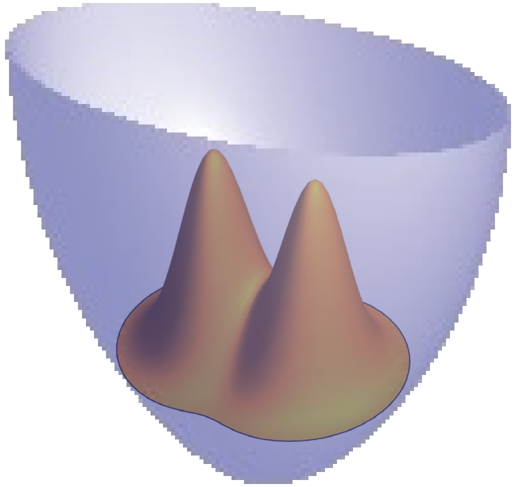
Electrons don't like each other : Impact of quantum dot shape on readout and exchange interactions



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Phys. Rev. B **104**, 195305 (2021)

Take home messages

-Unless you have very small and isotropic dots the single-particle picture is the wrong way of thinking about multiparticle states. Formation of Wigner molecules.

-ST splitting decreases exponentially with the dot length and the anisotropy only makes it faster

-Si dots are clearly more affected than GaAs and Ge dots

-Low-lying triplet states complicate PSB readout

-Low-lying triplet states limit exchange coupling

Intro: current status

-High single-qubit gate fidelities have been demonstrated in both electrons and hole qubits. See

Nature Nanotechnology **13**, 102-106 (2018)

Nature volume **569**, pages 532–536 (2019)

Nature Communications volume 11, Article number: 4144 (2020)

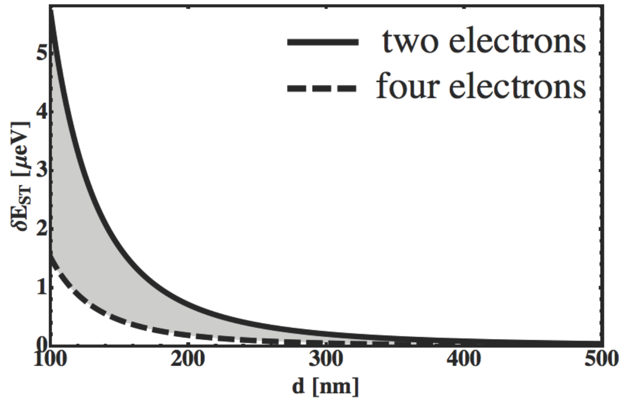
- Two-qubit gates beyond QEC threshold. See

arXiv:2107.00628

-Working four-qubit processor with holes

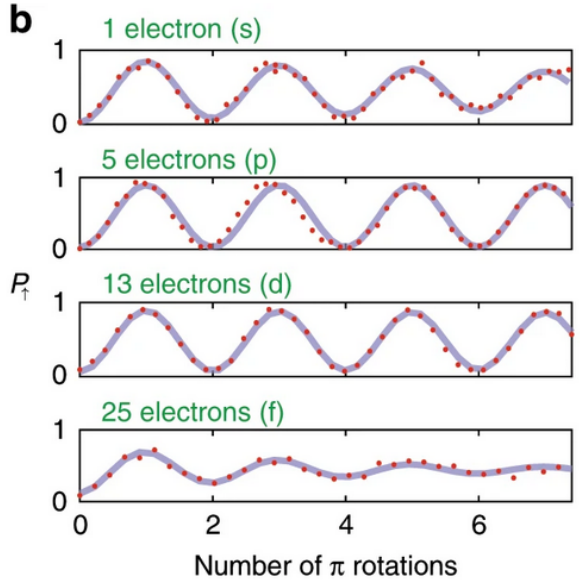
Nature **591**, 580–585 (2021)

Multi-particle states. Why do they matter?



-Multi-electron states may screen part of the charge noise

Validity of the single-particle description and charge noise resilience for multielectron quantum dots
Phys. Rev. B **91**, 155425 (2015)
All-Microwave Control and Dispersive Readout of Gate-Defined Quantum Dot Qubits in Circuit Quantum Electrodynamics
Phys. Rev. Lett. **122**, 206802 (2019)



-Enhanced dipolar coupling

Coherent spin control of s-, p-, d- and f-electrons in a silicon quantum dot
Nature Communications **11**, Article number: 797 (2020)

-Multiple coherent oscillations

Coherent Control and Spectroscopy of a Semiconductor Quantum Dot Wigner Molecule
Phys. Rev. Lett. **127**, 127701 (2021)

Goal: understand Coulomb effects in QD and its consequences on SC qubits

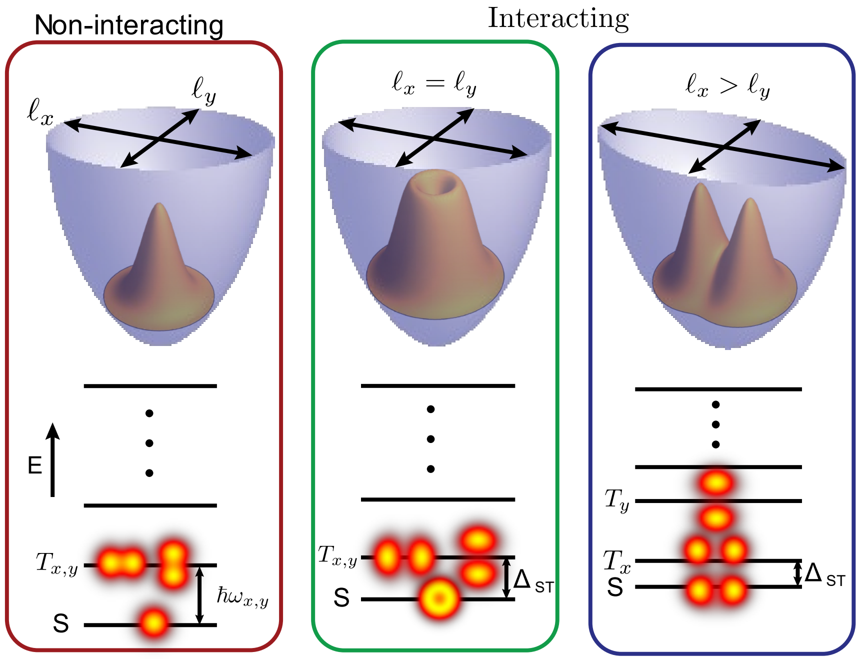
-Focus on 2-particle problem (holes or electrons)

-We will make use of Hooke's model:

Coulomb repulsion + harmonic confinement

-2D and single-band approximation

-General model that can be applied to different materials



Hooke’s atom model

$$H = \sum_{i=1,2} \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m(\omega_x^2 x_i^2 + \omega_y^2 y_i^2) + \frac{e^2}{4\pi\varepsilon r}$$

$$H_R = \frac{\mathbf{p}_R^2}{4m} + m(\omega_x^2 X^2 + \omega_y^2 Y^2)$$

$$H_r = \frac{\mathbf{p}_r^2}{m} + \frac{1}{4} m(\omega_x^2 x^2 + \omega_y^2 y^2) + \frac{e^2}{4\pi\varepsilon r}$$

We take x as the weakest confinement direction

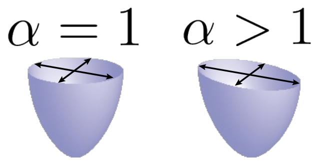
$$\ell_x = \sqrt{\hbar/(m\omega_x)}$$

$$E_{orb} = \hbar\omega_x$$

$$E_{ee} = e^2/(4\pi\varepsilon\ell_x)$$

Wigner ratio: $\lambda_W = E_{ee}/E_{orb}$

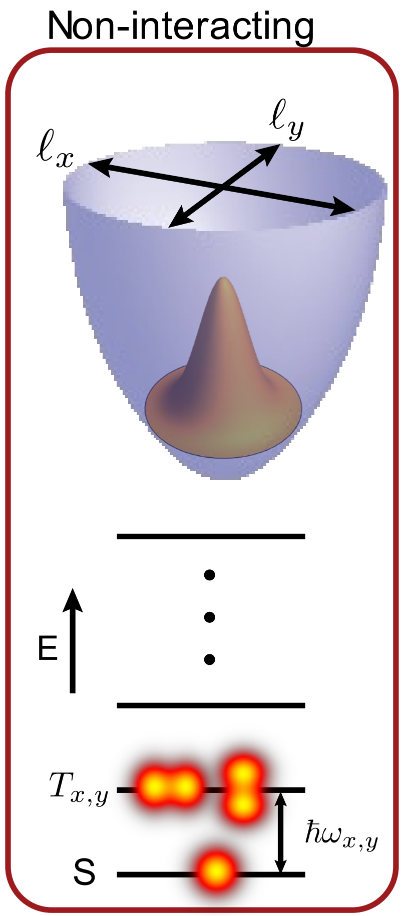
Anisotropy: $\alpha = \omega_y/\omega_x$

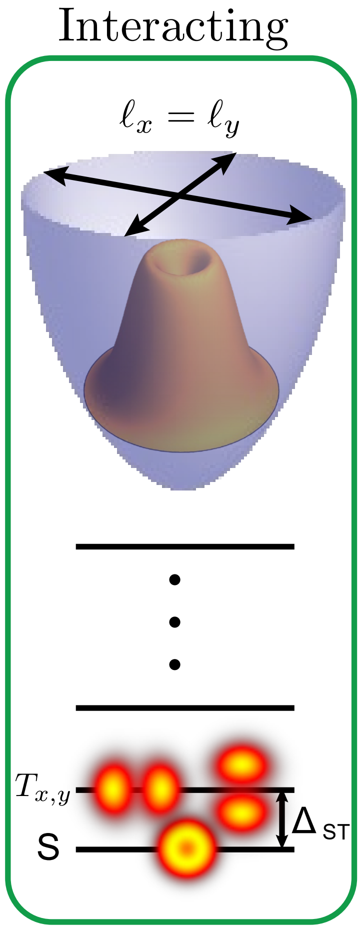


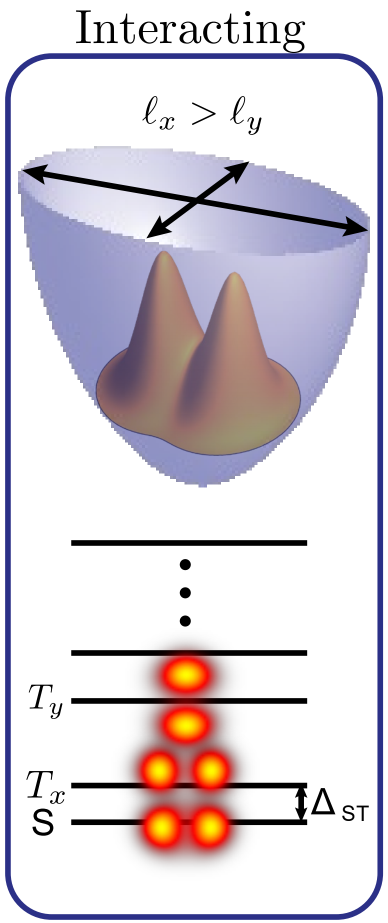
$$(x', y') = (x/\ell_x, y/\ell_x)$$

$$H'_r = -\partial_{x'}^2 - \partial_{y'}^2 + \frac{1}{4}(x'^2 + \alpha^2 y'^2) + \frac{\lambda_W}{|r'|}$$

Spectral compression & single-particle approximation breakdown







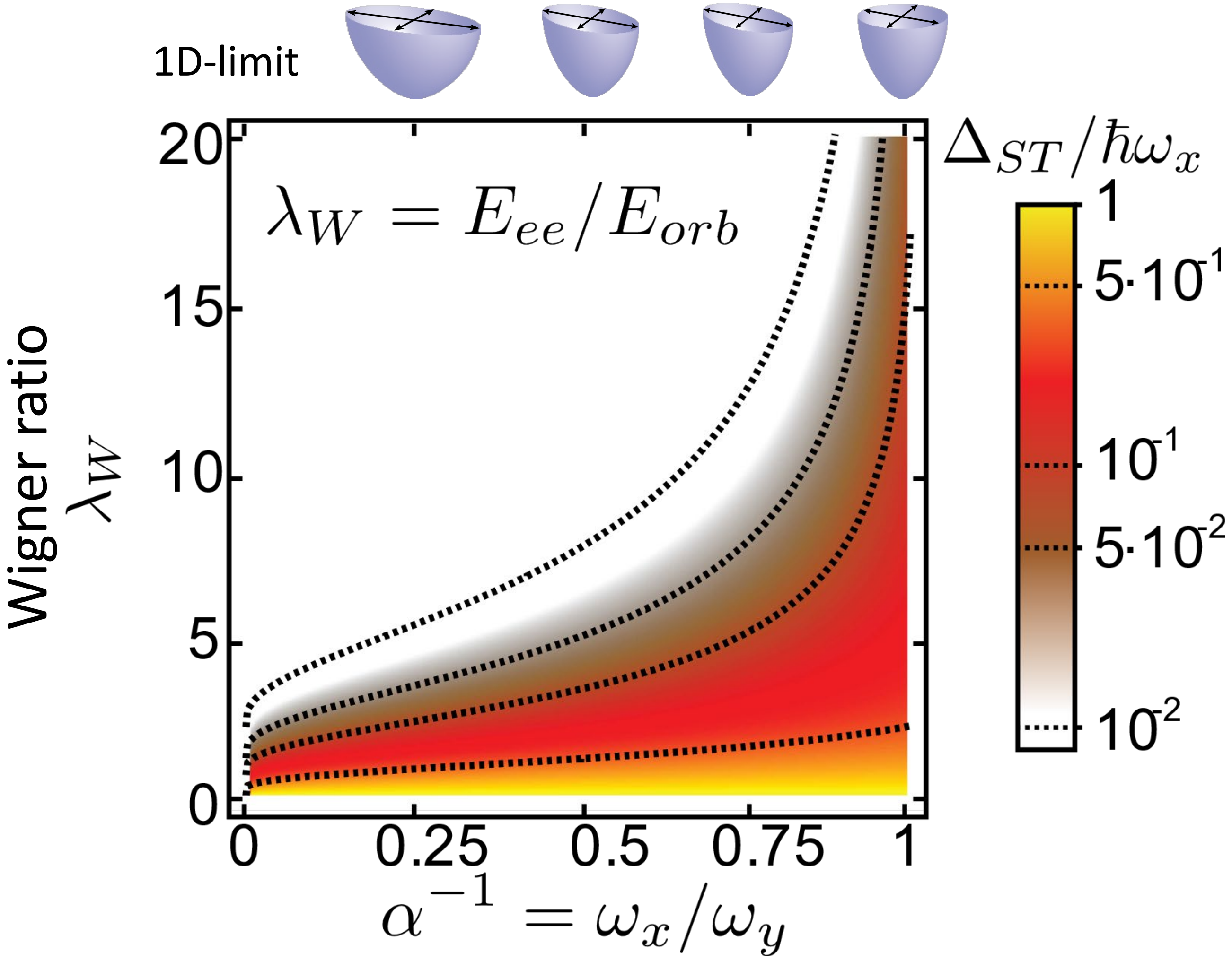
$$\Delta_{ST} \leq \hbar\omega_x$$

ST-splitting is reduced

-The Coulomb repulsion induces a reduction of the ST-splitting

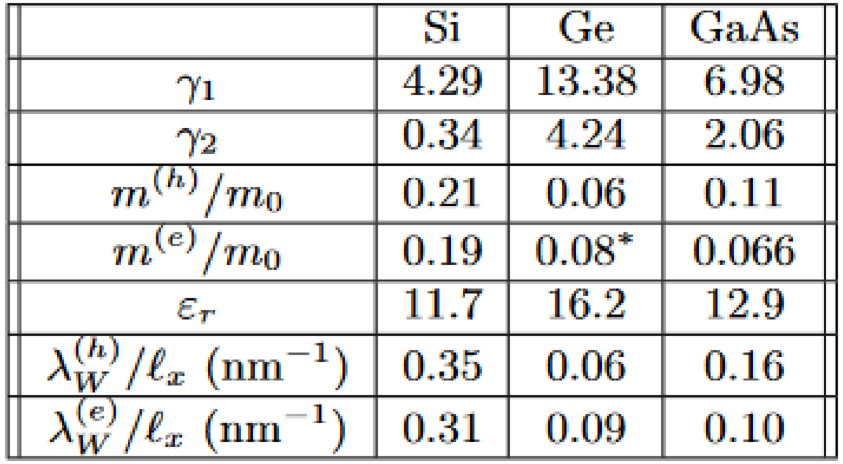
-The higher the interaction (larger dot) the larger the reduction

-The anisotropy quickly enhances this effect

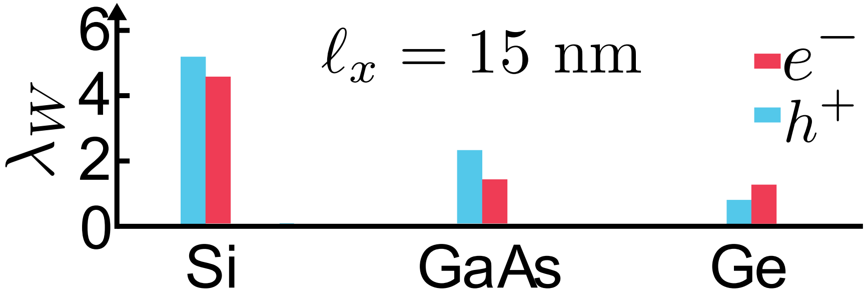


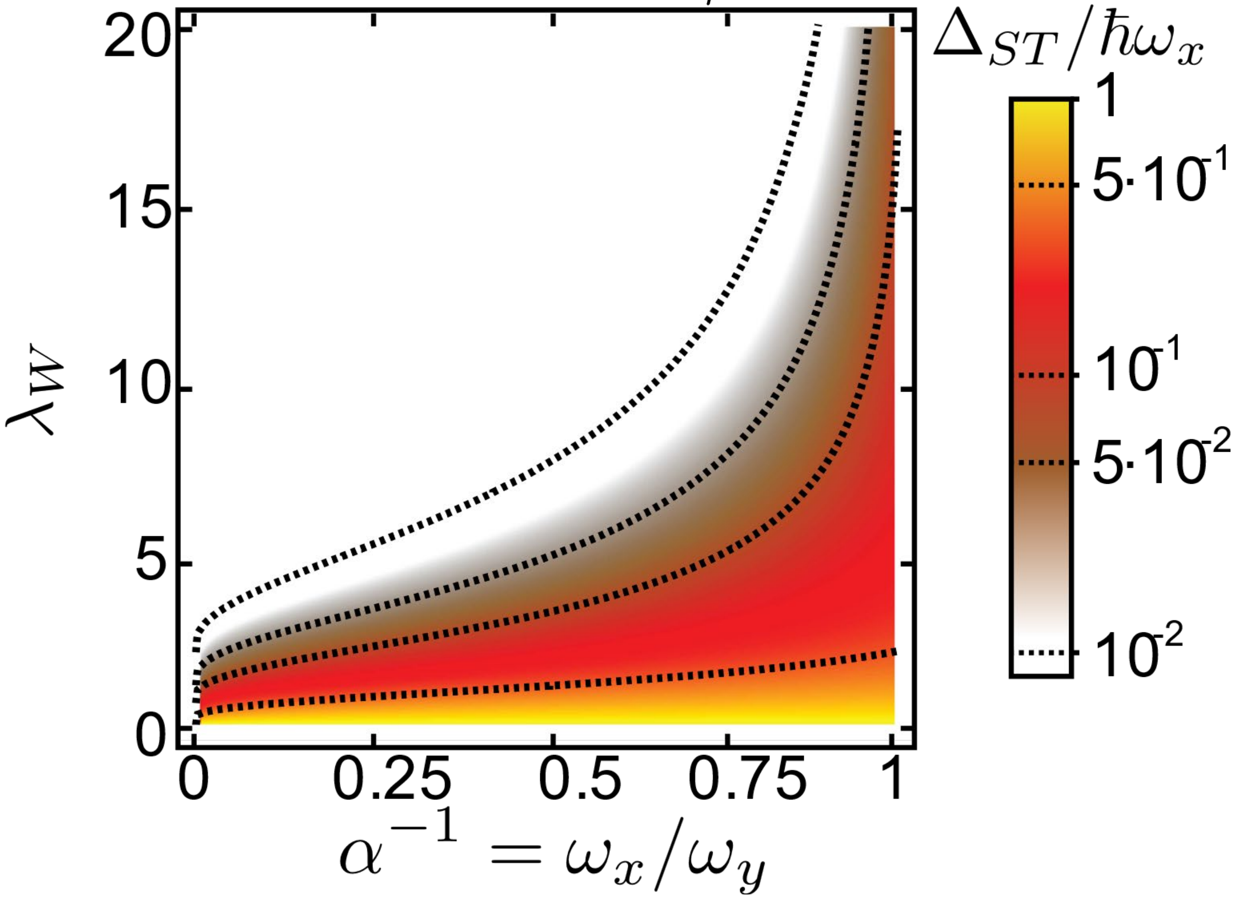
Silicon is the most affected

The reason is the large effective mass + low permittivity $\lambda_W \propto \frac{m_{\mathrm{eff}}}{\varepsilon_r}\ell_x$



	Si	Ge	GaAs
γ_1	4.29	13.38	6.98
γ_2	0.34	4.24	2.06
$m^{(h)}/m_0$	0.21	0.06	0.11
$m^{(e)}/m_0$	0.19	0.08*	0.066
ε_r	11.7	16.2	12.9
$\lambda_W^{(h)}/\ell_x$ (nm^{-1})	0.35	0.06	0.16
$\lambda_W^{(e)}/\ell_x$ (nm^{-1})	0.31	0.09	0.10





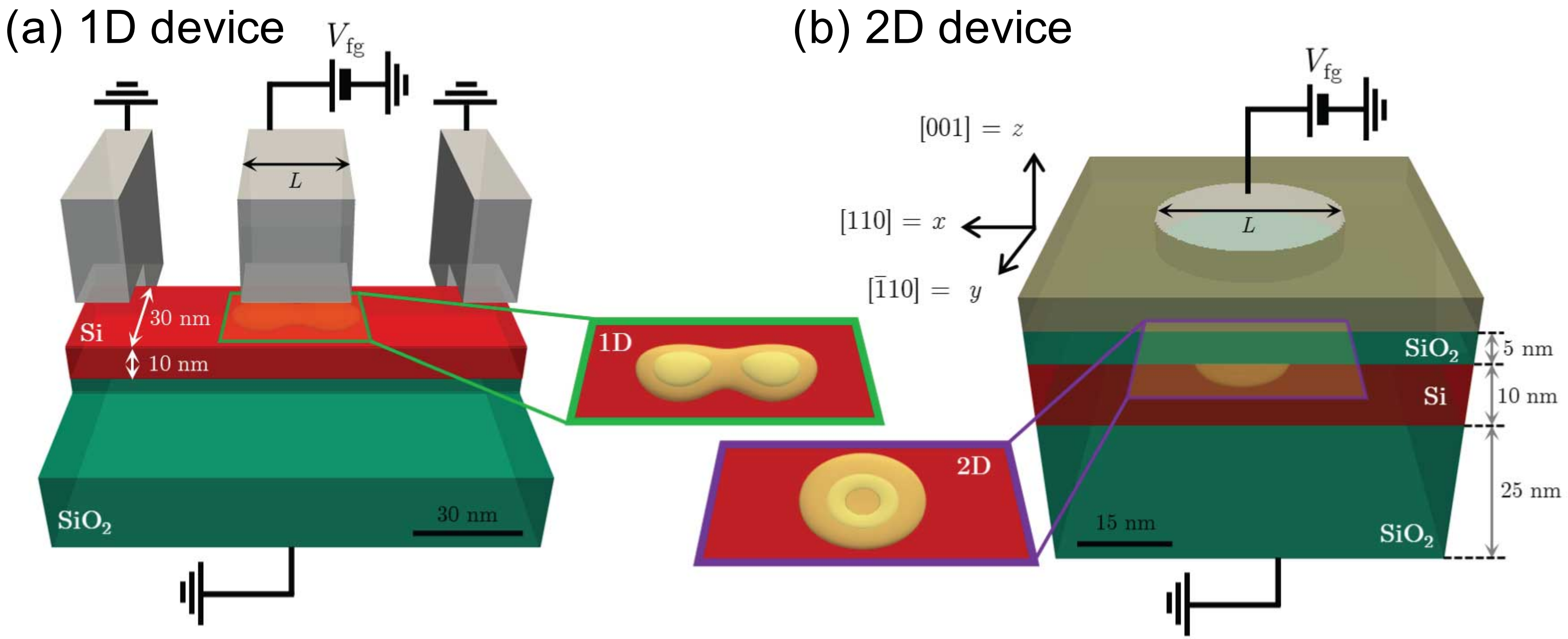
Comparison with realistic devices

- Poisson solver for the electrostatics

- 4KP band calculation for the single-hole simulations

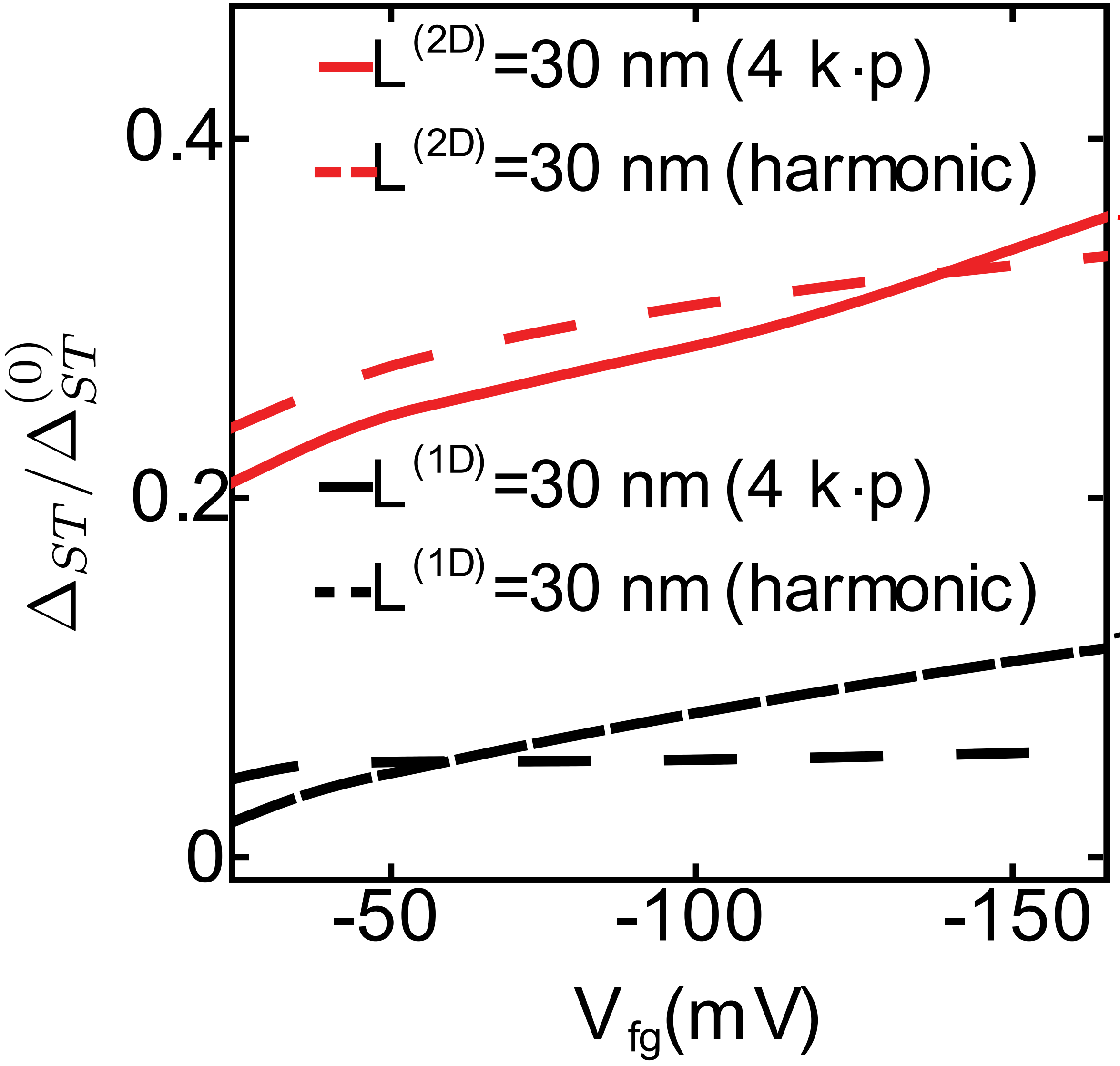
- TB for the single-electron simulations

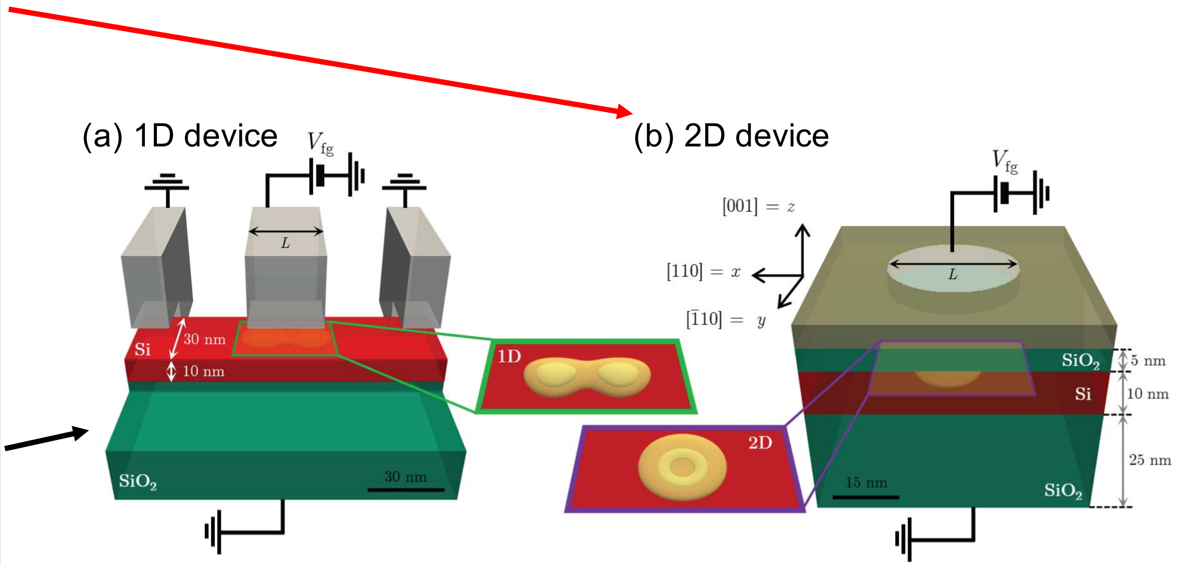
- Full CI to extend to 2-particle states


(a) 1D device

(b) 2D device

Simple model agrees with simulations

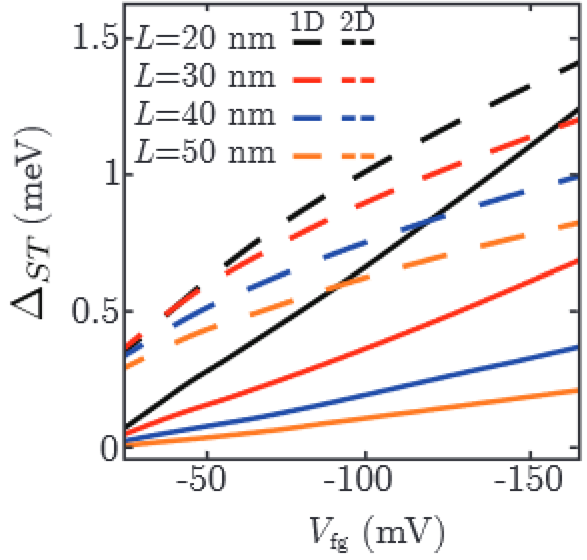


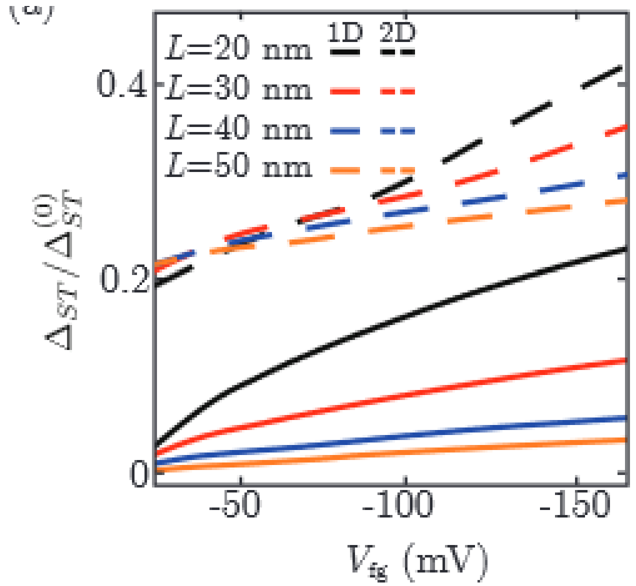


Singlet-triplet splitting decays fast with gate length

-2-hole results show fast ST decay with L

-Strengthening the confinement with gates mitigates the decay



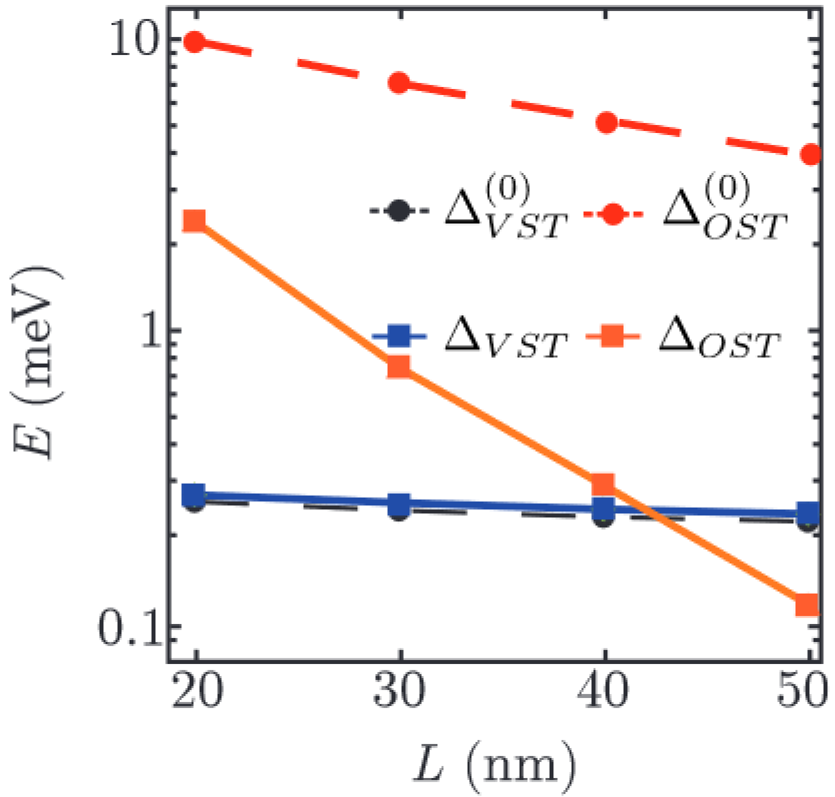


What about valleys?

-Used TB to obtain two-electron spectrum with valley states

-The valley triplet is mostly insensitive to molecularization even under disorder

-If the dot is too large, the orbital triplet will go lower than the valley triplet anyways



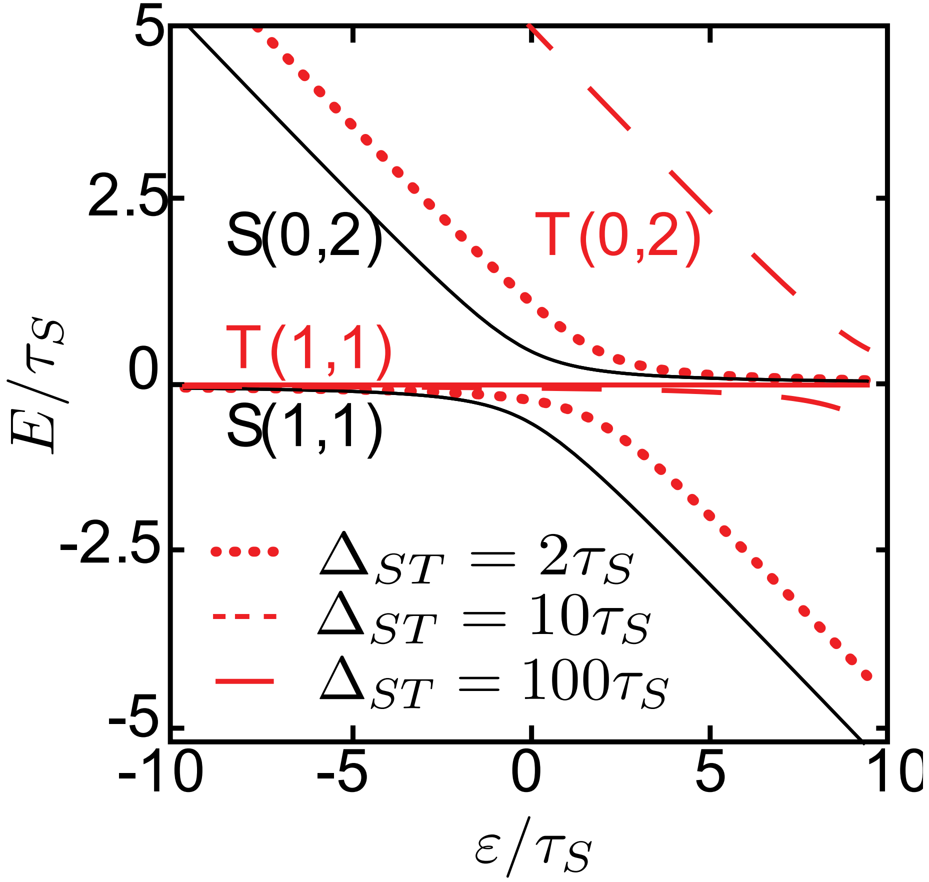
PSB readout: what happens if I have a low triplet state?

-Using PSB for readout requires going to (1,1)/(0,2) anticrossing

-If the qubit is in S state, a charge transition occurs

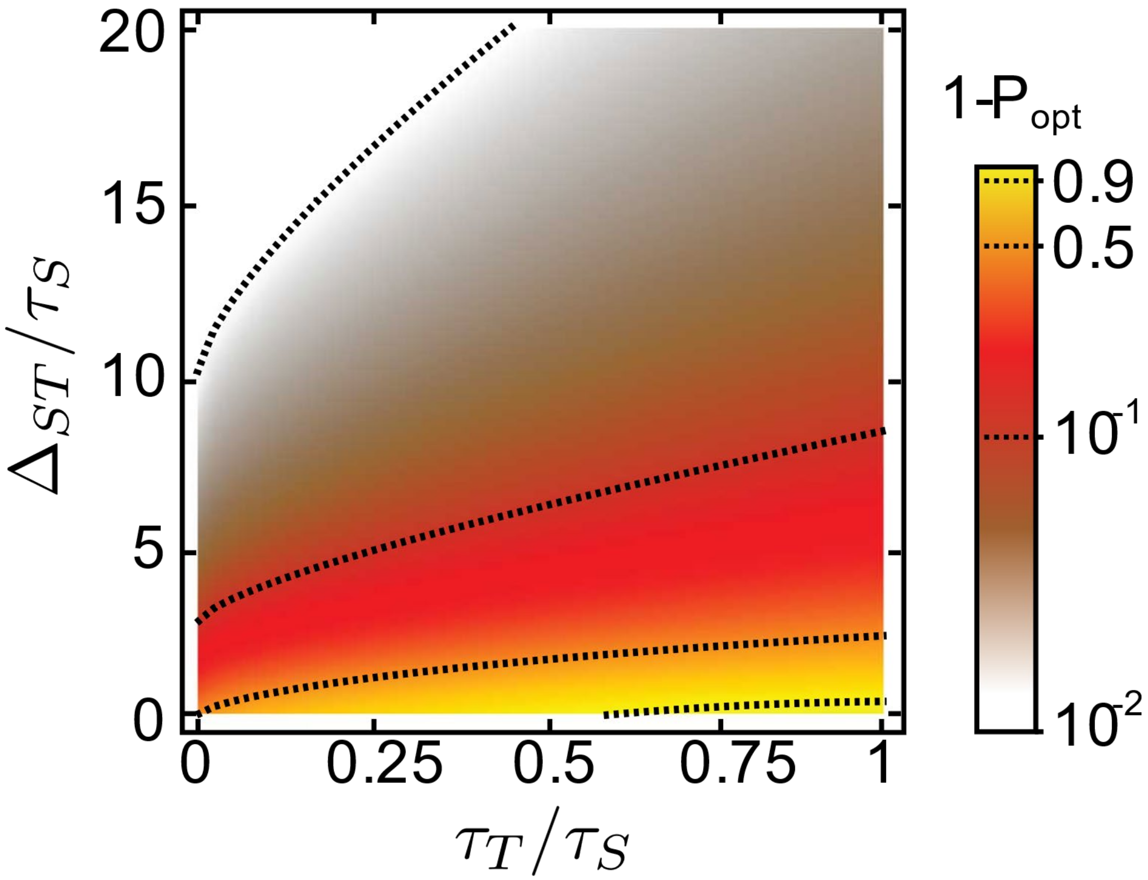
-If the qubit is in the T state, there should be no charge signature

-A low triplet may yield false readouts of singlet states



Readout may be hampered even at optimal positions

$$P_{\mathrm{opt}} = P_{S(1,1)\to S(0,2)}(\varepsilon_{\mathrm{opt}}) - P_{T(1,1)\to T(0,2)}(\varepsilon_{\mathrm{opt}})$$

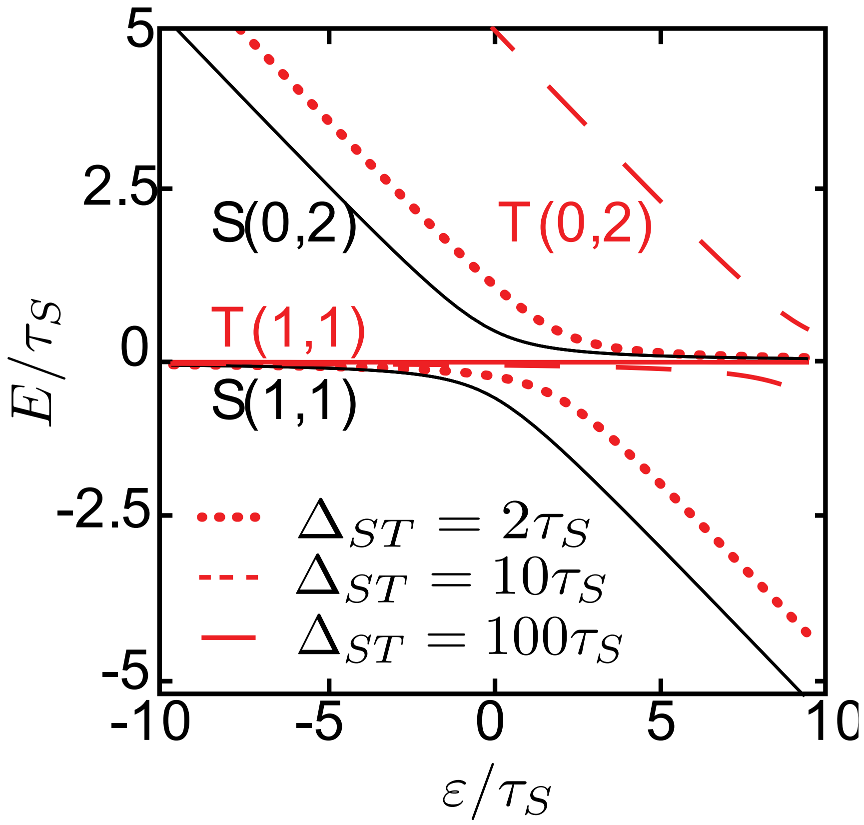


Effects on the exchange interaction

-The exchange coupling is just $J = E_T - E_S$

-The singlet state is bent with respect to the triplet state by the presence of excited singlets

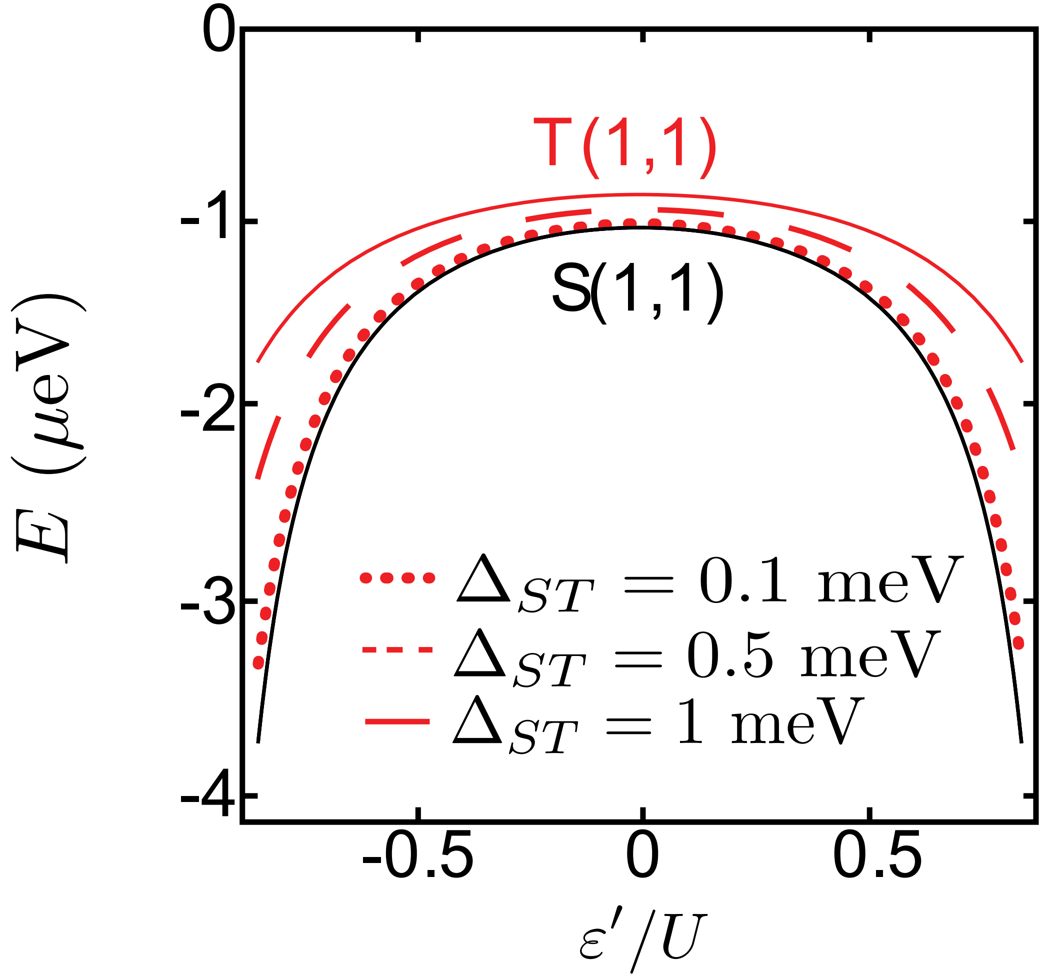
-Low-lying triplets bend the triplet energy in a similar way, limiting J



$$J = J_\infty - \frac{1}{2}\left(\varepsilon - \Delta_{ST} + \sqrt{(\varepsilon - \Delta_{ST})^2 + 4\tau_T^2}\right)$$

What about the SOP?

-At the SOP the qubits are insensitive to charge noise



$\tau_S = \tau_T = 50\ \mu eV$

Charging energy U=5 meV

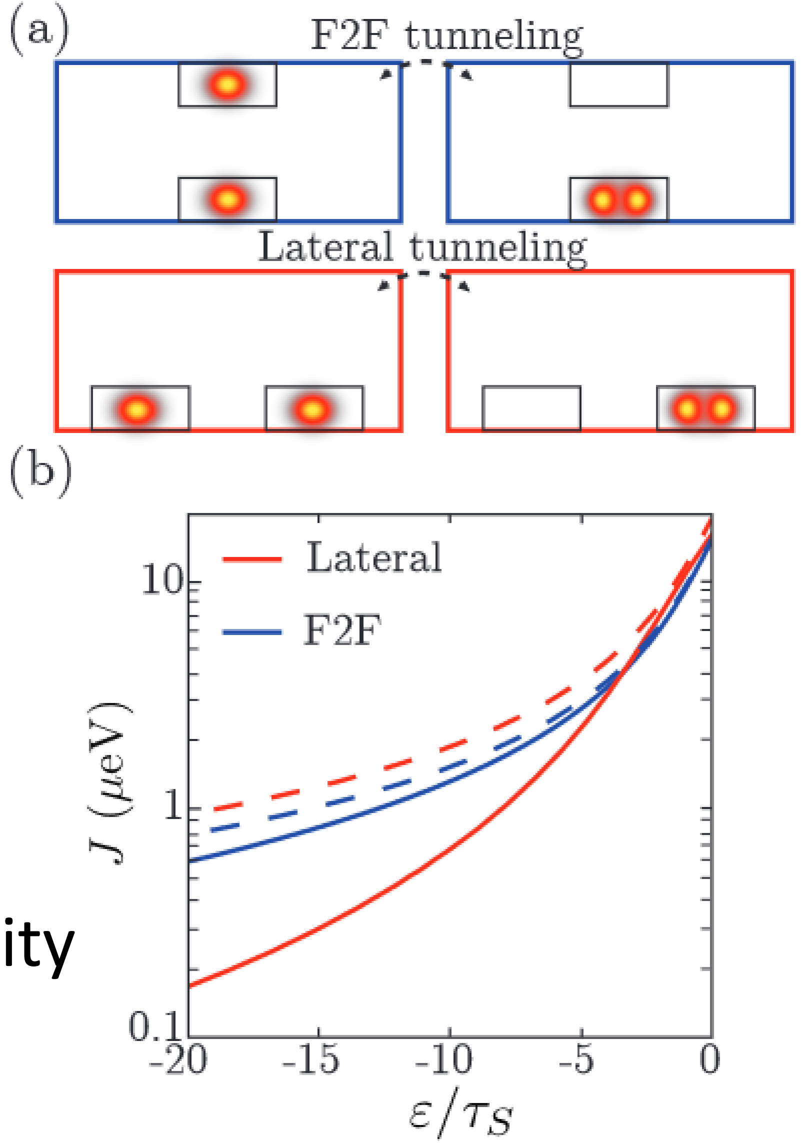
Impact of dot connectivity: face to face vs lateral

-In F2F the T(1,1) configuration has a negligible tunnel coupling to the T(0,2):

Bending is limited

-In the lateral configuration, T(1,1) loves to go to T(0,2)

Highest bending



Dashed for T(0,2) at infinity

Solid for realistic T(0,2)

Take home messages

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-ST splitting decreases exponentially with the dot length and the anisotropy only makes it faster

-Si dots are clearly more affected than GaAs and Ge dots

-Low-lying triplet states complicate PSB readout

-Low-lying triplet states limit exchange coupling

Smaller + isotropic dots are the easiest way to avoid this