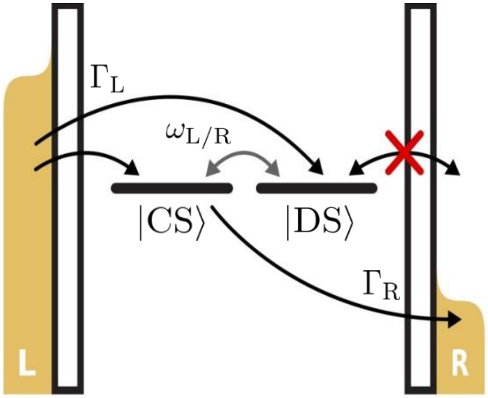
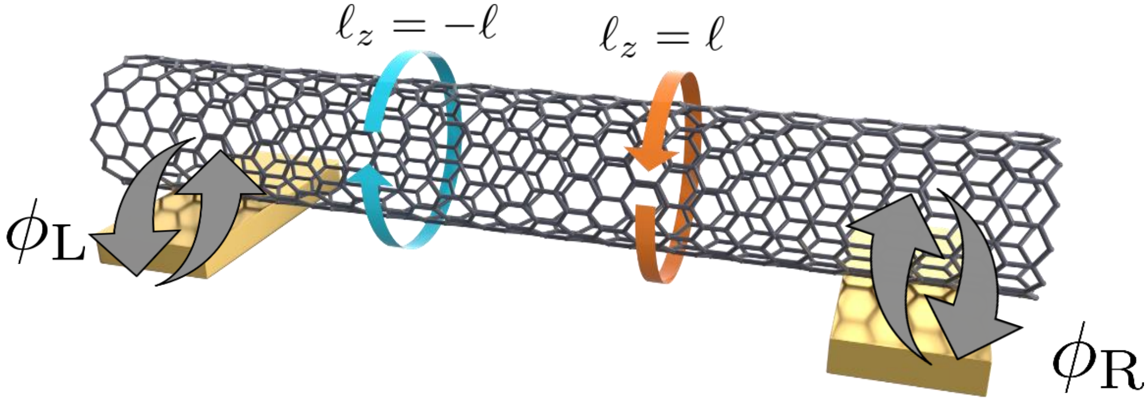
Dark states in a carbon nanotube quantum dot

II. Theory



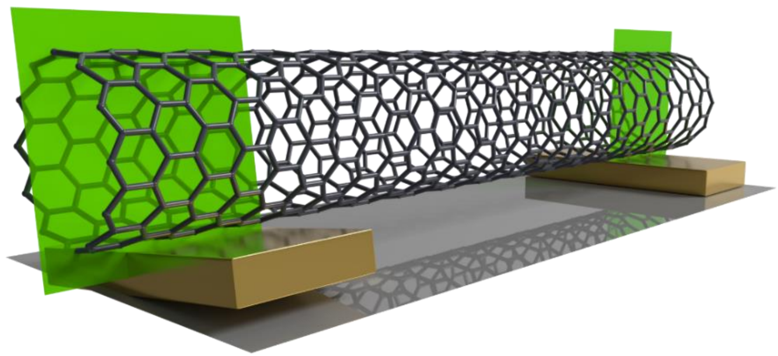


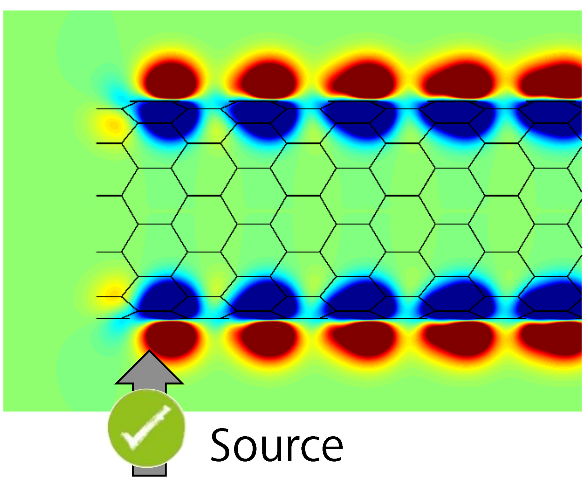
Michael Niklas, Michael Schafberger, Andrea Donarini, Nicola Paradiso, Christoph Strunk, and Milena Grifoni
University of Regensburg

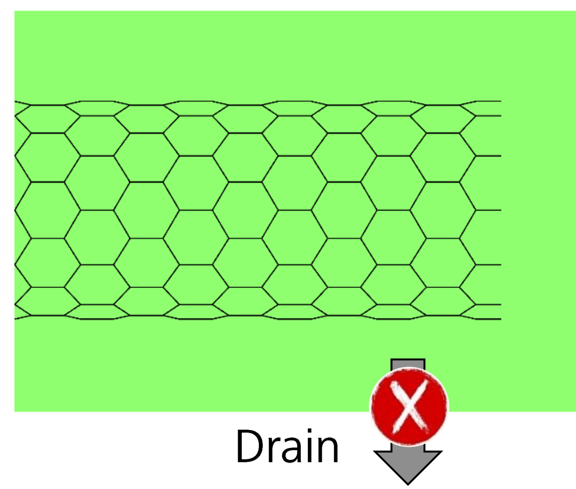
Universität Regensburg

Dark state wave function

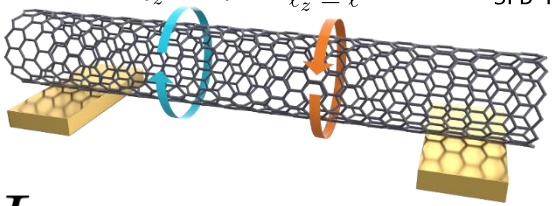
$$|\mathrm{DS}\rangle = \frac{1}{\sqrt{2}}\left[e^{i\ell\phi_\alpha}|\ell_z = \ell\rangle - e^{-i\ell\phi_\alpha}|\ell_z = -\ell\rangle\right]$$







Model: open quantum system



$$H = H_{\text{CNT}} + H_{\text{leads}} + H_{\text{tun}}$$

$$H_{\text{CNT}} = \sum_{m\ell_z} (m\epsilon_0 - \xi)\,\hat{n}_{m\ell_z} + \frac{U}{2}\hat{N}^2 + J\sum_m \left(\hat{\mathbf{S}}_{m\ell} \cdot \hat{\mathbf{S}}_{m-\ell} + \frac{1}{4}\hat{n}_{m\ell}\hat{n}_{m-\ell} \right)$$

Level spacing ($m\epsilon_0$); V_{g} (ξ); Constant interaction ($\frac{U}{2}\hat{N}^2$); Exchange interaction for zig-zag class CNTs (J term)

$$H_{\text{leads}} = \sum_{\alpha\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\alpha\mathbf{k}\sigma} c_{\alpha\mathbf{k}\sigma}$$

$$H_{\text{tun}} = \sum_{\alpha\mathbf{k}m\ell_z\sigma} t_{\alpha\mathbf{k}m\ell_z} d^\dagger_{m\ell_z\sigma} c_{\alpha\mathbf{k}\sigma} + \text{h.c.}$$

Includes the geometry of the contacts.
Is treated perturbatively

Transport

The dynamics is calculated via a generalized master equation for the reduced density matrix

$\rho = \mathrm{Tr}_{\mathrm{leads}}\left(\rho_{\mathrm{tot}}\right)$

$$\dot{\rho} = \overbrace{-\frac{i}{\hbar}[\hat{H}_{\mathrm{CNT}},\rho]}^{\text{Coherent dynamics}} \overbrace{-\frac{i}{\hbar}[\hat{H}_{\mathrm{LS}},\rho]}^{\text{Effective internal dynamics}}$$
$$+ \underbrace{\mathcal{L}_{\mathrm{tun}}[\rho]}_{\text{Tunnelling dynamics}} + \underbrace{\mathcal{L}_{\mathrm{rel}}[\rho]}_{\text{Phenom. relaxation}} := \mathcal{L}[\rho]$$

$$\mathcal{L}_{\mathrm{rel}}[\rho] = -\Gamma_{\mathrm{rel}}\left(\rho - \sum_{NFm} \rho^{\mathrm{th},NF}_{mm} |NFm\rangle\langle NFm| \sum_{En} \rho^{NE}_{nn}\right)$$

$\mathcal{L}[\rho^{\infty}] \equiv 0$ defines the stationary reduced density matrix.

Tunnelling Liouvillean

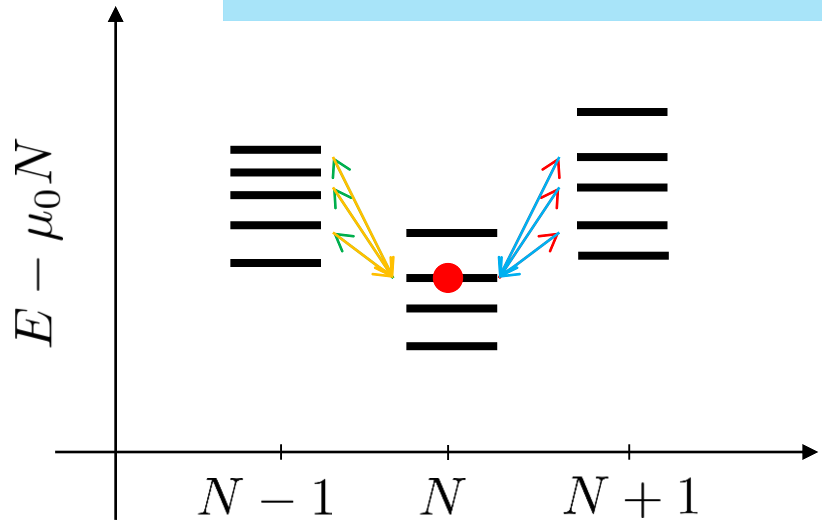
SFB 1277

$$\mathcal{L}_{\text{tun}}\rho^{NE} = -\frac{1}{2}\sum_{\alpha\sigma}\sum_{ij}\Big\{\mathcal{P}_{NE}\Big[d^\dagger_{i\sigma}\Gamma^\alpha_{ij}(E-H_{\text{CNT}})f^-_\alpha(E-H_{\text{CNT}})d_{j\sigma}+$$

$$+d_{j\sigma}\Gamma^\alpha_{ij}(H_{\text{CNT}}-E)f^+_\alpha(H_{\text{CNT}}-E)d^\dagger_{i\sigma}\Big]\rho^{NE}+H.c.\Big\}$$

$$+\sum_{\alpha\sigma}\sum_{ijE'}\mathcal{P}_{NE}\Big[d^\dagger_{i\sigma}\Gamma^\alpha_{ij}(E-E')\rho^{N-1E'}f^+_\alpha(E-E')d_{j\sigma}+$$

$$+\,d_{j\sigma}\Gamma^\alpha_{ij}(E'-E)\rho^{N+1E'}f^-_\alpha(E'-E)d^\dagger_{i\sigma}\Big]\mathcal{P}_{NE}$$



$$\mathcal{P}_{NE} := \sum_i |NEi\rangle\langle NEi|$$

Tunnelling rate matrix

SFB 1277

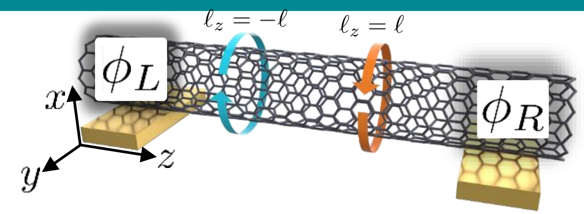
$$I_\alpha = \sum_{NE\sigma ij} \mathcal{P}_{NE}\Big[d_{j\sigma}\Gamma^\alpha_{ij}(H_{\mathrm{CNT}} - E)f^+_\alpha(H_{\mathrm{CNT}} - E)d^\dagger_{i\sigma}$$
$$-d^\dagger_{i\sigma}\Gamma^\alpha_{ij}(E - H_{\mathrm{CNT}})f^-_\alpha(E - H_{\mathrm{CNT}})d_{j\sigma}\Big]\mathcal{P}_{NE}$$

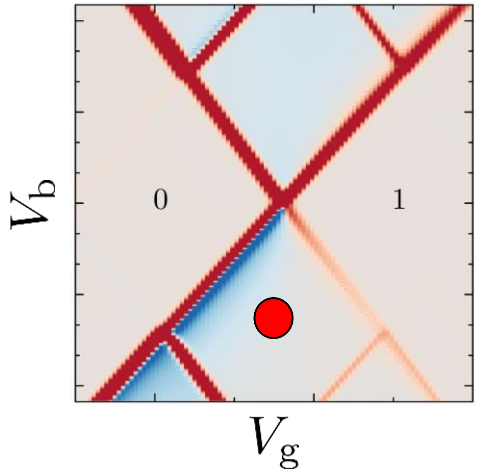
Current operator

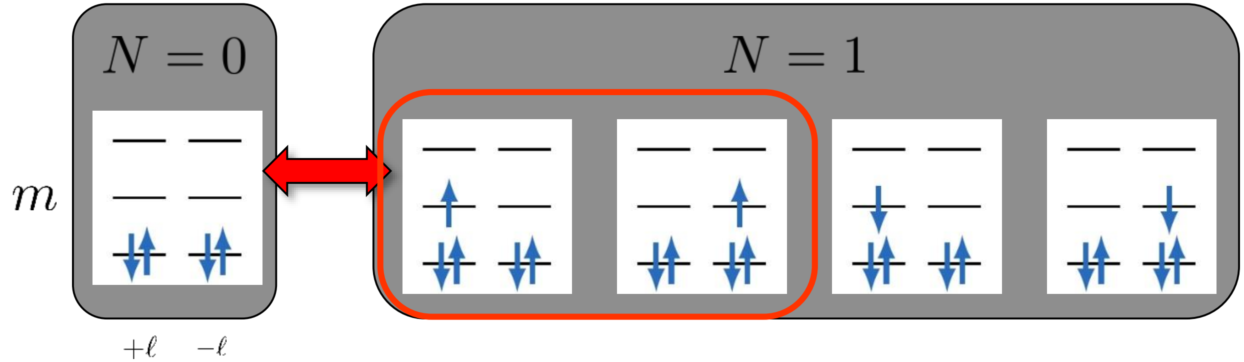
$$\Gamma^\alpha_{ij}(\Delta E) = \frac{2\pi}{\hbar}\sum_{\mathbf{k}}(t_{\alpha\mathbf{k}i})^* t_{\alpha\mathbf{k}j}\delta(\epsilon_{\mathbf{k}} - \Delta E)$$

Single particle tunnelling rate matrix

One particle dark state

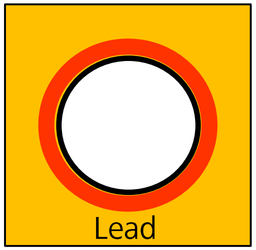




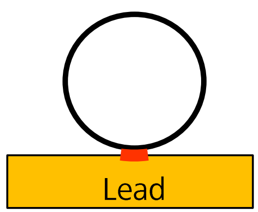


$$\Gamma^{\alpha}_{\ell_z \ell'_z}(E_1 - E_0) = \frac{2\pi}{\hbar} \sum_{\mathbf{k}} (t_{\alpha \mathbf{k} \ell_z})^* t_{\alpha \mathbf{k} \ell'_z} \delta(\epsilon_{\mathbf{k}} - E_1 - E_0)$$

$$\mathbf{\Gamma}^{\alpha} = \Gamma^{\alpha} \begin{pmatrix} 1 & a e^{2i\ell\phi_\alpha} \\ a e^{-2i\ell\phi_\alpha} & 1 \end{pmatrix}$$



$0 \leq a \leq 1$

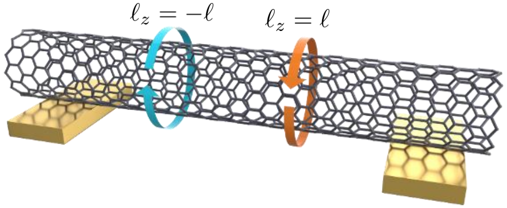


Atomically localized tunneling
or
Surface Γ-point approximation
(i.e. $k_x \approx k_F \quad k_y, k_z = 0$)

$a = 1$

SFB 1277

One particle dark state



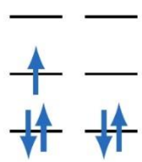
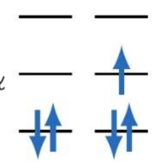
Angular momentum basis

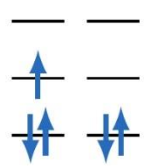
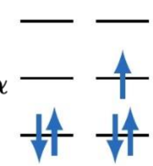
$$\Gamma^\alpha \underbrace{\begin{pmatrix} 1 & e^{2i\ell\phi_\alpha} \\ e^{-2i\ell\phi_\alpha} & 1 \end{pmatrix}}_{\mathcal{R}_\alpha}$$

Dark and coupled state basis

$$\Gamma^\alpha \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}$$

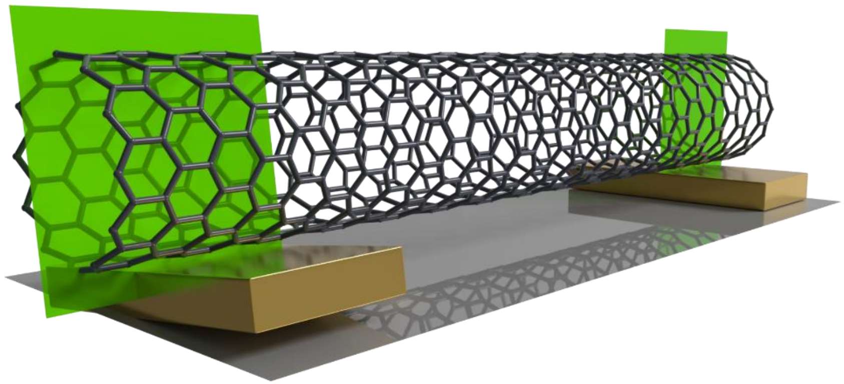
The basis $\{|DS\rangle, |CS\rangle\}$ **diagonalizes** one of the tunnelling rate matrices

$$|DS,\uparrow\alpha\rangle = \frac{1}{\sqrt{2}}\Big(e^{i\ell\phi_\alpha}$$  $$- e^{-i\ell\phi_\alpha}$$  $$\Big)$$

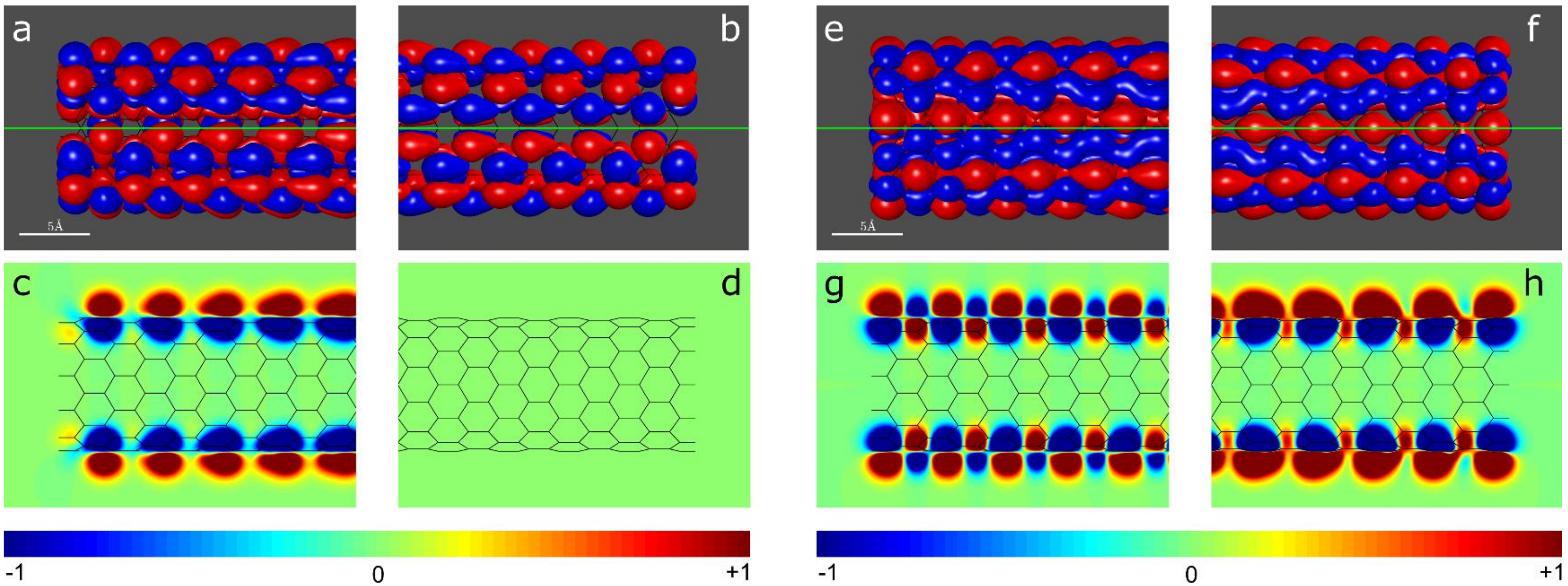
$$|CS,\uparrow\alpha\rangle = \frac{1}{\sqrt{2}}\Big(e^{i\ell\phi_\alpha}$$  $$+ e^{-i\ell\phi_\alpha}$$  $$\Big)$$

The dark state is defined with respect to a **specific** lead

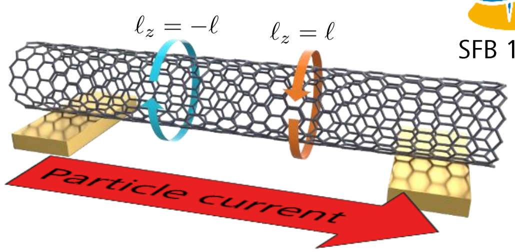
One particle dark state in a CNT (12,0)



$|DS, \mathrm{Right}\rangle$ $\quad$ $|CS, \mathrm{Right}\rangle$



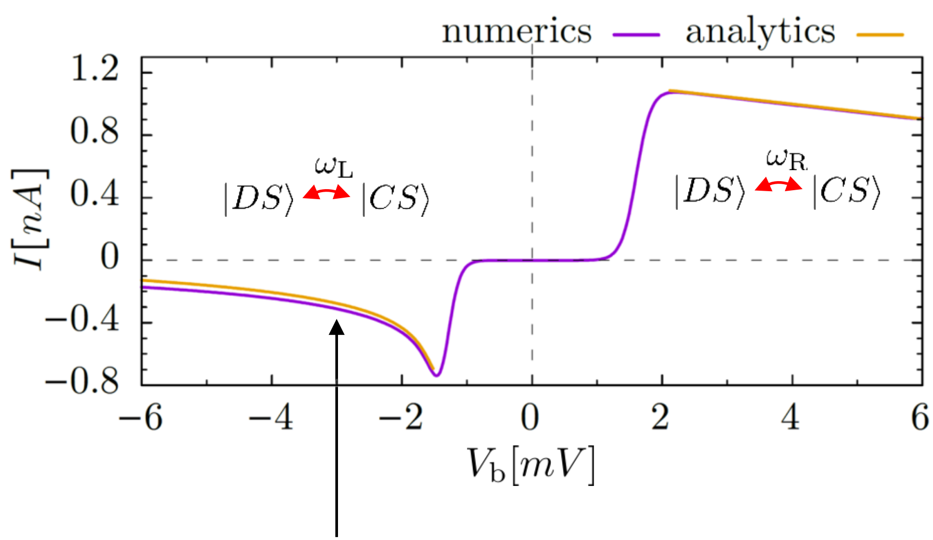
Lamb-shift like precession

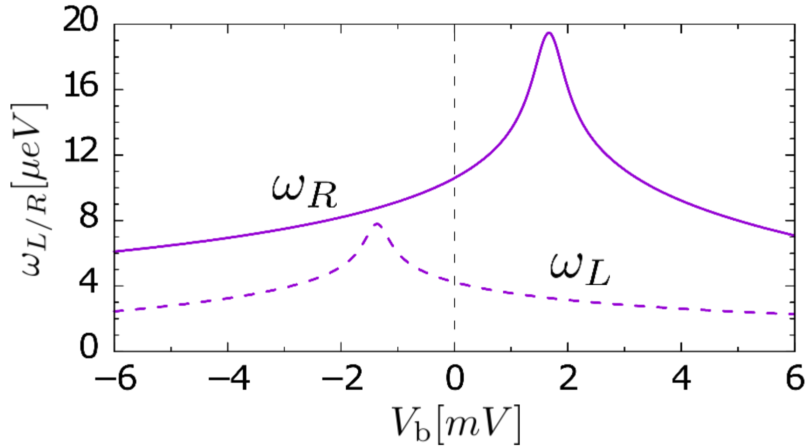


$$\dot{\rho} = -\frac{i}{\hbar}[H_{\mathrm{CNT}}, \rho] - \frac{i}{\hbar}[H_{\mathrm{LS}}, \rho] + \mathcal{L}_{\mathrm{tun}}[\rho] + \mathcal{L}_{\mathrm{rel}}[\rho]$$

$$H_{\mathrm{LS}} = \frac{\hbar}{2}(\omega_L \mathcal{R}_L + \omega_R \mathcal{R}_R)$$

$$\left[\mathcal{R}_\alpha, \, |DS, \alpha\rangle\langle DS, \alpha|\right] = 0$$ ➡ Only the **source** contribution perturbs the dark state





$$I = \frac{8e\Gamma_R \omega_L^2 \cos^2 \Delta\phi}{\Gamma_R^2 + 4(\omega_L - \omega_R)^2 + 2\omega_L \cos^2 \Delta\phi \, [\omega_L \Gamma_R / \Gamma_L + 4\omega_R]}$$

$$\Delta\phi = \frac{\phi_L - \phi_R}{2}$$

Closing remarks

SFB 1277

Interference occurs between the **degenerate** angular momentum states of a **zig-zag class** carbon nanotube

Spatially confined tunneling mixes angular momentum states providing a non-diagonal **tunnelling rate matrix**

The **dark state** is the eigenvector of the tunneling rate matrix with zero eigenvalue

The **Lamb-shift like** precession perturbs the dark state and explains the **bias voltage asymmetry**

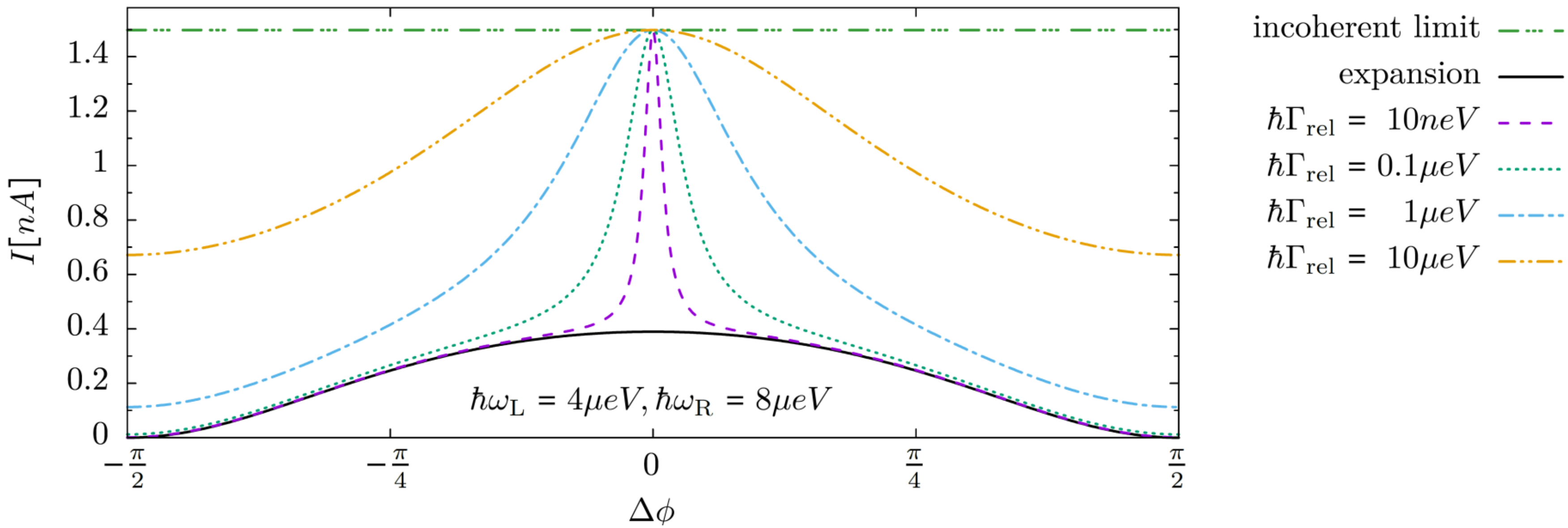
Thank you for your attention

Current vs. tunneling phases

SFB 1277

$$I = \frac{8e\Gamma_R \omega_L^2 \cos^2 \Delta\phi}{\Gamma_R^2 + 4(\omega_L - \omega_R)^2 + 2\omega_L \cos^2 \Delta\phi \, [\omega_L \Gamma_R / \Gamma_L + 4\omega_R]}$$

$$\Delta\phi = \frac{\phi_L - \phi_R}{2}$$



$$I(\Delta\phi = 0) = \frac{4e\Gamma_L\Gamma_R}{4\Gamma_L + \Gamma_R}$$

incoherent current through 4 degenerate levels

Effects of exchange interaction

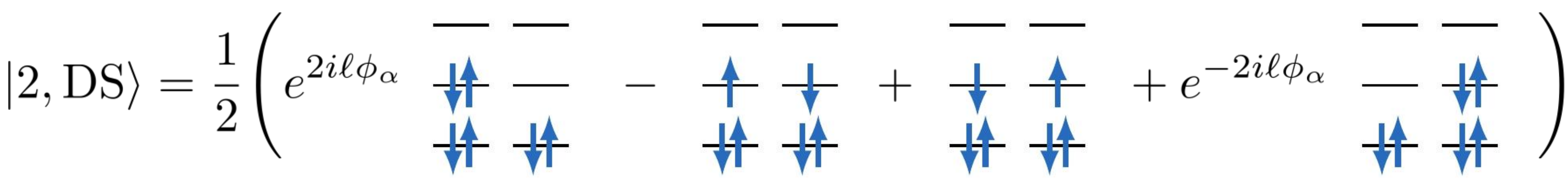
$$H_{\mathrm{CNT}} = \sum_{m\ell_z} (m\epsilon_0 - \xi)\, \hat{n}_{m\ell_z} + \frac{U}{2}\hat{N}^2 + J\sum_m \left(\hat{\mathbf{S}}_{m\ell} \cdot \hat{\mathbf{S}}_{m-\ell} + \frac{1}{4}\hat{n}_{m\ell}\hat{n}_{m-\ell}\right)$$

$J = 0$

2-particle groundstate is 6-fold degenerate

➡ new dark state possible

$|2, \mathrm{DS}\rangle = \frac{1}{2}\Big(e^{2i\ell\phi_\alpha}$ … $-$ … $+$ … $+\, e^{-2i\ell\phi_\alpha}$ … $\Big)$

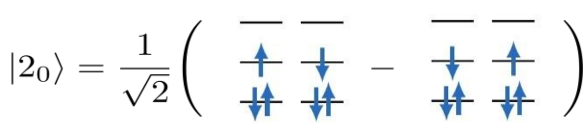


➡ interference also at 1↔2 particle resonance

$J > \Gamma$

2-particle groundstate is the inter-valley singlet

$|2_0\rangle = \frac{1}{\sqrt{2}}\Big($ … $-$ … $\Big)$



➡ no 2 particle dark state is possible