The IQubits project for quantum computing in Si and SiGe MOSFETs

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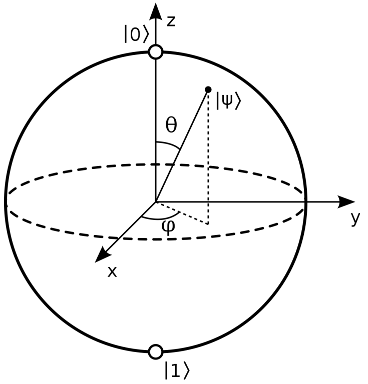
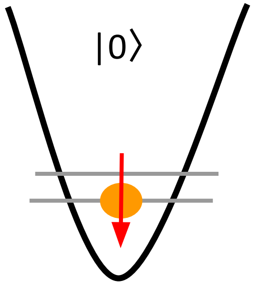
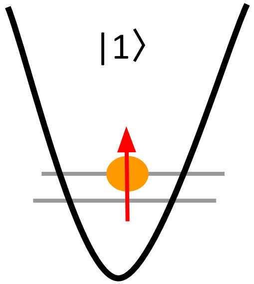
https://www.iqubits.eu

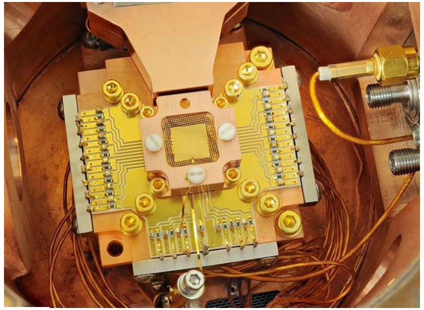
CNRNANO MODENA

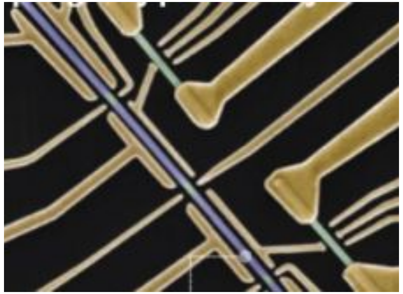
A NEW ROUTE FOR THE SPIN QUBIT

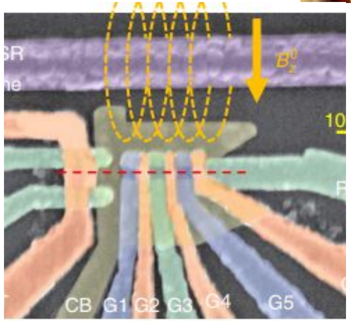


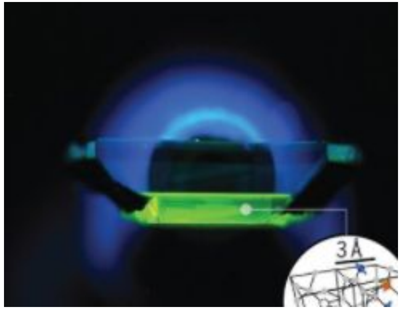








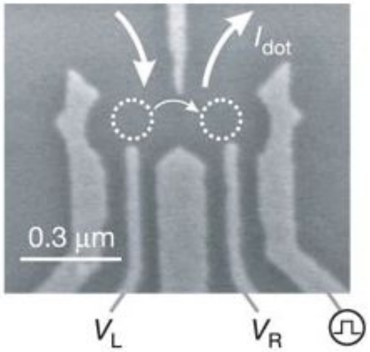




A NEW ROUTE FOR THE SPIN QUBIT

OLD PARADIGM

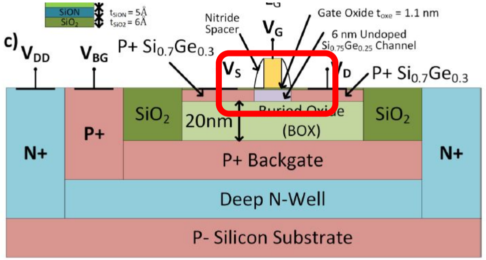
- QD in III-V semiconductor heterostructures
- Device implementations developed within academic-scale laboratories
- Magnetically controlled spin manipulation



F. H. L. Koppens et al., *Nature volume 442, pages766–771 (2006)*

NEW PARADIGM

- Silicon
- Commercial devices with industrial fabrication as starting point
- Fully-electrical control of the spin qubit



S. Bonen *et al.*, *IEEE Electron Device Lett.*, 40, 127-130 (2019)

SILICON AS HOST MATERIAL

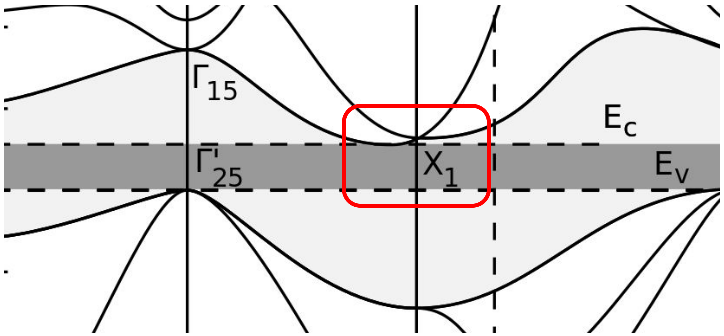
WEAK HYPERFINE INTERACTION

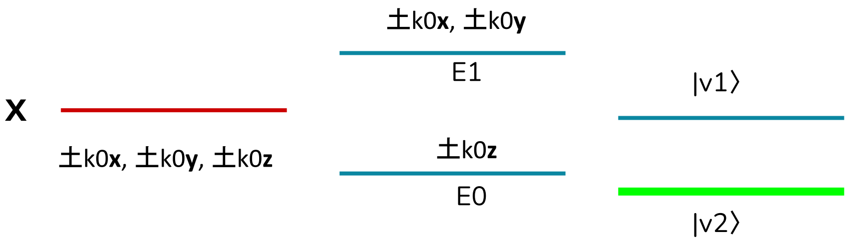
- No nuclear spin in most abundant isotope ^{28}Si
- % Improved by isotopic purification

ELECTRON AND HOLE SPIN QUBIT

- CB: Valley splitting @ X
- VB: HH-LH splitting @ Γ

ELECTRON SPIN QUBITS





6 degenerate CB valleys

z-confinement

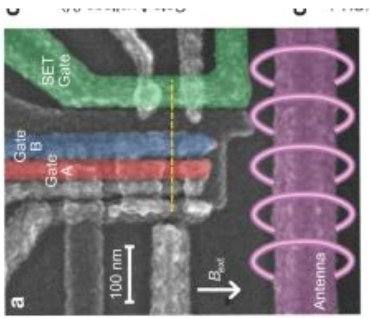
+ sharpness

- vertical confinement + valley splitting due to sharp interfaces or dopants
- **weak SO coupling in CB**

→ spin qubit

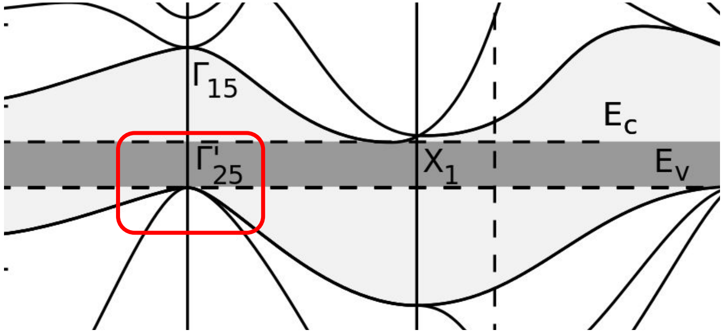
→ not sensitive to charge noise

→ **magnetically-driven spin manipulation**



J Yoneda, *Nat. Comm. 12 4114 (2021)*

HOLE SPIN QUBITS

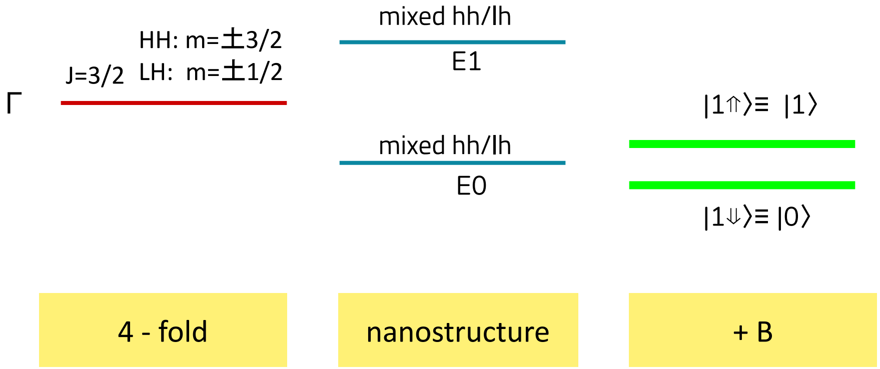


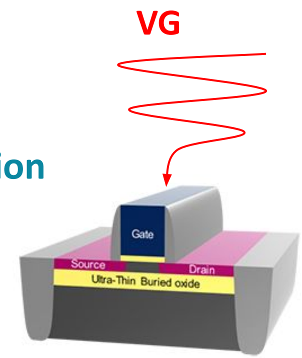
- HH, LH states degenerate at **k**=0
- Splitting of J=3/2 bands due to size quantization
- static B to lift Kramers degeneracy
- **large SO coupling**

→ pseudo-spin qubit

→ sensitive to charge noise

→ **all-electrical spin manipulation**





SILICON AS HOST MATERIAL

- **WEAK HYPERFINE INTERACTION**
  - No nuclear spin in most abundant isotope ^{28}Si
  - % Improved by isotopic purification
- **ELECTRON AND HOLE SPIN QUBIT**
  - CB: Valley splitting @ X
  - VB: HH-LH splitting @ Γ
- **EXPLOIT TECHNOLOGICAL ADVANCES**
  - Control on **quality** of lithography
  - **High-density** of components and interconnections
  - **Co-integration** feasible in **CMOS** platforms

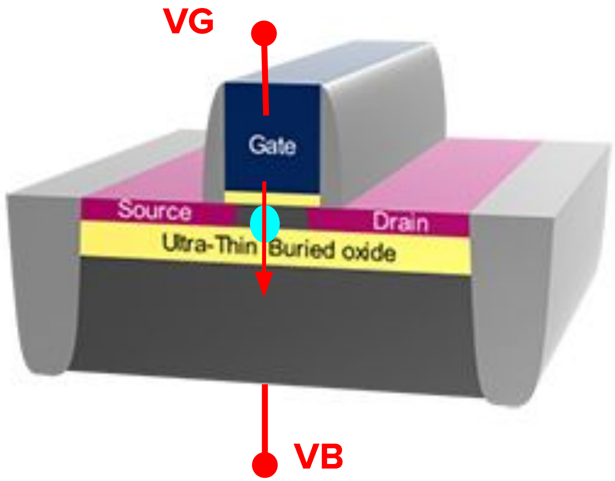
ideal for large arrays of QDs → error correction codes

IQUBITS PROJECT collaborative R.I.A. funded by Horizon 2020 [FET-Open programme]

OBJECTIVES: integration + scaling

- proposes ***commercial*** devices for spin qubit
- qubit ***co-integrated*** with control electronics (spin manipulation, readout…)

Fully-Depleted- Silicon-On Insulator (FDSOI) MOSFETs
Si and SiGe UNDOPED channel



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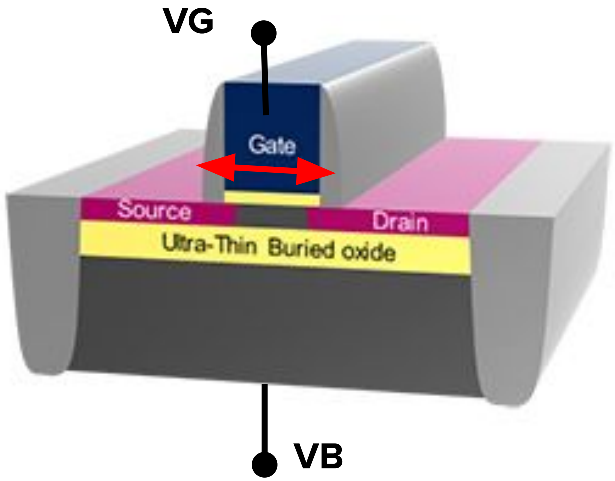
Ultra-scaled devices
10 nm channel length (increase ΔE)



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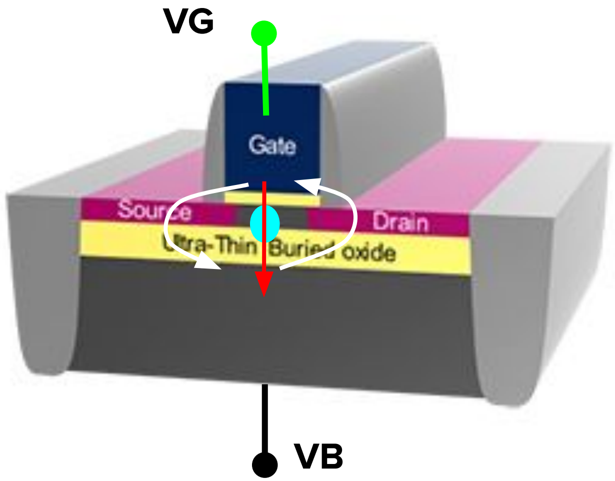
Fully-Depleted- Silicon-On Insulator (FDSOI) MOSFETs
Si and SiGe UNDOPED channel

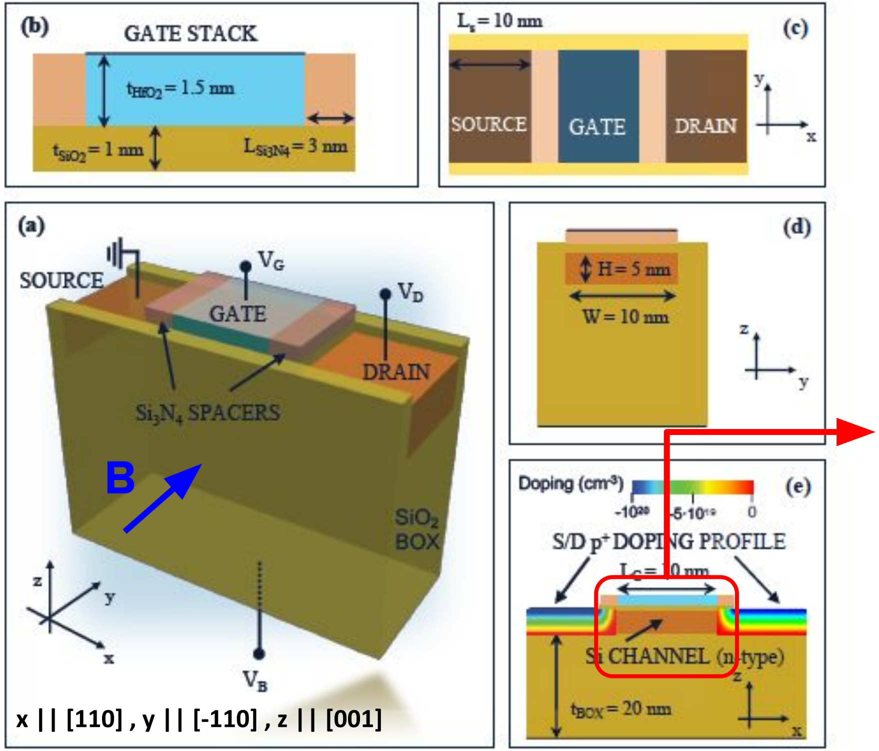
Ultra-scaled devices
10 nm channel length (increase ΔE)

Multi-scale simulation
From device electrostatic up to qubit operations

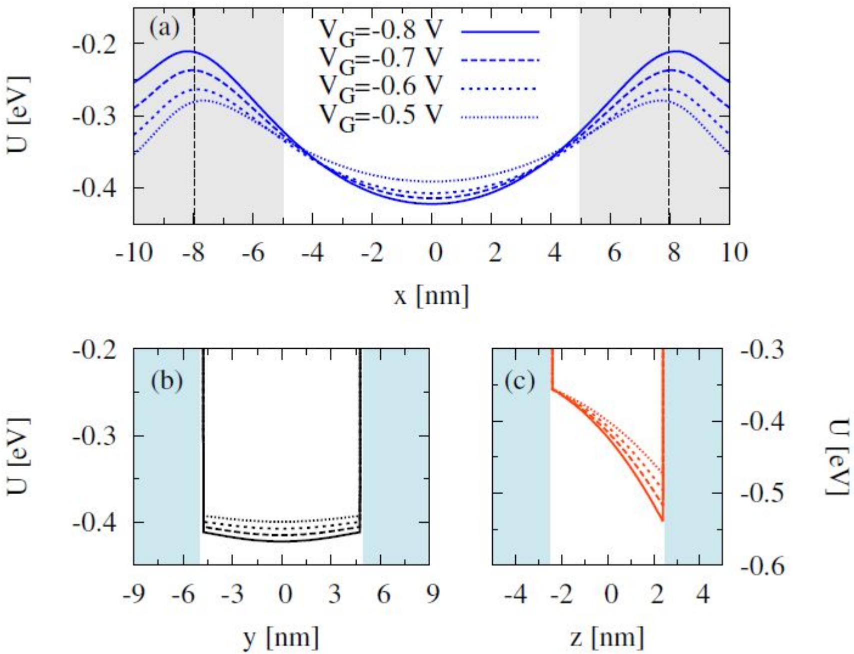


DOWNSCALED Si FDSOI pMOSFETs

Ginestra (MDLab)

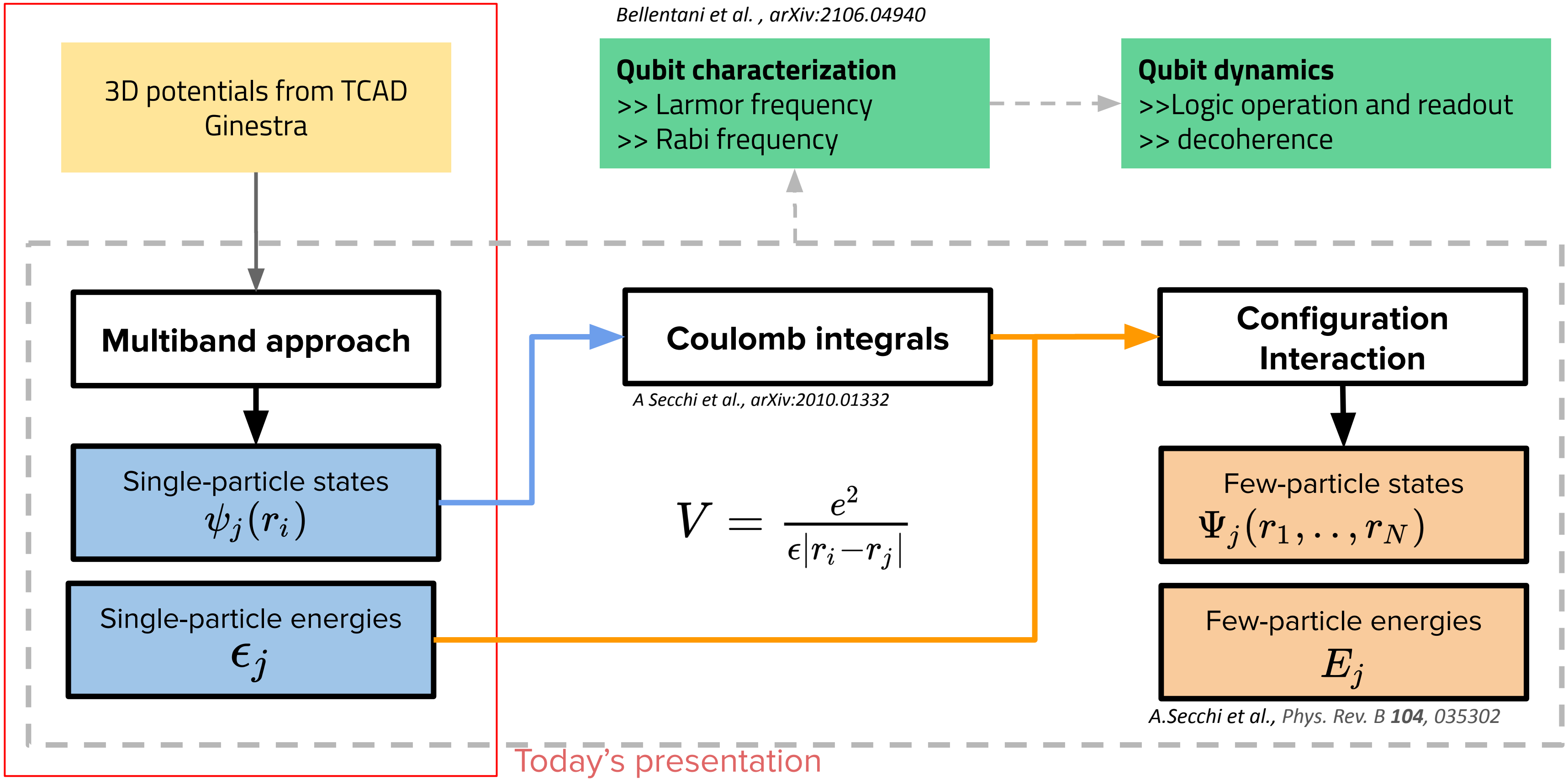


Lz= 5nm, Lx=10 nm, W=10-40 nm



Bellentani et al. , arXiv:2106.04940 (2021)

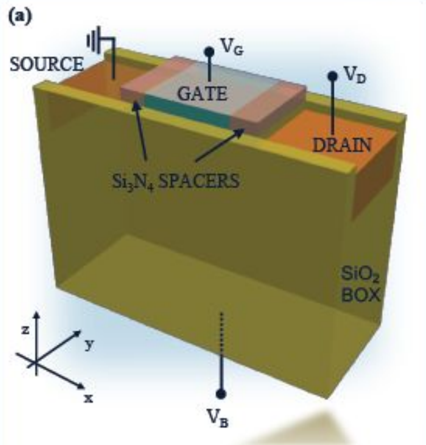
NUMERICAL APPROACH FOR HOLE SPIN QUBIT



Towards hole-spin qubits in Si pMOSFETs within a planar CMOS foundry technology

L. Bellentani[1], M. Bina[2], S. Bonen[3], A. Secchi[1], A. Bertoni[1], S. Voinigescu[3], A. Padovani[2], L. Larcher[2], and F. Troiani[1]
[1] S3, Istituto Nanoscienze-CNR, Modena, Italy
[2] Applied Materials - MDLx Italy R&D, Reggio Emilia, Italy and
[3] Edward S. Rogers Snr. Department of Electrical and Computer Engineering, University of Toronto, Toronto, Canada

- **QD formation** in the Si channel of downscaled pMOSFETs
- **Initialization** of the qubit in the ground state
- **Fully-electrical spin manipulation**



x || [110] , y || [-110] , z || [001]

6X6 k.p MODELING IN THE EFA SCHEME

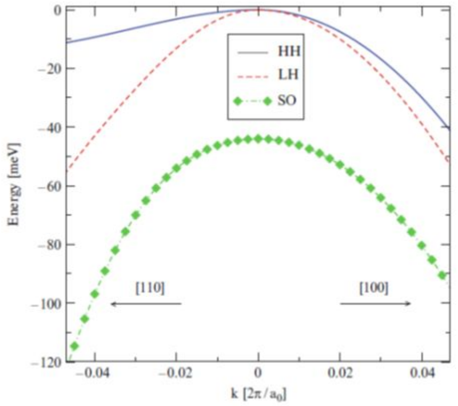
- Second-order perturbation of k.p Hamiltonian at **k**=0 + **Hso** for diamond lattice

- Basis set @ Γ→ p-like orbitals (l=1) + spin (s=1/2) → J=3/2, J=1/2

$$\{|b\rangle\} = \{|\tfrac{3}{2},+\tfrac{3}{2}\rangle, |\tfrac{3}{2},+\tfrac{1}{2}\rangle, |\tfrac{3}{2},-\tfrac{1}{2}\rangle, |\tfrac{3}{2},-\tfrac{3}{2}\rangle, |\tfrac{1}{2},+\tfrac{1}{2}\rangle, |\tfrac{1}{2},-\tfrac{1}{2}\rangle\}$$

hh+ lh+ lh- hh- so

Δ= 44 meV



- **Luttinger Kohn Hamiltonian** for basis with x||[110], y||[-110], z||[001]

$$\mathcal{H}_{\mathbf{k}} \equiv \begin{pmatrix} P_{\mathbf{k}}+Q_{\mathbf{k}} & -S_{\mathbf{k}} & \tilde{R}_{\mathbf{k}} & 0 & -\frac{1}{\sqrt{2}}S_{\mathbf{k}} & \sqrt{2}\tilde{R}_{\mathbf{k}} \\ -S^*_{\mathbf{k}} & P_{\mathbf{k}}-Q_{\mathbf{k}} & 0 & \tilde{R}_{\mathbf{k}} & -\sqrt{2}Q_{\mathbf{k}} & \sqrt{\frac{3}{2}}S_{\mathbf{k}} \\ \tilde{R}^*_{\mathbf{k}} & 0 & P_{\mathbf{k}}-Q_{\mathbf{k}} & S_{\mathbf{k}} & \sqrt{\frac{3}{2}}S^*_{\mathbf{k}} & \sqrt{2}Q_{\mathbf{k}} \\ 0 & \tilde{R}^*_{\mathbf{k}} & S^*_{\mathbf{k}} & P_{\mathbf{k}}+Q_{\mathbf{k}} & -\sqrt{2}\tilde{R}^*_{\mathbf{k}} & -\frac{1}{\sqrt{2}}S^*_{\mathbf{k}} \\ -\frac{1}{\sqrt{2}}S^*_{\mathbf{k}} & -\sqrt{2}Q_{\mathbf{k}} & \sqrt{\frac{3}{2}}S_{\mathbf{k}} & -\sqrt{2}\tilde{R}_{\mathbf{k}} & P_{\mathbf{k}}+\Delta & 0 \\ \sqrt{2}\tilde{R}^*_{\mathbf{k}} & \sqrt{\frac{3}{2}}S^*_{\mathbf{k}} & \sqrt{2}Q_{\mathbf{k}} & -\frac{1}{\sqrt{2}}S_{\mathbf{k}} & 0 & P_{\mathbf{k}}+\Delta \end{pmatrix}$$

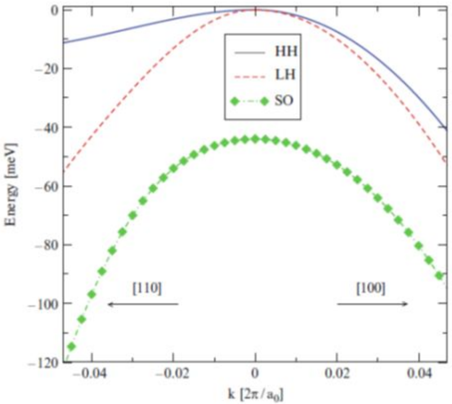
$$P_{\mathbf{k}} = \frac{\hbar^2}{2m_0}\gamma_1\left(k_x^2+k_y^2+k_z^2\right),$$

$$Q_{\mathbf{k}} = \frac{\hbar^2}{2m_0}\gamma_2\left(k_x^2+k_y^2-2k_z^2\right),$$

$$\tilde{R}_{\mathbf{k}} = \frac{\hbar^2}{2m_0}\sqrt{3}\left[-\gamma_3\left(k_x^2-k_y^2\right)+2i\gamma_2 k_x k_y\right],$$

$$S_{\mathbf{k}} = \frac{\hbar^2}{2m_0}2\sqrt{3}\gamma_3\left(k_x-ik_y\right)k_z .$$

6X6 k.p MODELING IN THE EFA SCHEME

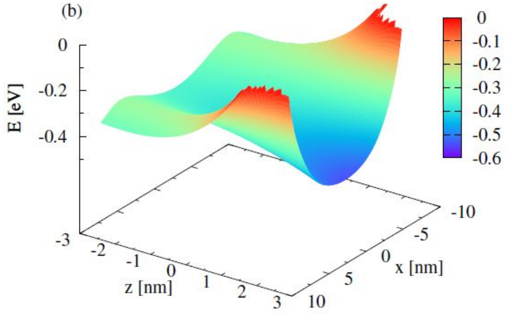


- **Envelope Function Approximation** for nano-confining potential U(**r**)

$$\mathcal{H}(\boldsymbol{r},\boldsymbol{k}) = \mathcal{H}_{\boldsymbol{k}} + U(\boldsymbol{r}) \xrightarrow{\text{LAPACK}} \Psi_m(\boldsymbol{r}) = \sum_b \psi_{m,b}(\boldsymbol{r})\langle \boldsymbol{r}|b\rangle$$

- Full-treatment of the magnetic contribution (Zeeman + vector potential)

U(**r**) [TCAD]

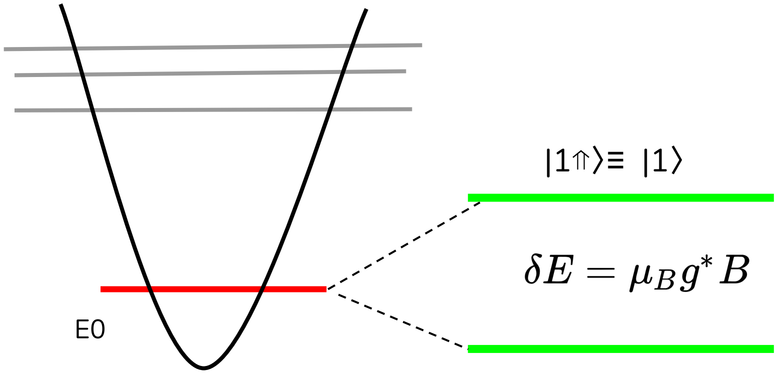


$$\mathcal{H}_{\boldsymbol{k}} \rightarrow \mathcal{H}_{\boldsymbol{k}-\frac{e}{h}\boldsymbol{r}\times\boldsymbol{B}/2} + \mathcal{Z} = \mathcal{H}_{\boldsymbol{k}} + \underbrace{\mathcal{Z} + \mathcal{H}_p + \mathcal{H}_d}_{H_B}$$

$\mathcal{H}_p \propto B$, $\mathcal{H}_d \propto B^2$

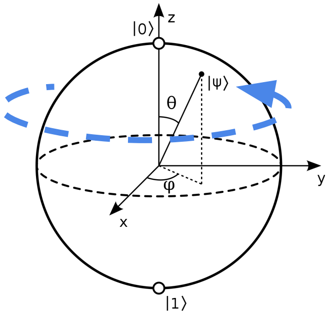
CHARACTERISTIC FREQUENCIES OF SPIN QUBIT

COULOMB BLOCKADE **+ B**



$$\delta E = \mu_B g^* B$$

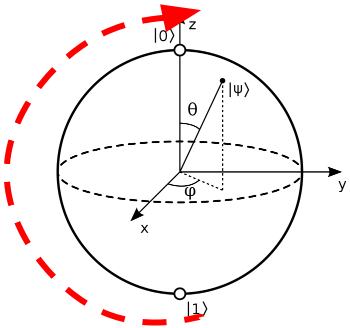
$$|\Psi(0)\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$



INITIALIZATION

Larmor frequency

$$f_L = \frac{\mu_B g^* B}{h}$$



SINGLE-QUBIT OPERATIONS

Rabi frequency

$$|\Psi(t)\rangle = e^{-i\omega_R \sigma_i t}|\Psi(0)\rangle$$

$$f_R = 2\pi\omega_R$$

ALL ELECTRICAL X,Y AND Z ROTATIONS

- *Electric-Dipole-induced Spin Resonance* (X, Y)

$$\delta VG(t) = V_{ac}\cos(2\pi f_L\, t + \phi)$$

$$\delta U(\boldsymbol{r}) = U_{VG+\delta VG(t)}(\boldsymbol{r}) - U_{VG}(\boldsymbol{r})$$

$$f_R^X = \frac{1}{h}|\langle 1 \Uparrow |\delta U(\boldsymbol{r})| 1 \Downarrow\rangle|$$

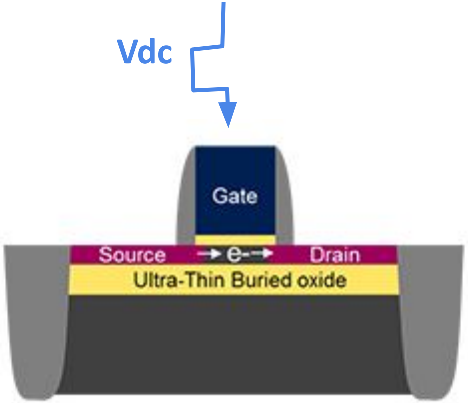
$$\phi = 0 \rightarrow X$$

$$\phi = \frac{\pi}{2} \rightarrow Y$$

- *DC pulse* (Z)

$$\delta VG(t) = V_{DC}$$

$$f_R^Z = \frac{1}{2h}|\langle 1 \Uparrow |\delta U(\boldsymbol{r})| 1 \Uparrow\rangle - \langle 1 \Downarrow |\delta U(\boldsymbol{r})| 1 \Downarrow\rangle|$$



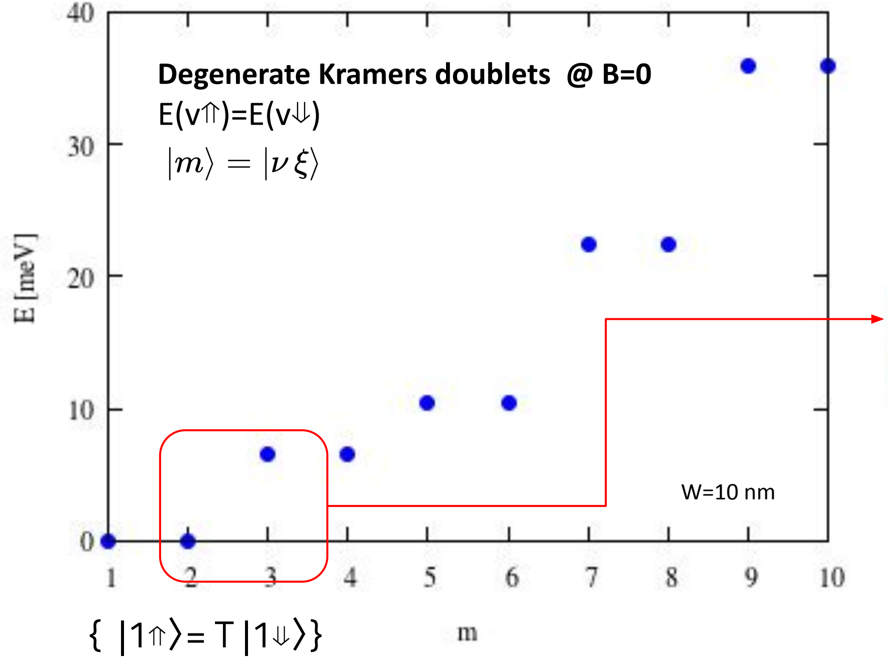
$$|\Psi(0)\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$

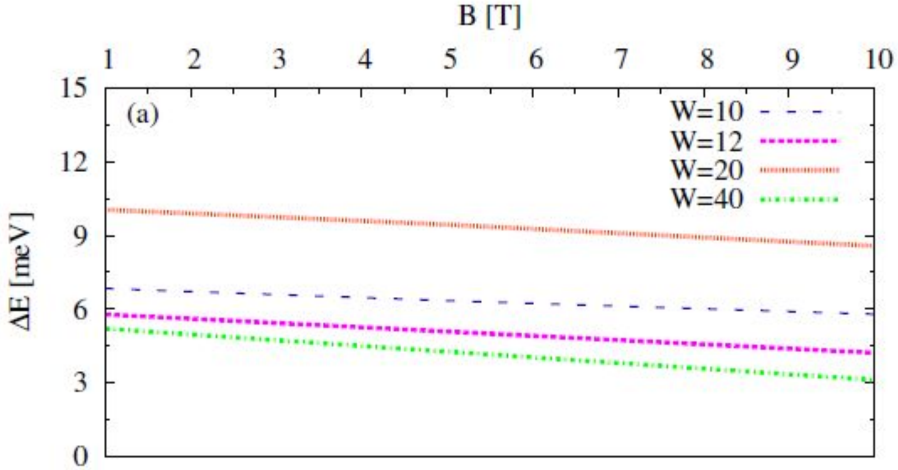
$$|\Psi(t)\rangle = e^{-i\omega_R\sigma_Z t}|\Psi(0)\rangle \quad |\Psi(t)\rangle = e^{-i\omega_R\sigma_X t}|\Psi(0)\rangle$$

QD FORMATION: SINGLE HOLE SPECTRUM

V_G [V]	$p^{hh}_{1,\xi}$ [%]	$p^{lh}_{1,\xi}$ [%]	$p^{so}_{1,\xi}$ [%]
-0.8	86.44	11.57	1.99
-0.6	83.14	14.56	2.30

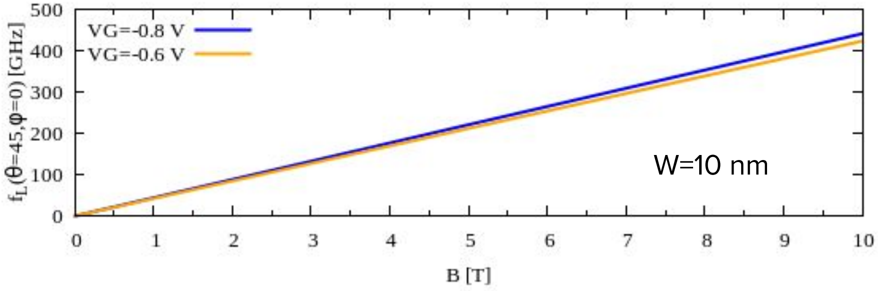
- Kramers doublets with HH/LX mixing
- **Large orbital splitting** ΔE=6.5 meV (75K)
- Ground doublet well isolated up to 10 T

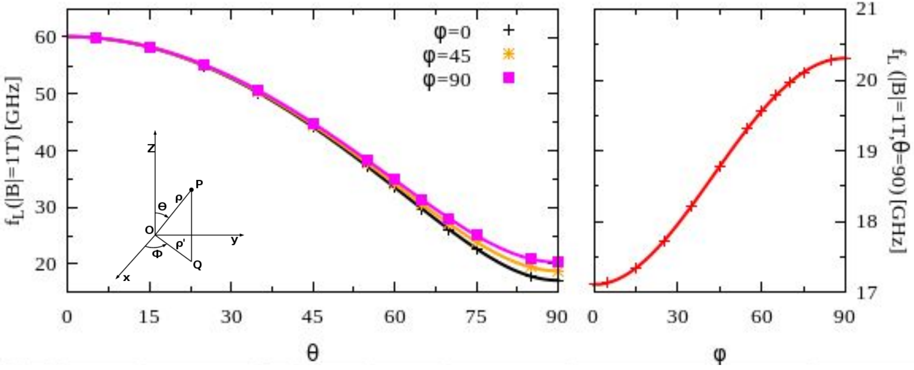




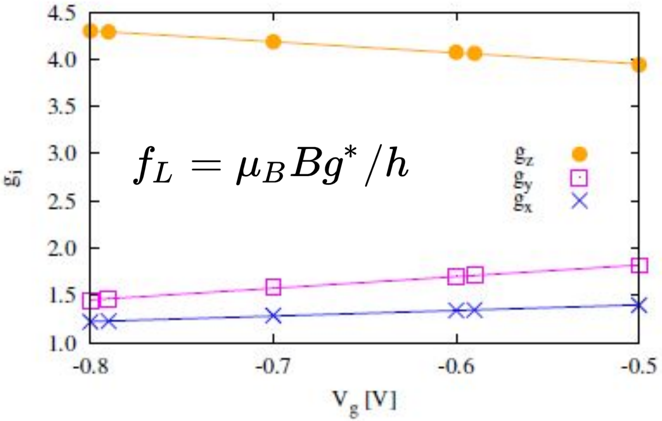
INITIALIZATION: LARMOR FREQUENCY

$$f_L(B,\theta,\phi) = (E_{1\Uparrow} - E_{1\Downarrow})/h$$



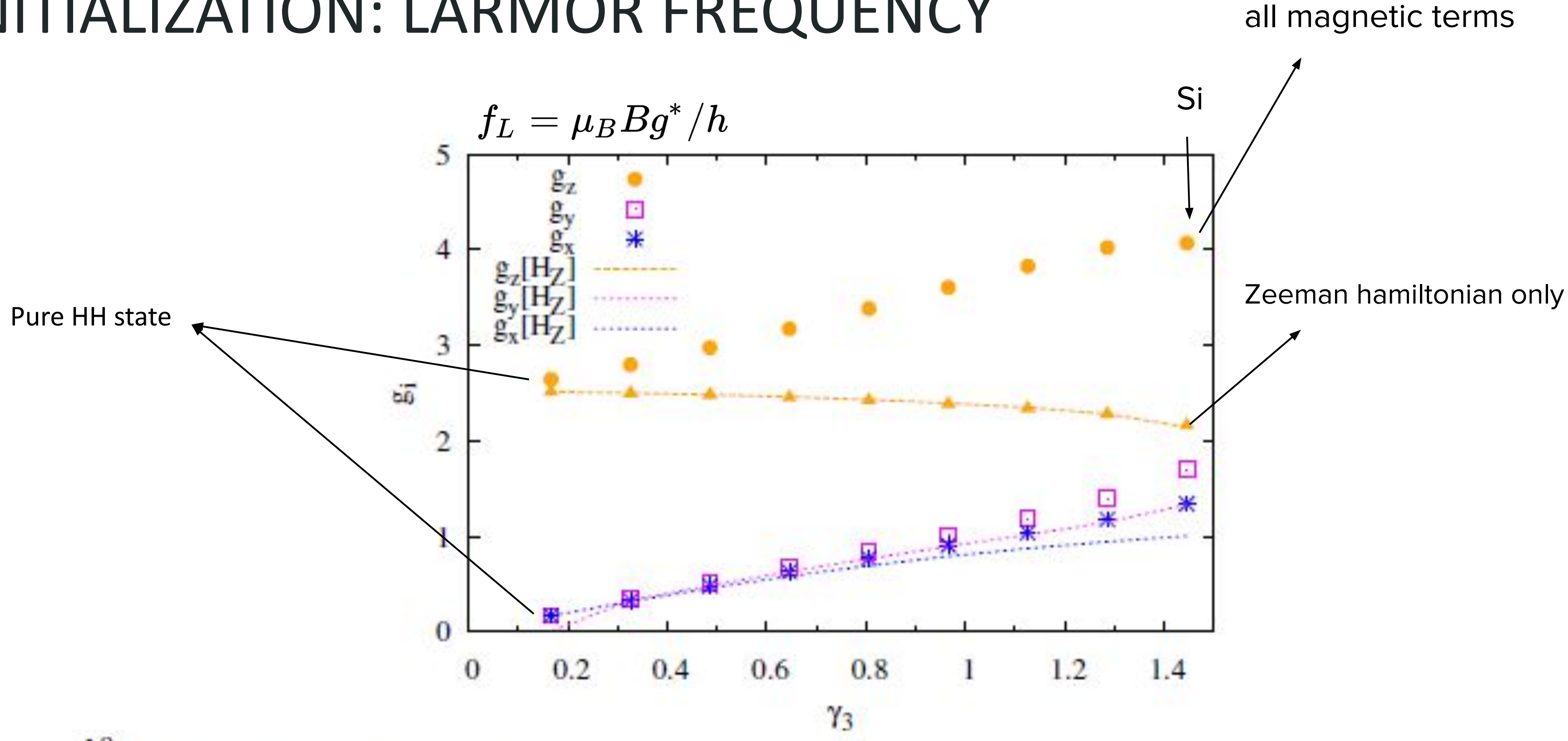


- Linear in B
- Linear in VG
- **60-20 GHz at B=1T → OK FOR EDSR**



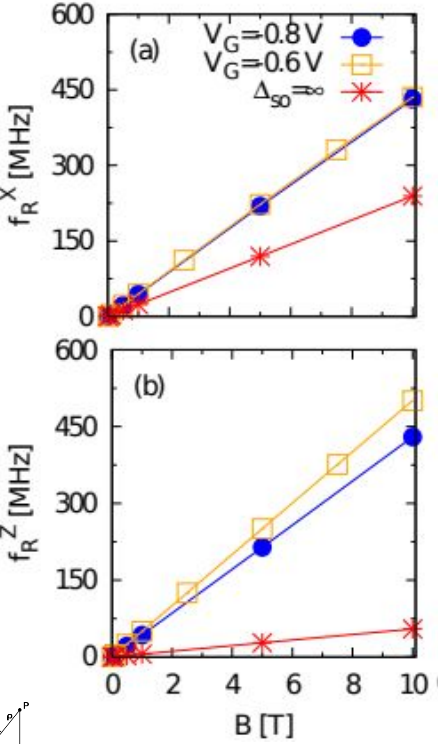
INITIALIZATION: LARMOR FREQUENCY

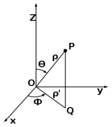
$$f_L = \mu_B B g^* / h$$



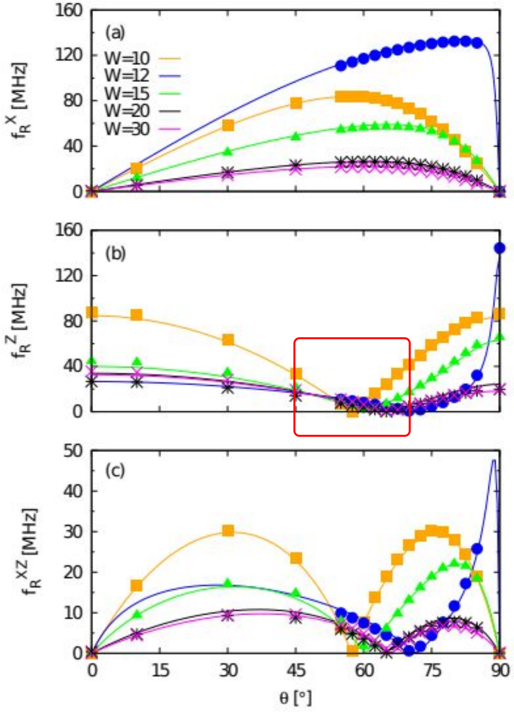
$$\widetilde{R}_{\boldsymbol{k}} = \frac{\hbar^2}{2m_0}\sqrt{3}\left[-\gamma_3\left(k_x^2 - k_y^2\right) + 2\mathrm{i}\gamma_2 k_x k_y\right] ,$$

SPIN MANIPULATION: RABI FREQUENCIES





B=1 T



- ≈ 100 MHz @ B=1 T
- SO non negligible
- Strongly anisotropic Rabi frequency
- almost anti-correlated fRX and fRZ

$$f_R^{XZ} = \left(\frac{1}{f_R^X} + \frac{1}{f_R^Z} \right)^{-1}$$

- fRZ=0 sweet spot against electrical noise
- Alternative Pauli Z-gate

$$Z(\phi) = Y(\pi/2)X(\phi)Y(-\pi/2)$$

INSIGHTS FROM THE G-MATRIX

- Linearity in B → Effective two-level description $H_B = \frac{1}{2}\mu_B {}^t\boldsymbol{\sigma} \cdot \hat{g}\boldsymbol{B} \quad \{|1 \Downarrow\rangle, |1 \Uparrow\rangle\}$
- Linearity in VG → g-matrix linearly perturbed $\hat{g}(VG) = \hat{g}(VG_0) + \hat{g}'(VG_0)\delta VG$

$$H(V_G, B; t) = \boldsymbol{\sigma} \cdot [\tfrac{1}{2}\mu_B \hat{g}(VG_0) \cdot \boldsymbol{B}] + \boldsymbol{\sigma} \cdot [\tfrac{1}{2}\mu_B \hat{g}'(VG_0) \cdot \boldsymbol{B}]\delta VG(t)$$

Larmor vector **ħΩ**

gate-voltage derivative **ħΩ'**

$$\boldsymbol{\Omega}' = \boldsymbol{\Omega}'_{\perp} + \boldsymbol{\Omega}'_{\parallel}$$

$$\Omega'_{\parallel} \rightarrow f_R^Z(B, \theta, \phi) = \frac{\mu_B B V_{ac}}{2hg^*} |(\hat{g}'\boldsymbol{b}) \cdot (\hat{g}\boldsymbol{b})|$$

$$\Omega'_{\perp} \rightarrow f_R^X(B, \theta, \phi) = \frac{\mu_B B V_{ac}}{2hg^*} |(\hat{g}'\boldsymbol{b}) \times (\hat{g}\boldsymbol{b})|$$

INSIGHTS FROM THE G-MATRIX

- **APPROX:** Diagonal g-matrix and g'-matrix (symmetries preserved)

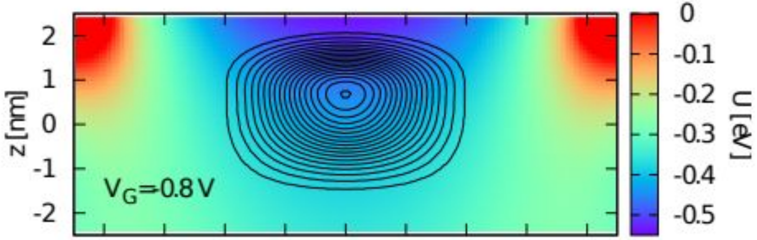
→ δVG modulates Zeeman split only (g-TMR)

$$\sigma_{yz} \approx 1\,,\ \sigma_{zx} \approx 1 \to \hat{g}(VG_0) = \begin{pmatrix} g_x & 0 & 0 \\ 0 & g_y & 0 \\ 0 & 0 & g_z \end{pmatrix}$$

$$\hat{g}'(VG^0) = \begin{pmatrix} g'_x & 0 & 0 \\ 0 & g'_y & 0 \\ 0 & 0 & g'_z \end{pmatrix}$$

$$\langle m|\sigma_{\alpha\beta}|m\rangle = \sum_b \sum_n |c^m_{\boldsymbol{n},b}|^2 (-1)^{n_\gamma}$$

V_G [V]	$\langle\sigma_{yz}\rangle$	$\langle\sigma_{zx}\rangle$	$\langle\sigma_{xy}\rangle$	$\langle\sigma_r\rangle$
-0.8	0.9655	0.9670	0.8548	0.8870
-0.6	0.9550	0.9692	0.8894	0.9289



INSIGHTS FROM THE G-MATRIX

$$\theta^{X}_{R,max} = \arctan\left(\sqrt{|g_\perp / g_\parallel|}\right)$$

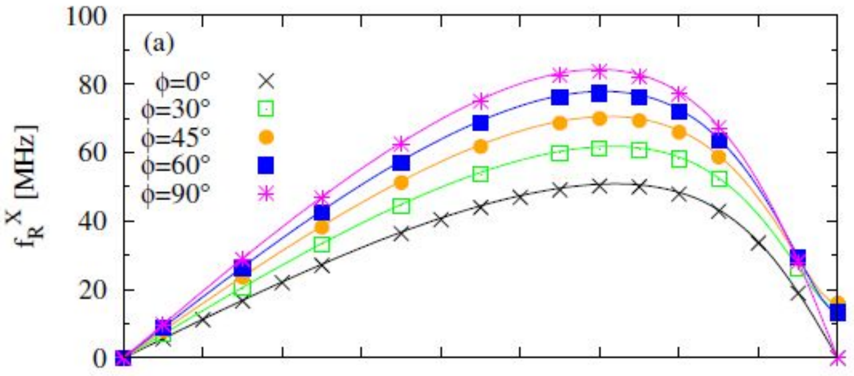
$$f_R^{X,max} = \frac{\mu_B B V_{ac}}{2h} \frac{|g'_\parallel g_\perp - g'_\perp g_\parallel|}{|g_\parallel| + |g_\perp|}$$

$$\theta^{Z}_{R,zero} = \arctan\left(\sqrt{|g_\perp g'_\perp / g_\parallel g'_\parallel|}\right)$$

$$f_R^{Z,max} = \frac{\mu_B B V_{ac}}{2h} \max_{\alpha \in x,y,z} |g'_\alpha|$$

- Rabi frequencies are dominated by g-TMR
- Optimal orientation for fast electrical control
- Anticorrelation between fRX and fRZ

$$g'_\perp \approx g'_\parallel \rightarrow \theta^{X}_{R,max} \approx \theta^{Z}_{R,zero}$$



Towards hole-spin qubits in Si pMOSFETs within a planar CMOS foundry technology

L. Bellentani[1], M. Bina[2], S. Bonen[3], A. Secchi[1], A. Bertoni[1],
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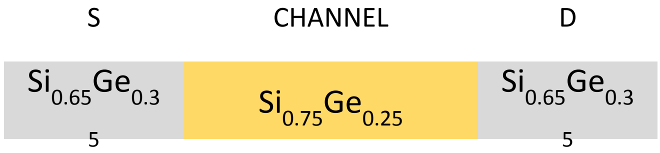
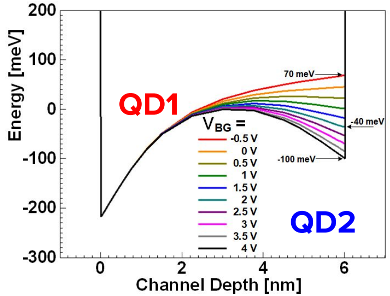
- ✓ **QD formation** in the Si channel of downscaled pMOSFETs
- ✓ **Initialization** of the qubit in the ground state
- ✓ **Fully-electrical spin manipulation**

+ SO is relevant
+ beyond Zeeman contribution are relevant
+ g-TMR dominates
+ sweet spots against electrical noise

TOWARDS SiGe DEVICES and DQDs

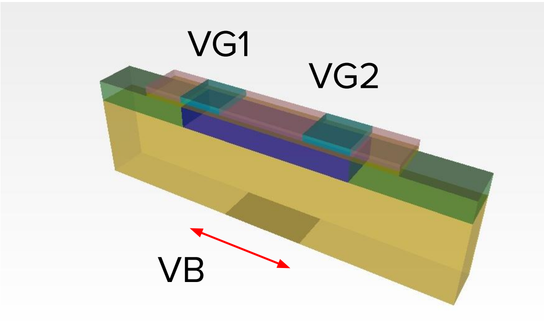


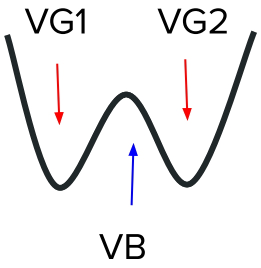
- Compatible with Si fabrication technique
- Higher carrier mobility
  - → increase energy mode splitting
  - → Relax lithographic requirements
- Compressive strain due to Ge concentration (Bir-Pikus Hamiltonian)
- No Ge nanoclustering in Si matrix



> *"High-throughput investigation of the electron transport properties in Si1-xGex alloys"*
> *BAMIDELE I. ADETUNJI, ANDREW SUPKA, MARCO FORNARI, AND ARRIGO CALZOLARI*

- Downscaled double QD SiGe devices
  - → horizontally vs vertically coupled QDs
  - → READOUT with gate reflectometry





RELATED WORK ON TWO-HOLE QUBITS

- Numerical and analytical investigation of interacting holes in Si/Ge DQDs

“*Interacting holes in Si and Ge double quantum dots: From a multiband approach to an effective-spin picture*”, A. Secchi, L. Bellentani, A. Bertoni, and F. Troiani Phys. Rev. B **104,** 035302 (2021)

- Numerical approach for Coulomb integrals with **interband scattering processes**

“*Inter- and intra-band Coulomb interactions between holes in Silicon nanostructures*”, A. Secchi, L. Bellentani, A. Bertoni, and F. Troiani arXiv:2010.01332 (2020)

$$V_{\{\nu\}} = \sum_{\{b\}} \int d\boldsymbol{r} \int d\boldsymbol{r}' \psi^*_{\nu_1,b_1}(\boldsymbol{r})\psi^*_{\nu_2,b_2}(\boldsymbol{r}')W_{\{b\}}(\boldsymbol{r}-\boldsymbol{r}')\psi_{\nu_3,b_3}(\boldsymbol{r}')\psi_{\nu_4,b_4}(\boldsymbol{r})$$

numerically demanding $\rightarrow$ Fourier transform method

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III-N growth and device development

CNR-Nano (S3, Modena)
DEVICE PHYSICS AND MODELLING
atomistic modeling of nanostructures and electric properties
simulation of quantum gates and readout/manipulation

MDLab
TCAD SIMULATION
device modelling and simulation of QD electrostatic

THANK YOU FOR YOUR ATTENTION







Related publications

- L. Bellentani, A. Secchi, A. Bertoni and F. Troiani, *Towards hole-spin qubits in Si pMOSFETs within a planar CMOS foundry technology, arXiv:2106.04940 (2021)*
- A. Secchi, L. Bellentani, A. Bertoni, and F. Troiani, *Interacting holes in Si and Ge double quantum dots: From a multiband approach to an effective-spin picture,* Phys. Rev. B 104, 035302 (2021)
- A. Secchi, L. Bellentani, A. Bertoni, and F. Troiani, *Inter- and intra-band Coulomb interactions between holes in Silicon nanostructures,* arXiv:2010.01332 (2020)

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