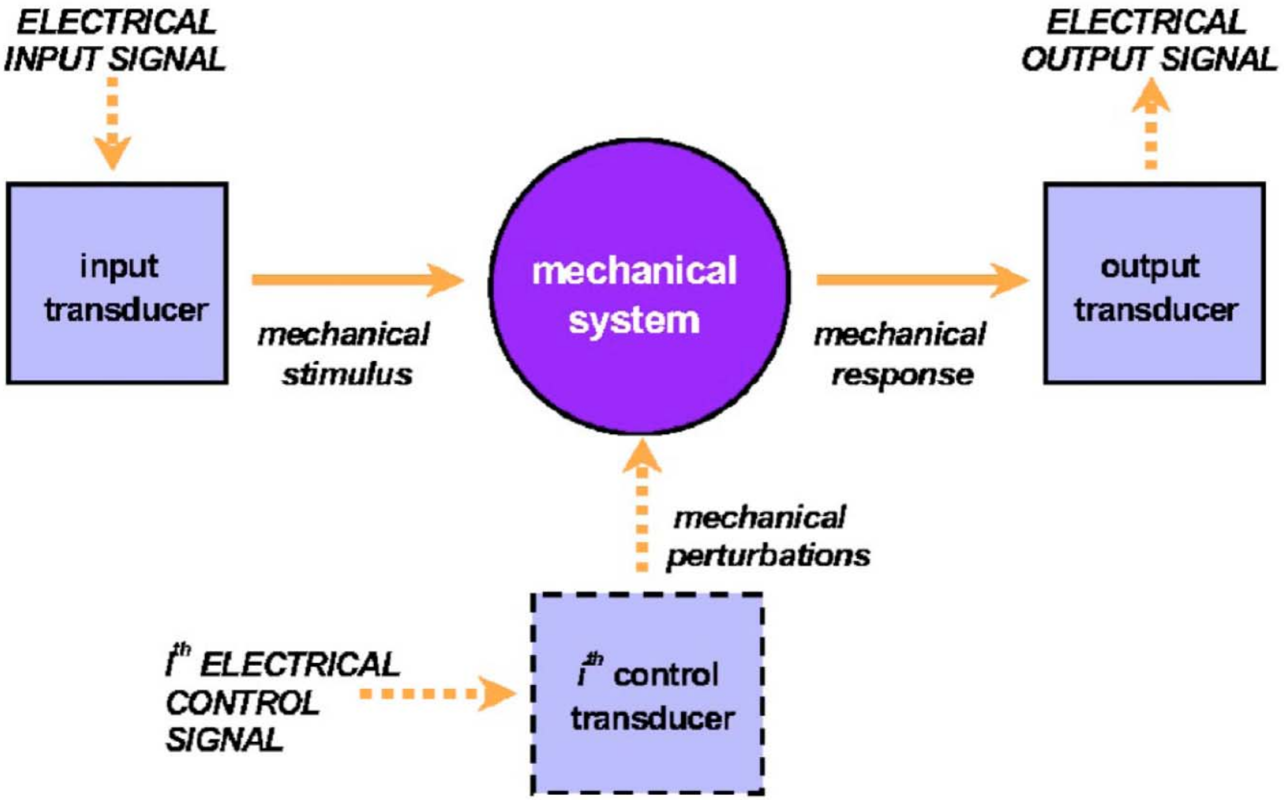
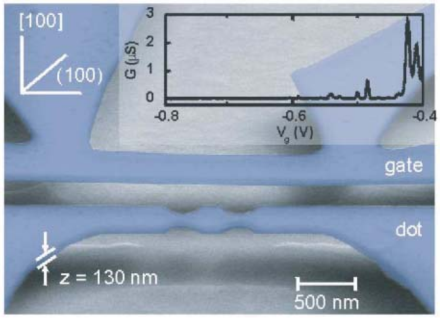
A. Donarini, A. Yar and M. Grifoni, *New Journal of Physics* **14**, 023045 (2012)

Nanoelectromechanical systems

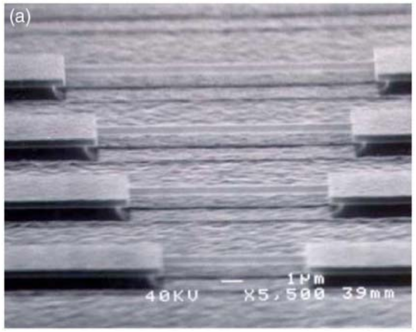


K. L. Ekinci and M. L. Roukes, *Rev. Sci. Instrum.* **76**, 061101 (2005)

Different realizations of NEMS

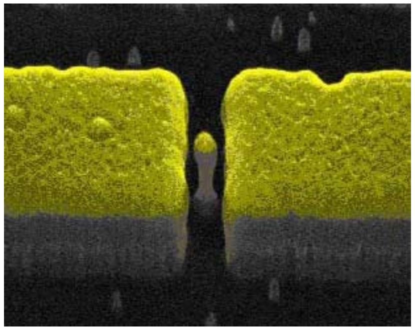


Weig et al. *PRL* **92**, 046804 (2004)

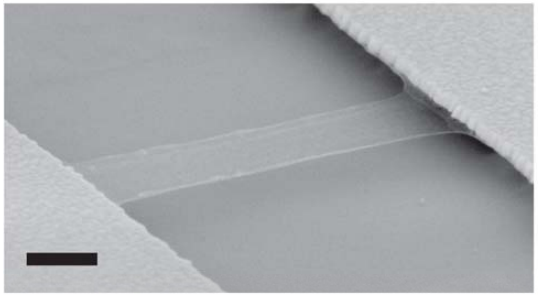


Ekinci and Roukes

Rev. Sci. Instrum. **76**, 061101 (2005)

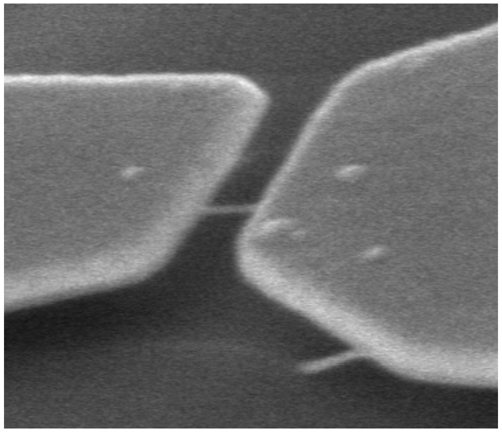


Kim et al. *New J. Phys.* **12**, 033008 (2010)



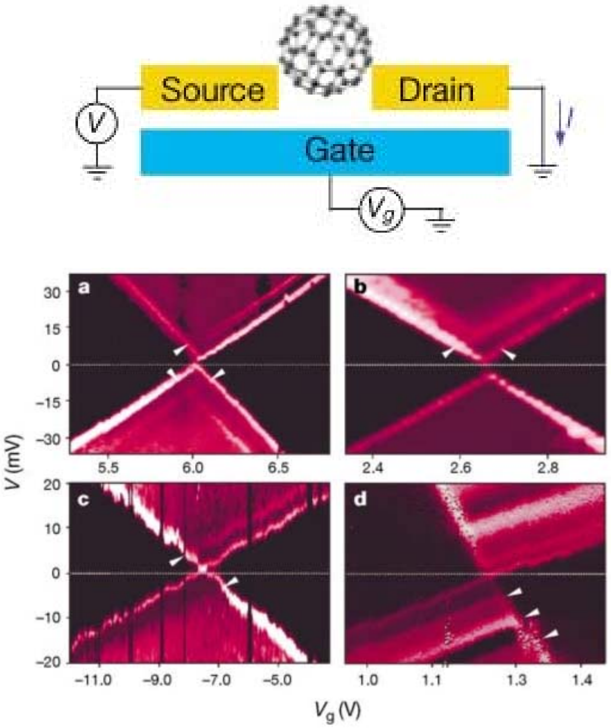
Eichler et al.

Nat. Nanotech. **6**, 339 (2011)

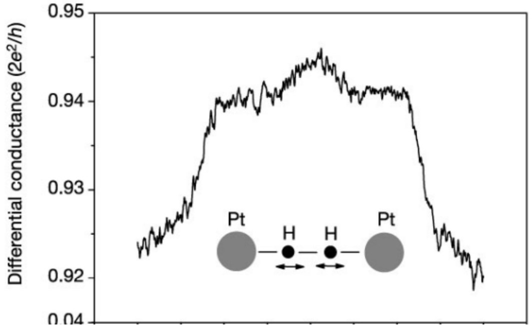


Sapmaz et al.

PRL **96**, 026801 (2006)

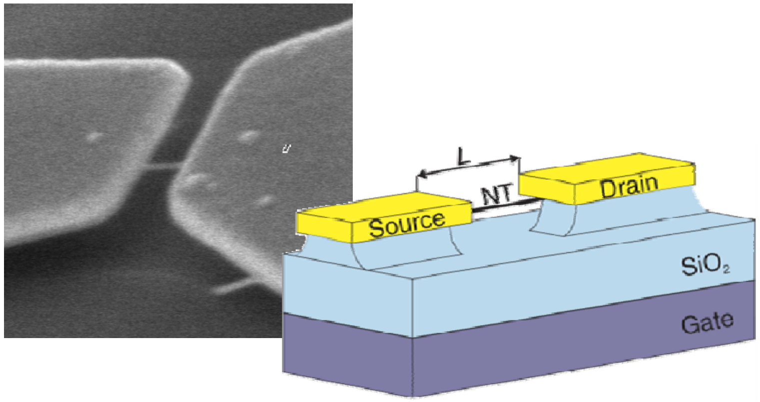


H. Park et al. *Nature* **407**, 57 (2000)

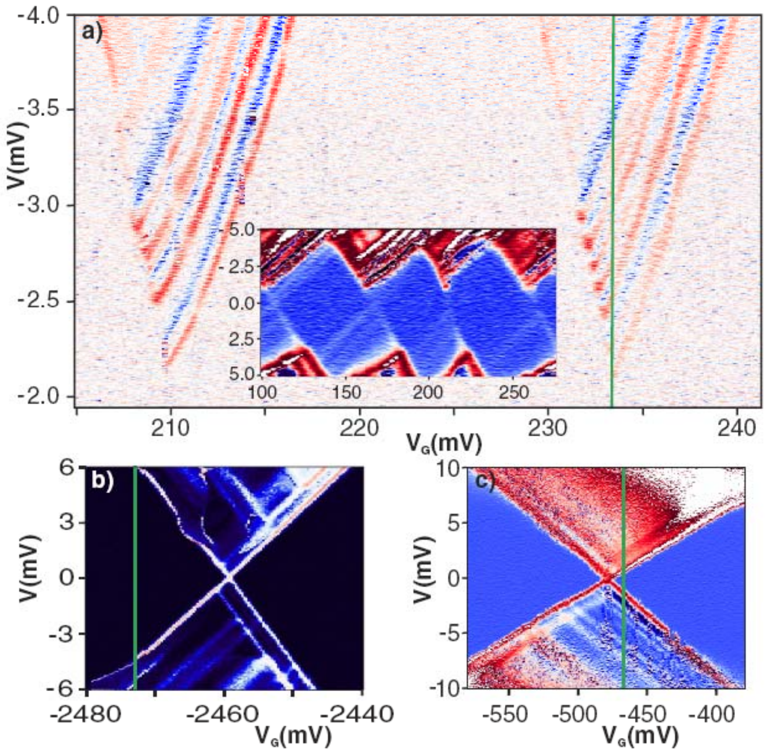


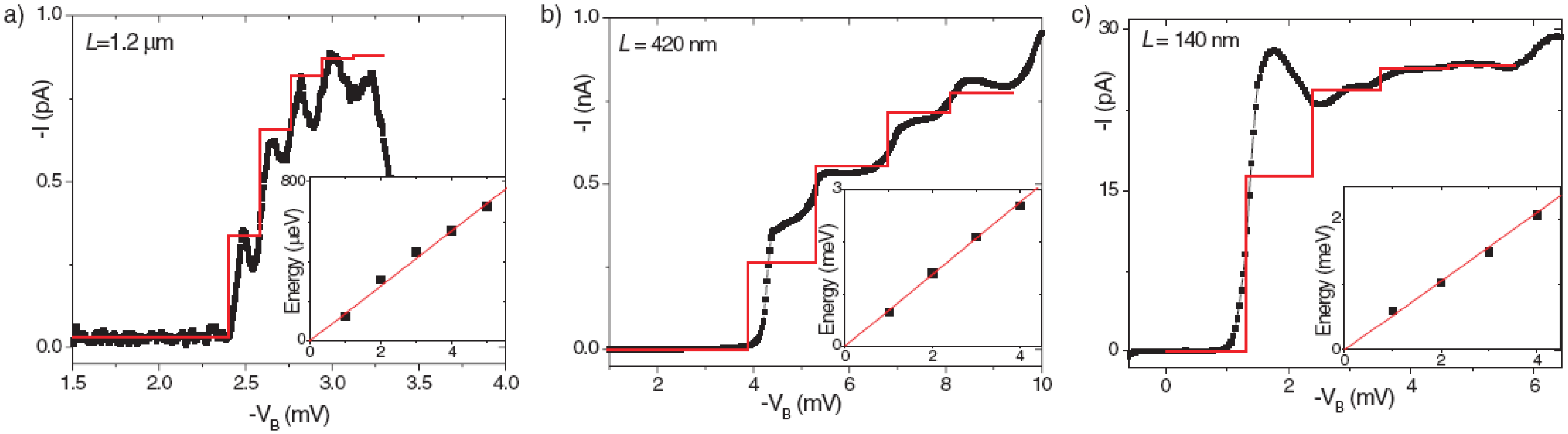
Smit et al. *Nature* **419**, 906 (2002)

Carbon nanotubes NEMS



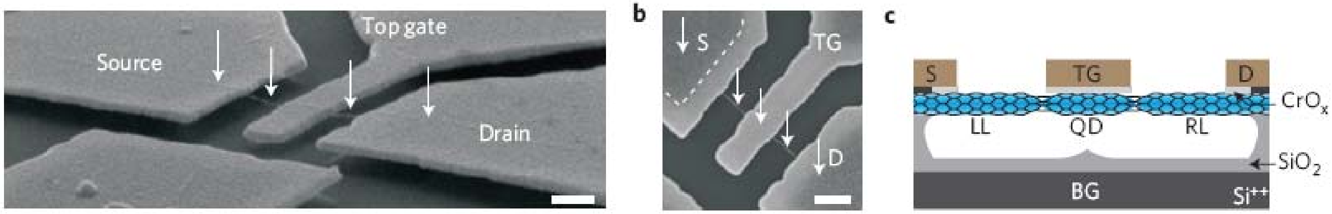
Sapmaz et al.
PRL **96**, 026801 (2006)

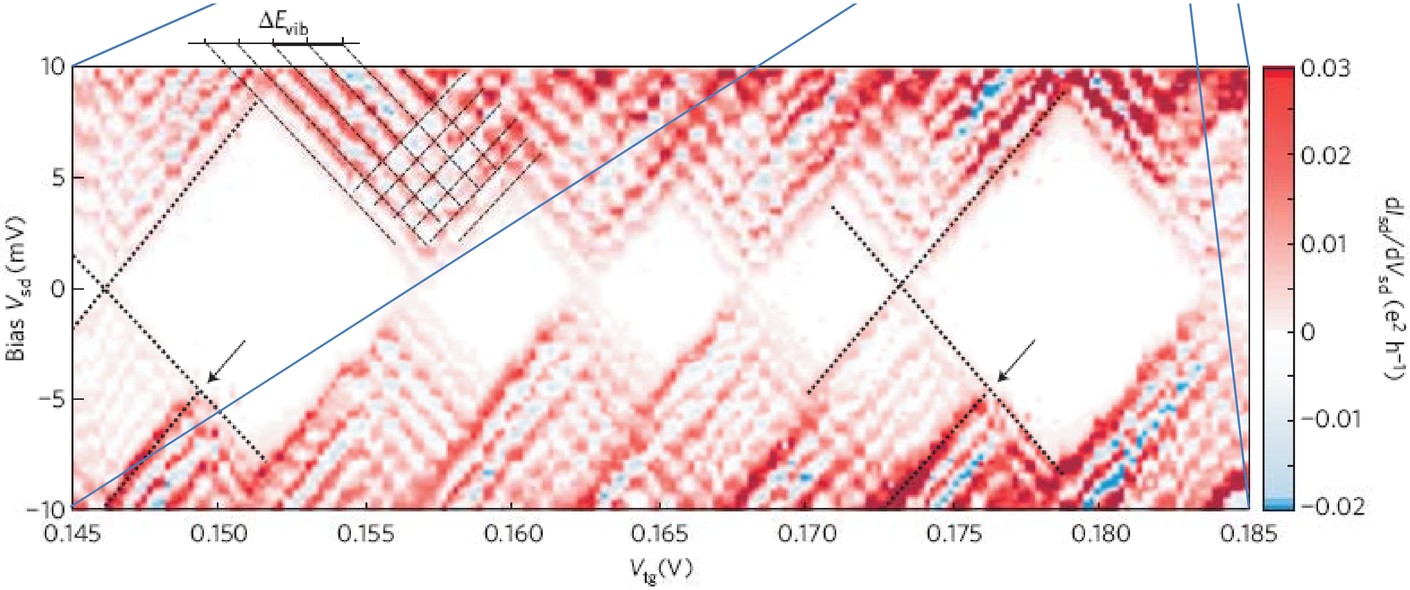




Carbon nanotubes NEMS

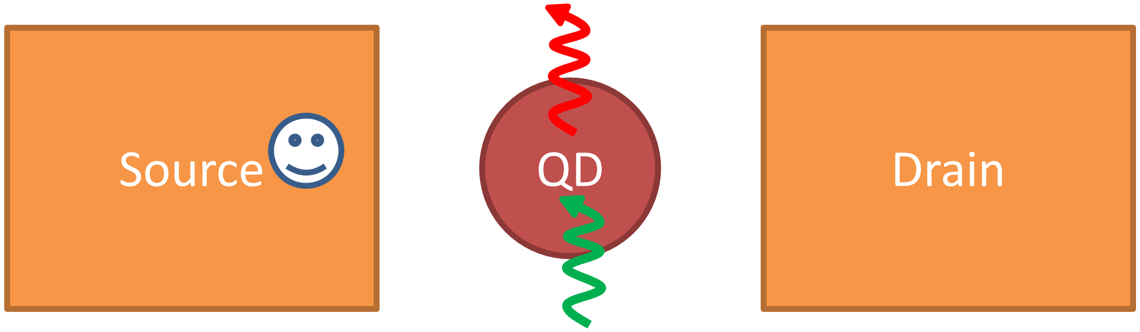
R. Leturcq et al. *Nat. Phys.* **5**, 327 (2009)

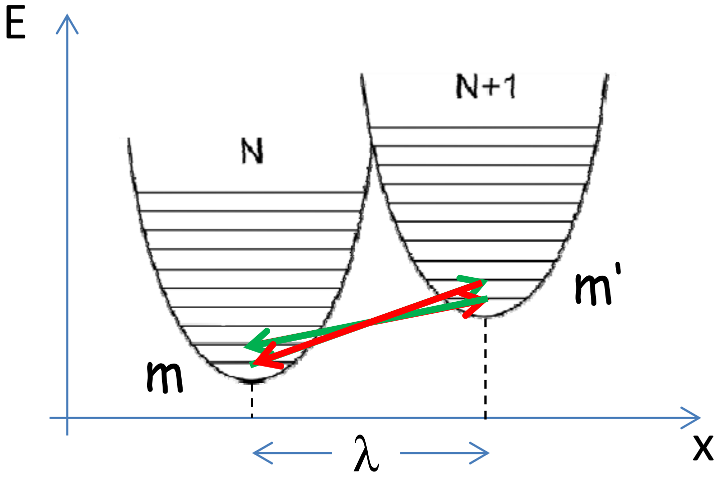


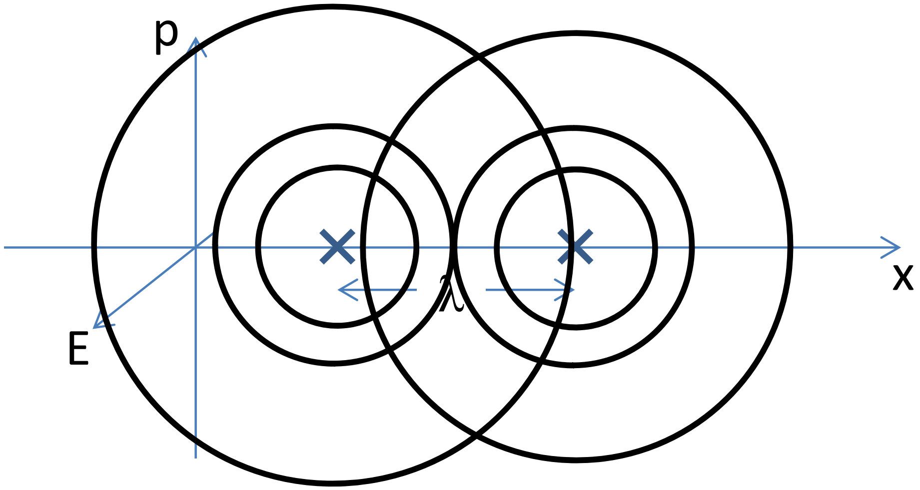


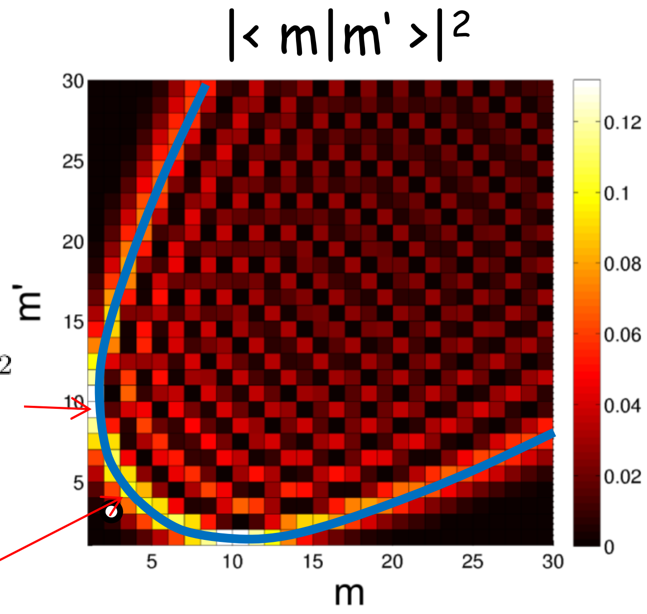
Franck Condon physics

$$H_S = \hbar\omega\left[(x^2+p^2) - 2n\lambda x\right] + \epsilon_0 n$$







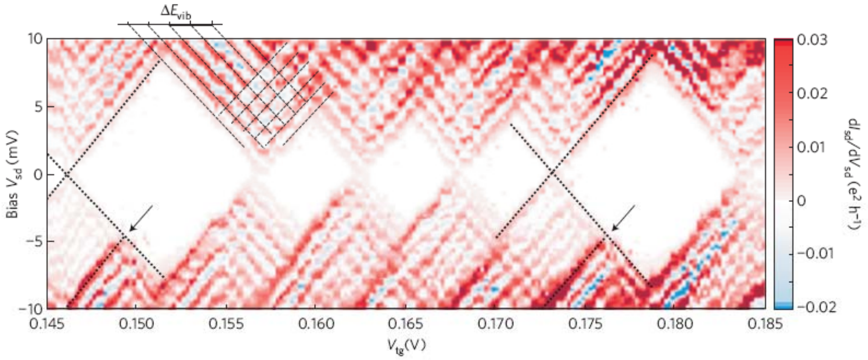


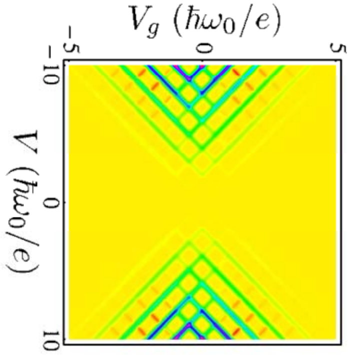
$m' = \lambda^2$
$m = 0$

$m = m' = (\lambda/2)^2$

Success of the „simple“ theory

1) It explains the **current blocking** at low bias (but above the Coulomb blockade threshold)

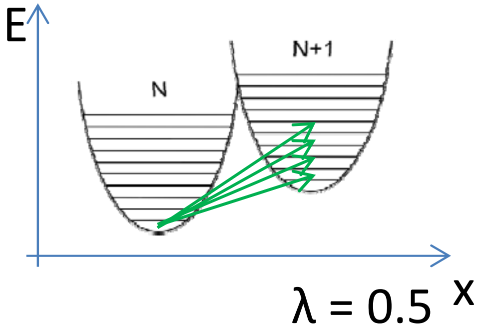




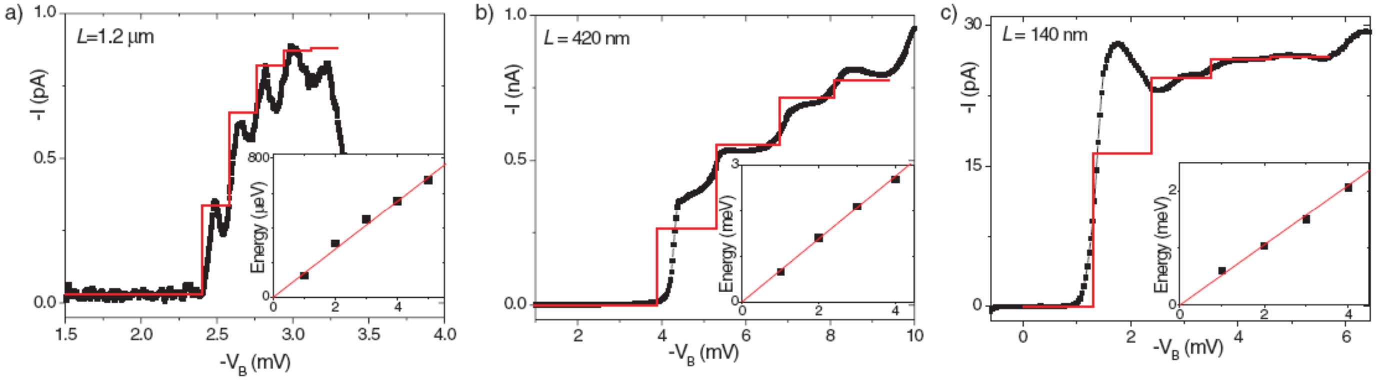
Koch and von Oppen
PRL **94** 206804 (2005)

2) Correctly predicts the **heights of the steps in the current** (for equilibrated phonons)

$$\delta I_n \propto |\langle 0|n\rangle|^2 = \frac{\lambda^{2n}}{n!}e^{-\lambda^2}$$



λ = 0.95 λ = 1.1 λ = 0.5



Sapmaz et al.
PRL **96**, 026801 (2006)

Opening of new questions

1) The **magnitude** of the dimensionless electron-phonon coupling.

$\lambda \approx 1$

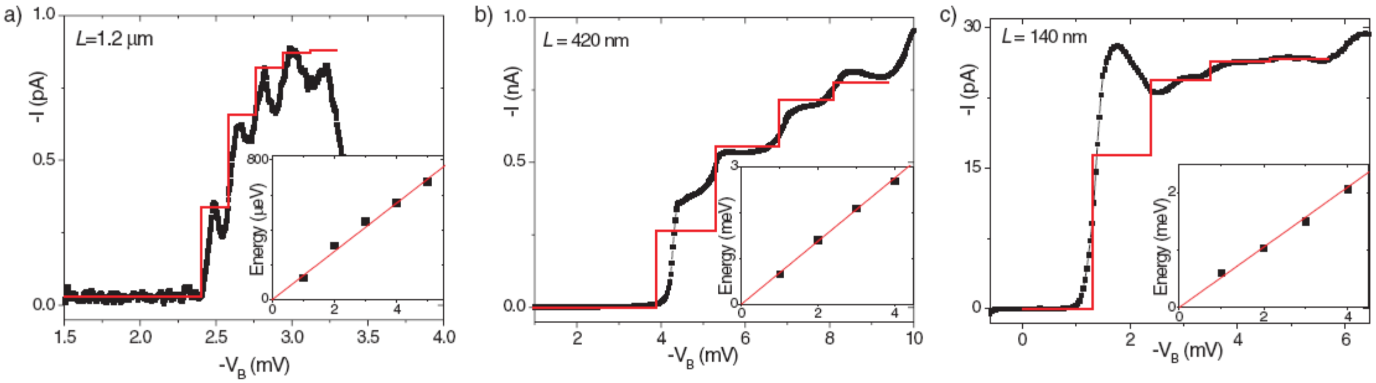
Anderson-Holstein model
fitting the experiments

$\lambda \approx 10^{-4}$

Microscopic
derivation

Izumida and Grifoni *New J. Phys.* **7** 244 (2005)
Flensberg *New J. Phys.* **8** 5 (2006)
Cavaliere et al *Phys. Rev. B* **81** 201303 (2010)

2) Missing explanation for the **current PEAKS** present in the experiments.



Importance of the geometry

Asymmetric Franck-Condon factors in suspended carbon nanotube quantum dots

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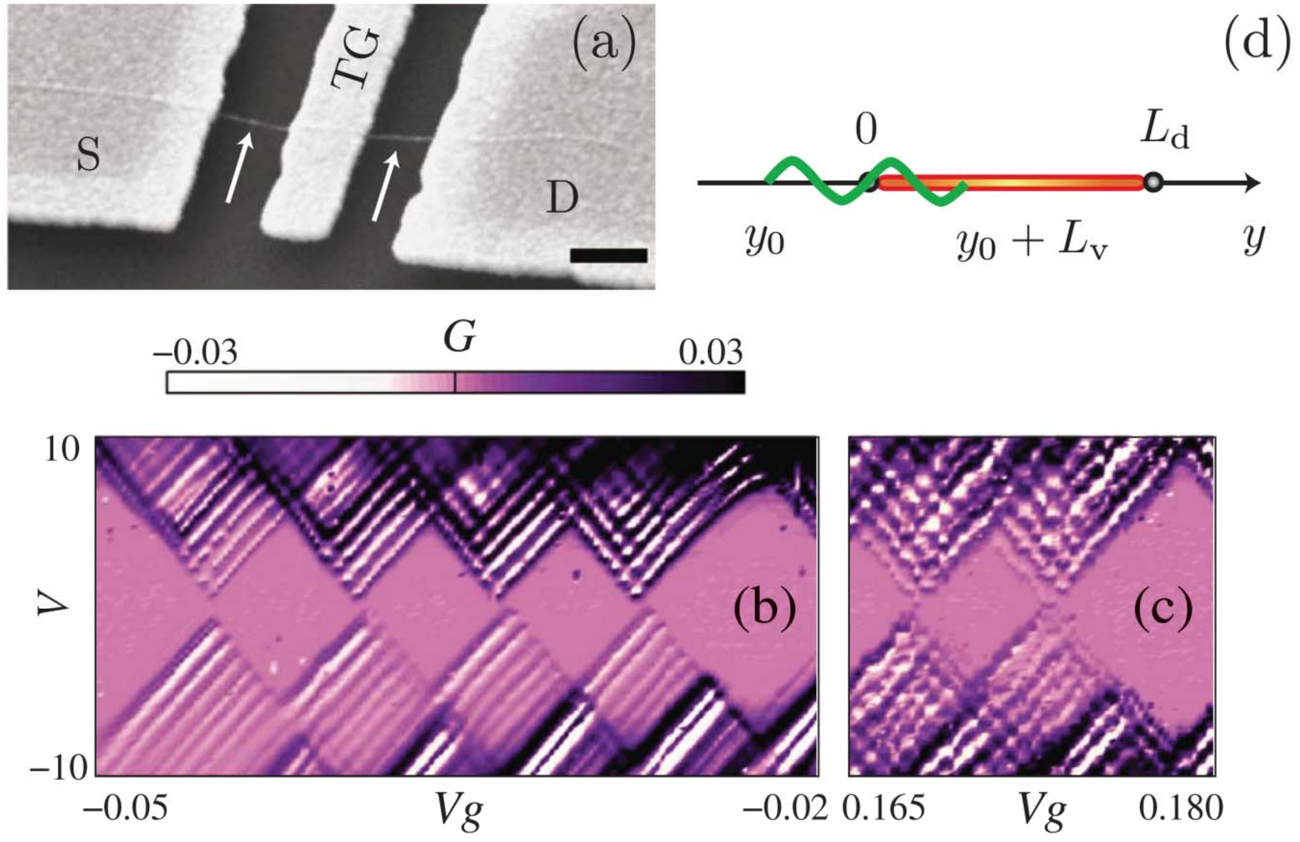

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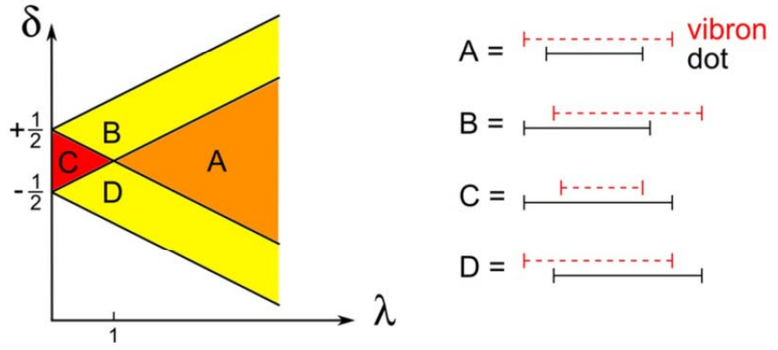
Short vibron close to the nanotube end ➡ **Position dependent** Franck-Condon factors

Strongly **screened** Coulomb interaction ➡ **Large** Franck-Condon factors

Only **one** stretching mode considered ➡ **Geometrical tunability** of the tunnelling amplitude and **NDC**

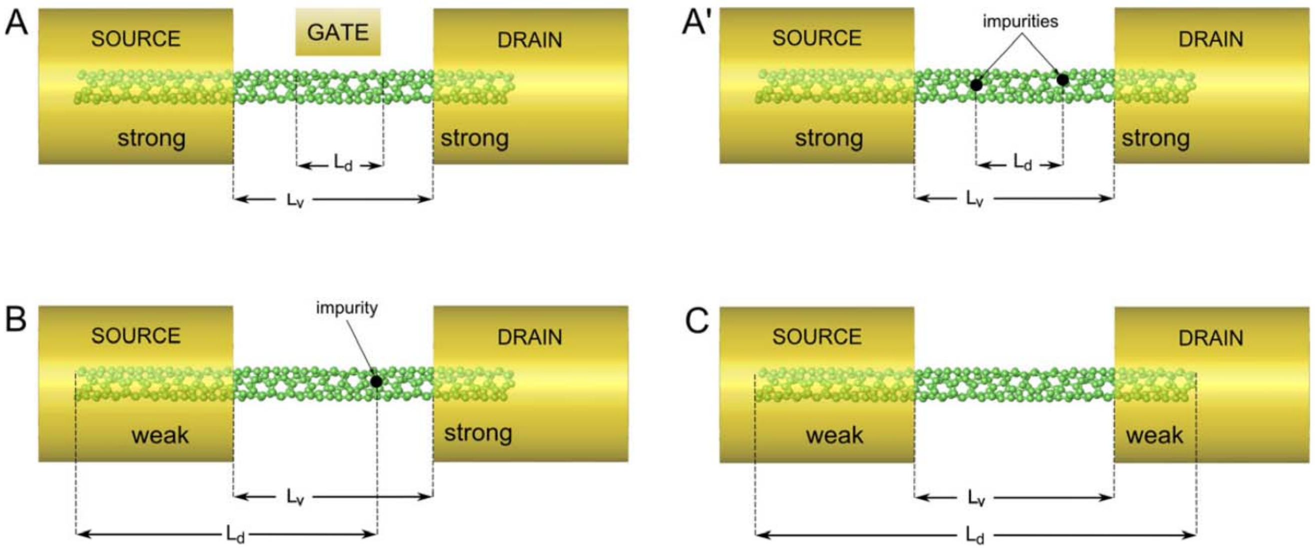
Extension of the model (i)

We studied the **entire** parameter space



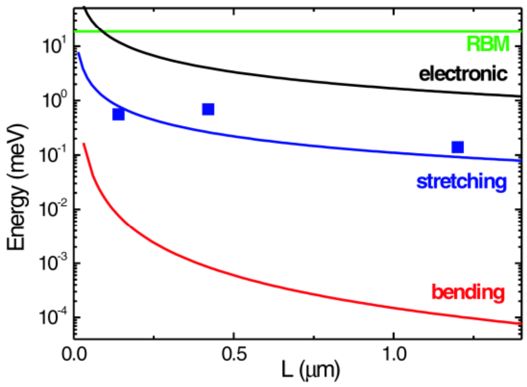
$$\lambda = L_{\rm v}/L_{\rm d}$$

$$\delta = (x_{\rm v} - x_{\rm d})/L_{\rm d}$$



Extension of the model (ii)

- We analyzed **multimode degenerate** vibronic configurations

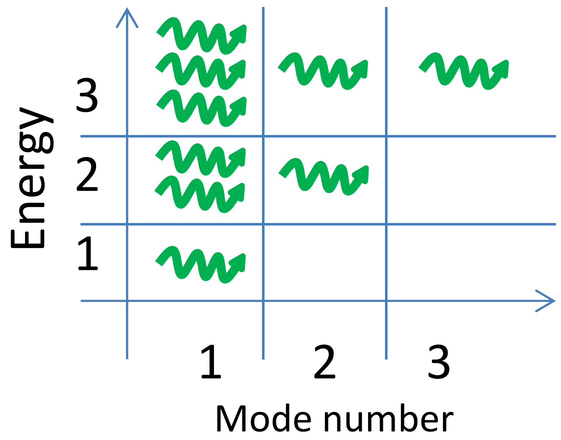


PRL **96**, 026801 (2006)

Degenerate states are a necessary condition for interference effects with associated negative differential conductance.

The stretching mode has **linear dispersion relation**

$$\omega_n = n\omega_1$$



- We considered **unscreened** Coulomb interaction on the nanotube

(Dimensionless e-e interaction strength $g_{c+} = 0.2$)

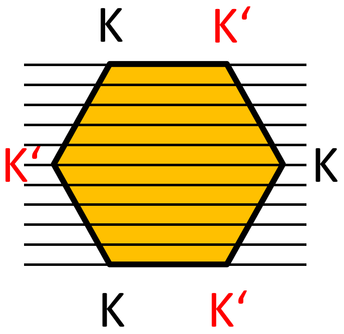
Low energy Hamiltonian of a SWCNT

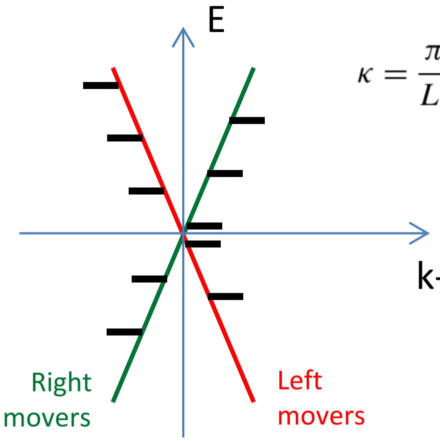
We consider the Hamiltonian of the form:

$$\hat{H}_{\mathrm{sys}} = \hat{H}_0 + \hat{V}_{\mathrm{ee}} + \hat{H}_{\mathrm{v}} + \hat{H}_{\mathrm{ev}}$$

Single particle: (metallic) nanotube with open boundary conditions

$$\hat{H}_0 = \hbar v_{\mathrm{F}} \sum_{r\sigma} r \sum_{\kappa} \kappa \hat{c}^{\dagger}_{r\sigma\kappa} \hat{c}_{r\sigma\kappa}$$





$$\kappa = \frac{\pi}{L_{\mathrm{d}}}(n_\kappa + \Delta)$$

Coulomb interaction: full form

$$\hat{V}_{\mathrm{ee}} = \frac{1}{2} \sum_{\sigma,\sigma'} \int \mathrm{d}\vec{r} \int \mathrm{d}\vec{r}' \hat{\Psi}^{\dagger}_{\sigma}(\vec{r}) \hat{\Psi}^{\dagger}_{\sigma'}(\vec{r}') U(\vec{r}-\vec{r}') \hat{\Psi}_{\sigma'}(\vec{r}') \hat{\Psi}_{\sigma}(\vec{r})$$

$$\hat{\Psi}_{\sigma}(\vec{r}) = \sum_{r\kappa} \varphi_{r\kappa}(\vec{r}) \hat{c}_{r\sigma\kappa}$$

Ohno potential $U(\vec{r}-\vec{r}') = U_0 \left[1 + \left(\frac{U_0 \epsilon |\vec{r}-\vec{r}'|}{\alpha} \right)^2 \right]^{-1/2}$

Tomonaga-Luttinger SWCNT

Different processes are represented by the **Coulomb Hamiltonian**:

Forward

~~Backward~~

Not too small tubes

~~Umklapp~~

Away from half filling

We can rewrite the Hamiltonian in the **Tomonaga Luttinger** form:

$$\hat{H}_0 + \hat{V}_{\mathrm{ee}} \approx \hat{H}_{\mathrm{TL}} = \hat{H}_{\mathrm{N}} + \sum_j \hat{H}_j$$

where

$$\hat{H}_{\mathrm{N}} = \frac{\varepsilon_0}{4} \sum_j \frac{\hat{N}_j^2}{2} + \varepsilon_\Delta \hat{N}_{c-} + E_{\mathrm{c}} \frac{\hat{N}_{c+}^2}{2}$$

Fermionic excitations

+

Charging effects

$$\hat{N}_{c+} = \textstyle\sum_{r\sigma} \hat{N}_{r\sigma}$$
$$\hat{N}_{c-} = \textstyle\sum_{r\sigma} \mathrm{sgn}(r) \hat{N}_{r\sigma}$$
$$\hat{N}_{s+} = \textstyle\sum_{r\sigma} \mathrm{sgn}(\sigma) \hat{N}_{r\sigma}$$
$$\hat{N}_{s-} = \textstyle\sum_{r\sigma} \mathrm{sgn}(r\sigma) \hat{N}_{r\sigma}$$

and

$$\hat{H}_j = \frac{\varepsilon_0}{g_j} \sum_{n \geqslant 1} n \, \hat{b}^{\dagger}_{j,n} \hat{b}_{j,n}$$

Bosonic excitations

$$\varepsilon_0 = \hbar v_{\mathrm{F}} \tfrac{\pi}{L_{\mathrm{d}}}$$
$$g_{c+} \approx 0.2$$
$$g_j = 1 \text{ for the other cases.}$$

Vibrons: a continuum model

$$\hat{H}_{\mathrm{v}} = \frac{1}{2}\int_{x_{\mathrm{v}}-\frac{L_{\mathrm{v}}}{2}}^{x_{\mathrm{v}}+\frac{L_{\mathrm{v}}}{2}} \mathrm{d}x \left[\frac{1}{\zeta}\hat{P}^2(x) + \zeta\, v_{\mathrm{st}}^2 \left(\partial_x \hat{u}(x)\right)^2\right]$$

Continuum model
for the **stretching motion**

$\zeta = 2\pi\, R M$

$M = 3.80 \times 10^{-7}\,\mathrm{kg\,m^{-2}}$

$v_{\mathrm{st}} = 2.4 \times 10^{4}\,\mathrm{m\,s^{-1}}$

where

$$\hat{u}(x) = \sqrt{\frac{\hbar}{\zeta\, v_{\mathrm{st}} L_{\mathrm{v}}}} \sum_{m \geqslant 1} \sin\left[k_m\left(x - x_{\mathrm{v}} + \frac{L_{\mathrm{v}}}{2}\right)\right] \frac{1}{\sqrt{k_m}} \left(\hat{a}_m^{\dagger} + \hat{a}_m\right)$$

Displacement field operator

$k_m = m\pi / L_{\mathrm{v}}$

$$\hat{P}(x) = \mathrm{i}\sqrt{\frac{\hbar\zeta\, v_{\mathrm{st}}}{L_{\mathrm{v}}}} \sum_{m \geqslant 1} \sin\left[k_m\left(x - x_{\mathrm{v}} + \frac{L_{\mathrm{v}}}{2}\right)\right] \sqrt{k_m} \left(\hat{a}_m^{\dagger} - \hat{a}_m\right)$$

Associated momentum

Finally

$$\hat{H}_{\mathrm{v}} = \sum_{m \geqslant 1} E_m \left(\hat{a}_m^{\dagger}\hat{a}_m + \frac{1}{2}\right) \qquad E_m = m\hbar v_{\mathrm{st}}\pi / L_{\mathrm{v}} \equiv m\hbar\omega.$$

Electron-vibron hamiltonian (i)

$$\hat{\rho}(\vec{r}) = \textstyle\sum_\sigma \hat{\Psi}^\dagger_\sigma(\vec{r})\hat{\Psi}_\sigma(\vec{r})$$

electron density

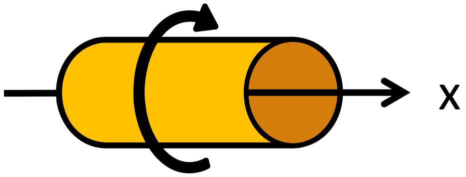
$$\hat{H}_{\rm ev} = \int \mathrm{d}\vec{r}\,\hat{\rho}(\vec{r})\hat{V}(\vec{r})$$

$$\hat{V}(\vec{r}) = g\partial_x\hat{u}(x)$$

deformation potential

$$g \approx 20\text{–}30\,\mathrm{eV}$$

3D to 1D



$$\hat{H}_{\rm ev} = g\sum_{m\geqslant 1}\left(\frac{\hbar k_m}{\zeta v_{\rm st}L_{\rm v}}\right)^{1/2}\underbrace{(\hat{a}^\dagger_m + \hat{a}_m)}_{\text{Vibronic coordinate}}\int_{\rm d\cap v}\mathrm{d}x\,\hat{\rho}_{\rm 1D}(x)\cos\left[k_m\left(x - x_{\rm v} + \frac{L_{\rm v}}{2}\right)\right]$$

Dot-vibron overlap

$$\hat{\rho}_{\rm 1D}(x) = \frac{\hat{N}_{c+}}{L_{\rm d}} + \frac{2}{\sqrt{\pi\hbar}}\partial_x\hat{\phi}_{c+}(x)$$

Density: **uniform** + **oscillating** components

$$\hat{\phi}_{c+}(x) = \sqrt{\frac{\hbar g_{c+}}{L_{\rm d}}}\sum_{n\geqslant 1}\sin\left[k_n\left(x - x_{\rm d} + \frac{L_{\rm d}}{2}\right)\right]\frac{1}{\sqrt{k_n}}\underbrace{(\hat{b}^\dagger_{c+,n} + \hat{b}_{c+,n})}_{\text{Plasmonic coordinate}}$$

$$k_n = n\pi/L_{\rm d}$$

Electron-vibron hamiltonian (ii)

$$\hat{H}_{\text{ev}} = I\sqrt{g_{c+}} \sum_{n,m\geqslant 1} \sqrt{nm}\, K_{nm}(\lambda,\delta)\, 2\hat{X}_n \hat{x}_m + I \sum_{m\geqslant 1} \sqrt{m}\, L_m(\lambda,\delta)\sqrt{2}\,\hat{N}_{c+}\hat{x}_m$$

Bare coupling constant

$$I = g\sqrt{\frac{\hbar\pi}{\zeta\, v_{\text{st}} L_{\text{d}}^2}}$$

Dimensionless geometric parameters

$$\lambda = L_{\text{v}}/L_{\text{d}}$$

$$\delta = (x_{\text{v}} - x_{\text{d}})/L_{\text{d}}$$

Plasmon and vibron coordinates

$$\hat{X}_n = \frac{\hat{b}_{c+,n} + \hat{b}^{\dagger}_{c+,n}}{\sqrt{2}} \qquad \hat{x}_m = \frac{\hat{a}_m + \hat{a}^{\dagger}_m}{\sqrt{2}}$$

Charge -vibron coupling ⇨

$$K_{nm}(\lambda,\delta) = \frac{1}{\lambda}\int_{x_{\min}}^{x_{\max}} \mathrm{d}x \left\{ \cos\left[\pi x\left(n + \frac{m}{\lambda}\right) - \frac{m\pi}{\lambda}\left(\delta + \frac{1-\lambda}{2}\right)\right] + \cos\left[\pi x\left(n - \frac{m}{\lambda}\right) + \frac{m\pi}{\lambda}\left(\delta + \frac{1-\lambda}{2}\right)\right]\right\}$$

Plasmon-vibron coupling ⇨

$$L_m(\lambda,\delta) = \frac{1}{\lambda}\int_{x_{\min}}^{x_{\max}} \mathrm{d}x \cos\left[\frac{m\pi}{\lambda}\left(x - \delta - \frac{1-\lambda}{2}\right)\right]$$

$$x_{\min} = \max[0, \delta + (1-\lambda)/2],$$
$$x_{\max} = \min[1, \delta + (1+\lambda)/2]$$

Energy scales

$L_\mathrm{d} = L_\mathrm{v} = 1\,\mu\mathrm{m}$

$R = 6.68\,\text{Å}$

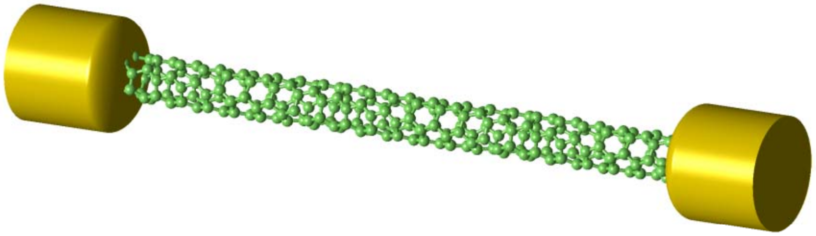
$M = 3.8 \times 10^{-7}\,\mathrm{kg\,m^{-2}}$

$g_{c+} = 0.2$

$v_\mathrm{F} = 8 \times 10^5\,\mathrm{m\,s^{-1}}$

$v_\mathrm{st} = 2.4 \times 10^4\,\mathrm{m\,s^{-1}}$

$g = 30\,\mathrm{eV}$



$$\left.\begin{array}{ll} \text{Lowest charged plasmon energy:} & \varepsilon_0/g_{c+} = 8.293\text{ meV} \\ \text{Lowest vibron energy:} & \hbar\omega = 0.050\text{ meV} \\ \text{Bare coupling constant:} & I = 0.088\text{ meV} \end{array}\right\} \hbar\omega,\, I \ll \varepsilon_0/g_{c+}$$

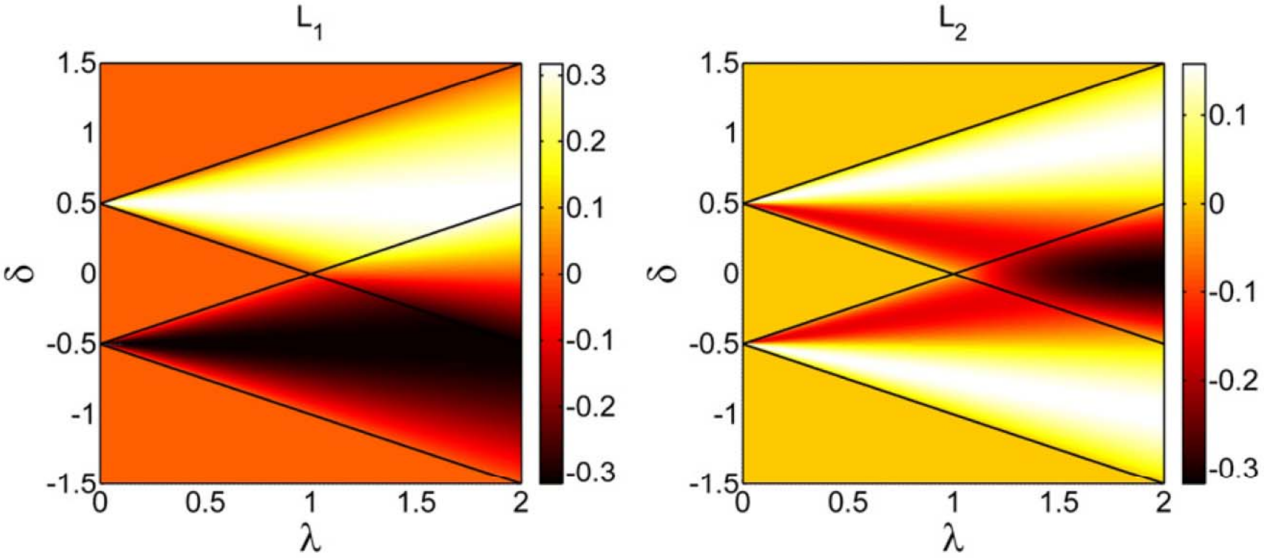
⬇

The electrical and the mechanical dynamics for an **isolated tube** are completely **independent**

BUT

The mechanical degree of freedom influences the **tunnelling dynamics** under specific geometrical conditions.

Charge-vibron coupling



$$\lambda = L_{\mathrm{v}}/L_{\mathrm{d}}$$

$$\delta = (x_{\mathrm{v}} - x_{\mathrm{d}})/L_{\mathrm{d}}$$

$$L_m^{(A)}(\lambda,\delta) = \frac{1}{m\pi}\left[\sin\left(m\pi\frac{1-2\delta+\lambda}{2\lambda}\right) + \sin\left(m\pi\frac{1+2\delta-\lambda}{2\lambda}\right)\right],$$

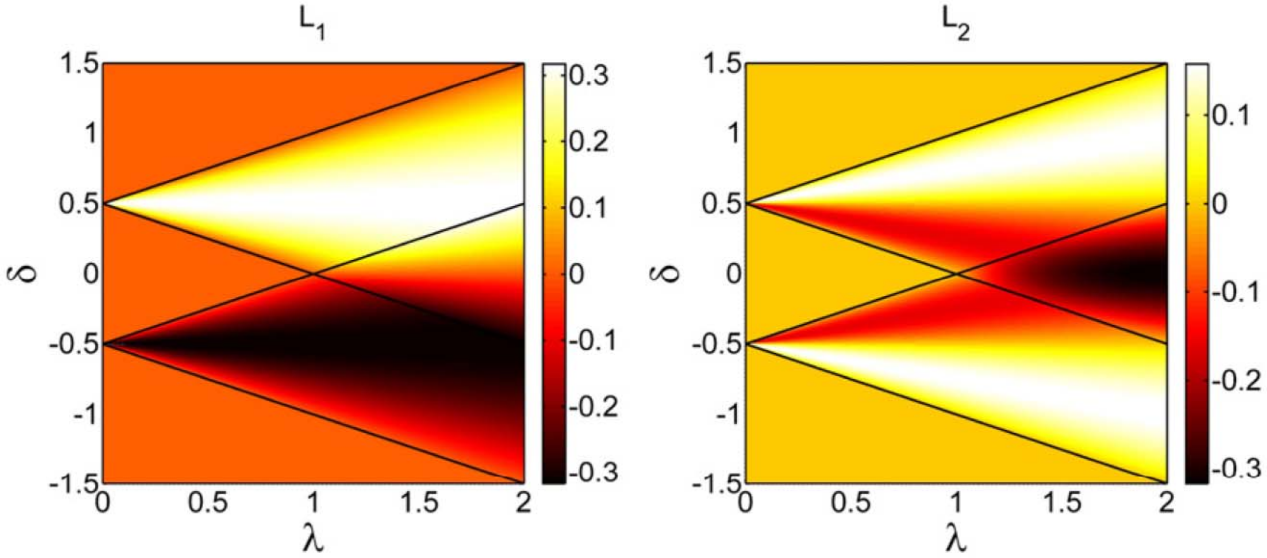
$$L_m^{(B)}(\lambda,\delta) = \frac{1}{m\pi}\sin\left(m\pi\frac{1-2\delta+\lambda}{2\lambda}\right),$$

$$L_m^{(C)}(\lambda,\delta) = 0,$$

$$L_m^{(D)}(\lambda,\delta) = \frac{1}{m\pi}\sin\left(m\pi\frac{1+2\delta-\lambda}{2\lambda}\right).$$

No **charge-vibron** coupling for vibrons **entirely inside** the dot

Charge-vibron coupling



$$\lambda = L_{\mathrm{v}}/L_{\mathrm{d}}$$

$$\delta = (x_{\mathrm{v}} - x_{\mathrm{d}})/L_{\mathrm{d}}$$

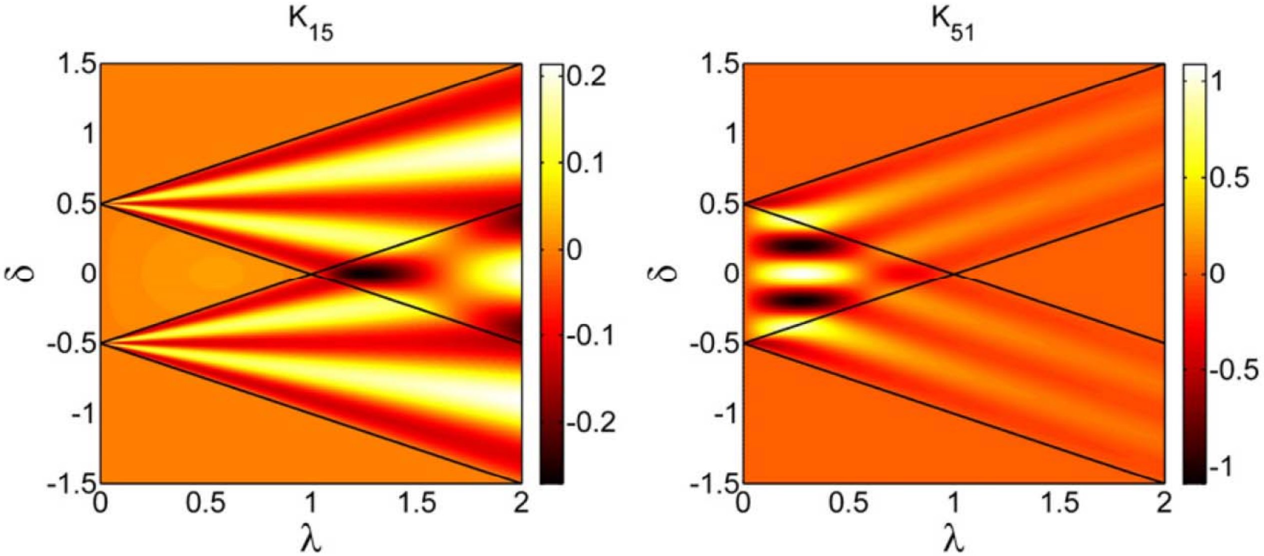
$$L_m(\lambda, \delta) = (-1)^m L_m(\lambda, -\delta)$$

➡ Only **even** modes couple to the charge in the **symmetric long** vibron regime

$$L_m\left(\lambda, \pm\frac{1}{2} + \alpha\lambda\right) = \frac{1}{m\pi}\sin\left[m\pi\left(\frac{1}{2} - \alpha\right)\right]$$

➡ Only **odd** modes couple to the charge in the **asymmetric short** vibron regime

Plasmon-vibron coupling



$$\lambda = L_{\mathrm{v}}/L_{\mathrm{d}}$$

$$\delta = (x_{\mathrm{v}} - x_{\mathrm{d}})/L_{\mathrm{d}}$$

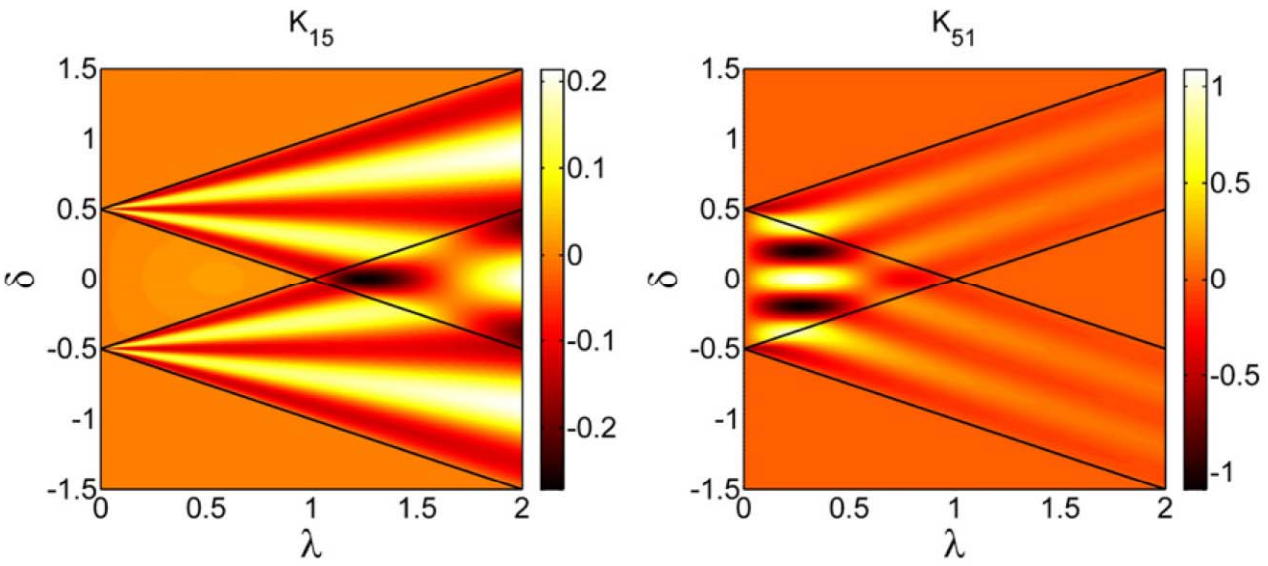
$$K_{nm}^{(A)}(\lambda,\delta) = -\frac{2m}{\pi(\lambda^2 n^2 - m^2)}\left[(-1)^n \sin\left(m\pi\frac{1-2\delta+\lambda}{2\lambda}\right) + \sin\left(m\pi\frac{1+2\delta-\lambda}{2\lambda}\right)\right],$$

$$K_{nm}^{(B)}(\lambda,\delta) = -\frac{2}{\pi(\lambda^2 n^2 - m^2)}\left[(-1)^n m \sin\left(m\pi\frac{1-2\delta+\lambda}{2\lambda}\right) + \lambda n \sin\left(\lambda n\pi\frac{1+2\delta-\lambda}{2\lambda}\right)\right],$$

$$K_{nm}^{(C)}(\lambda,\delta) = \frac{2\lambda n}{\pi(\lambda^2 n^2 - m^2)}\left[(-1)^m \sin\left(\lambda n\pi\frac{\lambda+2\delta+1}{2\lambda}\right) + \sin\left(\lambda n\pi\frac{\lambda-2\delta-1}{2\lambda}\right)\right],$$

$$K_{nm}^{(D)}(\lambda,\delta) = \frac{2}{\pi(\lambda^2 n^2 - m^2)}\left[(-1)^m \lambda n \sin\left(\lambda n\pi\frac{\lambda+2\delta+1}{2\lambda}\right) + m \sin\left(m\pi\frac{\lambda+2\delta-1}{2\lambda}\right)\right].$$

Plasmon-vibron coupling



$$\lambda = L_\mathrm{v}/L_\mathrm{d}$$

$$\delta = (x_\mathrm{v} - x_\mathrm{d})/L_\mathrm{d}$$

$$K_{nm}(\lambda,\delta) = 1/\lambda\ K_{mn}(1/\lambda, -\delta/\lambda)$$

→ Long vibron ↓ Short vibron = Vibron ⇄ Plasmon

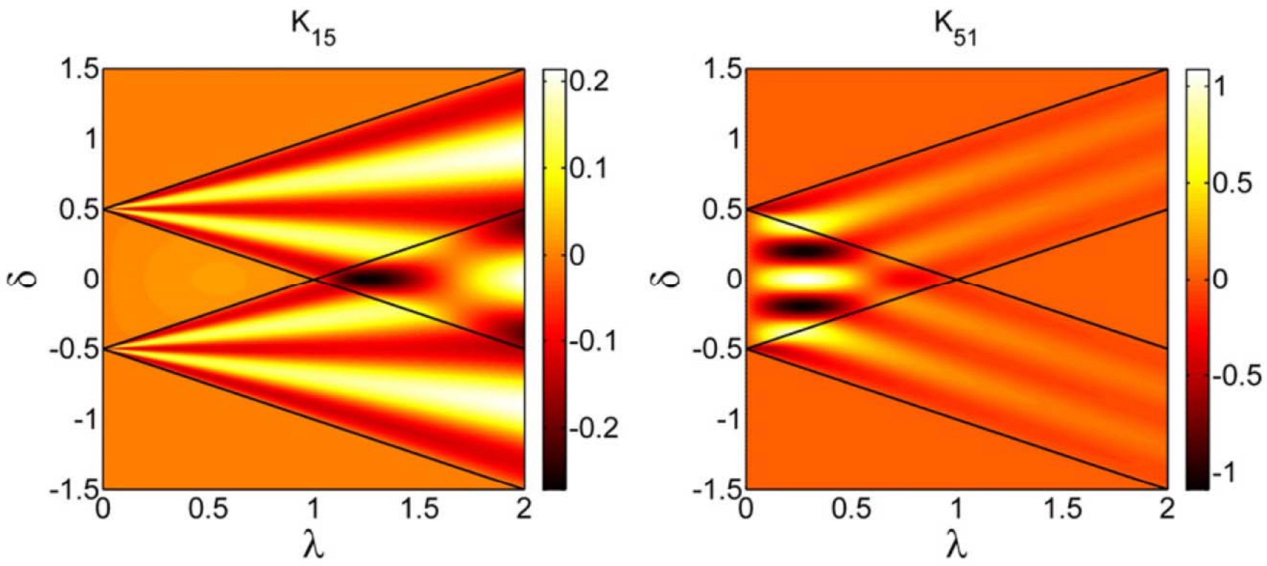
$$K_{nm}(\lambda,\delta) = (-1)^{n+m} K_{nm}(\lambda, -\delta)$$

→ **Parity** is **conserved** in **symmetric** junctions

$$\lim_{\lambda\to 1} K_{nm}(\lambda, 0) = \delta_{nm}$$

→ If dot and vibron **completely overlap** only vibron and polaron modes with the **same mode number** couple to each other

Plasmon-vibron coupling



$$\lambda = L_{\mathrm{v}}/L_{\mathrm{d}}$$

$$\delta = (x_{\mathrm{v}} - x_{\mathrm{d}})/L_{\mathrm{d}}$$

$$\lim_{\lambda \to \frac{m}{n}} K_{mn}(\lambda, \delta) = \begin{cases} \dfrac{n}{m} \cos\left[\dfrac{\pi}{2}(n - m - 2n\delta)\right], & \text{for } n < m \\ \cos\left[\dfrac{\pi}{2}(n - m - 2n\delta)\right], & \text{for } n > m \end{cases}$$

$k_m = k_n$

Different geometries maximize the coupling of **different modes**

$$K_{nm}\left(\lambda, \frac{1}{2} + \alpha\lambda\right) = \frac{2}{\pi m}(-1)^n \sin\left[m\pi\left(\frac{1}{2} - \alpha\right)\right] \quad \lambda \ll m/n$$

In the **short vibron** regime the e-v coupling is **constant** to **several plasmonic modes**

Diagonalization: the plasmon-vibrons

$$\hat{H}'_{\mathrm{sys}} = \sum_{n\geqslant 1} n\frac{\hbar\Omega}{2}\left(\hat{X}_n^2 + \hat{P}_n^2\right) + \sum_{m\geqslant 1} m\frac{\hbar\omega}{2}\left(\hat{x}_m^2 + \hat{p}_m^2\right)$$
$$+I\sqrt{g_{c+}}\sum_{n,m\geqslant 1}\sqrt{nm}\,K_{nm}2\hat{X}_n\hat{x}_m + I\sum_m \sqrt{m}L_m\sqrt{2}\hat{N}_{c+}\hat{x}_m,$$

$$\Omega = \pi v_{\mathrm{F}}/(g_{c+}L_{\mathrm{d}})$$
$$\omega = \pi v_{\mathrm{st}}/L_{\mathrm{v}}$$

As a quadratic form

$$\hat{H}'_{\mathrm{sys}} = \begin{pmatrix}\hat{\mathbf{X}}\\ \hat{\mathbf{x}}\\ \hat{\mathbf{P}}\\ \hat{\mathbf{p}}\end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \overset{\boldsymbol{\Delta}}{\begin{matrix} H_{\mathrm{pp}} & H_{\mathrm{pv}} \\ H_{\mathrm{vp}} & H_{\mathrm{vv}} \end{matrix}} & \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} \\ \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & \overset{\mathbf{1/2}}{\begin{matrix} H_{\mathrm{pp}} & 0 \\ 0 & H_{\mathrm{vv}} \end{matrix}} \end{pmatrix} \begin{pmatrix}\hat{\mathbf{X}}\\ \hat{\mathbf{x}}\\ \hat{\mathbf{P}}\\ \hat{\mathbf{p}}\end{pmatrix} + \hat{H}_{\mathrm{cv}}$$

Contraction

$$\hat{X}'_n = 1/\sqrt{n\hbar\Omega}\,\hat{X}_n, \quad \hat{x}'_m = 1/\sqrt{m\hbar\omega}\,\hat{x}_m,$$
$$\hat{P}'_n = \sqrt{n\hbar\Omega}\,\hat{P}_n, \quad \hat{p}'_m = \sqrt{m\hbar\omega}\,\hat{p}_m$$

Rotation

$$\hat{\xi}'_l = \sum_{n=1}^{N_{\mathrm{p}}} U^T_{ln}\,\hat{X}'_n + \sum_{m=1}^{N_{\mathrm{v}}} U^T_{lN_{\mathrm{p}}+m}\,\hat{x}'_m,$$
$$\hat{\pi}'_l = \sum_{n=1}^{N_{\mathrm{p}}} U^T_{ln}\,\hat{P}'_n + \sum_{m=1}^{N_{\mathrm{v}}} U^T_{lN_{\mathrm{p}}+m}\,\hat{p}'_m$$

Expansion

$$\hat{\xi}_l = \sqrt{\hbar\omega_l}\,\hat{\xi}'_l,$$
$$\hat{\pi}_l = 1/\sqrt{\hbar\omega_l}\,\hat{\pi}'_l$$

$$\boxed{\hat{H}'_{\mathrm{sys}} = \sum_l \frac{\hbar\omega_l}{2}(\hat{\xi}_l^2 + \hat{\pi}_l^2) + H_{\mathrm{cv}}}$$

Diagonalization: the polaron shift

$$\hat{H}'_{\text{sys}} = \sum_{l} \frac{\hbar\omega_l}{2}(\hat{\xi}_l^2 + \hat{\pi}_l^2) + H_{\text{cv}}$$

where

$$\hat{H}_{\text{cv}} = I\sqrt{2}\sum_{lm} mL_m\sqrt{\frac{\omega}{\omega_l}}U_{N_{\text{p}}+m,\,l}\,\hat{\xi}_l\hat{N}_{c+}.$$

$$\hat{\tilde{H}}'_{\text{sys}} = \text{e}^{-\hat{S}}\hat{H}'_{\text{sys}}\text{e}^{+\hat{S}}$$

$$\hat{S} = \text{i}\sqrt{2}\sum_{lm}\frac{I}{\hbar\omega_l}mL_m\sqrt{\frac{\omega}{\omega_l}}U_{N_{\text{p}}+m,\,l}\,\hat{\pi}_l\hat{N}_{c+}$$

⇓ Polaron transformation

$$\hat{\tilde{H}}'_{\text{sys}} = \sum_{l}\frac{\hbar\omega_l}{2}(\hat{\xi}_l^2 + \hat{\pi}_l^2) - \sum_{l}\frac{I^2}{\hbar\omega_l}\left(\sum_{m}L_m\sqrt{\frac{\omega}{\omega_l}}U_{N_{\text{p}}+m,\,l}\right)^2\hat{N}_{c+}^2$$

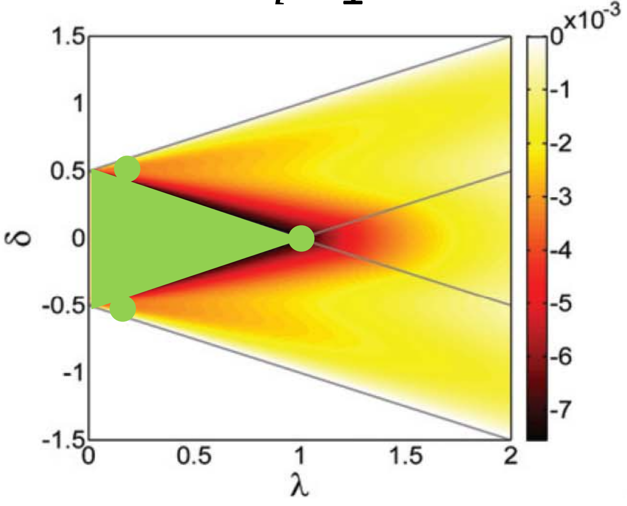
$$\boxed{E_{\vec{N},\vec{m}} = E_{\vec{N}} + \sum_{l}\hbar\omega_l\left(m_l + \frac{1}{2}\right) + \sum_{n,j\neq c+} n\varepsilon_0 m_{n,j}}$$

⇐ **The spectrum**

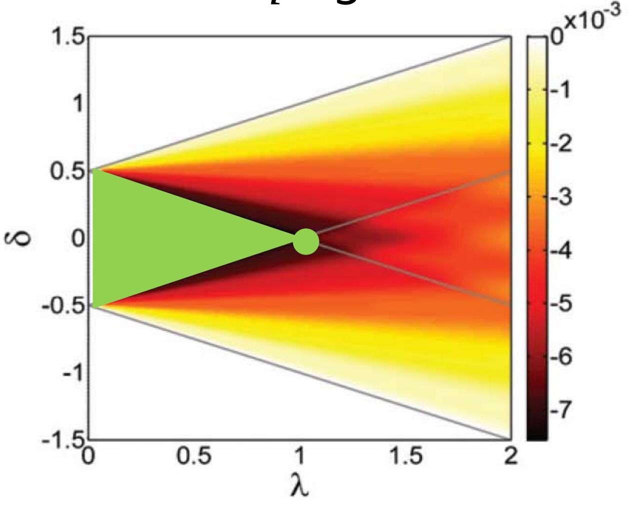
Spectrum

$$\frac{\omega_m - m\omega}{m\omega}$$

l = 1



l = 5



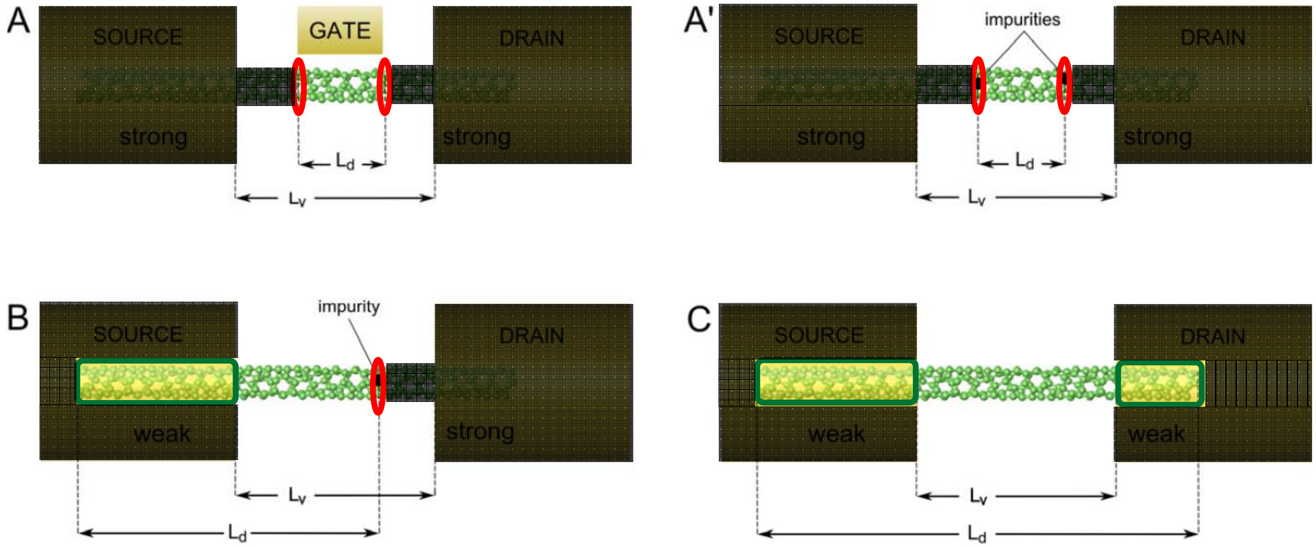
$$\frac{\omega_m - m\omega}{m\omega} \approx -\frac{2g_{c+}I^2}{\hbar^2\omega\Omega}$$

$$\hbar\omega_l = \sqrt{2\Delta_l} = n\hbar\sqrt{\frac{\Omega^2+\omega^2}{2} \pm \sqrt{\left(\frac{\Omega^2-\omega^2}{2}\right)^2 + \frac{4g_{c+}I^2\omega\Omega}{\hbar^2}}},$$

$$\omega_1 = \omega\sqrt{1 - \frac{4I^2g_{c+}}{\hbar^2\omega\Omega}\sum_{n=1}^{\infty}K_{n1}^2}$$

Tunnelling amplitudes

$$\langle \vec{N},\vec{m}|\hat{\Psi}^{\dagger}_{\sigma}(\vec{r})|\vec{N}',\vec{m}'\rangle$$



Localized **Extended**

tunnelling regions

Fermionic and bosonic fields

$\hat{\Psi}_{\sigma}(\vec{r}) \longrightarrow$ 3D to 1D

$$\hat{\psi}_{rF\sigma}(x) = \hat{\eta}_{r\sigma}\hat{K}_{rF\sigma}(x)\mathrm{e}^{\mathrm{i}\hat{\phi}^{\dagger}_{r\mathrm{F}\sigma}(x)}\,\mathrm{e}^{\mathrm{i}\hat{\phi}_{r\mathrm{F}\sigma}(x)}$$

$$\hat{K}_{rF\sigma}(x) = \frac{1}{\sqrt{2L_{\mathrm{d}}}}\mathrm{e}^{\mathrm{i}(\pi/L_{\mathrm{d}})\mathrm{sgn}(\mathrm{F})(r\hat{N}_{r\sigma}+\Delta)x}$$

$$\hat{\psi}_{rF\sigma}(x) \propto \hat{\eta}_{r\sigma}\hat{K}_{rF\sigma}(x)\prod_{n\geqslant 1}\mathrm{e}^{+\mathrm{i}P_n(x)\hat{X}_n-\mathrm{i}X_n(x)\hat{P}_n}$$

In terms of the plasmon operators

$$X_n(x) = \sqrt{\frac{2}{ng_{c+}}}\cos\left[\frac{n\pi}{L_{\mathrm{d}}}\left(x - x_{\mathrm{d}} + \frac{L_{\mathrm{d}}}{2}\right)\right],$$

$$P_n(x) = \sqrt{\frac{2g_{c+}}{n}}\mathrm{sgn}(\mathrm{F}r)\sin\left[\frac{n\pi}{L_{\mathrm{d}}}\left(x - x_{\mathrm{d}} + \frac{L_{\mathrm{d}}}{2}\right)\right]$$

Franck-Condon couplings (i)

$$|\vec{N},\vec{m}\rangle = \mathrm{e}^{\hat{S}}|\vec{N},\vec{m}\rangle_0,$$

Eigenstates: set of shifted vibron-plasmons

$$|\vec{N},\vec{m}\rangle_0 = \prod_l \frac{(\hat{\xi}_l - \mathrm{i}\hat{\pi}_l)^{m_l}}{\sqrt{2m_l!}}|\vec{N},0\rangle_0$$

$$\langle\vec{N},\vec{m}|\hat{\psi}_{rF\sigma}(x)|\vec{N}',\vec{m}'\rangle = {}_0\langle\vec{N},\vec{m}|\mathrm{e}^{-\hat{S}}\hat{\psi}_{rF\sigma}(x)\mathrm{e}^{+\hat{S}}|\vec{N}',\vec{m}'\rangle_0$$

$$\mathrm{e}^{-\hat{S}}\hat{\psi}_{rF\sigma}(x)\mathrm{e}^{+\hat{S}} \propto \hat{\eta}_{r\sigma}\hat{K}_{rF\sigma}\prod_l \mathrm{e}^{+\mathrm{i}\pi_l(x)\hat{\xi}_l - \mathrm{i}\xi_l(x)\hat{\pi}_l}$$

In terms of the vibron-plasmon operators

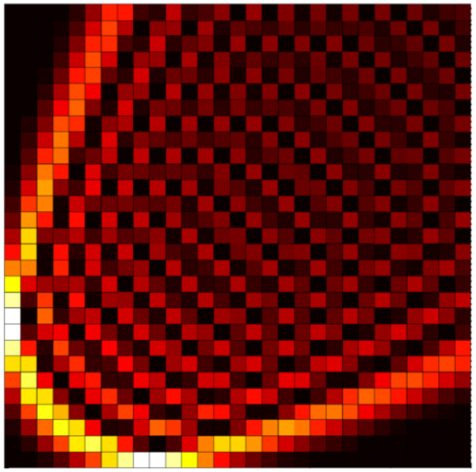
$$\xi_l(x) = -\frac{\sqrt{2}I}{\varepsilon_l}\sum_{m=1}^{N_\mathrm{v}}\sqrt{\frac{\hbar\omega}{\varepsilon_l}}mL_m U_{N_\mathrm{p}+m,\,l} + \sum_{n=1}^{N_\mathrm{p}}\sqrt{\frac{2\varepsilon_l}{n^2 g_{c+}\hbar\Omega}}U_{nl}\cos\left[\frac{n\pi}{L_\mathrm{d}}\left(x - x_\mathrm{d} + \frac{L_\mathrm{d}}{2}\right)\right],$$

$$\pi_l(x) = \sum_{n=1}^{N_\mathrm{p}}\sqrt{\frac{2g_{c+}\hbar\Omega}{\varepsilon_l}}U_{nl}\sin\left[\frac{n\pi}{L_\mathrm{d}}\left(x - x_\mathrm{d} + \frac{L_\mathrm{d}}{2}\right)\right].$$

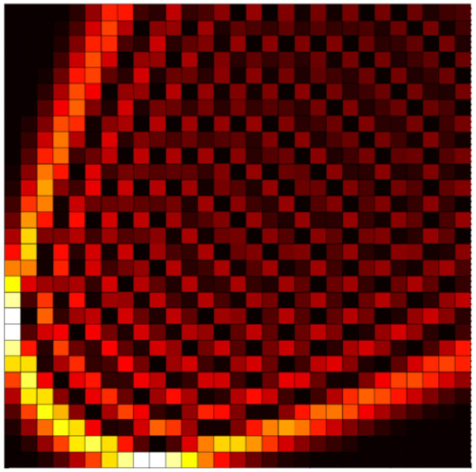
Franck-Condon couplings (ii)

$$\langle \vec{N}, \vec{m} | \hat{\psi}_{r\mathrm{F}\sigma}(x) | \vec{N}', \vec{m}' \rangle \propto \langle \vec{N} | \hat{\eta}_{r\sigma} \hat{K}_{r\mathrm{F}\sigma} | \vec{N}' \rangle \prod_{l} F(m_l, m'_l, \lambda_l)$$

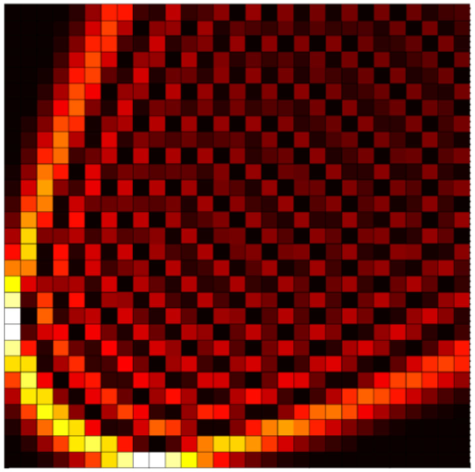
$$\lambda_l = -\frac{\xi_l - \mathrm{i}\pi_l}{\sqrt{2}}$$



x

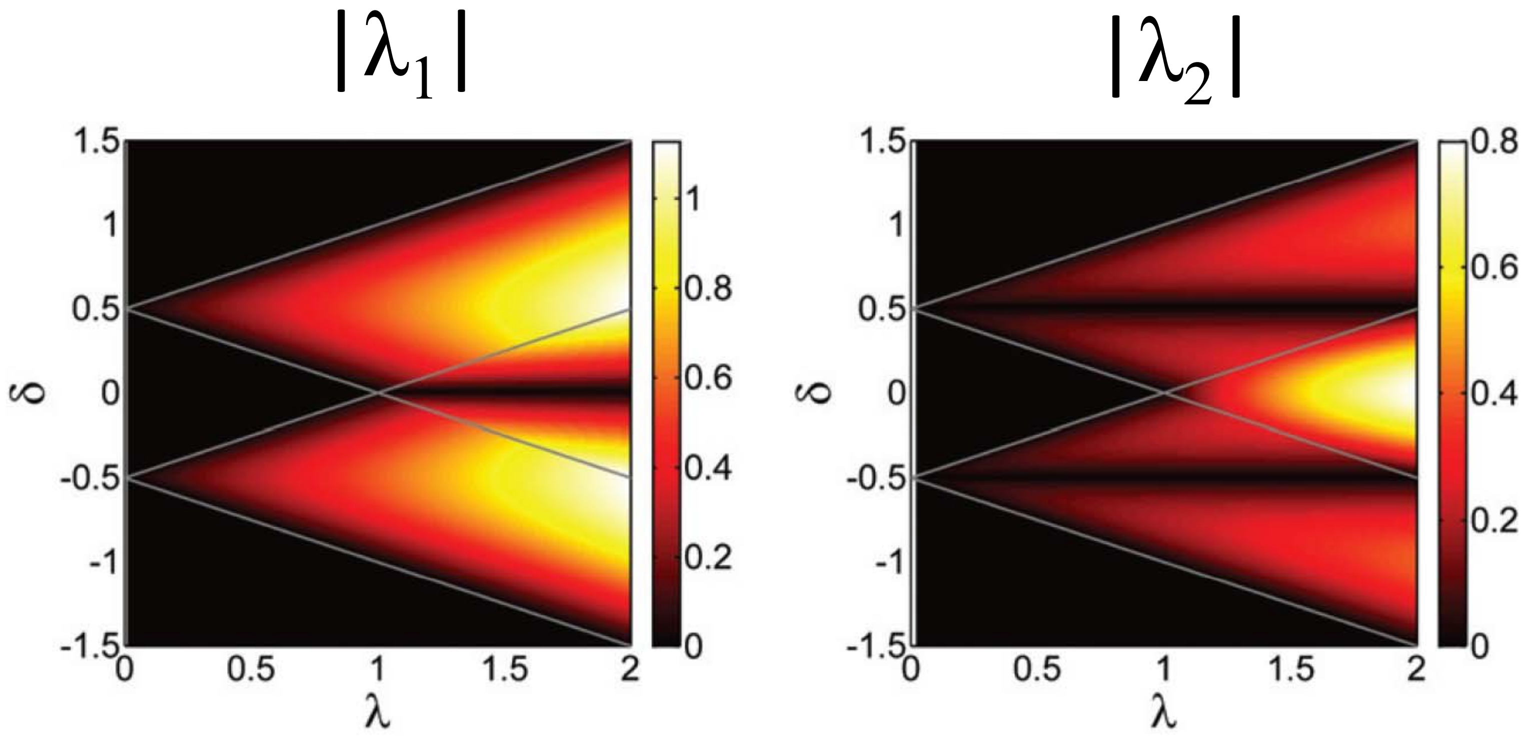


x

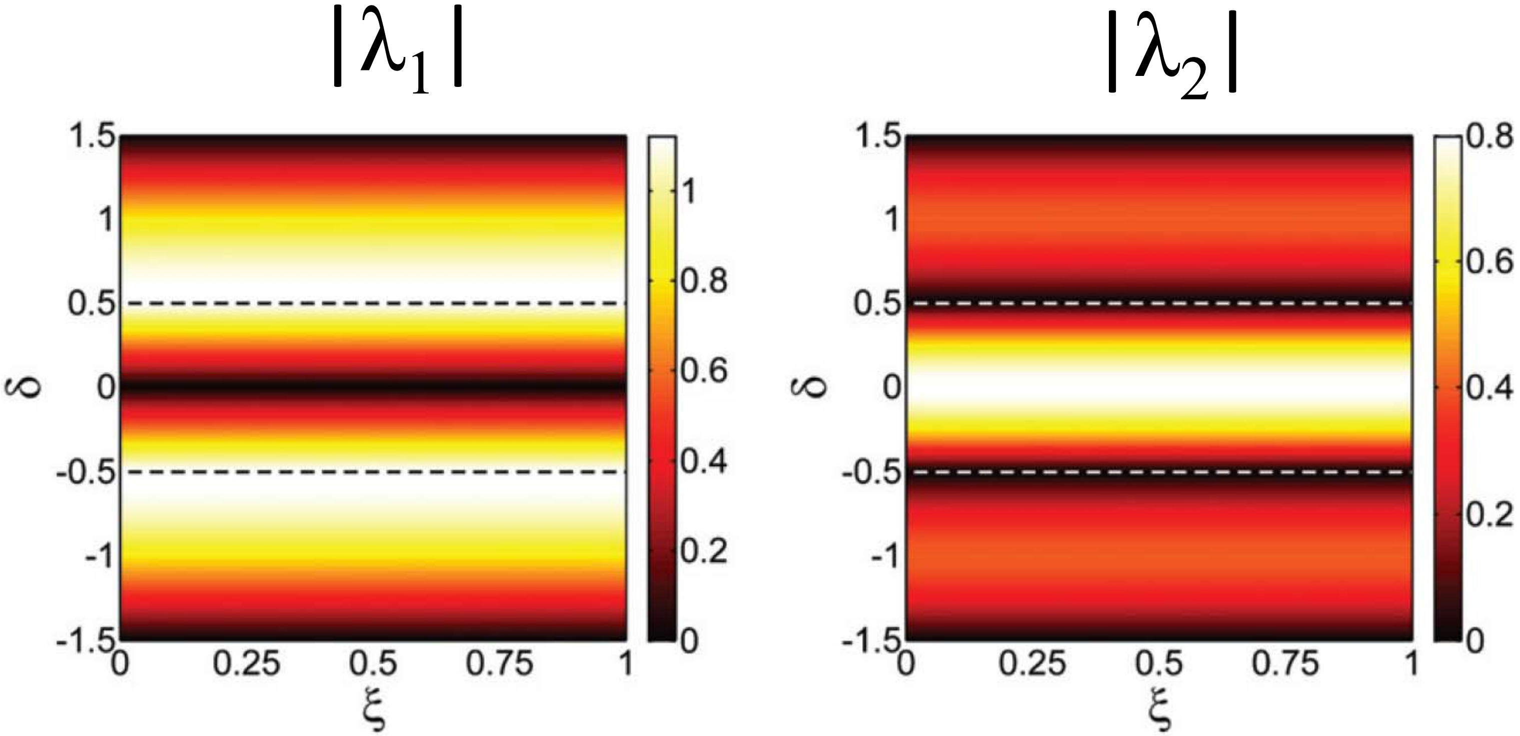


x …

Franck-Condon couplings (iii)

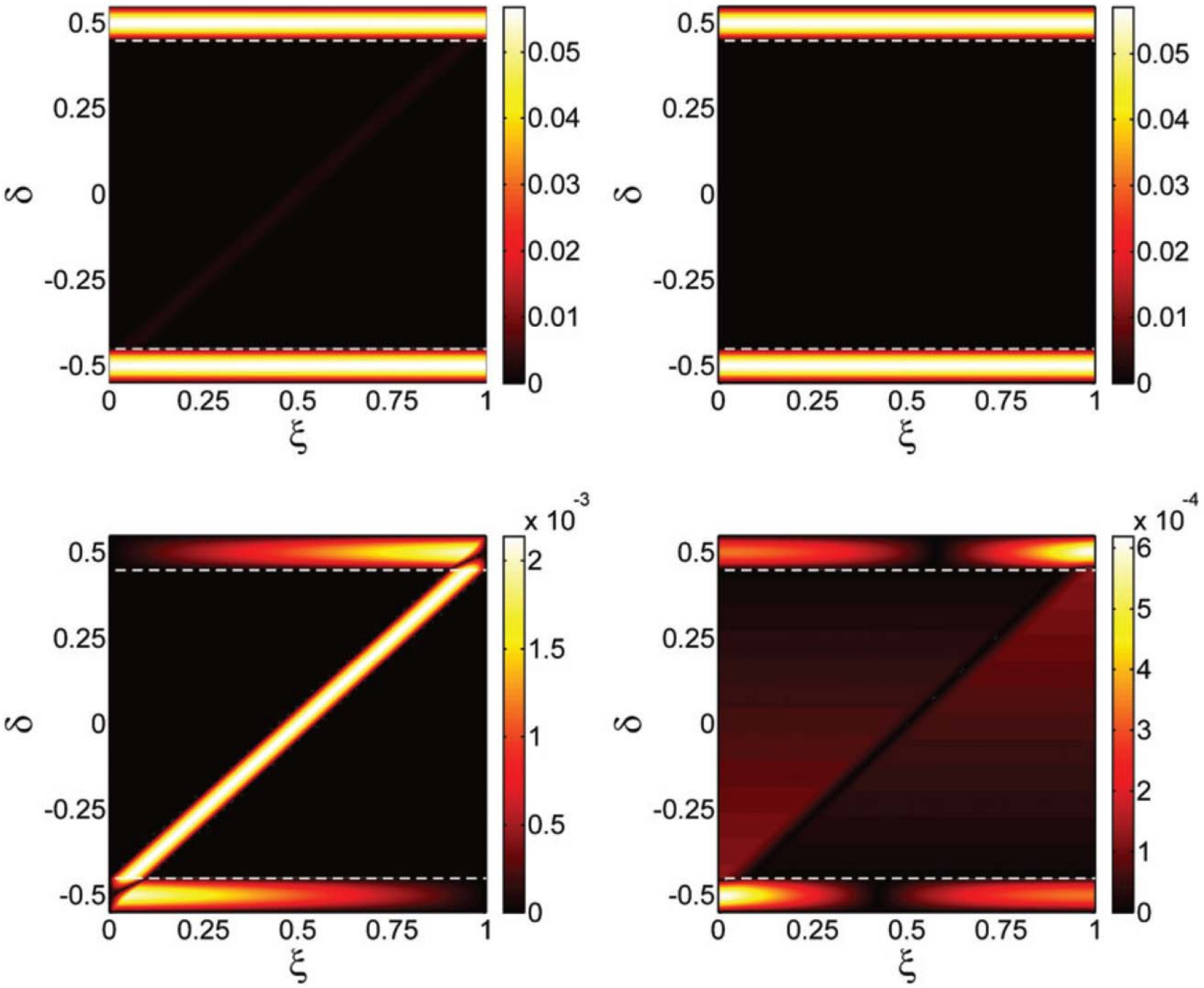


Long vibron regime



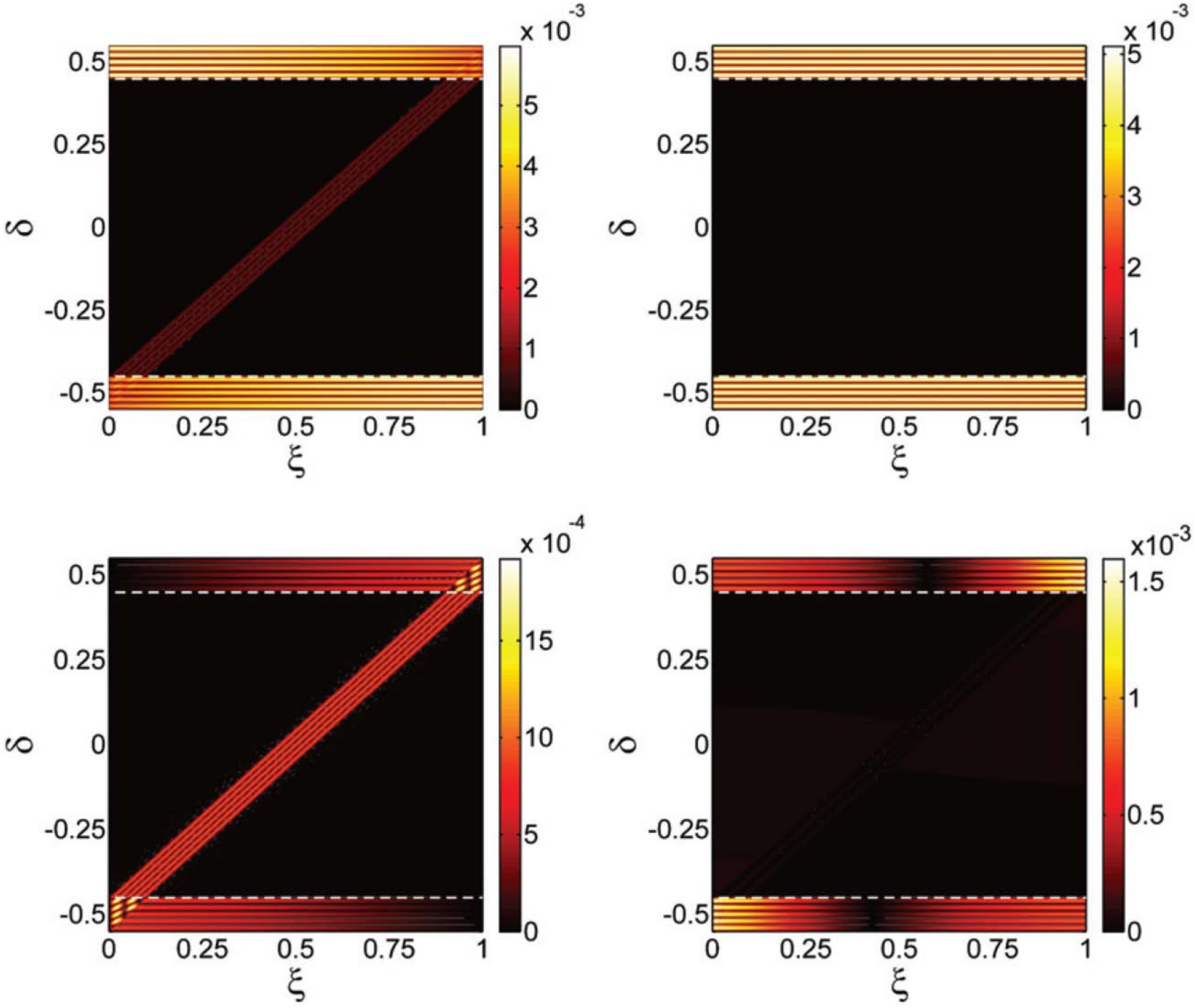
Short vibron regime (i)

$|\lambda_1|$



Short vibron regime (ii)

$|\lambda_5|$



Conclusions

1) We analyzed the spectrum and the effective Franck–Condon couplings of a suspended SWCNT quantum dot including **many vibronic modes** as well as **different dot–vibron geometrical configurations**.

2) In the low-energy description of the suspended SWCNT reduces to a **set of displaced plasmon–vibron** excitations.

3) The analysis of the coupling constants K_{nm} and L_m and of the Franck–Condon couplings on the entire geometrical parameters space allowed us to identify **different regimes**:

short symmetric vibron

long vibron

asymmetric short vibron

Three regimes

short symmetric vibron: the charge–vibron component vanishes and the Franck-Condon couplings are extremely small due to the energy scale separation between the plasmonic and vibronic modes that hinders the plasmon–vibron mixing. The Franck–Condon coupling is position dependent and is located around the position of the vibron.

long vibron: the charge–vibron coupling dominates the scenario giving substantially larger Franck–Condon couplings and independent of the position as in the simple Anderson–Holstein model. The Franck–Condon couplings are strongly dependent on the relative position of the vibron and the dot, leading to selection rules.

asymmetric short vibron:, the charge–vibron and plasmon–vibron contributions are of the same order and correspondingly one can distinguish the position-dependent contribution due to the plasmon–vibron mixing superimposed on the uniform polaron shift typical of the charge–vibron component of the coupling.

Thank you for your attention !