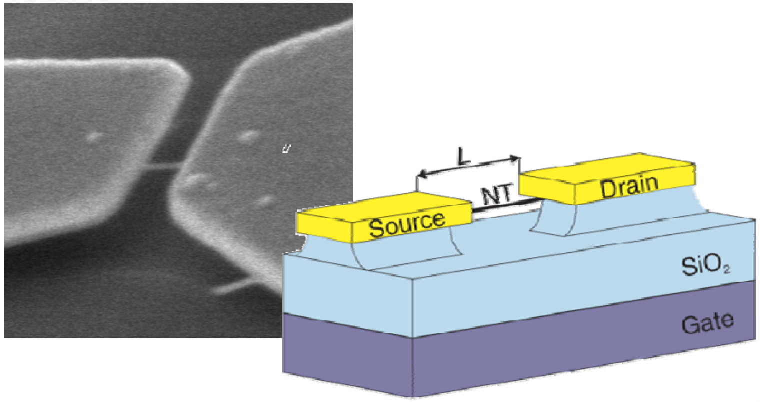
Spectrum and Franck-Condon factors of interacting SWCNT

Andrea Donarini

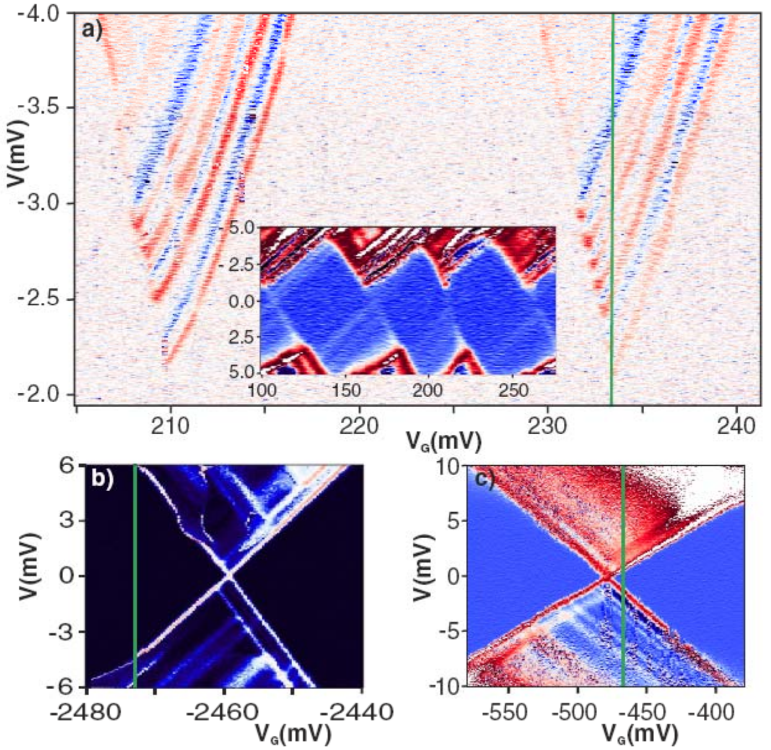
University of Regensburg - Germany

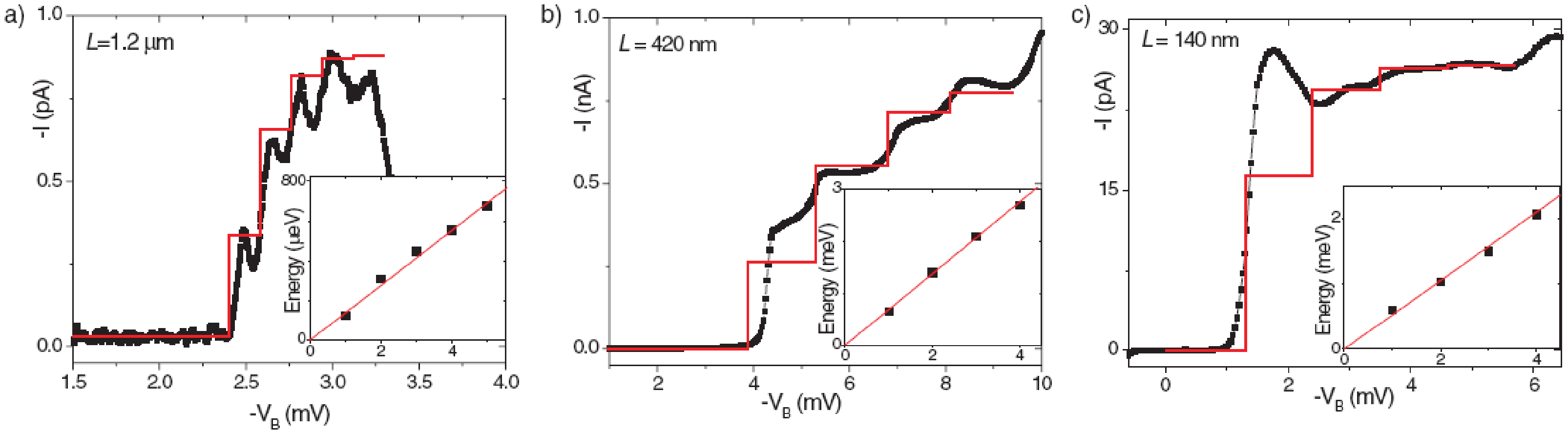
A. Donarini, A. Yar and M. Grifoni, *New Journal of Physics* **14**, 023045 (2012)

Carbon nanotubes NEMS



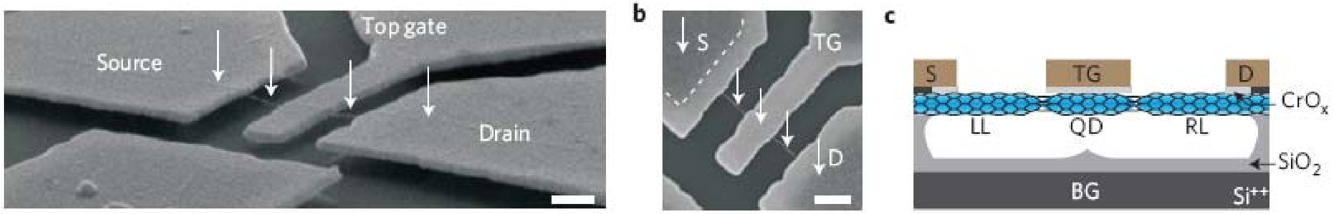
Sapmaz et al.
PRL **96**, 026801 (2006)

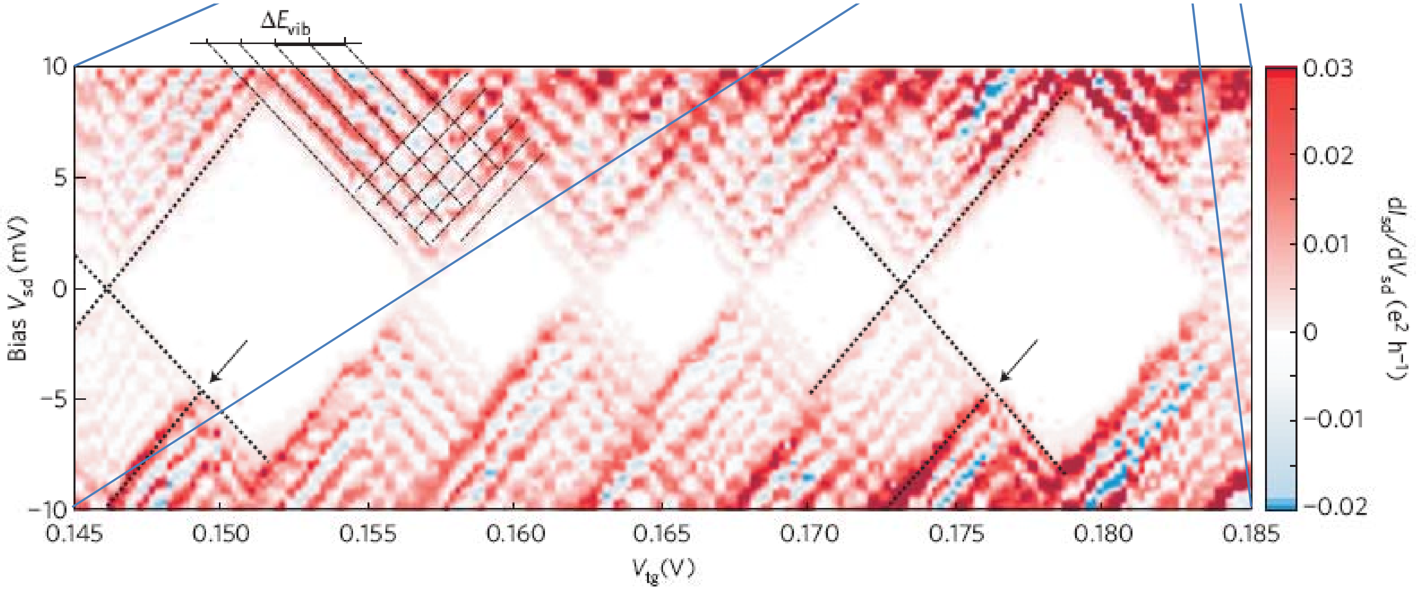




Carbon nanotubes NEMS

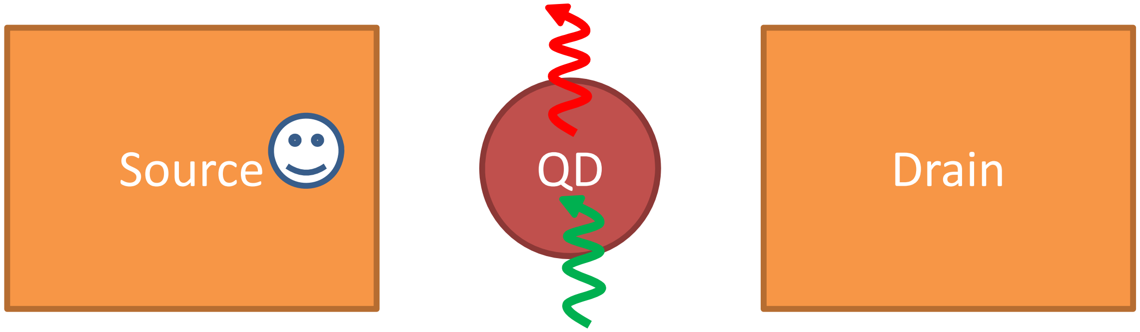
R. Leturcq et al. *Nat. Phys.* **5**, 327 (2009)

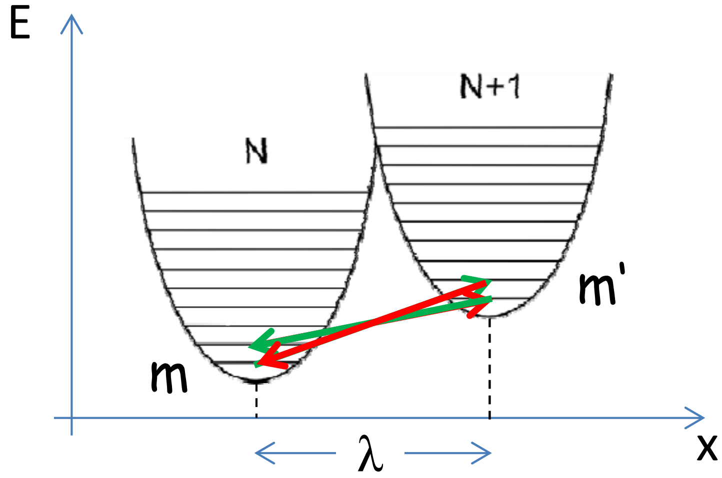




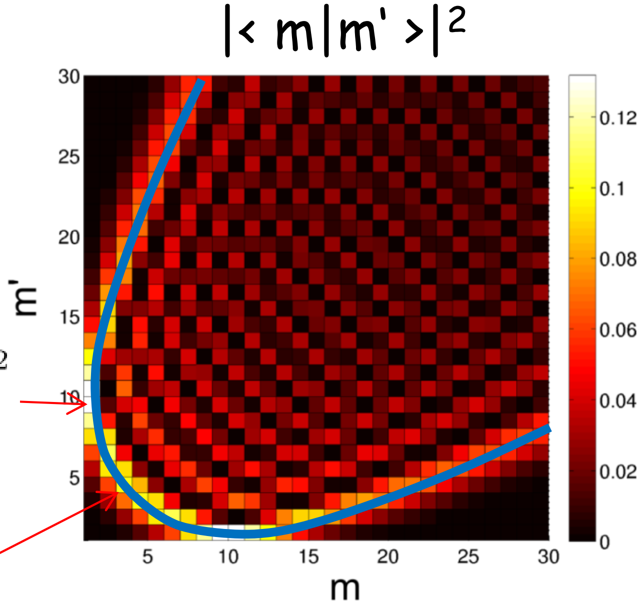
Franck Condon physics

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





Franck-Condon parabola

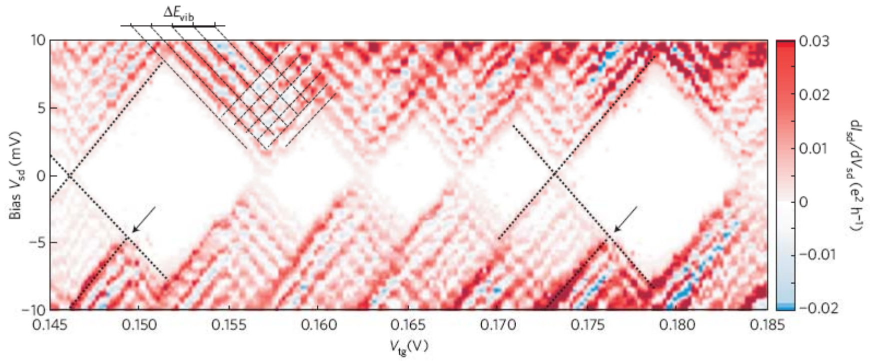


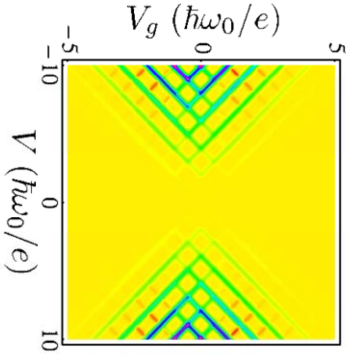
$m' = \lambda^2$
$m = 0$

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

Success of the simple theory

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

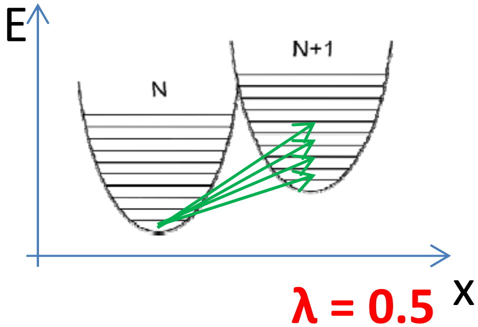




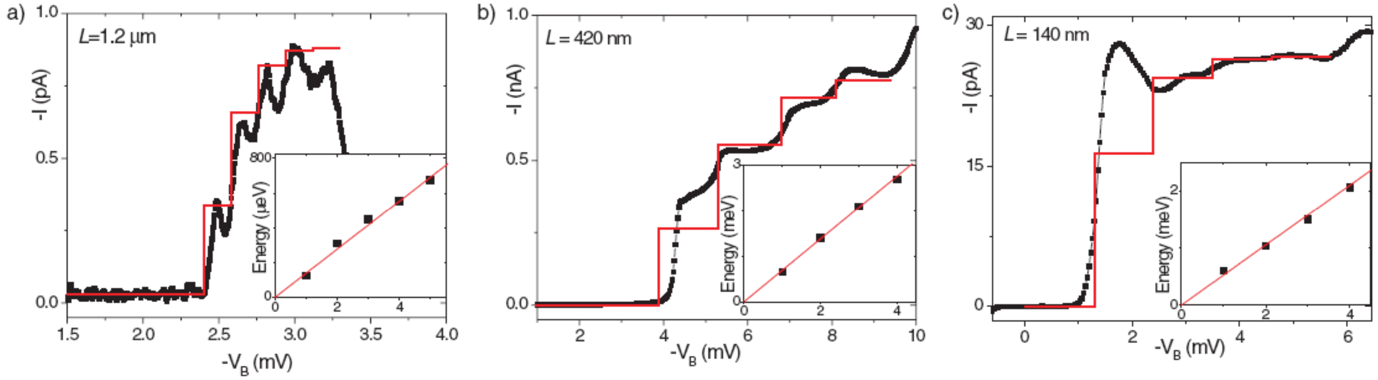
Koch and von Oppen
PRL **94** 206804 (2005)

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.

$\lambda \approx 1$

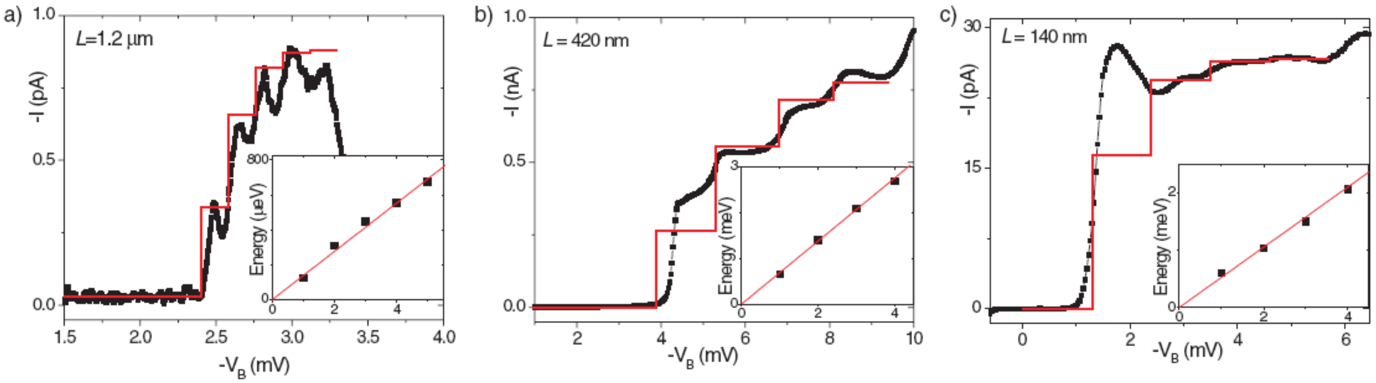
Anderson-Holstein model
fitting the experiments

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

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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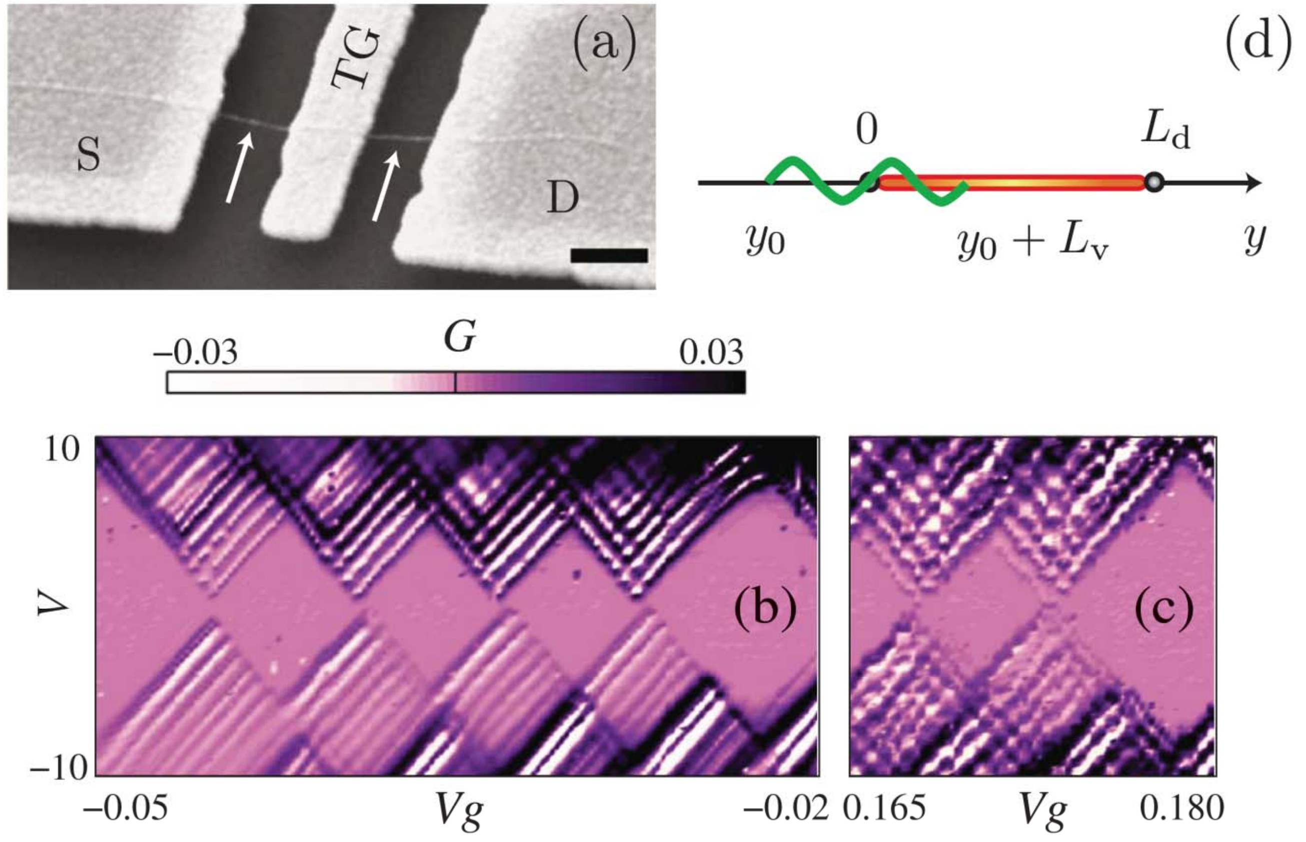

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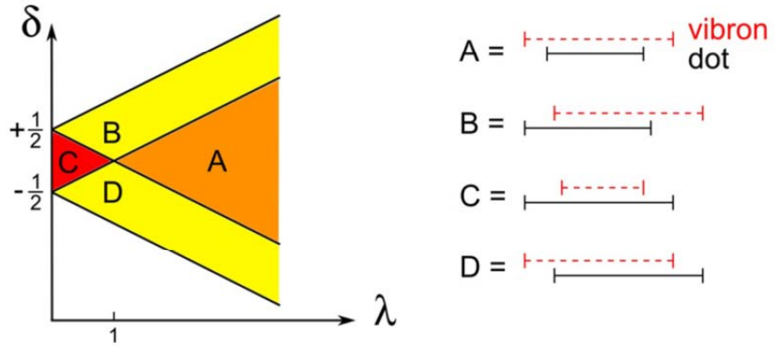
Short vibron close to the nanotube end ➡ **Position dependent** Franck-Condon factors

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

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

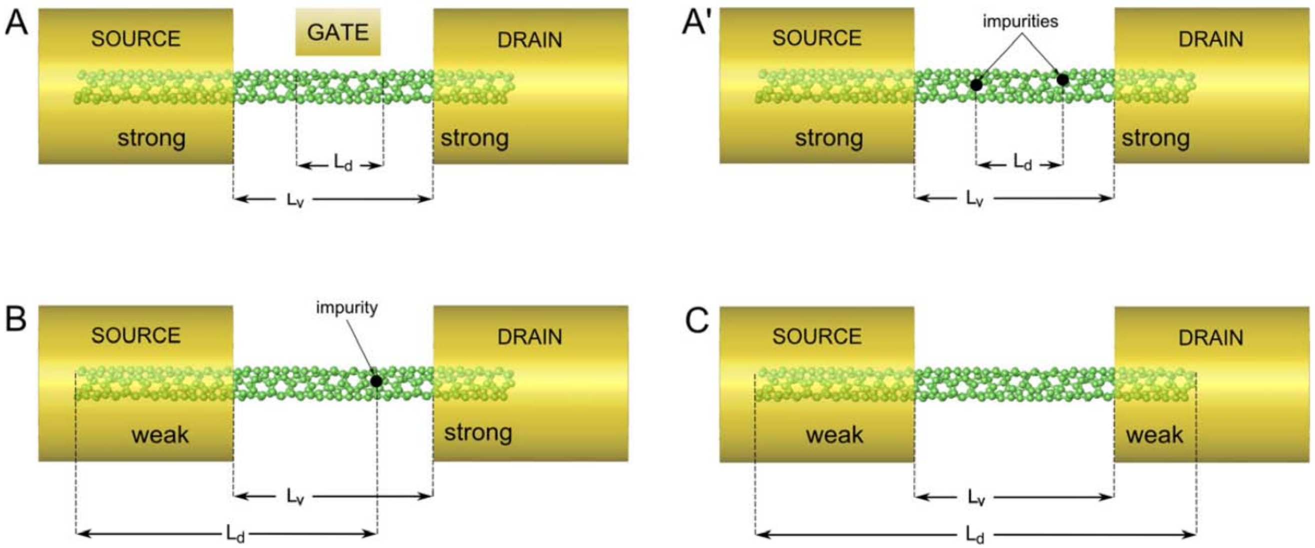
Extension of the model (i)

We studied the **entire** geometrical parameter space



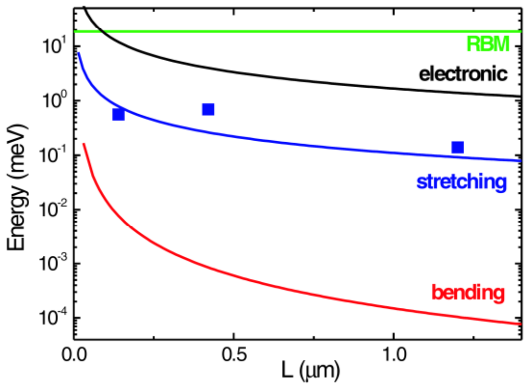
$$\lambda = L_{\rm v}/L_{\rm d}$$

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



Extension of the model (ii)

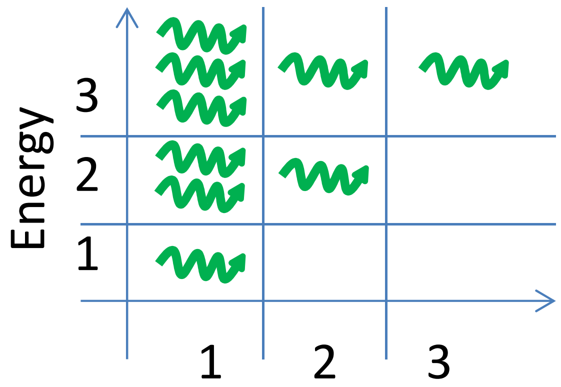
We analyzed **multimode degenerate** vibronic configurations



PRL **96**, 026801 (2006)

The stretching mode has **linear dispersion relation**

$$\omega_n = n\omega_1$$



Mode number

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

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:

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

where

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

Tomonaga-Luttinger liquid

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

$\varepsilon_0 = \hbar v_{\rm F} \frac{\pi}{L_{\rm d}}$

$g_{c+} \approx 0.2$

$g_j = 1$ for the other cases.

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

Continuum model
for the **stretching motion**

$\zeta = 2\pi RM$

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

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

Electron-vibron hamiltonian

We write the electron-vibron coupling in terms of **density and deformation potential** which leads to the following hamiltonian

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

Bare coupling constant

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

Dimensionless geometric parameters

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

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

Plasmon and vibron coordinates

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

Plasmon-vibron coupling ⇨

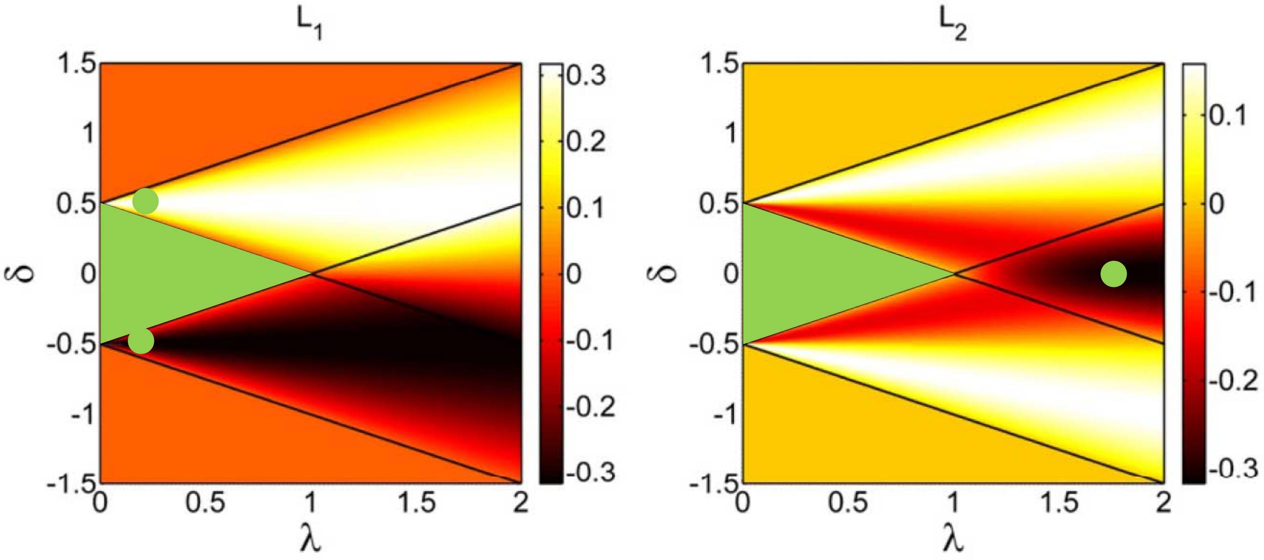
$$K_{nm}(\lambda, \delta) = \frac{1}{\lambda}\int_{x_{\min}}^{x_{\max}} \mathrm{d}x \left\{ \cos\left[\pi x\left(n + \frac{m}{\lambda}\right) - \frac{m\pi}{\lambda}\left(\delta + \frac{1-\lambda}{2}\right)\right] + \cos\left[\pi x\left(n - \frac{m}{\lambda}\right) + \frac{m\pi}{\lambda}\left(\delta +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

Charge-vibron coupling ⇨

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

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

Charge-vibron coupling

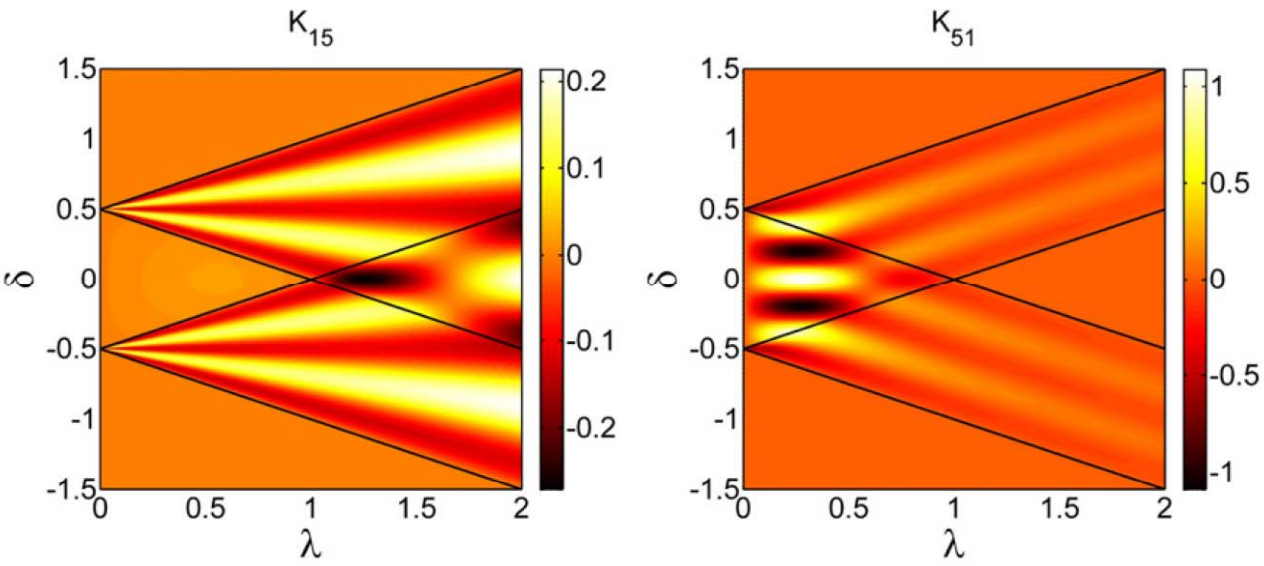


$$\lambda = L_{\mathrm{v}}/L_{\mathrm{d}}$$

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

- **No charge-vibron** coupling for vibrons **entirely inside** the dot
- Only **even** modes couple to the charge in the **symmetric long** vibron regime
- Only **odd** modes couple to the charge in the **asymmetric short** vibron regime

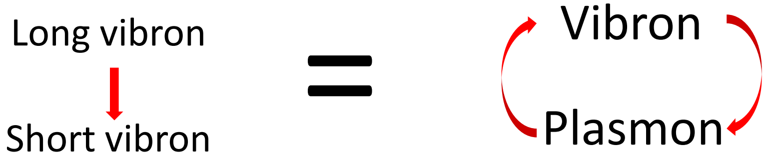
Plasmon-vibron coupling



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

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

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



Long vibron

Short vibron

=

Vibron

Plasmon

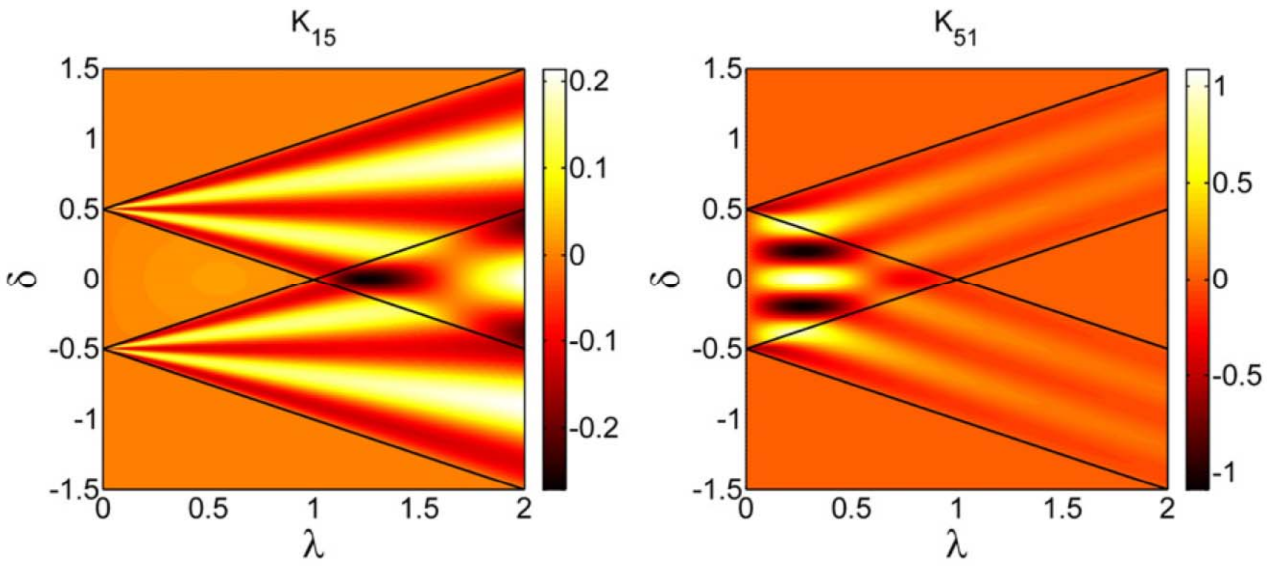
$$K_{nm}(\lambda,\delta) = (-1)^{n+m} K_{nm}(\lambda, -\delta)$$

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**

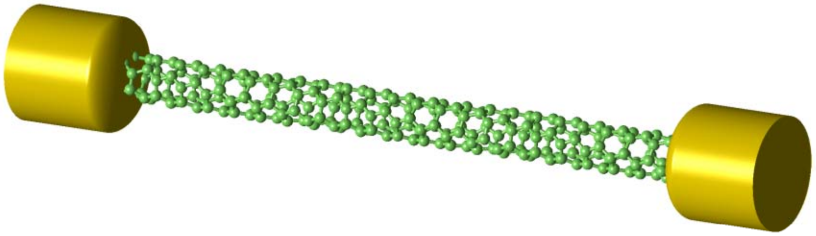
Energy scales

$L_d = L_v = 1\,\mu\text{m}$ $\quad v_F = 8 \times 10^5\,\text{m}\,\text{s}^{-1}$

$R = 6.68\,\text{Å}$ $\quad v_{st} = 2.4 \times 10^4\,\text{m}\,\text{s}^{-1}$

$M = 3.8 \times 10^{-7}\,\text{kg}\,\text{m}^{-2}$ $\quad g = 30\,\text{eV}$

$g_{c+} = 0.2$



Lowest charged plasmon energy: ε_0/g_{c+} = 8.293 meV

Lowest vibron energy: $\hbar\omega$ = 50 μeV

Bare coupling constant: I = 88 μeV

$$\hbar\omega,\, I \ll \varepsilon_0/g_{c+}$$

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.

Diagonalization

The Hamiltonian can be written in terms of quadratic form

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

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

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

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

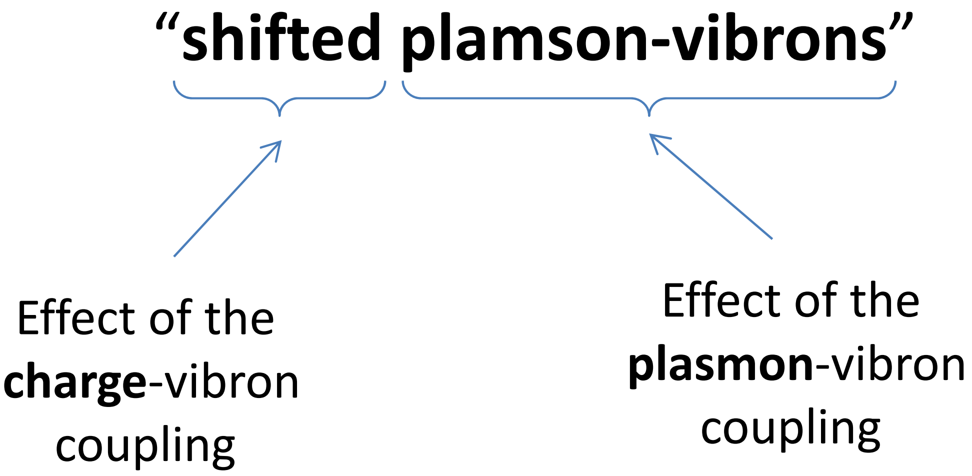
Polaron transformation

⇩

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

Effective description

The low energy excitations of a suspended SWCNT are



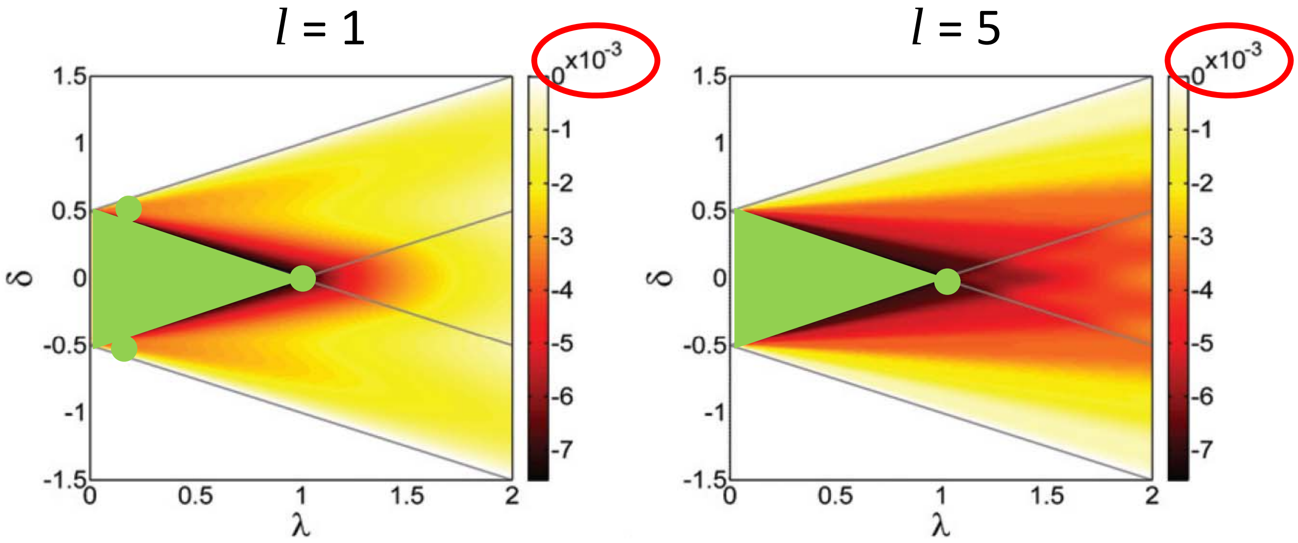
“shifted plamson-vibrons”

Effect of the
charge-vibron
coupling

Effect of the
plasmon-vibron
coupling

Spectrum

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



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

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

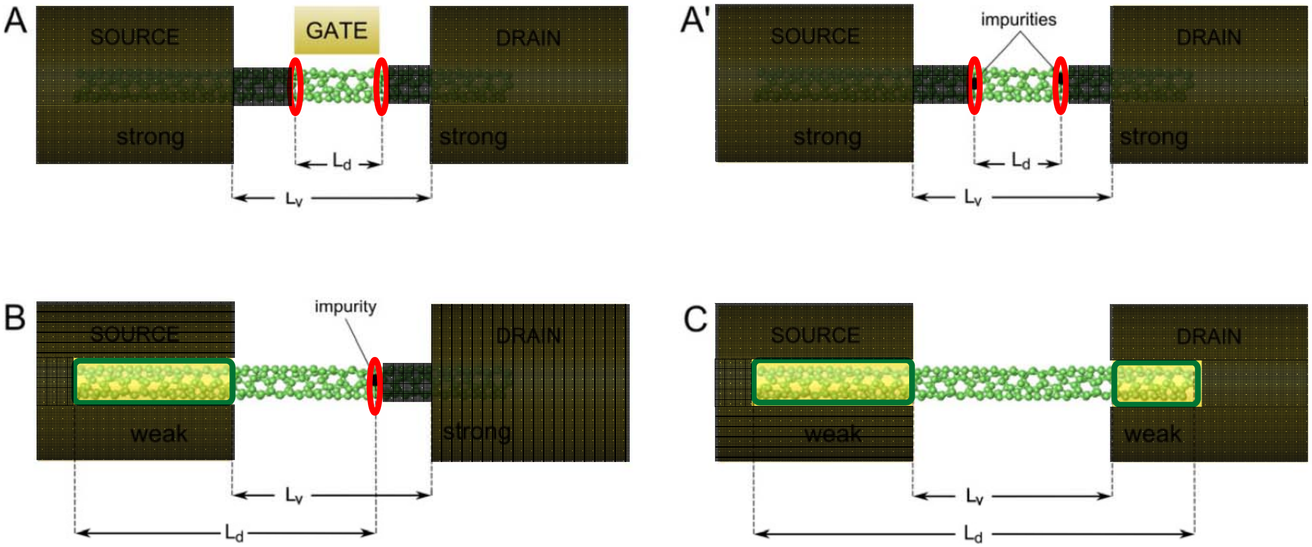
Wentzel-Bardeen singularity

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

A very modest renormalization for unscreened Coulomb interaction

Tunnelling amplitudes

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



Localized **Extended**

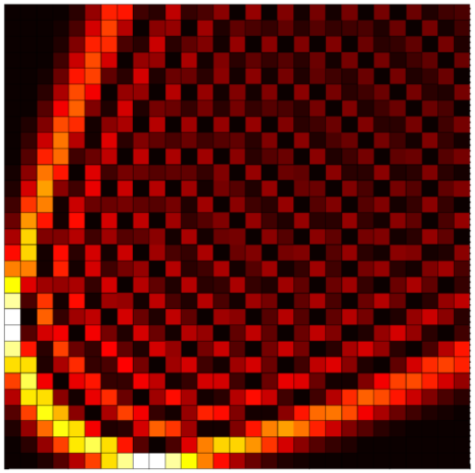
tunnelling regions

Multiple Franck-Condon parabolas

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

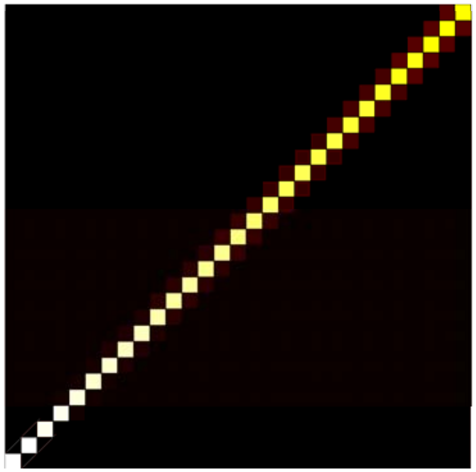
The tunnelling amplitude is a **product** of **different Franck-Condon parabolas**
With **different couplings** λ_l for the different vibron-plasmon modes

Mode 1



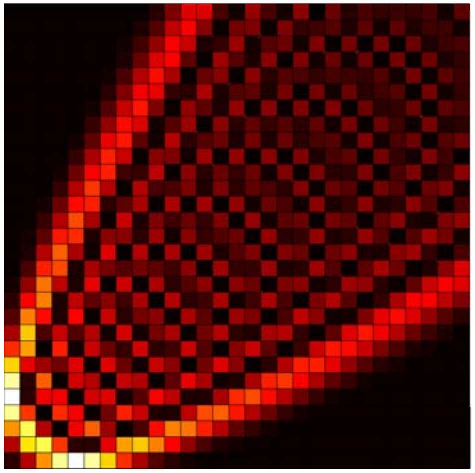
X

Mode 2



X

Mode 3



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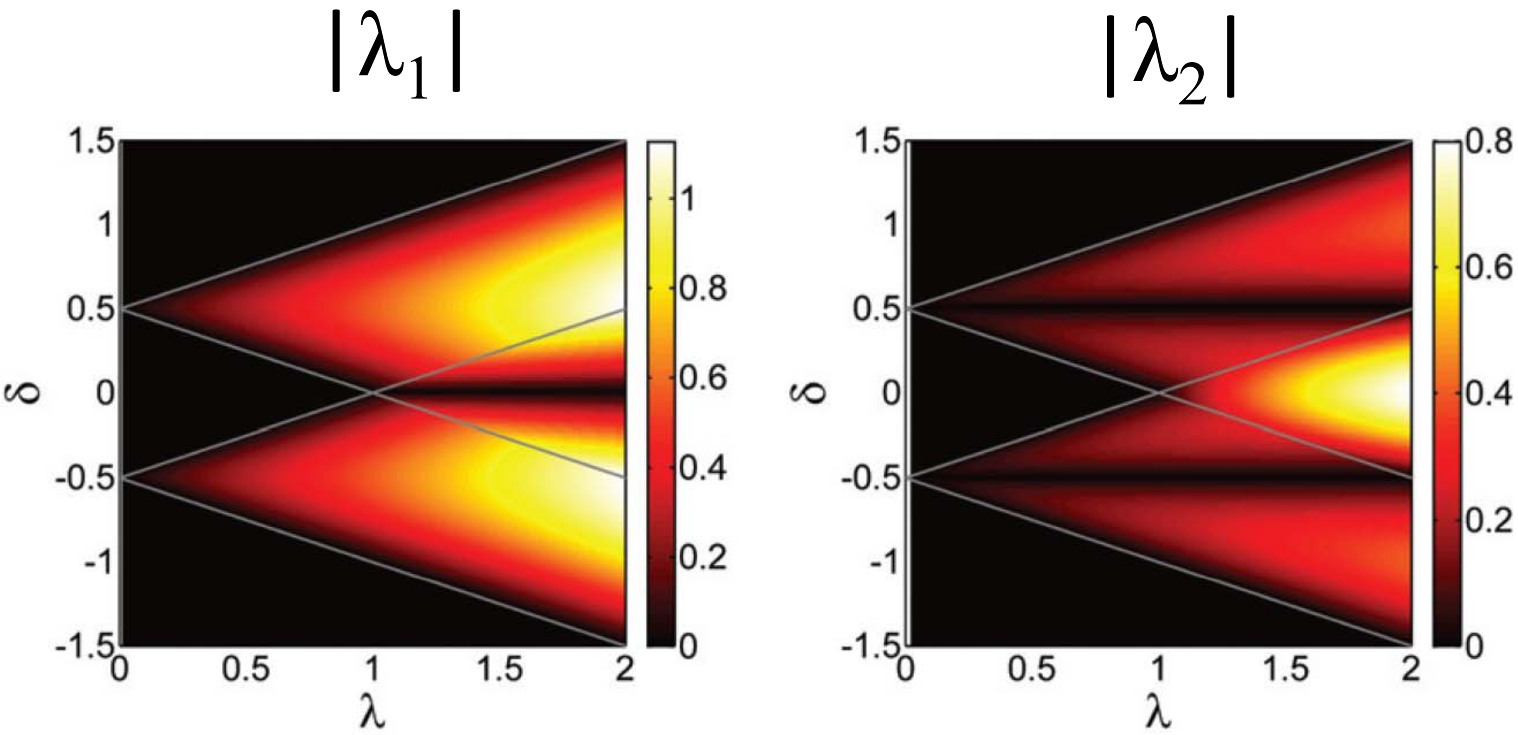
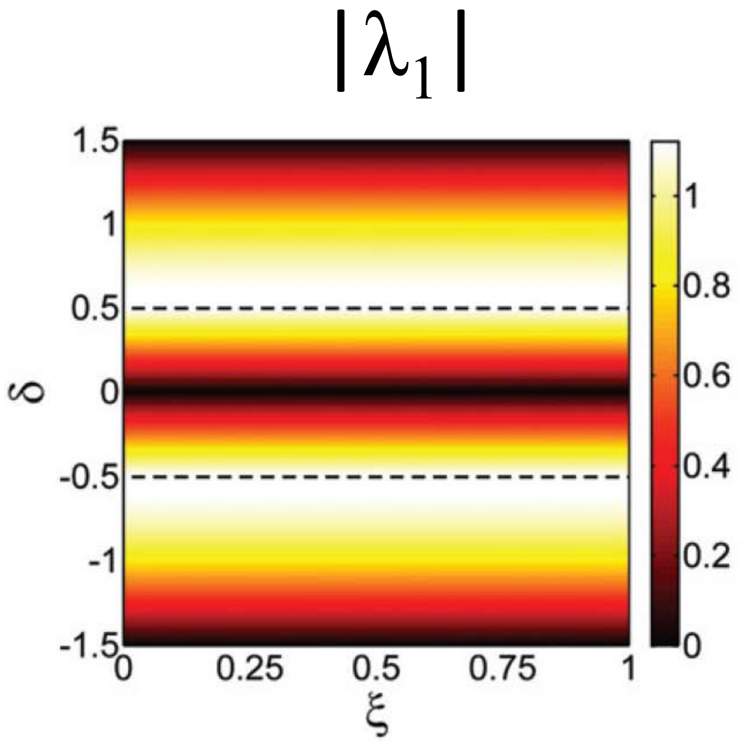
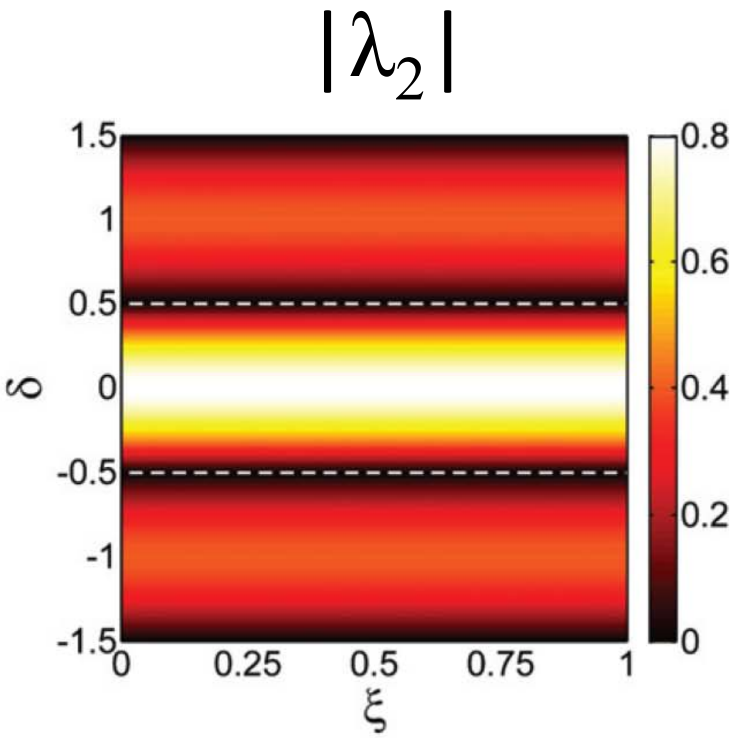
Franck-Condon couplings



Strong dependance on the **GEOMETRY** of the junction

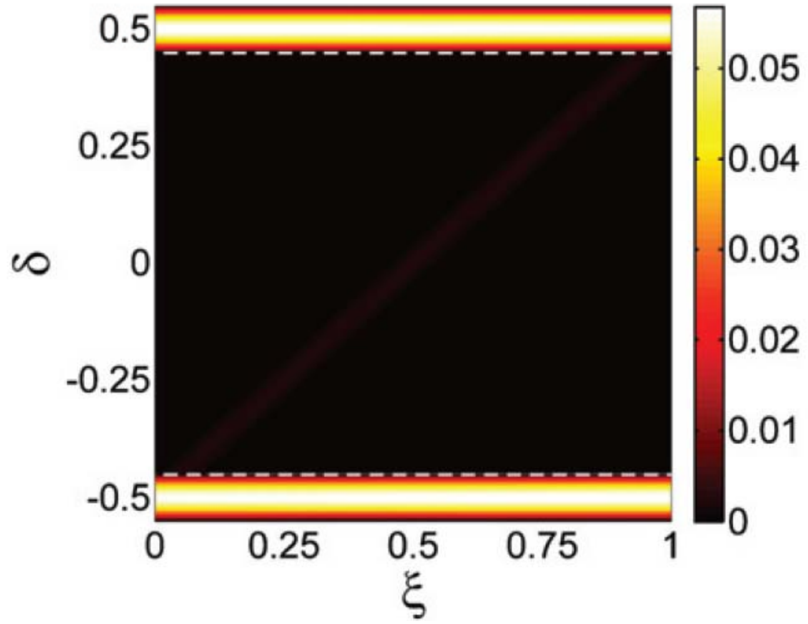
Long vibron regime


$|\lambda_1|$

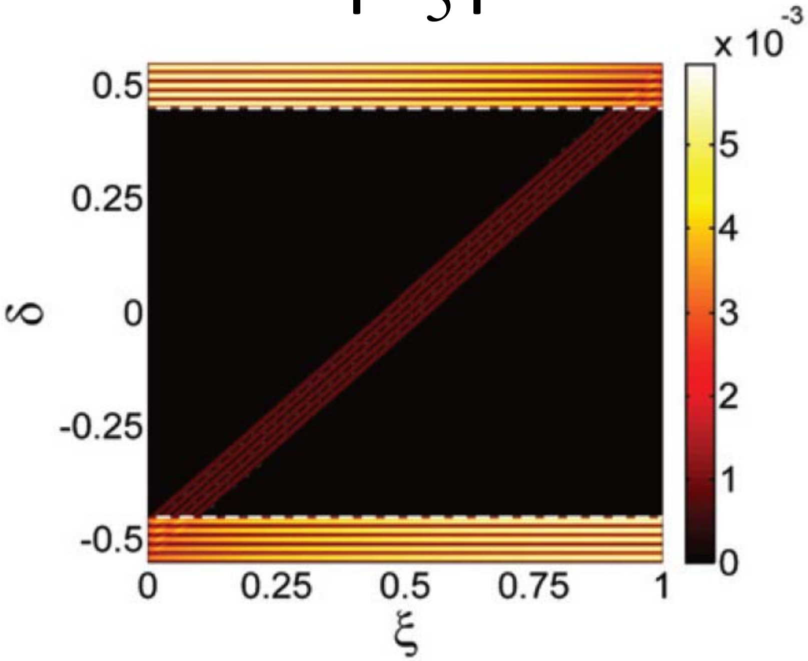

$|\lambda_2|$

Large FC factors,
Independent of the tunnelling position

Short vibron regime



$|\lambda_1|$



$|\lambda_5|$

Small FC factors,
Mimic position and shape of the vibron-plasmon mode

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**:

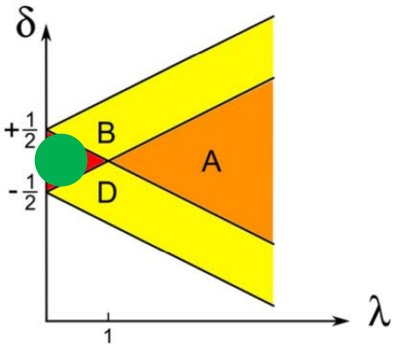
short symmetric vibron

long vibron

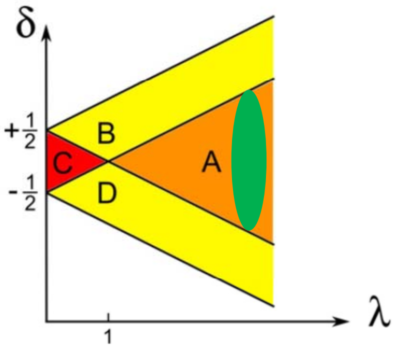
asymmetric short vibron

Three regimes

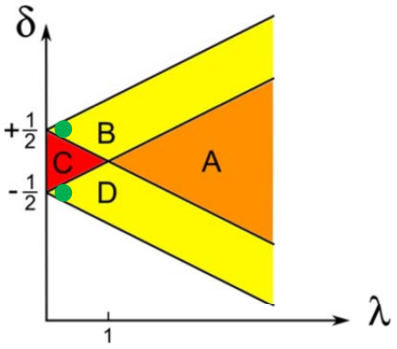
short symmetric vibron: the charge–vibron component vanishes and the Franck-Condon couplings are **extremely small** due to the **energy scale separation** between the plasmonic and vibronic modes that hinders the plasmon–vibron mixing. The Franck–Condon coupling is position dependent and is located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



short asymmetric 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 !

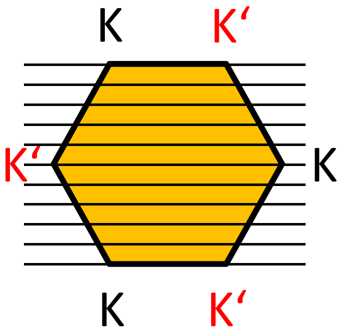
UR Low energy Hamiltonian of a SWCNT

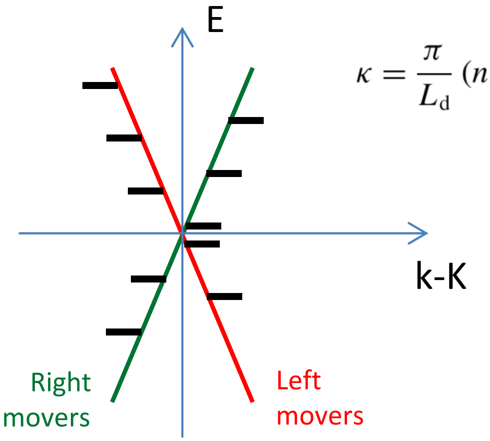
We consider the Hamiltonian of the form:

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

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

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

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

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

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**

$\zeta = 2\pi RM$
$M = 3.80 \times 10^{-7}\,\mathrm{kg\,m^{-2}}$
$v_{\mathrm{st}} = 2.4 \times 10^4\,\mathrm{m\,s^{-1}}$

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)

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

3D to 1D

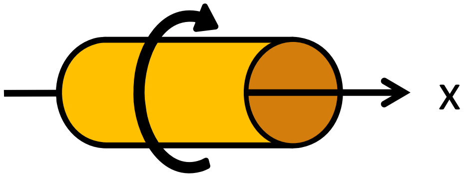
$$\hat{\rho}(\vec{r}) = \sum_\sigma \hat{\Psi}^\dagger_\sigma(\vec{r})\hat{\Psi}_\sigma(\vec{r})$$

electron density

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

deformation potential

$$g \approx 20\text{–}30\,\text{eV}$$



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

Dot-vibron overlap

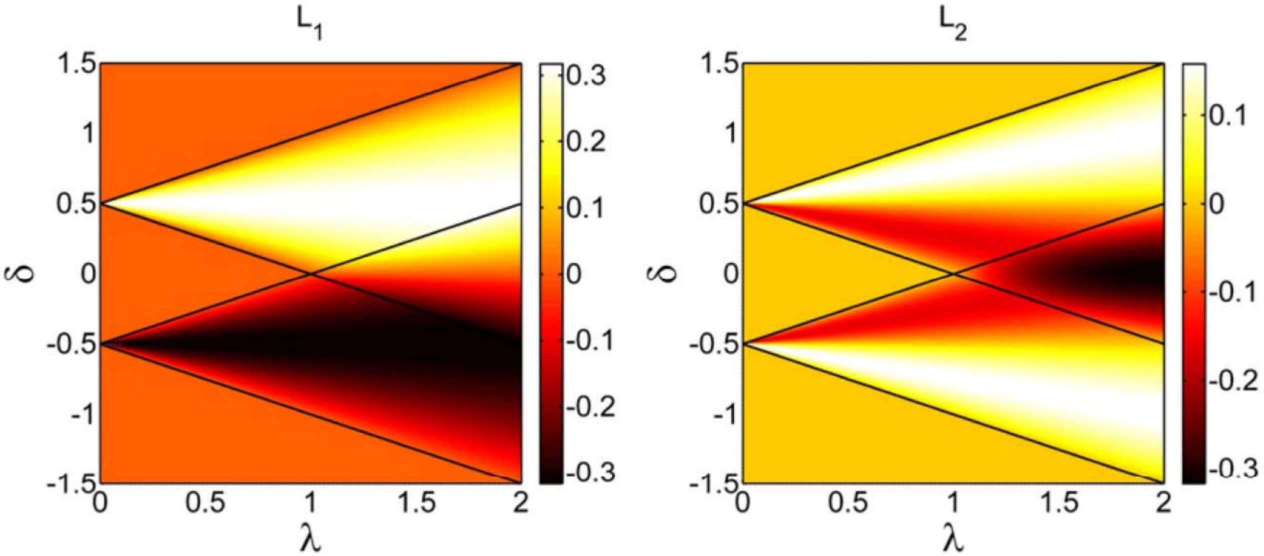
$$\hat{\rho}_{1\text{D}}(x) = \frac{\hat{N}_{c+}}{L_{\text{d}}} + \frac{2}{\sqrt{\pi\hbar}}\partial_x\hat{\phi}_{c+}(x)$$

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

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

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

Charge-vibron coupling



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

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

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

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

Fermionic and bosonic fields

$$\hat{\Psi}_{\sigma}(\vec{r}) \xrightarrow[\text{3D to 1D}]{} \hat{\psi}_{rF\sigma}(x) = \hat{\eta}_{r\sigma}\hat{K}_{rF\sigma}(x)\mathrm{e}^{\mathrm{i}\hat{\phi}^{\dagger}_{r\mathrm{F}\sigma}(x)}\,\mathrm{e}^{\mathrm{i}\hat{\phi}_{r\mathrm{F}\sigma}(x)}$$

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

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

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

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

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

Diagonalization: the polaron shift

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

where

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

Polaron transformation

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

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

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

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

The spectrum